Development of a geometallurgical framework for iron ores - A mineralogical approach to particle-based modeling

Mehdi Amiri Parian

Mineral Processing
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Mehdi Amiri Parian

Doctoral Thesis in Mineral Processing
Division of Minerals and Metallurgical Engineering
Luleå University of Technology
SE-971 87 LULEÅ
Sweden
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The demands for efficient utilization of ore bodies and proper risk management in the mining industry have resulted in a new cross-disciplinary subject called geometallurgy. Geometallurgy connects geological, mineral processing and subsequent downstream processing information together to provide a comprehensive model to be used in production planning and management. A geometallurgical program is an industrial application of geometallurgy. Various approaches that are employed in geometallurgical programs include the traditional way, which uses chemical elements, the proxy method, which applies small-scale tests, and the mineralogical approach using mineralogy or the combination of those. The mineralogical approach provides the most comprehensive and versatile way to treat geometallurgical data. Therefore, it was selected as a basis for this study.

For the mineralogical approach, quantitative mineralogical information is needed for both the deposit and the process. The geological model must describe the minerals present, give their chemical composition, report their mass proportions (modal composition) in the ore body and describe the ore texture. The process model must be capable of using mineralogical information provided by the geological model to forecast the metallurgical performance of different geological volumes and periods. A literature survey showed that areas, where more development is needed for using the mineralogical approach, are: 1) quick and inexpensive techniques for reliable modal analysis of the ore samples; 2) ore textural characterization to forecast the liberation distribution of the ore when crushed and ground; 3) unit operation models based on particle properties (at mineral liberation level) and 4) a system capable of handling all this information and transferring it to production model. This study focuses on developing tools in these areas.

A number of methods for obtaining mineral grades were evaluated with a focus on geometallurgical applicability, precision, and trueness. A new technique developed called combined method uses both quantitative X-ray powder diffraction with Rietveld refinement and the Element-to-Mineral Conversion method. The method not only delivers the required turnover for geometallurgy but also overcomes the shortcomings if X-ray powder diffraction or Element-to-Mineral Conversion were used alone.

Characterization of ore texture before and after breakage provides valuable insights about the fracture pattern in comminution, the population of particles for specific ore texture and their relation to parent ore texture. In the context of the mineralogical approach to geometallurgy, predicting the particle population from ore texture is a critical step to establish an interface between geology and mineral processing. A new method called Association Indicator Matrix developed to assess breakage pattern of ore texture and analyze mineral association. The results of ore texture and particle analysis were used to generate particle population from ore texture by applying particle size distribution and breakage frequencies. The outcome matches well with experimental data specifically for magnetite ore texture.

In geometallurgy, process models can be classified based on at which level the ore is defined, i.e. the feed stream to the processing plant and each unit operation, and what information subsequent streams carry. The most comprehensive level of mineral processing models is the particle-based one which includes practically all necessary information on streams for modeling unit operations. Within this study, a particle-based unit operation model was built for wet low-intensity magnetic separation,
and existing size classification and grinding models were evaluated to be used at particle level. A property-based model of magnetic beneficiation plant was created based on one of the LKAB operating plants at mineral and particle level, and the results were compared. Two different feeds to the plant were used. The results revealed that at the particle level, the process model is more sensitive to changes in feed property than any other levels. Particle level is more capable for process optimization for different geometallurgical domains.
The thesis presented here describes building and developing the mineralogical path to be used for geometallurgical modeling. The research based at Division of Minerals and Metallurgical Engineering, Luleå University of Technology and was carried out during 2012-2017. The work was funded by the Hjalmar Lundbohm Research Centre (HLRC).

I appreciate all helps from LKAB personal specifically Kari Niiranen, Andreas Fredriksson, Therese Lindberg, Mikko Kauppinen, and Axel Ståhlström. I am grateful to sample preparation crew at LKAB Kiruna namely Catrin Huuva, Ulrik Kalla, Emmeli Falk, Tomas Salmi and Peter Alanärä-Lassi (summer worker), for their positive attitude and their accurate work.

I kindly thank my colleagues Abdul Mwanga, Cecilia Lund, Jan Stener, Anders Sand, Bertil Pålsson, Pierre-Henri Koch, Tommy Karlkvist, and Lindsay Ohlin for the fruitful discussions.

Finally, I would like to thank my wife, daughter and my parents for their support, encouragement, and patience.

Mehdi Amiri Parian

Luleå, April 2017
List of papers and tools

The thesis is based on the following papers:


The list of papers not included in this thesis:


Tools developed:

A. MATLAB code: Element-to-Mineral Conversion and combined method for large datasets; used in paper I.

B. Stand-alone software: Grain Classifier; IncaMineral classification software to post-process data of IncaMineral system (C++); used in paper I and paper II.
C. MATLAB code: Image analysis for ore texture and polished sections - liberation and association analysis (MATLAB); used in paper III.

D. MATLAB code: Predicting particle population from ore texture by defining particle size distribution and breakage frequencies; used in paper III and paper IV.

E. MATLAB code & Stand-alone software: Export particle population in liberation form (From IncaMineral database or particle generation) to be used in HSC Chemistry software; used in paper II, III and IV.

My role in the papers included in the thesis:

I) The first author performed the sampling, sample preparation, modal quantification by different techniques as well as the development of the combined method to its final form. The paper was written by the first author and the other authors acted as supervisors and corrected the manuscript at different stages.

II) The sampling during the plant survey was done by LKAB personnel who also assisted in sample preparation. The process mineralogical analysis including preparing epoxy samples, automated mineralogy analysis, mass balancing and model development was conducted by the first author. The paper was written by the first author while the other authors acted as supervisors and corrected the manuscript at different stages.

III) The concept of developing the “Association Indicator Matrix” and forecasting particle population including fine sieving, epoxy sample preparations, optical microscopy and Auto-SEM analysis were done solely by the first author. Crushing and sieving of the ore texture samples was done by Abdul Mwanga. The paper was written by the first author and the other authors acted as supervisors and corrected the manuscript at different stages.

IV) Flowsheet drawing, set up of process models, calibrating model parameters as well as the simulations at different levels were done solely by the first author. The paper was written by the first author while the other authors acted as supervisors and corrected the manuscript at different stages.
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Chapter 1 - Introduction

1.1 Geometallurgical program and its approaches

Variation in feed quality of a plant has been a challenge for mineral processing operations. A prior understanding of the characteristics of the feed over the lifespan of the mining operation is the solution to successful circuit design, optimization, and troubleshooting. Also, demands for effective utilization of ore bodies and proper risk management in the mining industry have engendered an interest in geometallurgy. Several definitions have been proposed in the literature for geometallurgy (David, 2013; Dunham and Vann, 2007; Kittler et al., 2011; Lamberg, 2011). In this study, the following definition is used:

Geometallurgy is a cross-disciplinary subject that connects geological, mineral processing and subsequent downstream processing information together to provide a comprehensive and quantitative 3D model on the variability of the ore to be used for an efficient production planning and management.

Several key points that a geometallurgy study must possess are a cross-disciplinary approach, a focus on spatial variations in the ore body, a model to connect deposit information to the process and a final aim to be used in practice. A critical issue is to establish quantitative interfaces between the disciplines (i.e. geology and mineral processing) in a way that data content and structures are matching and ore characterization includes proper parameters which can be transferred along the process chain.

A geometallurgical program is an industrial application of geometallurgy. It provides a way to map the variation within the ore body, to handle the data and to forecast metallurgical performance at spatial and time level. The program also comprises a process to handle complex geological information and transfers them into geometallurgical domains to be used in process optimization, production planning, and business decision making. The program is an instrument which should evolve and change during the lifespan of a mine to ensure that geometallurgical domains address the variation properly in metallurgical performance.

Various approaches exist to establish a geometallurgical program (Kittler et al., 2011; Lishchuk, 2016). These include the conventional way, the proxy method, the mineralogical approach or a combination of these. The conventional approach heavily focuses on chemical assays and often neglects quantitative mineralogy. In the proxy approach, the main attempt is on finding correlations between the chemical composition of the ore and metallurgical performance in small-scale laboratory tests. Thus, tests provide a proxy to important ore properties relevant to processing. The most comprehensive of these is the mineralogical approach where all components of the geometallurgical model are based on quantitative mineralogical information or mineralogical attributes. This means that the geological model can provide details on the mineralogy of an ore deposit at spatial level and mineral processing model can deal with ore textural and mineralogical information received from the geological model. Generally speaking, the mineralogical approach is known to be the most thorough option (e.g. Lamberg 2011; Bonnici et al. 2008). This is natural since minerals define the value of the deposit, the method of extraction, economic risk valuation, and the concentration method (Hoal et al., 2013). However, many geometallurgical programs are not benefiting from the full potential of mineralogy due to the high cost of quantitative mineralogy and the large number of samples required.
In principal, the process and the product requirements define which characteristics of an ore body are essential. Therefore, critical properties to be obtained for assigning geometallurgical domains can be selected first based on the processing circuit (David, 2007). For example, grindability and crusher work index are valid parameters for comminution circuits and mineral recovery and impurity levels in case of concentration circuit. Usually, the next step is to find a relation between geological dataset (chemical composition data) and results from metallurgical testing. This type of approach is towards a proxy approach to geometallurgy. The difficulty rises when the variation in the ore body is high or unknown, meaning that a significant number of samples need to be collected for the variability (metallurgical) tests in order to map the ore. In this case, the solution is often to carry out the tests on blends or the selected number of samples but in both cases the risk of missing information on variability increases.

A mineralogy-based geometallurgical model employs quantitative mineralogical information, both on the deposit and in the process. The geological model must describe the minerals present, give their chemical composition, report their mass proportions (modal composition) in the ore body and describe the ore texture. The process model must be capable of using mineralogical information provided by the geological model to forecast the metallurgical performance of different geological volumes, such as samples, ore blocks, geometallurgical domains or blends prepared for the plant feed for various periods from hourly and daily scale to weekly, monthly and annual production.

In a mineralogy-based approach to geometallurgy, the simulation environment must be capable of handling both size reduction and concentration circuit at the particle level. This means that comminution circuit model needs to provide particle size distribution, throughput and even more importantly, liberation information (i.e. particles). On the other hand, the concentration circuit model must operate at the same level (i.e. particle level), deliver liberation information for both tailing, and concentrate streams. This requires particle-based process models which have not been sufficiently developed.

1.2 Scope of the present work

This work focuses on building and developing a mineralogical path to be used within geometallurgical modeling. The mineralogical approach provides the most comprehensive and versatile way to treat geometallurgical data (Hoal et al., 2013). Therefore, it was selected as the basis for this study.

Lund (2013) studied the methods for mineralogical characterization of LKAB’s Malmberget iron ore to be used in geometallurgical modeling. According to this work, the areas where the mineralogical approach needs further development are:

1) Quick and inexpensive techniques for reliable modal analysis (i.e. analysis for mineral grades) of the ore.
2) Ore textural characterization for forecasting the liberation distribution of the ore when crushed and ground.
3) Unit operation models based on particle properties (at mineral liberation level).
4) A system capable of handling all this information and transferring it into a production model (Figure 1).

These issues have been raised in several other studies (Dominy and Connor, 2016; Dunham and Vann, 2007; Walters and Kojovic, 2006). This study focuses on addressing the above areas with a particular
reference to iron ore. Therefore, the objectives are defined as follows and some areas are knowingly left out of the scope:

- To develop a reliable modal analysis method for geometallurgy of iron ore.
  - The method should be fast, inexpensive, based on available techniques and be applicable in mines.
  - Develop a generic method to estimate the error in modal analysis.
- To develop a procedure for forecasting particle liberation from ore texture.
  - The method should be drawn up for meso-scale of ore texture.
  - The breakage behavior of ore texture should be characterized.
- To develop a particle-based model for magnetic separation.
  - The method should be based on particle properties as received in mineral liberation analysis.
  - The model should be verified with experimental data.
- To develop a geometallurgical simulation system to handle mineralogical data and predict the product based on that.

Geometallurgy is a wide research area and a study like this cannot cover all the parts. The following relevant topics were left outside of the scope of this study:

- Drill core scanning and related tools (macro-scale textural characterization and classification).
- Block modeling and geostatistics of geometallurgy.

<table>
<thead>
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<th>Geometallurgical program</th>
</tr>
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<tbody>
<tr>
<td>Ore</td>
</tr>
</tbody>
</table>
| 1) Reliable modal analysis  
  2) Ore texture quantification |
| Process                  |
| 3) Particle-based unit models and process model |
| Simulation Framework     |
| 4) Interface between ore and process |

Figure 1. Schematic workflow for establishing a mineralogical path in a geometallurgical program.

1.3 Thesis Overview

The main areas of the study i.e. modal analysis, ore textural study, and process models are separate problems. Therefore, they are described and solved separately in the thesis. A brief description of chapters is as follows:

In Chapter 2, earlier works within the scope of the present study are reviewed. The literature survey is focused on ore characterization and process models that are of interest to the geometallurgy of iron ore. Ore characterization methods, with a focus on applicability to iron ore, are reviewed, and the drawbacks of each method are pointed out. Moreover, process models for magnetic separation, hydrocyclone classification, flotation and comminution are briefly reviewed.

In Chapter 3, selected sample sets for experiments and the methodology used to approach research the subject are described in detail. The subsequent chapters are dedicated to the areas that were previously mentioned in the scope of present work. At the end of each of these chapters, the outcomes are discussed.
In Chapter 4, a new modal mineralogy method comprising a combination of Element-to-Mineral Conversion and X-ray diffraction is explained. Subsequently, a general error model applicable to modal analysis methods is introduced, and results of the various modal analysis methods are compared and discussed.

Chapter 5 describes ore textural studies on meso-scale and results that are obtained from investigating progeny particles of ore textures in size fractions. This includes changes in mineral associations, liberation, and exposed surface of minerals in particles and implication of any type of breakage.

Chapter 6 describes the approach to constructing a particle-based model by using plant survey liberation data around the primary magnetic separation stage. This kind of model can utilize liberation data and be coupled to any process model. This step is necessary towards establishing a simulation framework based on particle properties.

Chapter 7 demonstrates the application of the particle-based model in simulation and upgrading of existing unit models to work with particles. Also, possible extensions of a simulation framework for utilizing ore texture attributes and classifications are demonstrated.

Chapter 8 summarizes the result of this study and lists possible directions for future research.
2.1 Introduction

The basic ideas behind geometallurgy are simple and have been known for many years. However, geometallurgical approaches and applications have been improved by recent analytical and measurement innovations. Also, lessons have been learned from failures, and many researchers have acknowledged the multidisciplinary approach. The main aspects from several geometallurgical studies that researchers found important and critical are given in Table 1.

<table>
<thead>
<tr>
<th>Critical area</th>
<th>Main aspects</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample selection and sampling</td>
<td>• Sample representativity.</td>
<td>Ashley &amp; Callow (2000); Liebezeit et al. (2011);</td>
</tr>
<tr>
<td></td>
<td>• Data quality, error analysis, and model validation.</td>
<td>Liebezeit et al. (2011); Dominy et al. (2011);</td>
</tr>
<tr>
<td></td>
<td>• Small-scale tests.</td>
<td>Dominy et al. (2016); Kittler et al. (2011)</td>
</tr>
<tr>
<td></td>
<td>• Spatial variability in the deposit.</td>
<td></td>
</tr>
<tr>
<td>New tools and shortcut tests for geometallurgy</td>
<td>• Application of a new or modified measurement technique.</td>
<td>Walters (2009); Hallewell (2009); Vatandoost et al. (2009); Keeney &amp; Walters (2011)</td>
</tr>
<tr>
<td></td>
<td>• Small-scale and low-cost tests.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Ore textural classification and modeling.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Mineral quantification and mapping.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Multivariate analysis and modeling.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Geostatistical modeling of processing attributes.</td>
<td></td>
</tr>
<tr>
<td>Holistic and multidisciplinary approach</td>
<td>• Sustainability.</td>
<td>Dunham et al. (2011); Beniscelli (2011); Newton &amp; Graham (2011); Dominy &amp; Connor (2016); Dunham &amp; Vann (2007)</td>
</tr>
<tr>
<td></td>
<td>• Geometallurgy application during the whole cycle of a project.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Geometallurgical attributes and their additivity.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• The proxy approach towards geometallurgy.</td>
<td></td>
</tr>
<tr>
<td>Geometallurgy for circuit design, optimization,</td>
<td>• Shortcut tests for floatability and grindability.</td>
<td>Bulled &amp; McInnes (2005)</td>
</tr>
<tr>
<td>and simulation</td>
<td>• Geostatistical distribution metallurgical parameters.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Simulation to predict metallurgical performance block by block.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Geometallurgy application in flotation circuit design and optimization.</td>
<td></td>
</tr>
<tr>
<td>Systematical and traditional geometallurgical</td>
<td>• Geostatistical distribution of assays.</td>
<td>Knight et al. (2011); Niiranen (2015); Liebezeit et al. (2016)</td>
</tr>
<tr>
<td>modeling</td>
<td>• Predictive equations based on assays.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Traditional approach toward geometallurgy.</td>
<td></td>
</tr>
<tr>
<td>GeoMet model based on ore texture, particles, and</td>
<td>• A geological model capable of delivering quantitative mineralogical data.</td>
<td>Lamberg et al. (2013); Lund (2013)</td>
</tr>
<tr>
<td>simulation</td>
<td>• Simulation of process at particle level.</td>
<td></td>
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</table>

Geometallurgical issues differ from one deposit to another. Therefore, no single template can be applied to all projects. There is no merit to applying the most comprehensive and expensive approach
if a simpler and a more cost-effective approach can address the geomeallurgical issues. However, objectives in geometallurgy are more or less the same regardless of commodity or ore type. The main purposes of geometallurgy are to quantify the ore regarding spatial variability, behavior in processing and economic value. This includes a creation of a base terminology and ore descriptions so that everyone in the project in different disciples can understand the terms (Ashley and Callow, 2000).

2.2 Geometallurgy of iron ores

Magnetite, hematite, and goethite are the most abundant and economic iron ore minerals. The cut-off grade for iron ore is around 25-30 % Fe and the iron ore products commonly have 55-65 % Fe. The products are usually in the form of lump, concentrate, pelletized or sintered fines. Marketable iron ore must satisfy required specifications of products (Table 2).

Table 2. Some physical and chemical composition requirements for Iron ore products.

<table>
<thead>
<tr>
<th>Iron ore product</th>
<th>Typical physical properties of concern*</th>
<th>Typical chemical composition requirement for blast furnace *</th>
</tr>
</thead>
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<tr>
<td>Lump, Pellet, Sinter</td>
<td>Particle size, moisture level, tumble index (TI), abrasion index (Al), decrepitation index (DI), reduction degradation index (RDI), and reducibility index (RI)*</td>
<td>Fe &gt; 63%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>P &lt; 0.1%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>S &lt; 0.2%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Al₂O₃ &lt; 3.5%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>SiO₂ &lt; 3%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Ti &lt; 1%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Mn &lt; 2%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cr &lt; 1%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Ni &lt; 0.5%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>As, Cu, Zn, Pb &lt; 0.1%</td>
</tr>
</tbody>
</table>

Table 2. Some physical and chemical composition requirements for Iron ore products.

* Description of indices and their application can be found in Clout & Manuel (2015) and LKAB (2014).

The iron ore products are further processed in a blast furnace. Only around 10% of the world’s iron ore is treated by direct reduction technology (Lu, 2015). The iron ore product used for direct reduction iron (DRI) process must have at least 67% Fe. Product quality in the case of iron ore normally means restrictions for certain impurities, the most serious being phosphorous, sulfur, silica and aluminum. Respectively, these impurities originate from apatite, sulfide minerals, and silicate minerals (such as quartz, feldspars, pyroxenes, amphiboles, and micas). Details on deleterious effects of the gangue and trace elements on downstream processes can be found e.g. in Clout & Manuel (2015). Also, certain physical properties of the product for transportation and downstream processes are necessary.

Iron ore beneficiation plants are high throughput operations, meaning that economy is often dictated by the capability of processing large production volumes at low costs per ton of final product. The quality of the product, the iron concentrate, varies widely from operation to another from the relatively low grade of direct shipping ores (>55 % Fe) to very high purity of iron pellets and other special products (>67 % Fe). The former ones are often hematite ores whereas the latter are mostly magnetite ore. Iron ore mines and their processing plants traditionally use chemical analysis in resource and reserve estimates, and in grade and product quality control.

As all iron ores are heterogeneous, maintaining reasonable recovery as well as having low impurity contents in the final product requires good knowledge of the ore body and a systematic way to manage the natural variability of the resource in production. This can be reached through employing a geometallurgical program. The most important parameters that are considered for a geometallurgical program that affect the production in iron ore operations are throughput, product quality, and recovery. Examples of such studies are briefly described below, and summaries are listed in Table 3.
A geometallurgical model was built for the Hannukainen iron ore deposit to predict the concentrate quality and iron recovery (SRK Consulting (UK), 2014). An iron recovery function was established based on Davis Tube Recovery (DTR) tests done on geometallurgical samples and correlations drawn between the metallurgical response and the feed assay. The DTR is a conventional laboratory test for magnetite ore deposits. Many similar applications of DTR test have been reported in the literature (Farrell et al., 2011; Gerber et al., 2015; Leevers et al., 2005).

An empirical method has been developed to predict the SiO₂ grade of the concentrate from Luossavaara-Kiirunavaara AB’s (LKAB) concentrator plants for the Kiruna iron ore deposit (Niiranen, 2006; Niiranen and Böhm, 2013, 2012; Niiranen and Fredriksson, 2012). The method requires lab-scale comminution and Davis Tube tests. Particle size distribution, energy consumption, chemical analysis of the samples tested are gathered in a database and used for determining correlations among desired parameters. The results are then used for predicting the silica content of the iron ore concentrates.

Geometallurgical studies on Nkout (Cameroon) and Putu (Liberia) iron ore deposits were conducted using QEMSCAN analysis and metallurgical tests (Anderson, 2014). A linear regression model was used to correlate iron head grade to iron oxide liberation, iron oxide content, and grade of some gangue minerals. Metallurgical tests included DTR test followed by wet high-intensity magnetic separation tests for the tailings from the DTR test. There is no indication that the information was used for developing a geometallurgical model.

A geometallurgical model has been applied to Carol Lake iron ore deposit to predict the variation in the milling plant energy consumption and throughput. This was achieved through routinely drill core sampling and hardness test conducting. The CEET (Comminution Economic Evaluation Tool, Kosick et al. (2001)) model was used to forecast mill energy consumption based on the hardness of each block. The results were reconciled with the latest mined ores and used to update the CEET model. A better understanding of the ore body, improved mine planning, consistency of ore hardness delivered to the plant, reduced downtime losses, and improved seasonal operation were considered as the remarks of the project (Bulled et al., 2009).

BHP Billiton West Australian Iron Ore conducts a geometallurgy program for its iron ore deposits in the Pilbara (Wright et al., 2013). Within its geometallurgical program a systematic approach is used as follows:

1. The drill holes are planned to capture variability in the deposits.
2. Various physical properties of products are measured on drill cores.
3. The data from previous steps are collected in a structured database.
4. Linear regression and correlation are developed and used for predicting geometallurgical parameters (such as grade of Fe, SiO₂, P, Al₂O₃, etc.).
5. Block estimation is done based on the algorithm developed in the previous step.

Future activities to improve the geometallurgical program were described as adding process specific variables and mineralogy.

Gomes et al. (2016) performed a geometallurgical study for the Pau Branco Mine. The geometallurgical model uses concentration factors of elements to predict the product quality of iron lumps. The overall gains after applying the geometallurgical model were described by an increase of
iron ore lump reserve, reduction of mine operational costs and overall positive impact on the net present value (NPV).

Lund et al. (2013) developed a preliminary geometallurgical model of LKAB’s Malmberget iron ore based on the mineralogical approach. In the preliminary geometallurgical model, each sample and block involves information on minerals present, their chemical composition, modal composition and ore textural type. Ore textural archetypes defined in the study were used to forecast particle types produced when the block is comminuted. The developed geological model of Malmberget was based on a mineralogical approach and was allowed to provide quantitative information including liberation distribution of the plant feed to the process.

At the Kings Valley mine, in Australia, product predictive models using multivariate regression analysis were developed within a geometallurgical study for channel iron deposit (CID) and detrital iron deposit (DID) ore types. The models were used to assess product quality as well as to estimate the processability of different material types. Additionally, a yield model of each ore type was proposed based on upgrading factors which considers feed and product grades. It was noted that further metallurgical test work is required to validate the regression models (Vatandoost et al., 2013).

Rio Tinto broadened the use of their standard classification scheme (i.e. using geological observations to predict metallurgical behavior) and applied the Material Type Classification Scheme (MTCS) to predict metallurgical behavior and product quality (Paine et al., 2016). Different case studies demonstrated the outcome of the applied technique for predicting changes in throughput, ore quality and recovery of various products.

Besides the cases listed above, limited information (e.g. company info pages, reports on limited work where the geometallurgical program is mentioned) is available on further deposits where a geometallurgical program has been developed. All this indicates that geometallurgy is gradually becoming a part of the product management within the ores in production. International standards, like JORC (The Australasian Institute of Mining and Metallurgy, 2012) and NI-43-101 (CSA, 2016) both mention variation or variability in ore to be covered in the feasibility studies, but do not explicitly define the term geometallurgy. However, it is becoming more and more common that geometallurgy is included as a separate item or chapter in deposit studies.

Table 3. Iron ore geometallurgical programs (published). √ = Considered.

<table>
<thead>
<tr>
<th>Iron ore deposit</th>
<th>Throughput</th>
<th>Product quality</th>
<th>Recovery</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kiruna (Sweden)</td>
<td>√</td>
<td>√</td>
<td>-</td>
<td>Niiranen (2015)</td>
</tr>
<tr>
<td>Malmberget (Sweden)</td>
<td>-</td>
<td>√</td>
<td>√</td>
<td>Lund (2013)</td>
</tr>
<tr>
<td>Hannukainen (Finland)</td>
<td>-</td>
<td>√</td>
<td>√</td>
<td>SRK Consulting (2014)</td>
</tr>
<tr>
<td>Carol Lake (Canada)</td>
<td>√</td>
<td>-</td>
<td>-</td>
<td>Bulled et al. (2009)</td>
</tr>
<tr>
<td>Pilbara deposits (Australia)</td>
<td>-</td>
<td>√</td>
<td>-</td>
<td>Wright et al. (2013)</td>
</tr>
<tr>
<td>Kings deposit (Australia)</td>
<td>-</td>
<td>√</td>
<td>√</td>
<td>Vatandoost et al. (2013)</td>
</tr>
<tr>
<td>Nkout &amp; Putu (Cameroon &amp; Liberia)</td>
<td>-</td>
<td>√</td>
<td>√</td>
<td>Anderson (2014)</td>
</tr>
<tr>
<td>Pau Branco Mine (Brazil)</td>
<td>-</td>
<td>√</td>
<td>-</td>
<td>Gomes et al. (2016)</td>
</tr>
<tr>
<td>Rio Tinto Iron Ore</td>
<td>√</td>
<td>√</td>
<td>√</td>
<td>Paine et al. (2016)</td>
</tr>
</tbody>
</table>

2.3 Ore characterization in geometallurgy

The essential and most important part of a geometallurgical program is the ore characterization. The ore characterization includes mineralogical studies, measurement of physical properties, and
metallurgical test work of ore samples (drill core samples or composites). It reveals the behavior of ore in the process and provides criteria for process design and production management. Methods and techniques for ore characterization have been improved to offer faster, comprehensive and more accurate results. This includes novel mathematical algorithms and image processing techniques as well as instruments such as scanning electron microscopy and hyperspectral imaging.

Distinguished areas in ore characterization are known to be mineralogy and ore metallurgical attributes. In the following, the methods and techniques used in these areas are briefly reviewed.

2.3.1 Methods for obtaining mineralogical information
Knowledge on the grades of valuable elements and their variation alone is not sufficient for geometallurgy. Firstly, the distribution of the valuable elements is complex in several ore types. For example, in nickel sulfide ores, it is important to know the distribution of nickel between non-sulfides and the different sulfide minerals (Newcombe, 2011). Similarly, in the process design and optimization for porphyry copper ore beneficiation, it is critical to know how much of the total copper is hosted by different sulfide and oxide minerals (Gregory et al., 2013). Secondly, the gangue minerals also play a crucial role in processing. For example in lateritic nickel ores, the gangue minerals have a direct effect on the acid consumption and permeability of the leaching heaps (David, 2008). In refractory and trace mineral ores, like gold and platinum group element ores, the gangue mineralogy defines the entire plant performance. Therefore, elemental grades are not necessarily the best attribute to use for the estimation of recovery and ultimate value. Besides, much of the sustainability and energy efficiency dimensions of geometallurgy are driven by mineralogy. Moreover, mineral grades are additive, which makes their geostatistical modeling relatively straightforward (Vann et al., 2011).

Different levels of mineralogical and chemical information (as summarized in Table 4) are routinely used for ore characterization in geometallurgical programs. They can be divided into the following types according to increasing complexity and details: (1) elemental composition, (2) qualitative mineralogy, (3) quantitative mineralogy, and (4) mineral textures (Jones, 1987; Lamberg et al., 2013). To gather this information into a geometallurgical program, the most cost- and time-efficient analysis methods should be selected. Examples of the methods used in mineralogical characterization are (2) identification of minerals by X-ray diffraction (XRD), (3) analysis of mineral grades by quantitative X-ray diffraction (Monecke et al., 2001), and (4) deriving mineral liberation information by automated mineralogy based on scanning electron microscopy (SEM) (Fandrich et al., 2007). When considering different methods for obtaining the mineralogical information, the trueness and precision of the information must be known. Only then, a selection of the most appropriate method can be made.
Table 4. The level of information and analysis methods commonly used in geometallurgy.

<table>
<thead>
<tr>
<th>Level</th>
<th>Analysis result</th>
<th>Commonly used analysis methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Elemental composition</td>
<td>Chemical composition of samples</td>
<td>X-ray fluorescence spectroscopy (XRF); Dissolution/Laser ablation + Atomic absorption spectroscopy (AAS) / Inductively coupled plasma optical emission spectrometry (ICP-OES) / Inductively coupled plasma mass spectrometry (ICP-MS)</td>
</tr>
<tr>
<td>2. Qualitative mineralogy</td>
<td>List of minerals present in samples, lithology</td>
<td>X-ray diffraction (XRD); Optical microscopy</td>
</tr>
<tr>
<td>3. Quantitative mineralogy</td>
<td>Bulk mineralogy, i.e. mass proportion of minerals in samples (modal composition)</td>
<td>Quantitative XRD; Element-to-Mineral Conversion (EMC); SEM-based automated mineralogy (MLA, QEMSCAN, IncaMineral, etc.); Optical image analysis; Hyperspectral imaging (SisuRock); X-Ray Computed Tomography (XCT); Mineral selective analysis methods (SATMAGAN, diagnostic leaching, etc.)</td>
</tr>
<tr>
<td></td>
<td>Chemical composition of minerals (as an extra measure to evaluate mineral grade against elemental grade)</td>
<td>Electron probe microanalysis (EPMA) with energy-dispersive spectrometer (EDS)/ Wavelength-dispersive spectrometer (WDS)</td>
</tr>
<tr>
<td>4. Ore texture</td>
<td>Mineral grain sizes, grain shapes, associated minerals (rock samples), liberation distribution of minerals in samples (particulate samples)</td>
<td>SEM-based image analysis (MLA, QEMSCAN, TIMA, Mineralogic, IncaMineral, RoqSCAN); Optical image analysis; Electron backscatter diffraction (EBSD); Hyperspectral Imaging (SisuRock); X-Ray Computed Tomography (XCT)</td>
</tr>
</tbody>
</table>

In a mineralogical approach to geometallurgy, information of the mineral grades is required for the entire ore body (Lamberg, 2011). Thus, the number of samples to be analyzed for mapping the ore variation in a geometallurgical project is usually very large (>10 000; Richardson et al. 2004). When selecting a method, one must consider several factors such as the costs, required time, availability, reliability, trueness, and precision. Particularly the information on the precision of the method is frequently not available for the material to be studied.

**Automated mineralogy**

Automated mineralogy based on scanning electron microscopy (SEM) and optical image analyses (OIA) from polished samples are the known techniques for mineral identification, estimating mineral grades, and liberation, and for ore textural study. SEM-based automated mineralogy is commonly regarded as the most reliable way of estimating mineral grades. However, the method requires careful and tedious sample preparation and the method itself is costly and time-consuming (Lastra and Petruk, 2014). On the other hand, OIA-based automated mineralogy has the lower cost and is less time demanding. CSIRO (Donskoi et al., 2013) reported an OIA-based automated mineralogy which has been used for iron ore characterization. In high-grade samples, the OIA system results were close to the SEM-based
automated mineralogy (QEMSCAN), but in lower grade samples and low resolutions, the OIA results drifted away from the true values (i.e. results from QEMSCAN and XRD).

Alternative methods such as quantitative XRD by Rietveld analysis (Mandile and Johnson, 1998) and the Element-to-Mineral Conversion (EMC) method (Herrmann and Berry, 2002; Lamberg et al., 1997; Lund et al., 2013; Paktunc, 1998; Whiten, 2007) allow for simpler and faster sample preparation and can even be non-destructive. Additionally, if the aim is the estimation of mineral grade, they may offer better value than automated mineralogical analysis system only if they can fulfill the requirements on trueness and precision.

**Element-to-Mineral Conversion (EMC)**

The Element-to-Mineral Conversion, EMC, is a traditional and straightforward way to estimate mineral grades by simultaneously solving a set of mass balance equations formulated between chemical elements and minerals. The method is restricted to relatively simple mineralogy where the number of minerals is not larger than the number of analyzed components, and the chemical composition of the minerals (mineral matrix) is known. The set of equations in matrix form can be written in the following form:

\[
A \times x = b;
\]

where

\[ A : \text{Matrix of chemical composition of minerals (known)} \]
\[ b : \text{Vector of analyzed chemical composition (known)} \]
\[ x : \text{Vector of mass proportion of minerals (unknown)} \]

The unknown \( x \) can then be determined e.g. by using the non-negative least squares method (Lawson and Hanson, 1995). The EMC can be improved by using additional mineral selective analysis methods such as bromine-methanol leaching for nickel ores (Penttinen et al., 1977), copper phase analysis for copper ores (Lamberg et al., 1997) and Satmagan analysis for iron ores (Stradling, 1991).

The EMC should not be confused with normative mineralogy methods such as the CIPW Norm or the Cation Norm (Cross et al., 1902) which aims at allocating chemical compositions into minerals based on the order of mineral formation in rock. These techniques are frequently used in geochemistry and petrology for the classification of rocks. They suffer mainly from a preset mineral list with stoichiometric mineral compositions as well as from limitations when exotic minerals are present, which is common in ore deposit characterization. Additionally, they do not necessarily provide the mineral grades in weight percentages. Hence, they are not suitable for geometallurgical purposes.

Weighted least square method can be applied to improve bulk mineralogy estimation by the EMC. The method requires an initial guess and weight factors to find a solution. Usually, the initial guess is selected from results of another method such as qualitative XRD and weight factors are calculated from the standard deviation of the analysis result. A combination of the XRD Rietveld and EMC has been used by Berry et al. (2011). They applied a non-negative least square algorithm with weighted values to estimate mineral grades. Their combined method was partially successful in overcoming the limit of determination of the Rietveld analysis that was initially posed by the XRD measurement. However, using calculated weighting factors in the method not necessary gives the best solution.
**Quantitative x-ray diffraction**

Quantitative XRD methods include Known Addition, Absorption-Diffraction, Mineral Intensity Factors (MIFs) and Full-pattern-fitting (Kahle et al., 2002). The Rietveld method is a full-pattern-fitting method and is regarded as a standardless method (Rietveld, 1969). Moreover, sample preparation, measurement, and data analysis are considerably fast. Depending on the sample preparation, measurement conditions (X-ray source, data acquisition time) and crystallinity of the minerals, the detection limit can be as low as 0.5 weight percent. Demonstration of using the XRD Rietveld method for modal analysis exists in the literature (Gentili et al., 2015; König et al., 2012, 2011; König and Spicer, 2007; Paine et al., 2011; Santini, 2015).

**Spectral logging and imaging**

Hyperspectral drill core logging and imaging technologies are a recognized method for mineralogical and ore type characterization. Reflectance spectroscopy, both in the visible and infrared wavelength range, is a fast and cost-effective technique to acquire quantitative mineralogy. Complementary information can be retrieved from Raman spectroscopy in addition to hyperspectral imaging when characterizing common iron oxide minerals and gangue minerals (Ramanaidou et al., 2015). Examples of application of such a technique in mineralogical studies can be found in the literature (Bonifazi et al., 2013; Konrad et al., 2015; Macrae et al., 2008; Ramanaidou and Wells, 2011; Yang et al., 2011).

2.3.2 **Ore texture characterization**

Ore texture characterization concepts in geology focus on the geological aspects of the texture such as formation and genesis (Craig, 2001; Nyström and Henriquez, 1994). However, from a geometallurgical and process mineralogy point of view, ore texture characterization should be quantitative and provide quantitative information regarding progeny particles and their composition, i.e. on liberation distribution (Petruk, 1988). The effect of ore texture on beneficiation and other downstream processes is recognized and has been evaluated in mineral processing (Bonifazi et al., 1990; Donskoi et al., 2008; Gaspar, 1991). Qualitative or categorical geological classification is not sufficient for mineral processing. The mineralogical approach to geometallurgy requires information on ore textures to enable quantitative evaluation of mineral liberation distribution and the required crushing and grinding energies for mineral liberation. The terminology for describing mineral liberation used by various authors tends to be confusing; the following definitions are used here (see Figure 2):

<table>
<thead>
<tr>
<th>Term</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle</td>
<td>A unity consisting of single or multiple grains and single or multiple phases (particles 1, 2 and 3).</td>
</tr>
<tr>
<td>Grain</td>
<td>A unit consisting of only one mineral that has a clear interfacial surface with other grains (A and B grains in particles 1 and 3).</td>
</tr>
<tr>
<td>Liberated particle</td>
<td>A particle consisting of only one phase (Particles 2 and 3).</td>
</tr>
<tr>
<td>Degree of liberation</td>
<td>Mass proportion of mineral of interest as liberated particles in the particulate material.</td>
</tr>
<tr>
<td>Mineral liberation</td>
<td>a) An action where minerals are liberated (comminution).</td>
</tr>
<tr>
<td></td>
<td>b) A broad term which describes the mode of occurrence of mineral in particulate material.</td>
</tr>
<tr>
<td>Liberation distribution</td>
<td>Mass distribution of mineral of interest in a particle population.</td>
</tr>
</tbody>
</table>

The definition of what encompasses ore texture varies among geologists and metallurgists (Leigh, 2008). A comprehensive review of definitions for ore textures is given by Vink (1997) and Bonnici.
The common definition for ore texture refers to volume, grain size, shape, spatial distribution and association of each mineral in the ore, thus in unfractured material. The other issue is in what scale textural information needs to be collected. The term microtexture is used for grain-scale features like mineral inclusions in another grain, mesotexture for hand specimen sizes, and macrotextures for scales larger than meso-scale (Richmond and Dimitrakopoulos, 2005). Ore texture is a generic term that refers to all scales.

**Figure 2. Composite and liberated particles.**

Ore texture measurement is commonly performed on thin sections, polished slabs, or drill cores depending on the required scale and details for intact ore or particulate samples. Optical microscopy, scanning electron microscopy (SEM), hyperspectral imaging, and x-ray diffraction mapping are common methods to acquire spatial distribution of phases in the sample. The mineral map is generated, and parameters of interest are calculated. Image analysis tools are commonly used to measure and quantify ore textural attributes (Nguyen, 2013; Pérez-Barnuevo et al., 2012; Zhang and Subasinghe, 2012).

### 2.3.3 Physical and metallurgical properties of ore

Ideally, all laboratory- and pilot-scale mineral processing tests can be used in a geometallurgical study. However, the large number of samples to be tested, the cost and time for conducting the tests, and being able to use small amounts of sample for the trials limit the selection of metallurgical tests for a geometallurgical study. This means that the tests must be suitable to be performed on drill core samples in large quantities in a relatively short time.

A geometallurgical model can benefit from measured physical properties of the ore while drilling or measured on drill cores. Despite the fact that many of the measured physical properties are not directly utilized in the geometallurgical program, they can still be used to establish a proxy relation to properties of interest. For example, a good prediction of ore hardness (crushability and grindability) has been reported by correlating drill core logging data against ore hardness (Hunt et al., 2013; Keeney and Nguyen, 2014; Nguyen et al., 2016; Vatandoost et al., 2009).

Many mineral processing properties of ores are collected based on systematic metallurgical tests that relate ore characteristics to process performance such as recovery, grade, throughput, energy consumption, particle size distribution and impurities (Kojovic et al., 2010; Lamberg et al., 2013). For example, a review of small-scale tests to characterize ore hardness, crushability, and grindability, can be found in Mwanga et al. (2015). Other frequently used tests for geometallurgy of magnetite ore include Davis Tube Recovery (DTR) test (Farrell et al., 2011; Leevers et al., 2005; McQuiston and Bechaud, 1968), Low-Intensity Magnetic Separation (LIMS) tests (Koenig and Broekman, 2011; Sundberg, 1998), floatability tests (Alexander and Collins, 2008; Franzidis, 2010). In addition, including the environmental impact of ore beneficiation has been acknowledged in recent geometallurgical studies (Becker et al., 2015; Opitz et al., 2016).

### 2.4 Process models for simulation of magnetite ore beneficiation plants

Minerals and particles are the fundamental elements in mineral processing operations and simulation. Both mineral and particle properties define the selection of a process and the process performance.
However, the full potential of using particles in mineral processing simulation has not been accomplished yet. This has been partly due to lack of analyzing instruments to collect information at particle level as well as the lack of mass balancing techniques and data reconciliation methods capable of working at the mineral liberation level. Also, unit operation models which predict the behavior of individual (also multiphase) particles based on their properties are largely missing.

The development of automated mineralogy (Gu et al., 2014) has facilitated collecting particle level information. Additionally, data reconciliation and mass balancing techniques improved from the traditional approach of balancing solids and elements (Hodouin, 2010) to reconciling and adjusting particle populations (Lamberg and Vianna, 2007). These developments have built a foundation to take mineral processing unit models and simulation to a new level.

As to the level of details, mineral processing predictive models can be divided into three categories whether the smallest block in the simulation is an entire processing circuit (black box model), a section (e.g. comminution circuit) or a single unit (e.g. individual flotation cells). In geometallurgy, it is common to use models that predict the full process with simple equations. For example in Hannukainen iron ore deposit, the iron recovery into the iron concentrate is defined with a simple equation based on iron and sulfur head grade (Equation (2), SRK Consulting (2014)).

\[ R_{re} = 98.5 \times (1 - e^{0.06 \times (Fe - 6)}) \times (-1.96 \times (S/Fe) + 1) \]  

(2)

Models describing a section are also common especially when throughput or comminution energy usage is being forecasted (comminution circuit). Geometallurgical models going to unit operation level are rare. This is mainly due to the difficulty of obtaining quantitative results from geology to work at unit level as well as the lack of interface to connect geological data to the mineral processing unit.

Another way of classifying the models is based on the level of detailness for describing the process streams. A stream has a flowrate of bulk mass, elements, minerals, and particles. A bulk stream can be considered as a set of sub-streams each representing a particle size class. The flow information that defines a stream, from lowest to the highest level of detailedness, are total solids, chemical elements, minerals, and particles. Obviously, the study goal determines the selection of the level and size information. For instance, sized solids (i.e. total solids flow of a narrow particle size class) are often used to model and simulate comminution circuits whereas bulk mineral information is common in froth flotation.

Other critical dimensions of a process model are what input parameters it takes, what the limitations are and how it was developed. Empirical models are solely based on observed data without using physical or chemical principals governing the system. Phenomenological (Semi-empirical) models are based on the data, but the theory of the process is to some extent used to correlate the equations and parameters in use. Finally, the fundamental models are solely based on physical and chemical properties and sub-processes in the system without the need of experimental data. Fundamental models that consider all involving elements in the process, have not yet found their place in mineral processing simulation. This is mainly due to a large number of sub- and micro-processes taking place even in simple mineral unit operations (e.g. pumping), the significant number of particles in the system and huge demand on computational resources.

The selection of a modeling level comes with certain restrictions (Table 5) that limit its usability when expanding it outside the scope where the model is created and calibrated. For instance, while a model at total solids flowrate level (i.e. tons per hour of total ore, concentrate, tailing, etc.) is enough for
equipment sizing in the basic engineering stage of an ore project, it cannot be used for estimating the performance of a separator unit. At the grindability type level, the material is divided into grindability types, e.g. hard and soft, and these types will behave differently in comminution circuit. Clearly, the feed stream that is defined only by grindability types cannot be adopted directly, for example, in a magnetic separation model, which at least requires elemental or mineral distribution information. At minerals by behavioral types (in bulk or by size) level, each mineral is divided into behavioral type classes for a certain processing phase. For example in flotation modeling, the floatability component approach divides each mineral into fast floating, slow floating and non-floating type class (Runge and Franzidis, 2003). Broadly speaking, these classes correlate to different liberation classes (Welsby et al., 2010). However, these behavioral type classes in various separation stages, e.g. magnetic separation, are not applicable since the classes are explicitly defined for a certain separation stage. At particle level (or mineral liberation level), the assumption is that similar particles (regarding the particle’s attributes such as composition and texture) behave similarly regardless of from which part of the ore they originate.

In a process or circuit simulation, the ideal situation is where all unit operation models work at the same level. If not, then transformation functions or models must be used where some of the required stream properties are generated based on existing information of the stream and additional information required by a model.

Table 5. Modeling levels and their limitations in minerals processing. The model is valid and can be extended outside the calibration point as long as the feed stream assumptions are met.

<table>
<thead>
<tr>
<th>Level</th>
<th>Feed stream assumptions</th>
<th>Example of application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk (B)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solids (BS)</td>
<td>Each particle will behave identically regardless of its size and composition</td>
<td>Solid splitter model, equipment scale-up, basic engineering</td>
</tr>
<tr>
<td>Element (BE)</td>
<td>Mineralogy, particle size distribution, and liberation distribution are fixed</td>
<td>Recovery function model for elements</td>
</tr>
<tr>
<td>Mineral (BM)</td>
<td>Particle size distribution and liberation distribution are unchanged</td>
<td>Mineral splitter model</td>
</tr>
<tr>
<td>Behavioral type (BB)</td>
<td>Particle size distribution is unchanged. Similar behavioral types will behave identically</td>
<td>Gravity separation model</td>
</tr>
<tr>
<td>Sized (S)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solids (SS)</td>
<td>Each particle of given size will behave identically</td>
<td>Commination model, Size classification model, equipment scale-up</td>
</tr>
<tr>
<td>Grindability type (SG)</td>
<td>Each particle type of given size will behave identically</td>
<td>Commination model</td>
</tr>
<tr>
<td>Element (SE)</td>
<td>Mineralogy and liberation distribution are unchanged</td>
<td>Recovery function model in size classes</td>
</tr>
<tr>
<td>Mineral (SM)</td>
<td>Liberation distribution is unchanged</td>
<td>Mineral splitter model in size classes</td>
</tr>
<tr>
<td>Behavioral type (SB)</td>
<td>Similar behavioral types will behave identically in narrow size fraction</td>
<td>Flotation model (fast and slow floating materials in size classes), Gravity separation model in size classes</td>
</tr>
<tr>
<td>Particle (SP)</td>
<td>Similar behavior of particles of same composition and size</td>
<td>Principally applicable to all unit models</td>
</tr>
</tbody>
</table>

This study focuses on geometallurgy of iron ore and flowsheet simulation. Process unit models to be studied are selected based on applicability at the particle level for iron ore beneficiation and flowsheet simulation. The task is to identify where appropriate models exist and where development is needed. A brief summary of the review outcomes is provided at the end of this chapter.
2.4.1 Magnetic separation models

Most of the unit operation models for mineral processing simulation are focused on design and operation of the unit with recommendations for improving their performance; this is true also for magnetic separators (Cui and Forssberg, 2003; Dobbins et al., 2009; Oberteuffer, 1974; Svoboda and Fujita, 2003). Models suitable for flowsheet simulation are quite a few, they are mostly empirical, and are rarely based on physical or chemical principles behind the process. In the following, various wet magnetic separator models are reviewed and compared against the modeling levels defined in Table 5.

In magnetite ore processing, the Davis Tube Recovery (DTR) test is traditionally used to develop recovery and grade models. Its development goes back to 1921, when a test previously performed manually was mechanized (Schulz, 1963). The model gives the concentrate quality and iron recovery based on iron grade in the feed. The approach has proved to be practical for judging the response of ore to magnetic separation. However, the model is valid (thus, can be extended outside the samples studied) if mineralogy, ore texture, and distribution of particle size and liberation in the feed remain unchanged. For example, a magnetite rich sample gives in the DTR test 97% recovery for iron, this value cannot be extended to ores where the main Fe mineral is hematite (mineralogy is different), where the grain size of magnetite is much finer (texture is different), similar comminution conditions give much coarser plant feed (particle size distribution) and the degree of liberation is much lower (liberation).

The empirical model of the wet high-intensity magnetic separator (WHIMS) by Dobby and Finch (1977) indicates that the recovery of particles into the magnetic concentrate is dependent on the magnetic susceptibility and size of particles. Experimental test work is required to determine the distribution of particle size and magnetic susceptibility in the feed. Their empirical model was defined as follows:

\[ R_M = C + B \times \log_{10} \left( \frac{M_1}{M_{50}} \right) \]  

where:

- \( R_M \): Recovery
- \( M_{50} \): Machine parameter (magnetic cut point at which the recovery is 50%)
- \( B \): Machine parameter
- \( C \): Constant determined based on \( B \) and \( M_{50} \)
- \( M_1 \): An empirical parameter calculated from a formula that is related to mass fraction of magnetic material in the feed, and magnetic and hydrodynamic forces (King, 2012)

Davis and Lyman (1983) defined the feed stream using a binary system of magnetic and non-magnetic particles split into size classes and studied the effect of several operational variables like feed rate, drum speed, and magnetite/non-magnetite particle size distribution on an Eriez full-scale high gradient wet magnetic separator. A two-component model for the magnetic loss was described based on operational variables. The model lacks the ability to forecast the concentrate grade.

King and Schneider (1995) developed an empirical magnetic separator model that uses particle properties and therefore can forecast the behavior of each particle separately. In the model, the distribution of any given particle between the concentrate and tailing is a function of the volumetric
abundance of the magnetic phase in the particle. The following formula describes the fraction of particles that ends up in the tailings stream:

\[ t(g_v, d) = \alpha(d) + (1 - \alpha(d))r(g_v) \]  

(4)

where

- \( t \): Recovery of particle in the tailing
- \( g_v \): Volumetric abundance of the magnetic phase in the particle
- \( d \): Particle size
- \( \alpha(d) \): Bypass fraction of particles based on size that reports directly to the tailing
- \( r(g_v) \): Primary classification function based on volumetric grade of magnetic phase in the particle

The by-pass function (i.e. material that by-passes the magnetic separation and reports to the tailing) is modeled from experimental data using the reciprocal of a natural exponential function with two coefficients. The primary classification function is modeled by a Rosin-Rammler distribution function and is only a function of particle composition, or more exactly the volumetric grade of the magnetic phase in a particle. The model was implemented in the MODSIM simulation software. However, the size of a particle function was not considered in classification.

The magnetic separator model in the USIM PAC simulator is defined based on the recovery of minerals in size fractions also called as simple distribution or split model. The user defines recoveries to the magnetic concentrate for each mineral by particle size fraction based on experimental results. An application example was given in the context of designing an iron ore beneficiation plant in Kiruna where a statistical model for a wet low-intensity magnetic separator (WLIMS) was developed (Söderman et al., 1996). The authors simplified the model by assuming that recovery of magnetite per size class is not affected by minor changes in the head grade, feed rate or particle size distribution of the feed.

Rayner and Napier-Munn (2000) developed a model to predict the percentage loss of magnetic particles for a wet drum magnetic separator in a dense medium application. The model is represented by a flocculation rate and a residence time (Rayner and Napier-Munn, 2003a). The feed stream is described by the behavior type for magnetic particles and ferrosilicon as the dense medium. The size of the particles was not considered in the model.

A simplified approach called pseudo-liberation approach for simulating the effect of liberation in WLIMS was proposed by Ersayin (2004). The assumption behind the model was that increasing the grade of magnetite in the feed would result in decreasing the degree of liberation of gangue minerals. For a given ore and a plant, the pseudo-liberation model uses empirical data and cubic spline functions to generate a plant-operating surface as a magnetic separator model.

Metso reported a model for the LIMS that couples discrete element method (DEM), computational fluid dynamics (CFD) and finite element method (FEM; Murariu 2013). In the model, each particle is supposedly treated separately. But details on how the model predicts the behavior of particles in the unit operation are not given. According to Murariu (2013), the model can be used to study the effect of operational parameters and geometry of LIMS on the separation efficiency.

The models, as summarized in Table 6, can fairly predict the metallurgical performance of a magnetic separator unit. The majority of the models have been developed for optimization purposes with strict
adaption to the feed type. Moreover, the available models are not capable of making use of particle level information. The closest one to provide such a feature is the King and Schneider (1995) model. However, the model considers particle size only for calculating the bypass to the tailings. Thus, particles of similar composition behave identically regardless of their particle size.

Table 6. Magnetic separator models including model level (according to Table 5) and considered operational parameters.

<table>
<thead>
<tr>
<th>Model</th>
<th>Level</th>
<th>Feed properties used in model</th>
<th>Input given by user</th>
<th>Output</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>DTR function</td>
<td>BE, Empirical</td>
<td>Iron grade</td>
<td>Empirical functions</td>
<td>Iron recovery</td>
<td>Schulz (1963)</td>
</tr>
<tr>
<td>Dobby and Finch</td>
<td>SB, Empirical</td>
<td>Magnetic susceptibility and particle size distribution of the feed</td>
<td>Machine and calibration parameters</td>
<td>Recovery in size class</td>
<td>Dobby and Finch (1977)</td>
</tr>
<tr>
<td>Davis and Lyman</td>
<td>BB, Empirical</td>
<td>Feed rate of magnetics (dry)</td>
<td>Drum speed, feed and squeeze pan clearances</td>
<td>Magnetite loss, Concentrate density</td>
<td>Davis and Lyman (1983)</td>
</tr>
<tr>
<td>King and Schneider</td>
<td>SP, Empirical</td>
<td>For each particle: magnetic volumetric grade, particle size</td>
<td>By-pass function</td>
<td>Recovery of particles</td>
<td>King and Schneider (1995)</td>
</tr>
<tr>
<td>Rayner and Napier-Munn</td>
<td>BM, Phenomenological</td>
<td>Volumetric feed rate, gangue fraction, magnetic volume susceptibility, magnetic density, the volume of solids</td>
<td>Slurry viscosity in pickup zone</td>
<td>Magnetite loss in tailing</td>
<td>Rayner and Napier-Munn (2003b)</td>
</tr>
<tr>
<td>Metso</td>
<td>SP, Fundamental</td>
<td>Not specified</td>
<td>Not specified</td>
<td>Not specified</td>
<td>Murariu (2013)</td>
</tr>
</tbody>
</table>

2.4.2 Size classification models

Screening or hydrodynamic classifiers generally are employed for particle size classification in mineral processing. In screening the separation of particles is affected by their sizes (as well as the size and the shape of the aperture in the screen) while hydrodynamic classifiers use the motion of particles. Hydrocyclone and spiral classifier fall into the second category. For hydrodynamic classifiers, the particle properties are fundamentally required to model classifiers while for screens, the size distribution of particles can be sufficient.

The schematic drawing of a typical hydrocyclone is shown in Figure 3. Several reviews of the hydrocyclone models and their applications are available in the literature (Barrientos and Concha, 1990; Chen et al., 2000; Frachon and Cilliers, 1999; Heiskanen, 1997; Kraipech et al., 2006; Svarovsky, 2000). In a context of flowsheet simulation in mineral processing, the number of suitable hydrocyclone models is limited. This is because solution from fundamental modeling of hydrocyclone is computationally intensive (Nageswararao et al., 2004). The remaining models are empirical or
phenomenological models that require experimental work to obtain material specific constants. Common models of these types are reviewed shortly in the following.

Figure 3. Schematic view of a hydrocyclone.

Plitt’s hydrocyclone model (Flintoff et al., 1987; Plitt, 1976) is probably the most popular model used in the simulation of mineral processing circuits. The original Plitt’s model was revised by Flintoff et al. (1987) to have no dependency to feed size. Instead, the model uses factors for calibration to the feed data as follows:

\[ d_{50c} = F_1 \times \frac{39.7 \times D_c^{0.46} D_i^{0.6} D_o^{1.21} \eta^{0.5} e^{0.063 \phi}}{D_u^{0.71} h^{0.38} Q^{0.45} \left( \frac{\rho_s - 1}{1.6} \right)^{0.15}} \]  

(5)

\[ m = F_2 \times 1.94 \times \left( \frac{D_i h}{Q} \right)^{0.15} e^{\frac{1.58 - \phi}{4.14}} \]  

(6)

\[ P = F_3 \times \frac{1.88 \times Q^{1.8} e^{0.0055 \phi}}{D_c^{0.37} D_i^{0.54} h^{0.28} (D_u^{2} + D_o^{2})^{0.87}} \]  

(7)

\[ S = F_4 \times \frac{18.62 \times \rho_s^{0.24} \left( \frac{D_*}{D_c} \right)^{3.31} h^{0.54} (D_u^{2} + D_o^{2})^{0.36} e^{0.0054 \phi}}{D_c^{1.11} \rho^{0.24}} \]  

(8)

The parameters in the equations are:

- \( \phi \): Volumetric concentration of solids in the feed slurry (%)
- \( F_1, F_2, F_3, F_4 \): Calibration factors
- \( D_c \): The Apex diameter (cm)
- \( D_i \): The cyclone inlet diameter (cm)
- \( D_o \): The vortex finder diameter (cm)
- \( D_e \): The cylindrical section diameter (cm)
- \( h \): Free vortex height in cyclone (cm)
- \( Q \): Volumetric flowrate of feed slurry (l/min)
- \( \rho_s \): Density of the solid phase (g/cm\(^3\))
- \( \rho_c \): Density of the cyclone feed slurry (g/cm\(^3\))
- \( \eta \): Viscosity of the carrier fluid (cP)
- \( m \): Sharpness of separation
- \( P \): Cyclone inlet pressure (kPa)
- \( d_{50c} \): The corrected cut size
- \( k \): Hydrodynamic exponent

- \( S \): The volumetric flow split, i.e. volumetric flowrate in underflow / Volumetric flowrate in overflow
Lynch and Rao (1975) developed the first widely used empirical hydrocyclone model. The model uses the correlations between the geometry of the hydrocyclone and flowrates. The general form of the model is as follows:

\[
\log_{10} d_{50c} = F_1 D_o - F_2 D_o + F_3 D_i + F_4 C_w - F_5 Q_f + F_6
\]

(9)

\[
Q_f = F_7 D_o^{0.73} D_i^{0.86} P^{0.42}
\]

(10)

\[
R_f = \frac{F_8 D_o}{W_f} - F_9 \frac{1}{W_f} + F_{10}
\]

(11)

where the parameters are:

\(D_o\): The vortex finder diameter (cm)
\(D_i\): The Apex diameter (cm)
\(D_c\): The cyclone inlet diameter (cm)
\(W_f\): Mass flowrate of water in feed (t/h)
\(Q_f\): Volumetric flowrate of feed slurry (l/min)
\(C_w\): Solids weight percent in feed
\(F_{1-10}\): Calibration factors
\(fR\): Water reporting to underflow (%)

Another empirical model for flowsheet simulation is of Nageswararao hydrocyclone model. In the development of the Nageswararao model, dimensionless variables were selected to predict the performance of industrial classifiers. In his model parameters defined in parenthesis, \([\ ]\), \([\ ]\), \([\ ]\) are used for scale factors, design variables, and operating variables, respectively (Nageswararao, 1995).

\[
Q = K_1 \left[D_c^{0.907} \left(\frac{D_o}{D_c}\right)^{0.67} \left(\frac{D_i}{D_c}\right)^{0.45} \left(\frac{L_c}{D_c}\right)^{0.20} \left(\frac{P}{\rho_p}\right)^{0.50}\right]
\]

(12)

\[
\frac{d_{50c}}{D_c} = K_2 \left[D_c^{0.65} \left(\frac{D_o}{D_c}\right)^{0.52} \left(\frac{D_i}{D_c}\right)^{-0.47} \left(\frac{D_L}{D_c}\right)^{-0.40} \left(\frac{L_c}{D_c}\right)^{0.20} \left(\frac{P}{\rho_p g D_c}\right)^{0.22} \left(\frac{\rho_s g D_c}{\rho_p g D_c}\right)^{0.91}\right]
\]

(13)

\[
R_f = K_3 \left[D_c^{0.06} \left(\frac{D_o}{D_c}\right)^{-1.19} \left(\frac{D_i}{D_c}\right)^{2.40} \left(\frac{D_L}{D_c}\right)^{-0.50} \left(\frac{L_c}{D_c}\right)^{0.22} \left(\frac{P}{\rho_p g D_c}\right)^{-0.53} \left(\frac{\rho_s g D_c}{\rho_p g D_c}\right)^{0.27}\right]
\]

(14)

\[
R_f = K_4 \left[D_c^{0.06} \left(\frac{D_o}{D_c}\right)^{-0.96} \left(\frac{D_i}{D_c}\right)^{1.83} \left(\frac{D_L}{D_c}\right)^{-0.25} \left(\frac{L_c}{D_c}\right)^{0.22} \left(\frac{P}{\rho_p g D_c}\right)^{-0.31} \left(\frac{\rho_s g D_c}{\rho_p g D_c}\right)^{-0.24}\right]
\]

(15)

where the parameters are:

\(D_c\): The cylindrical section diameter (cm)
\(K_{1-4}\): material specific constants dependent
\(\theta\): Full cone angle of cyclone (Rad)
\(P\): Cyclone inlet pressure (kPa)
\(\rho_p\): Density of the cyclone feed slurry (g/cm³)
\(g\): The acceleration due to gravity (cm/s²)
\(\lambda\): is \(\beta/(\alpha - \beta)\), \(\beta\) being the volumetric fraction of solids in the feed slurry
\(R_f\): Water reporting to underflow (%)
Asomah & Napier-Munn (1997) presented a model for inclined (not vertical) hydrocyclone. The model is similar to previous models, but it takes the angle of inclination and feed viscosity into the consideration. However, no data is available for the validation of the model in large-scale operations. The empirical model is formulated as follows:

\[
d_{50c}^c = F_1 D_c^{0.23} \left( \frac{P_{40}}{D_o} \right)^{-0.46} \left( \frac{D_o}{D_c} \right)^{0.95} \left( 1 - V_{c} \right)^{1.29} \left( \frac{1.39}{180} \right) R_{e}^{-0.16} A^{0.72} e^{-\frac{2.94}{180}}
\]

\[
R_{i} = F_1 D_c^{0.47} \left( \frac{P_{40}}{D_o} \right)^{-0.21} \left( \frac{D_o}{D_e} \right)^{-1.81} \left( \frac{L}{D_c} \right)^{0.29} \left( 1 - V_{c} \right)^{0.83} R_{e}^{-0.18} A^{-0.48} e^{-\frac{2.18}{180}}
\]

\[
m = F_1 D_c^{0.15} \left( \frac{D_o}{D_c} \right)^{1.05} \left( \frac{D_u}{D_c} \right)^{-0.16} \left( \frac{\mu_u}{\mu_w} \right)^{-0.85} \left( \frac{\rho_s - \rho_p}{\rho_s} \right)^{-2.18} R_{e}^{-0.11} A^{0.43} e^{-\frac{0.29}{180}}
\]

\[
P = F_1 Q_{c}^{2.00} D_c^{-1.48} \left( \frac{\rho_s}{\rho_p} \right)^{0.44} (D_p D_o)^{-1.54} \left( \frac{L_c}{D_c} \right)^{-0.46} A^{0.25} e^{-\frac{0.46}{180}}
\]

where the parameters are:

- \( D_o \): The cylindrical section diameter (cm)
- \( D_e \): The vortex finder diameter (cm)
- \( D_s \): The Apex diameter (cm)
- \( D_i \): The cyclone inlet diameter (cm)
- \( L_c \): The length of the cylindrical section (cm)
- \( A \): Cone angle of cyclone (degree)
- \( \alpha \): Cyclone inclination from vertical (degree)
- \( \rho_s \): Density of the cyclone feed solid (kg/l)
- \( \rho_p \): Density of the cyclone feed slurry (kg/l)
- \( \mu_u \): Slurry viscosity (cP)
- \( \mu_w \): Water (fluid) viscosity (cP)
- \( F_{1-4} \): Calibration factors
- \( d_{50c} \): Corrected separation size (\( \mu \)m)
- \( P \): Cyclone inlet pressure (kPa)
- \( R_{i} \): Water reporting to underflow (%)
- \( \rho_{50} \): Size 40% feed material passing (cm)
- \( V_{c} \): Feed volume fraction of solids

Svarovsky (1984) presented a hydrocyclone model based on a dimensional analysis which involved relationships between Stokes, Euler, and Reynolds number and defined as follows:

\[
Stk_{50} = \frac{(\rho_{50} - \rho_l) v_c d_{50}^2}{18 \times \mu D_c}
\]

\[
Eu = \frac{\Delta P}{\left( \frac{\rho_l v_c^2}{2} \right)}
\]

\[
Re = \frac{D_c v_c \rho_l}{\mu}
\]

\[
v_c = \frac{4 \times Q_c}{\pi D_c^2}
\]

where the parameters are:

- \( Stk_{50} \): Stokes number for cut size \( d_{50} \)
- \( \rho_{50} \): Solids density
- \( \rho_l \): Liquid density
- \( D_c \): The internal diameter of a hydrocyclone
- \( v_c \): Characteristic velocity
However, Svarovsky’s model was developed with small cyclones and dilute slurries and has not been widely used in mineral processing (King, 2012).

An example of a hydrocyclone model that used for considering particles and ore texture is a study by Donskoi et al. (2005). He used revised Plitt’s hydrocyclone model (Flintoff et al., 1987) in USIM PAC simulation package and defined a various class of particles (density based) in size fractions as a separate phase. This data was used to predict recovery of minerals, total iron, and masses in the hydrocyclone underflow.

A common method of representing separation efficiency by size is by efficiency curve (Napier-Munn et al., 2005). It relates mass proportion of each particle size in the feed which reports to the particle size. None of the above-listed models can truly treat particles individually and give different behavior for particles being similar in size but different in composition (density).

### 2.4.3 Comminution models

In iron ore beneficiation, the purpose of the comminution is mostly to liberate iron ore minerals from gangue minerals. Further comminution to finer than liberation is unnecessary unless there is a particle size requirement for the product such as fine magnetite concentrate for pelletizing process. Comminution equipment in the mineral industry are many and differ in design and application. It is not possible nor is the objective of this study to cover all crushing and grinding models. Emphasize is given on models which are capable of delivering stream properties for flowsheet simulation instead power consumption, operating conditions or optimization. This means size distribution and liberation models which can be applied for size reduction processes. Considering modeling levels given in Table 5, only sized level models are valid here.

In the most simplified case, particle size distribution of discharge stream can be modeled by fitting particle size distribution functions such as Rosin-Rammler, lognormal or logistic distribution (see King 2012) for the product. Based on the experimental work and observations the best distribution function can be selected to model particle size distribution of the discharge stream. The distribution functions as such cannot forecast how the size distribution will be if there are changes in grinding conditions, residence time or material properties (like feed particle size distribution, mineralogy, or ore texture). Some studies (Mwanga, 2016) have used an approach where P80 from Bond equation has been used to forecast the full particle size distribution by Rosin-Rammler equation by keeping the parameter describing the steepness of the cumulative distribution curve fixed. This kind of model can be described as a forecast of particle size distribution experimentally.

Population balance model (Austin et al., 1984) is versatile and has a wider range of forecasting capability than the one described above. Once the model is calibrated, it can forecast the product particle size distribution even if the particle size distribution of the feed changes. It is based on the mass balances by particle size comprising a selection function (S) and the breakage function (B). The equation in cumulative form is defined as follows:

\[
\frac{\partial M(x,t)}{\partial t} = \int S(y)B(x,y)\frac{\partial M(y,t)}{\partial y}dy
\]
where:

\( M(x,t) \): Cumulative mass of particles finer than size \( x \)

\( S(y) \): The selection function which shows the mass fraction of size \( y \) which is going to be fragmented

\( B(x,y) \): The cumulative breakage function which is the fraction of particles of size \( y \) which are fragmented to give particles of size less than \( x \)

The equation (24) in discrete form changes to

\[
\frac{dM_i}{dt} = -S_i(t) + \sum_{j=1}^{i-1} b_{ij} S_j(t)
\]  

(25)

The most popular breakage function models are based on a mixture of two separate populations (Equation (26)). However, it can be even simplified as one population. A general and simplified representation of the selection function is in the form of equation (27).

\[
B(x,y) = K \left( \frac{x}{y} \right)^a + (1-K) \left( \frac{x}{y} \right)^b
\]

(26)

\[
S(x) = Kx^a
\]

(27)

If one takes simplified forms of selection and breakage functions, the solution of equation (24) becomes well-known Rosin-Rammler distribution.

\[
M(x,t) = M(x,0)e^{-Ax^t}
\]

(28)

Size-mass balance models can relatively well predict particle size distribution of a mill product even if the particle size distribution of the feed changes. However, the model is not capable of predicting neither mineral grades by size nor liberation distribution.

In the concept of liberation modeling, various approaches are known. The first approach is to model liberation independently from size reduction modeling and assuming that liberation process is related to the texture of the ore and the target size (Gaudin, 1939; Wiegel and Li, 1967). Usually, the main parameters in this liberation model are the average grade of phases and the size ratio between particles and grains. This approach is also called texture modeling and is achieved by superimposing particles mesh over texture image. This approach further developed from simple textures to consider a variety of ore textures (Barbery, 1991) or transformation of textures to simple forms (Meloy and Gotoh, 1985). In this, the key parameters are the volumetric grade of the ore mineral and the interfacial surface area between phases which is related to the grain size.

The second approach was developed by extending the theory of liberation (Andrews and Mika, 1976; Wiegel, 1976). These authors have considered the problem of simultaneously accounting for liberation and breakage in a batch mill. Other approaches have been reported in the literature such as integration of liberation, size reduction and process modeling (Bax et al., 2016; Khalesi, 2010).

The first part of liberation model is how the ore texture is defined or is characterized to be used for developing predictive liberation models. The second part of liberation model is how the mineral distribution in particles is defined. This can be described by distribution functions without measurement or measured by images analysis techniques. A majority of liberation models are based on binary system (i.e. an ore mineral embedded in a gangue matrix), and they lack the capability of forecasting multiphase particles. A comprehensive review of liberation models and their development
in 80’s and before was given by Barbery and Leroux (1988). Another important part of liberation modeling is how actually fragmentation (breakage) occurs. As discussed earlier, a simple approach is to superimpose particle patterns over textures. A recent review of mineral liberation and liberation in comminution is given by Mariano et al. (2016).

Practical implementation of mineral liberation models in the mineral processing is rare. This is because the models are mainly for binary systems and taking models to the multiphase system is too complicated. Nevertheless, in simplified ore textures (binary system) the models have been tested and compared against experimental data (Barbery and Leroux, 1988; Choi et al., 1986; Finch and Petruk, 1984; Hsih and Wen, 1994; Leigh et al., 1996; Schneider et al., 1991).

In simulation software of mineral processing, MODSIM has implemented complete Andrews-Mika liberation modeling. HSC Chemistry since version 7.1 (Outotec, 2012) has included liberation model as built-in comminution models. Traditional comminution models describe the product particle size distribution and internally the software forecast the liberation distribution of the product if the liberation information on the feed stream is given (Lamberg and Lund, 2012). This is done by keeping the liberation distribution within the size fractions unchanged, and the changes are applied only to mass proportions of different size fractions. As the mineral grades between the particle size fractions may be different, the shift in mass proportions of the particle size fractions would change the mineral grades in bulk. Therefore, there is an extra reconciliation step to conserve the bulk mineral balance between the feed and product.

2.4.4 Flotation models

It is known that kinetic model well describes the batch flotation results. In batch flotation modeling with its specific assumptions, such as perfect mixing, full particle suspension and capture efficiency, the rate of flotation is directly related to remaining floatable material in the cell (King, 2012). The flotation rate equation in differential form is:

\[ \frac{dC}{dt} = kC^n \]  \hspace{1cm} (29)

where \( n \) denotes the order of the equation. In the simplest form, the first order kinetic, the equation (29) becomes:

\[ C = C_0 e^{-kt} \]  \hspace{1cm} (30)

By the assumption that a fraction of each mineral is non-floatable and considering the ultimate recovery \( (R_\infty) \) the form of the equation in terms of recovery of the mineral in batch flotation and perfect mixer (industrial single tank cell) becomes:

\[ R = R_\infty \left( 1 - e^{-kt} \right) \]  \hspace{1cm} (31)

\[ R = \frac{kt}{1+kt} \]  \hspace{1cm} (32)

To find the constants, experimental data must be fitted with the equations. The extension of the first order kinetic model (Equation (31)) is the Klimpel model which has the rectangular rate distribution instead of uniform rate as the classic first order kinetic model (Dowling et al., 1985). The Klimpel (1980) kinetic model is defined as follows:
The Klimpel model has been used for analysis of more than 300 flotation tests at WEMCO® and was found to fit experimental data reasonably well (Parekh and Miller, 1999).

Kelsall (1961) presented a kinetic based flotation model consisting slow and fast floating rate constant. Comparing to classic first order kinetic model, Kelsall’s model was considered to offer a better estimate. Later his model modified by Jowett (1974) to consider ultimate recovery as follows:

$$R = R_\infty \left(1 - e^{-\frac{t}{kt}}\right)$$  \hspace{1cm} (33)

A comprehensive survey of flotation models can be found elsewhere (Dowling et al., 1985; Mavros and Matis, 1991; Runge and Franzidis, 2003; Wang et al., 2015). The other approaches of flotation modeling are the models considering environment effects. These models remark the relation between metallurgical performance and environment variables (Gorain et al., 1999; Mathe et al., 1998; Tabosa et al., 2016; Vera et al., 2002; Wang et al., 2016). Compared to other unit processing models, flotation models are more mature in reaching to particle level modeling (Lamberg and Vianna, 2007; Savassi, 2006; Welsby et al., 2010).

### 2.4.5 Summary of the process unit models for particle-based simulation

In the concept of particle-based simulation, a minimum requirement for a unit model is the capability to work at particle size level and address relevant particle properties for the unit process. This means some of the existing unit operation models can still be used in particle-based simulations with some considerations. For example, even though Efficiency Curve or Plitt’s hydrocyclone model is not particle-based in nature, the particle population can be used to generate the bulk information needed to calculate the cut size of a hydrocyclone. Mineral liberation information would be required in some areas, including magnetic separation and flotation. Regarding this study, magnetic separation model is needed to perform simulations at liberation level. The applicability and limitation of existing unit operation models for the mineralogical approach are summarized in Table 7.

<table>
<thead>
<tr>
<th>Area</th>
<th>Model</th>
<th>Considerations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Magnetic separation</td>
<td>King and Schneider (1995), Parian et al. (2016)</td>
<td>-</td>
</tr>
<tr>
<td>Comminution</td>
<td>HSC Chemistry: combined fixed particle size distribution and liberation model</td>
<td>Assumes liberation in narrow size fractions remains unchanged</td>
</tr>
<tr>
<td>Particle size classifier</td>
<td>Fixed particle size distribution</td>
<td>The only size of particles is considered to affect separation</td>
</tr>
<tr>
<td>Hydrocyclone</td>
<td>Efficiency curve/Efficiency curve by mineral</td>
<td>Does not take into account particle/mineral densities</td>
</tr>
<tr>
<td>Flotation</td>
<td>HSC Chemistry, Lamberg &amp; Vienna</td>
<td>Kinetic constants for multiphase particles deviates from linear behavior</td>
</tr>
</tbody>
</table>
3.1 Sample sets and sample preparation

Northern Sweden is known as a significant mining district in Europe with diverse styles of mineralization, including Fe oxide, Cu±Au and Au ores. In the area, more than 40 different iron ore deposits have been identified varying with respect to ore type, main ore minerals, and alteration features, etc. (Bergman et al., 2001).

One of the major companies that is active in mining and processing iron ore in Northern Sweden is LKAB. LKAB is operating in Kiruna, Malmberget and Svappavaara districts and has the world’s largest underground iron ore mines. The ore body of Kiruna is about four kilometers long and has a depth of two kilometers. The Malmberget mine consists of about 20 ore bodies and is mainly magnetite ore, but also hematite-bearing ore bodies exist. The recently opened Gruvberget mine in the Svappavaara ore field is operated as an open pit mine. Production from this mine together with the planned Leveäniemi and Mertainen mines close to Svappavaara account for about 25% of the company’s total output of iron ore in 2015.

In iron ores of Northern Sweden, from mineralogical and mineral processing point of view, the valuable iron-bearing minerals are magnetite and hematite, and the gangue minerals are apatite, amphiboles, feldspars, clinopyroxene and quartz. Garnet and calcite may be present in some of the deposits (Lund, 2013).

The sample selection for all experimental work for this study was done with collaboration with LKAB and the samples are from LKAB ore deposits and operations. The samples for each area of study are separate and vary mineralogically.

3.1.1 Sample set for modal analysis study

For modal analysis study, a total of 20 ore and process samples from the different iron ore deposits of LKAB were collected. The iron grade in the samples varied between 21-63%. The ore samples were classified as semi-massive hematite ore and massive magnetite ore (Niiranen, 2006).

Sample preparation started with crushing and splitting of the samples (Figure 4). One subsample was taken for the preparation of resin mounts to be used for automated mineralogy. The remaining part was pulverized in a swing mill and again split into two. One subsample was used for X-ray fluorescence analysis, and the second one was further ground with a swing mill to produce a very fine powder with a P_{80} of 20 microns for filling the back-loading holders with an opening diameter of 26 mm for X-ray powder diffraction analysis.
In ore projects, normally 0.3-2.0 m long drill core sections are collected for chemical assays and mineralogical study. However, crushed drill core has a wide size particle distribution, which is a problem both in sample preparation and in measurement to analyze mineral grades. In the preparation of resin mounts, crushed samples tend to segregate, i.e. large and dense particles are enriched in the lower part of the resin. This leads to a bias in the analysis of particle size distribution, mineral grades and mineral distribution (Kwitko-Ribeiro, 2012). Therefore, a common procedure is to first size the samples into narrow size fractions, which is a measure used to minimize analysis error when the focus is on quantitative textural measurements, i.e. liberation, etc.

When assaying a large number of samples (>10000), sizing is not an option since it multiplies the number of samples to be analyzed. In an analysis of polished section, using unsized samples introduces segmentation and stereological errors. The stereological error is less significant than segmentation error and is more influential in the liberation analysis than bulk mineralogy analysis as shown by Lastra and Petruk (2014). To minimize the segregation, the samples were “double sectioned,” also known as vertical sectioning. This technique is commonly used in several mineralogical laboratories and has been validated to reduce the sample segregation significantly (Kwitko-Ribeiro, 2012). In double-sectioning samples were initially mold in resin and after hardening sawed into slices. The slices were after that arranged in another mold in a way that they show the sedimentation profile towards the side to be analyzed (Kwitko-Ribeiro, 2012).

### 3.1.2 Sample set for ore textural study

Various AQ (core diameter 27 mm) and BQ drill cores (36.5 mm) of iron ore with variation in ore textures were selected for the ore textural study. The samples were cut along the core axis and were scanned by the flatbed scanner. Afterward, the drill cores were cut in intervals of two centimeters. Two pieces were used for preparing epoxy block; other pieces went through the crushing process. These pieces were crushed in laboratory jaw crusher with closed side setting opening of 3.35 mm. The crushing product was sieved, and subsamples of each size fraction were selected to make epoxy samples for particle measurements (Figure 5).
3.1.3 Sample set for model development and simulation framework

Plant survey data was used for developing the WLIMS model and simulation framework of the process. The plant survey was done at one of the LKAB’s iron ore processing plants in Kiruna, Northern Sweden. While the plant was operating at steady state, selected streams in the plant were sampled during a two hours’ period. The sampling protocol at LKAB was followed. Incremental sampling was performed around the circuit during the sampling period. Samples were taken at 10-minute intervals and added to the same bucket after each sampling interval. The cutter width was at least three times the diameter of the largest particles in the stream to minimize the sampling error. Before sampling, a dummy sample was taken, and the sampler was emptied out before taking the proper sample.

Additionally, all the available information from the process control system was recorded during the sampling period. For two of the streams, sampling was repeated to find the standard deviation and ensure the quality of the sampling.

The survey samples were prepared according to the procedure shown in Figure 6. The sample preparation was started with weighting the samples in the wet and dry state (steps 2-4), followed by deagglomeration and splitting on a rotary splitter to produce subsamples for further sizing, ensuring there was 5 – 10kg per sample to assure sufficient coarser particles per sample (step 5). The pulp samples were dried at room temperature (3). The first split was stored for later usage (8), the second for bulk chemical analysis by X-ray fluorescence (XRF) (6) and the third for wet sieving (7) followed by drying. Sieving provided four particle size fractions: +125, -125+63, -63+38, -38 µm. Each size fraction from sieving (9) was split into two parts, one for an XRF analysis (11) and the other one for preparing resin mounts for optical and scanning electron microscopy.
3.2 Analytical methods and approaches

The analytical methods and approaches are structured separately, and each part is discussed in relation to the objective of the area.

3.2.1 Modal analysis

Several types of iron ore samples were used to compare different methods of analyzing bulk mineralogy, i.e. mineral grades, to be applied in geometallurgy and process mineralogy. A new method called Combined EMC, and XRD (or shorter: Combined method) was developed in order to overcome some of the shortcomings in Element-to-Mineral Conversion and quantitative XRD by Rietveld analysis. Practically, the algorithm that was used for combined method can be applied for any other method of modal mineralogy to adjust the mineral grades to match closely with the chemical composition of given sample. Additionally, a model for describing precision and trueness in the analysis of mineral grades is presented. The model covers the whole grade range (0-100 wt%), is easy to use and informative.

Element-to-Mineral Conversion

Based on the information available (elemental assays and chemical composition of minerals), mineral grades can be calculated by the non-negative least square method. However, here the system of linear equations is underdetermined by having twelve unknowns (mineral grades) and nine equations (reliable elemental assays and Satmagan). Therefore, mathematically this system of linear equations does not have a unique solution not even when the non-negativity constraint is added. Practically this means that mineral grades are calculated for nine phases and other phases, the solution gives zero grades.

Chemical analyses of the samples (Table 8) were done at chemical laboratory of LKAB using the company’s standardized methods. X-ray fluorescence spectrometry (MagIX FAST, PANalytical) was used for the eleven major and minor elements. Divalent iron was analyzed by the titrimetric method (ISO 9035:1989) and the mass proportion of magnetic material was measured with the Saturation
Magnetic Analyzer (Satmagan) model 135 (Stradling, 1991). A calibration of the Satmagan analysis was done to give similar results as with the titrimetric Fe\(^{2+}\) method; i.e. for a pure magnetite sample, the Satmagan value was 24.3%.

Table 8. Chemical analyses of samples as wt% by XRF and Satmagan (Sat.) method.

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<th>Si</th>
<th>P</th>
<th>K</th>
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* Margin of error (± 2δ) for XRF assays can be calculated by \(±0.013 \times \sqrt{x}\) where x is the elemental assay.

**X-ray powder diffraction**

The first trial of the X-ray powder diffraction analyses was done at Luleå University of Technology (LTU) using a PANalytical Empyrean X-ray diffractometer equipped with a copper tube, Pixel3D detector, and pyrolytic graphite monochromator. The 2θ range was from 5 to 75° with a step size of 0.02°. These conditions resulted in a total measurement time of 150 minutes for a single XRD scan. Mineral phases were identified using HighScore Plus Version 3 software package and the Crystallography Open Database (COD). In the Rietveld refinement background correction, scale factors, unit cells, preferred orientations, and profile variables were included.

X-ray diffraction and Rietveld refinement with a copper tube and monochromator on the iron ore samples led to underestimation of iron mineral phases (Parian and Lamberg, 2013). This was mainly due to microabsorption and also fluorescence radiation of the iron ore samples by copper tube (Villiers and Lu, 2015). Therefore, samples were reanalyzed at the Geological Survey of Finland (GTK) with PANalytical CubiX\(^3\) industrial XRD system equipped with Cobalt tube and X'Celerator detector. Phase identification and Rietveld refinement afterward were same as described previously.

Additionally, two of the samples were measured several times in Helmholtz-Institute for Resource Technology in Freiberg, Germany using PANalytical Empyrean, equipped with a Cobalt tube, monochromator, and Xe proportional counter detector. The step width and 2θ range were same as previous measurements. The Rietveld refinement of these data was done by BGMN (BGMN by
Bergmann et al., (1998)) and these data are used for estimating error for X-ray diffraction and Rietveld refinement.

Automated mineralogy

A Merlin SEM - Zeiss Gemini (FESEM, Luleå University of Technology, Sweden) with Oxford Instrument EDS detector and IncaMineral software was used for automated mineralogy analyses. The IncaMineral system combines backscattered detector images with EDS information in the analysis of automated mineralogy (Liipo et al., 2012). Within the IncaMineral software, the raw analysis data is stored in a database, and mineral identification and quantification can be done either during analysis or retrospectively. To obtain a reliable estimate, the number of particles analyzed for the mineral quantification was at least 10,000. In this study, mineral identification was done based on back-scattered information and EDS analysis. Developed software at the Luleå University of Technology (by author) was used for post-processing the data i.e. mineral identification, reporting mineral grades and chemical composition of a sample.

To confirm IncaMineral results quality, two resin mount samples were analyzed at the geometallurgy laboratory, Technical University of Freiberg by Mineral Liberation Analyzer (MLA) system, which was equipped with FEI Quanta 650F and two Bruker Quantax X-Flash 5030 energy-dispersive X-ray spectrometers.

The automated mineralogy analysis provided a mineral list, which includes more than 15 phases. In some of the samples, even several types of one mineral were found, e.g. several amphiboles. For geometallurgy, this is not practical, and some simplification is necessary. The simplification is also required for comparing the methods. Therefore, the main phases in the samples were classified into groups of albite (Ab), actinolite (Act), apatite (Ap), biotite (Bt), diopside (Di), orthoclase (Or), quartz (Qtz), andradite (Adr), scapolite (Scp), calcite (Cal), magnetite (Mgt) and hematite (Hem). In the grouping of the minerals and the selection of group representer, the similar behavior of the minerals in the iron processing plant, the similarity in their chemical compositions, and abundance of the mineral in the group were considered to streamline application and evaluation of the methods. For example, a group of actinolite consists of various amphibole minerals such as tremolite, actinolite, and hornblende. The chemical compositions of the minerals (Table 9) were provided by LKAB and partly taken from a previous study from LKAB’s mine in Malmberget (Lund, 2013). Analysis of mineral chemistry, in those studies, was carried out at the Geological Survey of Finland (GTK) using a CAMECA SX100 electron microprobe equipped with five WDS. This information was also verified by automated mineralogy as the IncaMineral system provides the chemical composition of each analyzed grain and based on that an average composition of each phase can then be approximately calculated.
The combined EMC-XRD method originated to overcome limitations of EMC and XRD. It takes mineral grades by the Rietveld analysis as an initial estimate and changes mineral grades to minimize the following function:

\[ f(x) = \| b - A \times x \| \]

where

- \( b \): The vector of chemical composition of the sample
- \( A \): The matrix of chemical compositions of minerals
- \( x \): The vector of mineral grades, i.e. unknown to be solved

The absolute minimum of \( f(x) \) would be the results of simple Element-to-Mineral Conversion method by the methods described before (e.g. NNLS). However, finding a local minimum of \( f(x) \) close to the original Rietveld values was found to be a more appropriate solution, and therefore the Levenberg-Marquardt algorithm (Bates and Watts, 1988) was used in the combined method. Additionally, the algorithm can be applied to adjust mineral grades results from other methods to agree with the chemical composition of the sample.

Optimizing functions in MATLAB were used for an advanced combination of XRD and XRF data for solving the mineral grades. This is referred to as the combined EMC-XRD method.

**Error analysis**

Trueness is defined as “the closeness of agreement between the expectation of a test result or measurement result and a true value” whereas precision is the repeatability (or reproducibility) of the measurement method. Accuracy means “closeness of agreement between a measured quantity value and a true quantity value of a measurand” (Reichenbächer and Einax, 2011). According to The International Vocabulary of Basic and General Terms in Metrology (VIM), accuracy is a qualitative concept and commonly regarded as a combination of trueness and precision. The trueness and

---

**Table 9. The chemical composition of minerals (“the mineral matrix”) as wt%.

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<th>O %</th>
<th>F %</th>
<th>Na %</th>
<th>Mg %</th>
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<th>Si %</th>
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<tr>
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<td>0.00</td>
<td>0.00</td>
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</tr>
</tbody>
</table>

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33
precision are normally expressed in terms of bias and standard deviation, respectively (Menditto et al., 2007). To validate a method result correctly, both terms must be considered.

Commonly standards or artificially mixed samples are used for evaluating the trueness. For the analysis of mineral grades, standards are not commonly available. As this study aims to assess different analysis methods of mineral grades for practical geometallurgy, the usage of a synthetic sample was avoided. Synthetic samples would not represent the original textures, complexity, and variation existing in natural specimens. Moreover, using synthetic samples would lead to underestimating the error in the analysis of ore samples in practice.

The alternative way to evaluate the trueness is to compare against a valid reference. However, the references such as XRF analysis for chemical analysis or SEM-based automated mineralogy for mineral grades cannot be regarded as true values. Therefore, when using these references for the estimation of the trueness, which is now unknown, instead of the term trueness the term closeness was selected to evaluate how close the results are compared to the references.

Here, the precision of the methods is addressed by the standard deviation. The estimate of the standard deviation is done by replicate samples and replicate analyses. Repeating only the measurement gives the repeatability and repeating the sample preparation and measurement gives the reproducibility. In this study, the standard deviation calculated for XRF and quantitative XRD by Rietveld analysis is a measure of reproducibility, while for automated mineralogy it is a measure of repeatability.

Based on bootstrapping technique Evans and Napier-Munn (2013) suggested that the standard deviation in an analysis of mineral grades is proportional to the square root of the total area of particles measured. Moreover, they conclude that the model reflects the relationship between standard deviation and number of particles measured. Similarly, the standard deviation of an estimated mineral grade can be calculated with the formula (Evans and Napier-Munn, 2013; Mann, 2010):

$$
\sigma = \sqrt{\frac{pq}{N}}
$$

where

- $\sigma$ : The standard deviation
- $p$ : The measured mineral grade
- $q$ : is the value of $(1 - p)$
- $N$ : The number of particles measured

Comparatively, the relationship between relative standard deviation and average mineral grade can be modeled as:

$$
RSD = ax^{-0.5}
$$

where

- $RSD$ : The relative standard deviation
- $a$ : Coefficient
- $x$ : The grade of mineral of interest
The formula suggests that the relative standard deviation is proportional to the square root of the grade. This model was used in the following to estimate the (relative) standard deviation of the measurements for any mineral grade.

The measurement of the closeness is challenging. The paired t-test is often used for comparing two methods (e.g. Benvie et al., 2013). However, the t-test can be used to compare whether two methods give the same average value, but it does not provide an easy way for estimating the magnitude of the differences respect to a reference method. Nevertheless, the t-test was not completely rejected, and it was used to validate the comparison of methods in two ways; by comparing mineral grades and back-calculated elemental grades against references. The selected references for evaluating mineral grades and chemical composition analyses were SEM-based automated mineralogy and XRF analysis, respectively.

For the measuring of closeness, a Root-Mean-Square-Deviation (RMSD) was used besides the t-test (Hyndman and Koehler, 2006). Principally, RMSD aggregates the magnitude of deviations from the reference value into a single value. Mathematically, it is a concept similar to the standard deviation, but the term is used to describe an average deviation from the reference. This is used as the degree of closeness and is expressed as follows:

\[
RMSD = \sqrt{\frac{\sum_{i=1}^{n} (\mu - x_i)^2}{n}}
\]  

(38)

\[
RELATIVE\ RMSD = 100 \times \frac{RMSD}{\mu}
\]  

(39)

where

\( n \): The number of measurements

\( \mu \): The reference value

\( x_i \): The measured value

\( \bar{\mu} \): The average of the reference values

The Relative RMSD can be calculated for each mineral and element with different methods. The method showing smallest variation around the reference value (i.e. a lower RMSD) is regarded as the closest to the reference.

3.2.2 Ore textural analysis

Routine analysis of ore textural samples is affected by required details, image resolution, time and cost of analysis. Optical and SEM-based automated mineralogy are the common methods of obtaining ore textural image. The image is usually treated by image processing tools to extract textural and mineralogical information.

Here, ore textural analysis was performed in optical and scanning electron microscopy. The aim was to analysis particulate and intact rock samples to generate the mineral map. Afterward, the mineral map was used for retrieving textural attributes and liberation. Therefore, for eight drill cores, mineral maps were created for intact ore and particulates samples after crushing. Crushed sample sieved and sized in 1.68-3.35 mm, 0.85-1.68 mm, 0.43-85 mm and 0.30-0.43 mm size fractions. Measurement of below 0.30 mm size fraction was skipped due to the high liberation of minerals in all samples.
**Image acquisition**

Image acquisition of ore texture was performed by mosaic capturing of field images by automated stage optical microscopy (Zeiss Axio Imager) and SEM backscatter detector (AZtec - Zeiss Merlin). The whole image of the samples was made by stitching field images using built-in programs. Minerals relating to specific gray level in backscatter image were identified by EDS analysis of the phases at that gray level. This data was used later in assigning phases in mineral maps.

**Image processing**

Image processing is a rapidly advancing area of retrieving information from images. The technique is used to classify objects in the image (such as grains, particles or phases) and retrieve a broad range of features. In an ore textural study, captured images are used for phase discrimination, calculation of object shape factors, mineral grades, and the association between phases. In this study, image processing sequences including phase discrimination, object separation, feature extractions were done by writing code in MATLAB. The code can analyze ore texture and particulate samples to give numeric ore textural features and liberation. The extension of the code can generate particle population from ore texture by defining breakage pattern and particle size distribution.

**Phase separation**

Phase separation began by assigning multiple threshold values according to a range of gray levels corresponding to each phase. The image pixel values matching each threshold interval were assigned a new value representing a phase. In particulate samples, the epoxy region was assigned a zero value for simpler processing of objects during imaging processing.

**Composition and liberation**

Obtaining a mineral map of ore texture or particulate sample facilitates the calculation of mineral grades and liberation. Commonly, the area of each phase (number of pixels occupied by the phase) in a particle or whole texture are calculated to obtain information on the composition of the particle. To convert this value to weight percentages, the density of the minerals is used as weight factors in the calculation of composition.

The other important factor that can be useful in characterizing breakage and also relevant in some aspect of mineral processing (such as flotation and leaching) is liberation by exposed surface area of particles. In each particle, this is calculated by normalizing measured shared boundary between phases and background (epoxy).

**Mineral association**

Association of minerals can be estimated based on the proportion of minerals in the particles. However, this approach for the intact ore texture only gives mineral grades of texture. Therefore, an alternative method is to calculate the interfacial surface area between minerals in the intact ore texture or particle as an indication of association.

An image can be considered as a matrix of pixel values. An easy and straightforward way of estimating the association in the image is using co-occurrence matrix. A mineral map with n phases (n pixel values) will have $n \times n$ size co-occurrence matrix. Each cell of the matrix, $C(i,j)$, is correspondence to the number of times that the cell $i$ is situated with cell $j$ in the defined offset. Here, for calculation of association, the co-occurrence matrix is the sum of cell values for 0-360° in intervals of 45° (Figure 7).
For example, for a simple case with three-pixel values as below with one-pixel distance offset, the corresponding co-occurrence for different orientation is as Table 10.

Therefore, the co-occurrence matrix for Figure 8 is:

\[
C = \begin{bmatrix}
12 & 22 & 13 \\
22 & 16 & 14 \\
13 & 14 & 18 \\
\end{bmatrix}
\]  

The co-occurrence matrix can be normalized to give an indication of association based on the abundance of a phase interfacial in the sample. This can be done by normalizing non-diagonal cells, row or column wise. This is called Association Indicator Matrix (AIM). For example, for above example, AIM is:

\[
AIM_c = \begin{bmatrix}
0 & 62.9 & 37.1 \\
61.1 & 0 & 38.9 \\
48.1 & 51.9 & 0 \\
\end{bmatrix}
\]

The non-diagonal values are the association indicators. For the above example, phase one has 62.9% association with phase two and 37.1% with phase three. In the particles, the exposed surface of
particles may consider in the calculation. This can be done by including the background (epoxy) as another phase. This also makes the calculation of the surface exposure of minerals straightforward.

**Limitations**

The optical image was planned to be used for discrimination of hematite and magnetite in the samples. Even though hematite and magnetite could be distinguished easily in the optical image, imperfect image stitching by built-in programs lead to incorrect registration of image objects (Figure 9). Additionally, uncorrected uneven illumination in the image fields presented another obstacle in the image processing of the data (Figure 10). These problems could have been fixed by correcting uneven illumination in the field images as well as aligning field images in a correct way. However, AZtec system for capturing backscatter images does not provide an easy way to access field images.

![Figure 9. Imperfect image registration. Optical image (left), BSE image (middle), Blend of Optical and BSE images (right).](image1)

![Figure 10. Uneven illumination effect in the stitched images (left side optical image, right side BSE image).](image2)

**3.2.3 Model development and simulation framework**

**Wet Low-Intensity Magnetic Separator (WLIMS) model development**

Chemical analyses of the plant survey samples were done at the chemical laboratory of LKAB. The data was used as a quick sanity check to evaluate the quality of modal mineralogy by automated mineralogy. Epoxy samples on size fractions were prepared at the Kemi University of Applied Science. Scanning electron microscopy (SEM) and automated mineralogy analysis on epoxy samples were done by using a Merlin SEM (FESEM - Zeiss Gemini) with Oxford Instrument EDS detector at Luleå University of Technology, Sweden.

On average, more than 20,000 particles were measured in each size fraction, which sums up to around 300,000 particles in three streams around primary magnetic separator. Identifying of minerals, reporting of mineral grades and back-calculating of chemical compositions were done by post-
processing the raw data (software developed by author). The mineral list shown in Table 11 was used as the reference for the program and back-calculation of the chemical composition of samples. The chemical composition of minerals was taken from Lund et al. (2013) and verified by EDS analysis.

Mass balancing, data reconciliation, particle tracking, LIMS modeling were done using the modeling and simulation software HSC Chemistry 9 by Outotec and MATLAB by Mathworks.

Table 11. Average chemical composition of minerals ("the mineral matrix") as wt% and their specific gravity (g/cm$^3$).

<table>
<thead>
<tr>
<th></th>
<th>Magnetite</th>
<th>Quartz</th>
<th>Apatite</th>
<th>Biotite</th>
<th>Albite</th>
<th>Actinolite</th>
<th>Calcite</th>
<th>Titanite</th>
<th>Ti-magnetite</th>
<th>Anhydrite</th>
</tr>
</thead>
<tbody>
<tr>
<td>F %</td>
<td>0.00</td>
<td>0.00</td>
<td>3.72</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>S %</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>23.55</td>
</tr>
<tr>
<td>Na %</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.02</td>
<td>5.11</td>
<td>0.02</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Mg %</td>
<td>0.01</td>
<td>0.00</td>
<td>0.07</td>
<td>10.26</td>
<td>0.00</td>
<td>10.09</td>
<td>0.00</td>
<td>0.00</td>
<td>1.94</td>
<td>0.00</td>
</tr>
<tr>
<td>Al %</td>
<td>0.05</td>
<td>0.00</td>
<td>0.00</td>
<td>6.91</td>
<td>10.78</td>
<td>0.99</td>
<td>0.00</td>
<td>0.00</td>
<td>2.60</td>
<td>0.00</td>
</tr>
<tr>
<td>Si %</td>
<td>0.00</td>
<td>46.72</td>
<td>0.00</td>
<td>19.60</td>
<td>33.98</td>
<td>25.30</td>
<td>0.00</td>
<td>14.32</td>
<td>0.02</td>
<td>0.00</td>
</tr>
<tr>
<td>P %</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>16.06</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>K %</td>
<td>0.00</td>
<td>0.01</td>
<td>0.00</td>
<td>6.55</td>
<td>0.00</td>
<td>0.11</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Ca %</td>
<td>0.00</td>
<td>0.01</td>
<td>40.39</td>
<td>0.00</td>
<td>0.04</td>
<td>7.55</td>
<td>37.17</td>
<td>20.44</td>
<td>0.02</td>
<td>29.43</td>
</tr>
<tr>
<td>Ti %</td>
<td>0.05</td>
<td>0.00</td>
<td>0.00</td>
<td>2.24</td>
<td>0.01</td>
<td>0.01</td>
<td>0.00</td>
<td>24.41</td>
<td>12.95</td>
<td>0.00</td>
</tr>
<tr>
<td>V %</td>
<td>0.04</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Mn %</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.04</td>
<td>0.01</td>
<td>0.04</td>
<td>0.00</td>
<td>0.00</td>
<td>0.71</td>
<td>0.00</td>
</tr>
<tr>
<td>Fe %</td>
<td>72.43</td>
<td>0.02</td>
<td>0.16</td>
<td>10.77</td>
<td>0.01</td>
<td>8.00</td>
<td>0.00</td>
<td>0.00</td>
<td>49.44</td>
<td>0.00</td>
</tr>
</tbody>
</table>

| S.g.*  | 5.2       | 2.7    | 3.2     | 2.9     | 2.6    | 3.0        | 2.7     | 3.6      | 5.2          | 3.0       |

Specific gravity

Simulation framework

The flowsheet was drawn in HSC Chemistry 9.1 Sim module and is used to demonstrate different levels of modeling according to Table 5. The newly made particle-based WLIMS model was also adapted in HSC Chemistry 9.1 Sim to be used for the simulation.
4.1 Introduction

Reliable analysis of mineral grades is a crucial part of resource characterization, process mineralogy, and geometallurgy. It is a prerequisite for deportment analysis, mineralogical mass balancing and modeling and simulation of mineral processing circuits. Recently, automated mineralogy has become the major method for the analysis of mineral grades. In geometallurgy, however, the method is far too expensive and time demanding. When there is a need for assaying mineral grades in thousands of ore samples, sizing to narrow size fractions is necessary, and the total number of samples for the analysis becomes enormous. Therefore, an alternative method is needed for better value. In the following results from different modal analysis methods obtained and compared.

4.2 Analysis of mineral grades in the iron ore samples

In iron ores, it is essential to have a good estimate of the magnetite-hematite ratio since this ratio defines the concentration technique used and in Malmberget iron operations it determines the process line the ore is fed into (Alldén Öberg et al., 2008). Furthermore, in Kiruna iron operations the apatite grade is used to classify the iron ores (Niiranen and Böhm, 2012). The phosphorous content of the final concentrate is a quality criterion; for instance, in the Low Phosphorous Sinter Feed (MAF) the maximum acceptable grade is 0.025% P (LKAB, 2014).

From a geometallurgical point of view, magnetite, hematite, and apatite are the most significant minerals in the iron operations in Northern Sweden. The analytical results for these minerals by different methods are compared in Table 12. It should be noted for the magnetite grade by EMC, Satmagan analysis was used while this was not used in the combined method. Distinguishing magnetite and hematite in automated mineralogy is challenging and requires careful and precise setting (Figueroa et al., 2011). For apatite, the detection limit of XRD can be as low as one wt%. However, the combined method should allow overcoming this limit by considering XRF analysis.

Having a good estimate of the gangue silicate minerals in the ore is crucial considering that silica is one of the quality requirements for an iron concentrate. The main silicate minerals in the samples are albite, actinolite, and biotite. Iron-bearing garnet, i.e. andradite, is found with calcite in certain deposits (Frietsch, 1980). Accessory and trace silicate minerals include scapolite, diopside, orthoclase and quartz. The silicate minerals are normally not considered when classifying the ores of LKAB (Niiranen and Böhm, 2012). However, the silica content of the final product must be below certain values, e.g. for Low Phosphorous Sinter Feed (MAF), the limit is 0.80% SiO₂ (LKAB, 2014). Adolfsson and Fredriksson (2011) observed that silica content in the concentrate does not directly correlate with the silica grade in the ore. This refers to that the silicate minerals do not all behave in the same way in iron ore processing. For example, biotite tends to be enriched in fine particle sizes (Westerstrand, 2013) where the separation efficiency in concentration is poor, while andradite can end up to concentrate if the magnetic separator is not properly tuned.
### Table 12. Analysis of mineral grades for the most significant minerals: magnetite, hematite, and apatite.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Magnetite (wt%)</th>
<th>Hematite (wt%)</th>
<th>Apatite (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EMC</td>
<td>XRD</td>
<td>CMB</td>
</tr>
<tr>
<td>1</td>
<td>88.57</td>
<td>89.6</td>
<td>88.27</td>
</tr>
<tr>
<td>2</td>
<td>60.12</td>
<td>74.6</td>
<td>72.43</td>
</tr>
<tr>
<td>3</td>
<td>70.90</td>
<td>78.9</td>
<td>78.17</td>
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<tr>
<td>4</td>
<td>26.95</td>
<td>29.4</td>
<td>27.84</td>
</tr>
<tr>
<td>5</td>
<td>71.31</td>
<td>79.9</td>
<td>79.38</td>
</tr>
<tr>
<td>6</td>
<td>12.86</td>
<td>12.0</td>
<td>15.09</td>
</tr>
<tr>
<td>7</td>
<td>1.25</td>
<td>0.0</td>
<td>1.06</td>
</tr>
<tr>
<td>8</td>
<td>2.08</td>
<td>0.0</td>
<td>0.84</td>
</tr>
<tr>
<td>9</td>
<td>2.91</td>
<td>0.0</td>
<td>0.90</td>
</tr>
<tr>
<td>10</td>
<td>2.08</td>
<td>2.70</td>
<td>79.94</td>
</tr>
<tr>
<td>11</td>
<td>2.49</td>
<td>0.0</td>
<td>1.58</td>
</tr>
<tr>
<td>12</td>
<td>81.18</td>
<td>85.1</td>
<td>79.79</td>
</tr>
<tr>
<td>13</td>
<td>86.44</td>
<td>84.6</td>
<td>85.17</td>
</tr>
<tr>
<td>14</td>
<td>64.89</td>
<td>66.2</td>
<td>64.01</td>
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<tr>
<td>15</td>
<td>66.27</td>
<td>66.6</td>
<td>65.60</td>
</tr>
<tr>
<td>16</td>
<td>26.75</td>
<td>28.2</td>
<td>26.52</td>
</tr>
<tr>
<td>17</td>
<td>49.76</td>
<td>49.3</td>
<td>50.53</td>
</tr>
<tr>
<td>18</td>
<td>75.04</td>
<td>78.0</td>
<td>76.36</td>
</tr>
<tr>
<td>19</td>
<td>96.87</td>
<td>98.3</td>
<td>96.39</td>
</tr>
<tr>
<td>20</td>
<td>83.33</td>
<td>82.2</td>
<td>83.26</td>
</tr>
</tbody>
</table>

**EMC:** Element-to-Mineral Conversion, **XRD:** Quantitative XRD by Rietveld analysis, **CMB:** Combined EMC-XRD, **AM:** SEM-based automated mineralogy

Considering iron ore processing, biotite, andradite and silicate minerals have significance. EMC underestimates the biotite and andradite grade (Table 13). This is due to the presence of many silicate minerals and the lack of enough assay variables to estimate them correctly. Comparing to automated mineralogy results, in some samples, the Rietveld analysis overestimated the biotite grade which could be due to preferred orientation and partly very low content resulting in high relative errors (Kleeberg et al., 2008). On the other hand, all methods gave more or less similar grades for other silicate mineral estimations, i.e. the sum of albite, actinolite, diopside, quartz and scapolite.

### Table 13. Analysis of mineral grades for biotite, andradite and other silicates, which includes scapolite, diopside, orthoclase, and quartz.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Biotite (wt%)</th>
<th>Andradite (wt%)</th>
<th>Other silicates (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EMC</td>
<td>XRD</td>
<td>CMB</td>
</tr>
<tr>
<td>1</td>
<td>4.32</td>
<td>1.4</td>
<td>4.75</td>
</tr>
<tr>
<td>2</td>
<td>114</td>
<td>0.8</td>
<td>1.72</td>
</tr>
<tr>
<td>3</td>
<td>1.07</td>
<td>0.0</td>
<td>0.35</td>
</tr>
<tr>
<td>4</td>
<td>1.39</td>
<td>1.7</td>
<td>2.05</td>
</tr>
<tr>
<td>5</td>
<td>0.86</td>
<td>0.0</td>
<td>0.29</td>
</tr>
<tr>
<td>6</td>
<td>0.00</td>
<td>0.0</td>
<td>0.00</td>
</tr>
<tr>
<td>7</td>
<td>0.00</td>
<td>0.0</td>
<td>0.00</td>
</tr>
<tr>
<td>8</td>
<td>0.00</td>
<td>0.0</td>
<td>0.00</td>
</tr>
<tr>
<td>9</td>
<td>0.00</td>
<td>0.0</td>
<td>0.92</td>
</tr>
</tbody>
</table>
4.3 Developing a grade-based error model

4.3.1 Precision of the analyses

Repeats and replicates were used for estimation of the standard deviation of the analyses. For establishing the error model for precision, the relative standard deviation against mineral grade was fitted with equation (37). In principle, the error model gives the coefficient of variation (i.e. relative standard deviation) for the mineral grade of interest (Figure 11). In general, a good fit between experimental data and model equation was achieved. Comparatively, the precision of the methods from the best to the worst are: 1) SEM-based automated mineralogy, 2) Element-to-Mineral Conversion, 3) quantitative XRD with Rietveld for simple mineralogy, 4) combined EMC-XRD, and 5) quantitative XRD with Rietveld for complex mineralogy. This means, for example, for an average ore sample with 70% magnetite (or hematite) the precision of the methods (i.e. uncertainty in 95% confidence level) vary from ±0.57 to ±3.68 wt%. This can be regarded as acceptable in geometallurgy. On the other hand, for average ore grade of 1 wt% such as apatite and biotite, the coefficient of variation is between 4 and 22% (standard deviation 0.04-0.22 wt%). The error is high for technical work like resource estimation or process mineralogy (Pitard, 1993) but the analysis quality is still good enough for geometallurgical purposes like domaining where acceptable error can be higher.
Figure 11. Relative standard deviation against mineral grades (CMB, AM, XRD). Curves for different methods derived from replicates and repeats. For Element-to-Mineral Conversion (EMC) and combined method (CMB) curves were generated using Monte Carlo simulation. For calculating the relative standard deviation of combined method, relative standard deviation of XRD with complex mineralogy was used. The dashed vertical line at 1% mineral grade shows the detection limit of XRD.

4.3.2 Closeness of the analyses

For quality control, two resin mounts analyzed by IncaMineral were also analyzed by Mineral Liberation Analyzer (MLA). Comparing analyzed minerals by IncaMineral against MLA analysis (Table 14), mineral grades by IncaMineral are close to MLA mineral grades, which suggest that the two methods are giving similar results.

Table 14. Comparing mineral grades by IncaMineral (INCA) system and Mineral Liberation Analyser (MLA) system. For INCA 95% confidence interval is given.

<table>
<thead>
<tr>
<th></th>
<th>Fe oxide (wt%)</th>
<th>Apatite (wt%)</th>
<th>Biotite (wt%)</th>
<th>Andradite (wt%)</th>
<th>Other silicates (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>MLA</td>
<td>INCA</td>
<td>MLA</td>
<td>INCA</td>
<td>MLA</td>
</tr>
<tr>
<td>A</td>
<td>89.90</td>
<td>89.83±0.68</td>
<td>1.12</td>
<td>1.01±0.07</td>
<td>1.74</td>
</tr>
<tr>
<td>B</td>
<td>77.53</td>
<td>77.68±0.63</td>
<td>3.62</td>
<td>3.33±0.13</td>
<td>1.95</td>
</tr>
</tbody>
</table>

Automated mineralogy analysis results were used as the reference values when comparing closeness of the methods. The paired t-test implies that XRD, combined EMC-XRD, and EMC do not give significantly different results compared to automated mineralogy (Table 15). On the other hand, relative RMSD shows that the difference between the automated mineralogy and EMC is relatively higher than that of the other methods (Figure 12 and Table 15). Relative RMSD reveals that XRD results for iron oxide are closest to automated mineralogy while paired t-test suggests XRD results are slightly positively biased.
Figure 12. Relative RMSD against mineral grades (EMC, XRD, CMB). Curves for different methods derived from fitting calculated RMSD for experimental data.

Table 15. The closeness of analysis methods for mineral grades by paired t-test and RMSD against automated mineralogy as the reference.

<table>
<thead>
<tr>
<th></th>
<th>t value</th>
<th></th>
<th></th>
<th>RMSD</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>XRD</td>
<td>CMB</td>
<td>EMC</td>
<td>XRD</td>
<td>CMB</td>
<td>EMC</td>
<td></td>
</tr>
<tr>
<td>Fe oxides</td>
<td>2.82*</td>
<td>1.81</td>
<td>2.20</td>
<td>4.77</td>
<td>6.31</td>
<td>8.76</td>
<td></td>
</tr>
<tr>
<td>Apatite</td>
<td>-0.07</td>
<td>-0.52</td>
<td>-0.31</td>
<td>1.80</td>
<td>1.56</td>
<td>1.54</td>
<td></td>
</tr>
<tr>
<td>Biotite</td>
<td>0.56</td>
<td>1.53</td>
<td>1.49</td>
<td>0.79</td>
<td>1.59</td>
<td>1.74</td>
<td></td>
</tr>
<tr>
<td>Andradite</td>
<td>-1.38</td>
<td>-2.06</td>
<td>-2.21</td>
<td>1.74</td>
<td>2.12</td>
<td>9.64</td>
<td></td>
</tr>
<tr>
<td>Other silicate</td>
<td>-0.16</td>
<td>0.63</td>
<td>2.00</td>
<td>1.63</td>
<td>1.61</td>
<td>2.41</td>
<td></td>
</tr>
<tr>
<td>t critical</td>
<td>±2.26</td>
<td>±2.26</td>
<td>±2.26</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* Absolute value of t is greater than critical value indicating statistically significant difference in results between automated mineralogy and the method

The alternative way of evaluating closeness was by regarding XRF analysis as the reference value and comparing back-calculated chemical compositions of the samples against it. Paired t-test results suggest that combined EMC-XRD and EMC methods give significantly different mean values for the chemical composition (Table 16). However, relative RMSD indicates all the methods in terms of deviations from XRF assays are in the same range (Figure 13). In other words, the deviation from the true (i.e. reference) value in all the methods is about equal.
Figure 13. Relative RMSD against elemental grades (AM, EMC, CMB, XRD). Curves for different methods derived from fitting calculated RMSD for experimental data.

Table 16. The closeness of analysis methods for elemental grades by paired t-test and RMSD against XRF analysis as the reference.

<table>
<thead>
<tr>
<th>Chemical Assays</th>
<th>t value by paired t-test</th>
<th>RMSD</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>XRD</td>
<td>CMB</td>
<td>EMC</td>
<td>AM</td>
<td>XRD</td>
</tr>
<tr>
<td>Na</td>
<td>1.39</td>
<td>1.27</td>
<td>-0.36</td>
<td>2.85*</td>
<td>0.35</td>
</tr>
<tr>
<td>Mg</td>
<td>-2.75*</td>
<td>-2.07</td>
<td>-3.43*</td>
<td>-1.06</td>
<td>0.36</td>
</tr>
<tr>
<td>Al</td>
<td>0.86</td>
<td>-0.34</td>
<td>2.17*</td>
<td>1.34</td>
<td>0.47</td>
</tr>
<tr>
<td>Si</td>
<td>2.40*</td>
<td>2.03</td>
<td>1.48</td>
<td>0.42</td>
<td>0.92</td>
</tr>
<tr>
<td>P</td>
<td>-3.69*</td>
<td>-5.52*</td>
<td>-5.40*</td>
<td>0.40</td>
<td>0.14</td>
</tr>
<tr>
<td>K</td>
<td>-0.06</td>
<td>4.35*</td>
<td>-0.23</td>
<td>0.25</td>
<td>0.26</td>
</tr>
<tr>
<td>Ca</td>
<td>-0.94</td>
<td>2.72*</td>
<td>1.77</td>
<td>0.81</td>
<td>0.60</td>
</tr>
<tr>
<td>Ti</td>
<td>0.78</td>
<td>1.75</td>
<td>-0.22</td>
<td>5.18*</td>
<td>0.18</td>
</tr>
<tr>
<td>V</td>
<td>-2.19*</td>
<td>-2.17*</td>
<td>-2.03</td>
<td>-1.52</td>
<td>0.06</td>
</tr>
<tr>
<td>Mn</td>
<td>-12.97*</td>
<td>-12.80*</td>
<td>-13.60*</td>
<td>-8.97*</td>
<td>0.08</td>
</tr>
<tr>
<td>Fe</td>
<td>-0.19</td>
<td>-1.17</td>
<td>2.57*</td>
<td>-1.42</td>
<td>1.91</td>
</tr>
<tr>
<td>Satmagan</td>
<td>0.47</td>
<td>0.12</td>
<td>-2.67*</td>
<td></td>
<td>1.12</td>
</tr>
</tbody>
</table>

* The absolute value of t is greater than the critical value indicating statistically significant difference between analyzed chemical composition (XRF) and back-calculated composition from the mineral composition.

4.4 Discussion on results of combined method and application of grade-based error model

Quantitative X-ray diffraction with Rietveld analysis has been proposed as a quick mineralogical method for geometallurgy. Challenges in the method are the detection limit and general doubts about its precision and trueness when there is complex mineralogy. Partially, these challenges can be overcome by proper sample preparation (Pederson et al., 2004). For iron ores, when there are significant variations in the grade of iron oxide, phyllosilicate, and minor phases in the samples, sample preparation needs to be adapted carefully for different grade ranges. Additionally, to obtain
best results from Rietveld refinement, the radiation source, the effective particle size to minimize micro-absorption, and the proper way of filling sample holder to minimize preferred orientation must be sensibly selected. When aiming for a practical solution in this study, not all these conditions were optimum.

A combined method using weighted values (Berry et al., 2011; Roine, 2009) provides an alternative to adjusting mineral grades to match the Rietveld analysis results and chemical assays, but its problem is how to define the weighting factors in order to get reliable results. Weighting factors can be set based on the uncertainties of the elemental and mineral grade, but still, this approach cannot overcome limitations such as XRD detection limit and high relative error in low mineral grades. The combined EMC-XRD method developed here does not use weighting factors but can still find the closest solution to match both the Rietveld analysis results and chemical assays. Knowing the error model, more constraints can be established for estimating mineral grades by combined method.

Any technique for the analysis of mineral grades in a geometallurgical program requires careful mineralogical study before the method is routinely applied. In combined method, the mineralogical study must provide information on the list of all possible minerals, their crystal structure, and their chemical composition. Additionally, to be able to apply the combined method, the minerals need to be grouped in a sensible way, i.e. groups consist of minerals with similarity in chemical composition as well as process behavior. Therefore, nature of the ore body and the process define the grouping of minerals, acceptable error, and eventually the method to be used.

However, combined method is not a universal solution for every situation. Principally, the algorithm for estimating mineral grades can take as many restrictive constraints as needed. Therefore, if several minor minerals are present in the sample but the information for calculating mineral grades is insufficient, the combined method requires additional constraints to converge to the optimal solution. In addition, the assumption used here is that the chemical composition of minerals is known and does not vary. Strictly speaking, this is not a realistic assumption, but it simplifies the complex situation for finding a bridge between elemental assays and mineral grades.

It is relatively rare to find error estimation for the analyses of mineral grades published in the literature and research reports. For quality control, the back-calculated chemical composition is often plotted against the analyzed ones (e.g. Berry et al., 2011; Hestnes and Sørensen, 2012). As these illustrations visualize the quality, they do not quantify how big the difference is. Paired t-test is used, but as was shown in the results, it fails in measuring how close the results are. In addition, it requires that standard deviations be equal and not dependent on the grade, which is an unrealistic assumption. Relative RMSD is an informative and efficient way of measuring the closeness. The calculation is similar to the standard deviation, which makes it straightforward and portable for several purposes like mass balancing and modeling.

The precision and degree of trueness of analysis for mineral grades are dependent on the abundance of a phase in a sample and the number of observations (counts) collected. In automated mineralogy, this depends on the number of particles and grains analyzed. In X-ray techniques (X-ray diffraction and X-ray fluorescence), the ratio of signal to noise, thus analysis time, plays the role. Here a simple equation was used to describe the standard deviation and the RMSD in the wide grade range where analysis conditions are the same as commonly used in process mineralogy. This approach is practical when individual standard deviations are needed for measurements. Examples of such problems are circuit mass balancing and Monte Carlo simulations.
The methods available for obtaining mineral grades either directly (such as quantitative XRD by Rietveld analysis and automated mineralogy) or indirectly (EMC and combined EMC-XRD) have different advantages and disadvantages. Table 17 summarizes the different methods and their applicability in geometallurgy. To be used for metallic ores, the detection limit must be lower than one wt%, which excludes XRD. In geometallurgical programs, the number of samples to be analyzed during developing a deposit model is high, several thousand in a year. Therefore, the requirements for sample preparation and analysis time and costs exclude the usage of automated mineralogy as a routine tool for the analysis of mineral grades in geometallurgy. Even though Element-to-Mineral Conversion has excellent repeatability, it suffers from poor trueness in most of the real geometallurgical cases. This is due to a larger number of unknowns (minerals) than known quantities (chemical elements assayed) which makes the system mathematically underdetermined. Hence, the combined method fulfills the requirements to be used in ore characterization and deposit modeling for geometallurgy.

The problem remaining is that with all methods the back-calculated chemical composition does not match perfectly with the chemical assays of the commodity elements. This makes adoption of mineral grades challenging as resource geologists and metallurgist have a long tradition to work with chemical assays, they find it difficult to take parallel mineralogical information that is not entirely consistent with chemical assays. Weighting can be a solution for that, but more work is needed to establish solid grounds for defining the weighting factors and controlling that weighing does not cause the mineral grades to drift too far away from the true mineral composition. For a selection of the best possible option further information regarding practical considerations such as sample preparation, costs, detection limit, and the information that method offers are necessary (Table 17).

Table 17. Comparison of different methods for obtaining mineral grades.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>XRD with Rietveld</th>
<th>Automated Mineralogy</th>
<th>EMC**</th>
<th>Combined</th>
</tr>
</thead>
<tbody>
<tr>
<td>Detection limit (wt%)</td>
<td>1</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td>Sample preparation time (minutes)</td>
<td>45</td>
<td>480</td>
<td>0</td>
<td>45</td>
</tr>
<tr>
<td>Analysis time (minutes)</td>
<td>90</td>
<td>240</td>
<td>0</td>
<td>90</td>
</tr>
<tr>
<td>Cost (approximate, US$)</td>
<td>60</td>
<td>200</td>
<td>0</td>
<td>60</td>
</tr>
<tr>
<td>Experienced operator needed</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Experienced mineralogist needed</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Precision*</td>
<td>9.0-21.8</td>
<td>3.6</td>
<td>5.2</td>
<td>10.6</td>
</tr>
<tr>
<td>Closeness (against XRF)*</td>
<td>38.4</td>
<td>32.5</td>
<td>21.6</td>
<td>24.7</td>
</tr>
<tr>
<td>Closeness (against AM)*</td>
<td>56.5</td>
<td>-</td>
<td>110.0</td>
<td>76.8</td>
</tr>
<tr>
<td>Additional information</td>
<td>Crystalline structure of minerals</td>
<td>Textural information (liberation, association, grain size, intergrowths, etc.)</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

**EMC method used here is a solution to the underdetermined situation. Closeness (against AM) is not representative of all EMC cases.

*Closeness and precision are the “a” of the model (equation 3). It gives relative standard deviation directly for the grade. The smaller the value is, the better is the method.
Chapter 5 - Ore texture characterization and relation to mineral liberation

5.1 Introduction

Ore texture and particle composition information is a critical part of the mineralogical approach to geometallurgy. The ore texture and the progeny particles after a breakage in the comminution are the missing link between geology and mineral processing in the concept of geometallurgy. Mostly, ore texture is quantified in terms of descriptors (such as covariance function, proximity function and linear intercept length distribution (Zhang and Subasinghe, 2012). However, these descriptors are mostly developed for binary systems, and there is no extension for three-dimensional ore texture volume. In this study, ore textures and particles are quantified by association indicator to show the trend of ore texture breakage in crushing.

5.2 Association Indicator for ore texture

The analysis of eight drill cores of iron ore in terms of modal composition and association indicator shows variations in ore textures (Table 18). The average grain size of gangue phases was estimated by optical image microscopy while grain size of magnetite and iron oxide (magnetite and hematite) was measured by image processing technique.

The association between magnetite and apatite in magnetite samples is in order of F > E > D1 > G while the association between apatite and magnetite is F > E > G > D1. This shows that even though D1 has the highest apatite grade but the association between magnetite and apatite is less than E and F samples with high-grade magnetite. Consideration of both modal composition and Association Indicator gives insight about the assemblage of phase in the texture. Approximately in all samples, apatite is highly associated with magnetite and iron oxide phases regardless of apatite or magnetite grade. Also, considering grain size of phases, except in D1 sample that has roughly even grain size distribution, in the rest of the samples magnetite and hematite grains have the coarsest size among existing phases.
<table>
<thead>
<tr>
<th>Sample</th>
<th>Phase</th>
<th>Grades (wt%)</th>
<th>Association Indicator Matrix (%)</th>
<th>Average grain size (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>Biotite</td>
<td>3.17</td>
<td>[− 47.11 21.44 31.45]</td>
<td>400</td>
</tr>
<tr>
<td></td>
<td>Amphibole</td>
<td>2.67</td>
<td>[34.64 − 24.43 40.92]</td>
<td>600</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>2.04</td>
<td>[17.82 27.77 − 54.41]</td>
<td>400</td>
</tr>
<tr>
<td></td>
<td>Magnetite</td>
<td>92.13</td>
<td>[20.87 36.86 42.28 −]</td>
<td>881</td>
</tr>
<tr>
<td>F</td>
<td>Quartz</td>
<td>0.17</td>
<td>[− 38.31 17.32 44.37]</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>Feldspar</td>
<td>1.10</td>
<td>[16.02 − 29.03 54.95]</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>1.35</td>
<td>[2.18 9.17 − 88.65]</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>Magnetite</td>
<td>97.38</td>
<td>[5.17 15.49 79.34 −]</td>
<td>894</td>
</tr>
<tr>
<td>G</td>
<td>Quartz</td>
<td>0.92</td>
<td>[− 59.82 3.89 36.28]</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>Feldspar</td>
<td>0.72</td>
<td>[51.18 − 6.86 41.96]</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>0.29</td>
<td>[15.48 31.67 − 52.85]</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>Magnetite</td>
<td>98.07</td>
<td>[36.87 48.68 13.45 −]</td>
<td>1905</td>
</tr>
<tr>
<td>D1</td>
<td>Quartz</td>
<td>5.52</td>
<td>[− 64.79 19.02 5.20 10.98]</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>Feldspar</td>
<td>12.88</td>
<td>[47.62 − 34.98 4.13 13.27]</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>7.24</td>
<td>[14.08 15.22 29.25 − 41.46]</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>Magnetite</td>
<td>64.09</td>
<td>[15.84 26.18 35.88 22.10 −]</td>
<td>504</td>
</tr>
<tr>
<td>A2</td>
<td>Quartz</td>
<td>2.18</td>
<td>[− 43.04 56.96]</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>1.87</td>
<td>[16.05 − 83.95]</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>Hematite</td>
<td>95.96</td>
<td>[20.10 79.90 −]</td>
<td>1486</td>
</tr>
<tr>
<td>A1</td>
<td>Quartz</td>
<td>4.23</td>
<td>[− 20.62 79.38]</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>3.86</td>
<td>[31.59 − 68.41]</td>
<td>500</td>
</tr>
<tr>
<td></td>
<td>Iron oxide</td>
<td>91.90</td>
<td>[64.35 35.65 −]</td>
<td>1218</td>
</tr>
<tr>
<td>B2</td>
<td>Quartz</td>
<td>3.48</td>
<td>[− 66.89 6.69 26.43]</td>
<td>400</td>
</tr>
<tr>
<td></td>
<td>Feldspar</td>
<td>2.32</td>
<td>[52.62 − 7.93 39.46]</td>
<td>400</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>1.88</td>
<td>[18.51 27.54 − 53.95]</td>
<td>600</td>
</tr>
<tr>
<td></td>
<td>Iron oxide</td>
<td>92.32</td>
<td>[27.45 52.18 20.38 −]</td>
<td>1629</td>
</tr>
<tr>
<td>C1</td>
<td>Feldspar</td>
<td>1.28</td>
<td>[− 40.06 59.94]</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>6.90</td>
<td>[19.13 − 80.87]</td>
<td>700</td>
</tr>
<tr>
<td></td>
<td>Iron oxide</td>
<td>91.82</td>
<td>[26.44 73.56 −]</td>
<td>1192</td>
</tr>
</tbody>
</table>

### 5.3 Association Indicator for particles

The AIM can be used for characterizing breakage behavior of particles and estimating the association of minerals based on the interfacial perimeter in the particle. The Association Indicator for particles is a unique way of assessing particle population. AIM values for different types of particle (Figure 14) are listed in Table 19. For example, particles P1 and P2 have a similar composition. However, they have different AIM values. In the AIM of particles, surrounding area of particles (e.g. epoxy, free space) is considered as an additional phase. In this way, the exposed surface of particles is considered in the AIM. The first row of AIM shows liberation by exposed surface.
As many of the samples have high iron oxide grade and mineral liberation is expected to be very high in these, only four of the samples with a high amount of gangue phases namely E, D1, A1, and C1 were selected for further studies.

![Figure 14. Particles with different composition and interfacial perimeter.](image)

Table 19. Comparison of Association Indicators for various types of particles according to Figure 14.

<table>
<thead>
<tr>
<th>Type</th>
<th>Composition</th>
<th>AIM</th>
<th>Type</th>
<th>Composition</th>
<th>AIM</th>
</tr>
</thead>
<tbody>
<tr>
<td>P1</td>
<td>[50 25 25]</td>
<td>[−0 50 8 42]</td>
<td>P2</td>
<td>[50 25 25]</td>
<td>[−0 50 25 25]</td>
</tr>
<tr>
<td></td>
<td>60 − 40 0</td>
<td></td>
<td></td>
<td>60 − 20 20 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>12 44 − 44</td>
<td></td>
<td></td>
<td>50 33 − 17</td>
<td></td>
</tr>
<tr>
<td></td>
<td>56 0 44 −</td>
<td></td>
<td></td>
<td>50 33 17 −</td>
<td></td>
</tr>
<tr>
<td>P3</td>
<td>[65 10 25]</td>
<td>[−0 67 0 33]</td>
<td>A</td>
<td>[100 0 0]</td>
<td>[−0 100 0 0]</td>
</tr>
<tr>
<td></td>
<td>61 − 24 15</td>
<td></td>
<td></td>
<td>100 − 0 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0 100 − 0</td>
<td></td>
<td></td>
<td>0 0 − 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>67 33 0 −</td>
<td></td>
<td></td>
<td>0 0 0 −</td>
<td></td>
</tr>
</tbody>
</table>

5.4 Ore texture and breakage characterization

Characterization of ore texture before and after breakage provides valuable insights about the fracture pattern in comminution, the population of particles for specific ore texture and their relation to parent ore texture. Characteristic of ore textures from simplest to more sophisticated way can be considered by analysis of particle size distribution after breakage, distribution of liberations and analysis of changes in associations. In the context of the mineralogical approach to geometallurgy, predicting the particle population from ore texture is a critical step to establish an interface between geology and mineral processing. This is also subject of interest in mineral processing for liberation analysis and comminution processes.

5.4.1 Particle size distribution after breakage

Particle size distribution of comminuted ore textures in one stage crushing, and 100% less than 3.35 mm are demonstrated in Figure 15. The crushed samples approximately have similar particle size distribution.

![Figure 15. Cumulative particle size distribution of particles after one stage crushing (left) and 100% crushing less than 3.35 mm (right).](image)
Modeling of particle size distribution of the comminuted sample is a well-established area and not new. However, to compare the size distributions numerically and also enable generating the particle size distribution for further purposes, the particle size distributions were fitted with Rosin-Rammler distribution function as follows:

\[
f(D) = 100 \times \left(1 - \exp\left(-\left(\frac{D}{D_{63.2}}\right)^n\right)\right)
\]

where

\(f(D)\): Cumulative weight percentage of particles passing size \(D\)
\(D\): The particle size
\(D_{63.2}\): The particle size where the distribution value is 63.2%
\(n\): A factor describing the spread of the distribution

The parameter values of particle size distributions (Table 20) suggests that more or less all the ore textures have similar size distribution. In general, textures with finer grain size distributions have wider particle size distributions (lower \(n\) values) such as D1 and F samples. This data is used later for generating particle size distribution for forecasting particles.

<table>
<thead>
<tr>
<th></th>
<th>One stage crushing</th>
<th>100% less than 3.35 mm crushing</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(D_{63.2})</td>
<td>(n)</td>
</tr>
<tr>
<td>E</td>
<td>1.90</td>
<td>1.31</td>
</tr>
<tr>
<td>D1</td>
<td>3.32</td>
<td>0.90</td>
</tr>
<tr>
<td>A1</td>
<td>2.47</td>
<td>1.09</td>
</tr>
<tr>
<td>C1</td>
<td>2.48</td>
<td>1.08</td>
</tr>
</tbody>
</table>

5.4.2 Distribution of particle types after breakage

The distribution of particle types in the samples shows that most of the samples have very high liberation even in the coarsest size fractions (Figure 16). Among the samples, D1 sample has the highest amount of locked particles. Iron oxide minerals are the major contributors to the liberated and locked particles.
5.4.3 Association Indicator distribution for locked particles

Distribution of particle Association Indicator has significance in defining the breakage behavior of particles. By comparing the Association Indicator in the intact sample and in crushed one conclusion on randomness versus degree of preference in breakage can be made. This value is an estimation how the breakage separates one phase from another compared to original ore texture.

Before analyzing the Association Indicator for different phases, it is important to understand how the breakage pattern affects the Association Indicator values. In simple cases as demonstrated in Table 21, when breakage is a phase-boundary fracture, phases reach a liberated state in coarse particle sizes. This means the interfacial area between phases disappears and consequently, Association Indicator values become zero. On the other hand, the association with the background (exposed surface) reaches to its maximum i.e. 100% Association Indicator value.

In a case of preferential breakage in one phase, Association Indicator value for the phase where breakage occurs decreases for non-liberated particle compared to original particle while Association Indicator value of the phase with no breakage remains same. In the case of boundary-region breakage, Association Indicator values for the phases decrease respect to parent particle while due to generating free surface Association Indicator values between phases and background increases. An indication of this type of fracture is observing a significant number of non-liberated particles in fine size fractions.
Table 21 A simple demonstration of the effect of breakage type on variation in AI values for particles. (A and B are phases and C is the background). DOL is the degree of liberation.

<table>
<thead>
<tr>
<th>Parent particle</th>
<th>Breakage</th>
<th>Progeny particles</th>
<th>AI change</th>
<th>DOL A</th>
<th>DOL B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parent particle</td>
<td>Breakage</td>
<td>Progeny particles</td>
<td>AI change</td>
<td>DOL A</td>
<td>DOL B</td>
</tr>
<tr>
<td>Parent particle</td>
<td>Breakage</td>
<td>Progeny particles</td>
<td>AI change</td>
<td>DOL A</td>
<td>DOL B</td>
</tr>
</tbody>
</table>

Looking at the distribution of Association Indicator values between phases, for example, magnetite and apatite in Figure 17, Association Indicator value for apatite-magnetite after breakage compared to ore texture has not been changed significantly, however for magnetite-apatite Association Indicator decreases in finer size fractions. These indicate that the breakage between magnetite and apatite (two major phases in D1 sample) is a combination of boundary-region and preferential in magnetite phase. The part that should not be neglected is the contribution of detachment breakage. Since the liberated particles are not considered in this graph, no conclusion can be made about this type of breakage. However, if the surface liberation of one phase increases dramatically simultaneously by decreasing particle size without leaving locked particles behind, that could be an indication of detachment process.

Figure 17. Distribution of Association Indicator values for magnetite and apatite in D1 sample.
To investigate changes of Association Indicator values for different phases, the term $AI_{50}$ is introduced. The $AI_{50}$ is the value of the Association Indicator for 50% of the population of locked particles (median value). AIM$_{50}$ is the Association Indicator Matrix filled for $AI_{50}$ values for each cell. AIM$_{50}$ can be generated for each size class of locked particles and compared against AIM of the original ore texture. This can be used to evaluate breakage and trend of separation of two specific phases from each other.

The graphs (Figure 18-21) show the changes in $AI_{50}$ values for different paired phases. $AI_{50}$ for a phase and background (epoxy) demonstrates the abundance of a phase free surface in locked particles. The trend along with the liberation of the phase show the generation of free surface for the specific phase in size fractions.

Figure 18. Changes in $AI_{50}$ from ore texture to size fractions for locked particles in E sample.

Figure 19. Changes in $AI_{50}$ from ore texture to size fractions for locked particles in D1 sample.
A significant trend in all samples is the association between iron oxide minerals and gangue phases. The AI50 value in size fractions decreases from intact ore to particles while the iron oxide free surface in locked particles increases. This indicates that in these samples, the breakage takes place preferentially in iron oxide phase. Additionally, increased mass proportion of free iron oxide particles (thus liberation degree) is another reason to support preferential breakage.

5.5 Forecasting particle population from ore texture

Ore texture mapping and breakage behavior of ore are the critical steps for forecasting the particle population. Experimental work and analysis that has been done on the ore textures can be utilized for forecasting particle population. The particle size distribution modeled by Rosin-Rammler equation.
along with the degree of breakage either preferential in phase or random estimated by breakage characterization are the main parameters for forecasting liberation distribution.

Simple assumptions can be made to reduce the complexity of forecasting particle population. For example, rectangular particle shapes which selectively or randomly positioned over ore texture is used to generate particles. The size of particles is taken from modeled particle size distribution. Schematically, the approach that is applied here is shown in Figure 22.

5.5.1 Assigning breakage frequency
To assign preferential breakage in a phase or entirely random breakage, breakage probability function was used for selecting pixels on the mineral map of ore texture. For example, if the breakage is known to be preferential in some specific phases, a probability function can be generated based on the degree of breakage to position random particles selectively over ore texture. To ensure that the particle has the surface exposure for that particular phase, the corner of the rectangle was selected for the anchor to position on the mineral map. For given ore texture D1, by random breakage and 100% preferential breakage in magnetite phase, the liberation distribution of magnetite in size fractions would be as Figure 23.
From the degree of liberation and AIM values in size fractions, the degree of breakage can be roughly estimated as Table 22. For example, the degree of liberation of D1 sample is around 74% for magnetite and 4% for apatite in the fine fractions while AIM$_{50}$ for these phases indicates that surface exposure of the phases in the locked particles is increasing in the fine fractions as well. This is suggesting that for the liberation of magnetite and apatite, preferential breakage in these phases is the main contributor. If we assume that the main breakages in the sample are either preferential in phases or random (no preferences in any way), it is safe to use the degree of liberations as a rough estimate to selectively position corner of rectangle particles over phases in mineral map. For the D1 sample, this would be 4% chance to place rectangular corner in apatite phase, 74% chance for magnetite phases and 21% chance to have no preferential positioning (random).

Table 22. The probability distribution for preferential breakage in a specific phase and random breakage established based on the degree of liberation.

<table>
<thead>
<tr>
<th>Phases</th>
<th>Preferential Breakage</th>
<th>E</th>
<th>D1</th>
<th>A1</th>
<th>C1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz</td>
<td>-</td>
<td>0.1</td>
<td>1.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Feldspar</td>
<td>-</td>
<td>0.1</td>
<td>-</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>Biotite</td>
<td>0.3</td>
<td>0.8</td>
<td>-</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Amphibole</td>
<td>0.0</td>
<td>-</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Apatite</td>
<td>1.2</td>
<td>4.4</td>
<td>5.0</td>
<td>5.2</td>
<td></td>
</tr>
<tr>
<td>Iron oxide</td>
<td>88.1</td>
<td>73.5</td>
<td>83.3</td>
<td>83.2</td>
<td></td>
</tr>
<tr>
<td>Random</td>
<td>10.4</td>
<td>21.1</td>
<td>10.4</td>
<td>11.1</td>
<td></td>
</tr>
</tbody>
</table>

Applying preferential and random breakage over ore textures yields particle population. Approximately one million particles were generated for each sample.

5.5.2 Adjusting liberation to match modal mineralogy
Generating particles by this method not necessary gives the same modal composition as the experimental work for some size fractions specifically for finer fractions. However, the liberation distribution is still close to the experimental liberation. The differences in modal composition and degree of liberation of some minerals could be due to the way that the particles are generated. In realistic breakage with classification stage, when particle breaks preferentially in one phase, non-liberated progeny particles are generated as well. This means that non-liberated particle still has a chance to break to fully liberated particles in finer size fractions, but this cannot be considered in the particle generation approach. In current particle generation, grade of the phase with highest preferential breakage increases in finer fractions. This specifically applies to the finest size fraction.
Possible explanation is the resolution of the mineral map which in certain point particle size reaches to. This means that many fine particles are consisting of only a few pixels or even one pixel. This can be fixed by the approach that was introduced by Lamberg & Vianna (2007) to adjust the mass proportion of particles to match modal composition. This is not a perfect solution, but it solves the inconsistency between liberation distribution of particles and modal composition. The modal composition of selected samples from experimental and texture breakage with the adjusted composition are listed in Table 23-26. In general, similar composition reached for all samples only by adjusting the mass proportion of particles.

Table 23. The modal composition of E sample from experimental (Exp.) and forecasted particles after adjusting liberation (Adj.).

<table>
<thead>
<tr>
<th>Fraction</th>
<th>Biotite (wt%)</th>
<th>Amphibole (wt%)</th>
<th>Apatite (wt%)</th>
<th>Magnetite (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;1680</td>
<td>1.64</td>
<td>1.57</td>
<td>1.51</td>
<td>1.52</td>
</tr>
<tr>
<td>850-1680</td>
<td>0.97</td>
<td>0.92</td>
<td>0.62</td>
<td>0.75</td>
</tr>
<tr>
<td>425-850</td>
<td>1.00</td>
<td>0.96</td>
<td>0.50</td>
<td>0.70</td>
</tr>
<tr>
<td>300-425</td>
<td>1.30</td>
<td>1.26</td>
<td>0.57</td>
<td>0.86</td>
</tr>
</tbody>
</table>

Table 24. The modal composition of D1 sample from experimental (Exp.) and forecasted particles after adjusting liberation (Adj.).

<table>
<thead>
<tr>
<th>Fraction</th>
<th>Quartz (wt%)</th>
<th>Feldspar (wt%)</th>
<th>Biotite (wt%)</th>
<th>Apatite (wt%)</th>
<th>Magnetite (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;1680</td>
<td>6.22</td>
<td>6.71</td>
<td>23.08</td>
<td>22.63</td>
<td>5.33</td>
</tr>
<tr>
<td>850-1680</td>
<td>3.63</td>
<td>4.08</td>
<td>13.02</td>
<td>12.49</td>
<td>5.64</td>
</tr>
<tr>
<td>425-850</td>
<td>1.50</td>
<td>1.51</td>
<td>2.07</td>
<td>2.58</td>
<td>7.15</td>
</tr>
<tr>
<td>300-425</td>
<td>1.50</td>
<td>1.76</td>
<td>2.78</td>
<td>3.22</td>
<td>7.28</td>
</tr>
</tbody>
</table>

Table 25. The modal composition of A1 sample from experimental (Exp.) and forecasted particles after adjusting liberation (Adj.).

<table>
<thead>
<tr>
<th>Fraction</th>
<th>Quartz (wt%)</th>
<th>Apatite (wt%)</th>
<th>Iron oxide (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;1680</td>
<td>6.67</td>
<td>6.46</td>
<td>3.90</td>
</tr>
<tr>
<td>850-1680</td>
<td>2.92</td>
<td>3.08</td>
<td>1.93</td>
</tr>
<tr>
<td>425-850</td>
<td>5.06</td>
<td>4.99</td>
<td>5.92</td>
</tr>
<tr>
<td>300-425</td>
<td>2.63</td>
<td>2.85</td>
<td>6.90</td>
</tr>
</tbody>
</table>

Table 26. The modal composition of C1 sample from experimental (Exp.) and forecasted particles after adjusting liberation (Adj.).

<table>
<thead>
<tr>
<th>Fraction</th>
<th>Feldspar (wt%)</th>
<th>Apatite (wt%)</th>
<th>Iron oxide (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;1680</td>
<td>1.52</td>
<td>1.49</td>
<td>3.26</td>
</tr>
<tr>
<td>850-1680</td>
<td>0.73</td>
<td>0.69</td>
<td>1.57</td>
</tr>
<tr>
<td>425-850</td>
<td>1.10</td>
<td>0.92</td>
<td>4.03</td>
</tr>
<tr>
<td>300-425</td>
<td>1.26</td>
<td>1.03</td>
<td>7.33</td>
</tr>
</tbody>
</table>

5.5.3 Comparing liberation of iron oxide minerals

As the major phase in the samples is iron oxide mineral and its liberation is critical for mineral processing plant performance, the iron oxide liberation distribution comparison is made between experimental and forecasted particles. Generally speaking, in most of the samples, the trend of iron oxide liberation is predicted well (Figure 24). However, particle population of magnetite ore samples
(E and D1) presents closer liberation distribution than those of iron oxide (both magnetite and hematite are present). In overall, this verifies that the primary ore texture is a major factor controlling the liberation distribution in crushing.

Figure 24. Liberation distribution of iron oxide minerals from experimental (left) and forecasted particles (right).

5.6 Discussion on ore texture characterization

Image processing methods are widely used for ore texture and particle characterization, however, liberation by composition and exposed surface are still the dominated methods for liberation and
particle characterization. One of the shortcomings of the existing methods for association and liberation distribution is the inability to compare the particle texture against the original ore texture numerically. Textural descriptors that are commonly used for particles (Pérez-Barnuevo et al., 2012) are to show the complexity of texture or identification, but they lack the capability to relate particles to the parent texture in a way that can be used for the breakage analysis and forecasting.

The Association Indicator Matrix (AIM) can be regarded as an extension of work by Lund et al. (2015) to account for a grade of mineral in the particle in the assessment of association. The suggested method could not consider phase boundaries or exposed surface. Therefore, the applicability of association index was limited especially when there were disseminated grains or inclusion in the particle. Current method accompanied by particle composition can store valuable information about the distribution of interfacial areas between phases and liberation distribution by composition and exposed surface.

The merits of Association Indicator over absolute value of interfacial area or common co-occurrence matrix are not only that it is less sensitive to scale, for example, due to fractal effect, but also values can be compared to different textures as well as particles and can be used as criteria for textural classification. The cell values in the AIM also give relevant information about how the phases are occurring in the ore texture. For example, if the AI value goes near 100%, it is an indication that one phase is mainly accompanied by another phase, for instance as inclusions.

The other potential strong point of AIM is the capability of evaluating the nature of breakage of given ore texture for further generation of full particle population. This was demonstrated by four drill core samples where liberation distribution of iron oxide minerals was compared. In general, results for magnetite samples were closer to experimental data. This could be because hematite and magnetite are lumped together in iron oxide samples, and same breakage frequency as magnetite was used for hematite.

The generated mineral map of ore texture from drill core mapping was used as an input for forecasting particles. The particle size distribution from crushing was used for generating various sizes of rectangles that were superimposed on the mineral map. For positioning the rectangles over the mineral map, breakage probability was used. The assumption was that the preferential breakage in the phase is the cause of the liberation of minerals and random breakage can yield both liberated and non-liberated particles. The obstacle in this approach is that grade of mineral with highest preferential in finer size fractions progressively increase. Therefore, liberation adjustment step was required to match modal composition in size fraction according to experimental.

The value of the developed method is that it links original texture and mineral liberation. The approach generates full particle population which can be used directly in particle-based process simulations.
6.1 Introduction

Missing mineral liberation information and a lack of mass balancing techniques for multiphase particles has hindered the development of unit operation process models to be based on particle properties (Table 5). Particle level information provides an excellent opportunity to relate particle properties to physical sub-processes and to develop a model for forecasting the performance of any unit operation. In the development of the particle-based model, first, the quality of data and measurements are assessed then the techniques used for relating particle properties to the recovery of the instrument are described. The presentation of the model in mathematical form and verification of model by using industrial data is followed after.

6.2 Quality of data and measurements

The standard deviation for XRF and automated mineralogy measurements in repeated samples were calculated according to the developed error model. The standard deviation for XRF assays follows the equation

\[ \text{STD}_{\text{XRF}} = \pm 0.007 \times \sqrt{x} \]  

where \( x \) is the elemental grade in wt%. Standard deviation for mineral grades measured by automated mineralogy follows the equation

\[ \text{STD}_{\text{AM}} = \pm 0.208 \times \sqrt{x} \]  

where \( x \) is the mineral grade in wt%. Equation (44) was used for setting standard deviations during mass balancing the data for minerals.

To evaluate the quality of automated mineralogy, back-calculated chemical compositions were compared against chemical assays (Figure 25). Generally, good overall correlation was observed. However, minor elements such as vanadium (V), manganese (Mn) and potassium (K) show a weak correlation between chemical assays and back calculations. This could be due to either error in XRF analysis at low concentration or inaccuracy in the chemical composition of minerals (Table 11).
Mass balancing and data reconciliation improve the reliability of measurements and can under certain circumstances even enable the estimation of unmeasured streams and variables. It is a requirement for estimating the metallurgical performance of the circuit (recovery calculations), for diagnosis of process bottlenecks, and for modeling the process. Well-established methods exist for mass balancing and data reconciliation of mineral processing data, and several software packages have been developed for performing these tasks (Hodouin, 2010).

Particle mass balancing also called particle tracking is the state-of-the-art technique as developed by Lamberg and Vianna (2007) for mineralogical mass balancing. It transfers the mass balancing concepts of conventional chemical assays to the mineral level and finally to the mineral liberation level. The method requires delicate considerations to provide consistent results and to overcome missing liberation data. The following steps need to be included when extending the mass balancing to the particle level (i.e. mineral liberation level):

1) Bulk mass balance by minerals
2) Sized mass balance by minerals
3) Particle mass balance (by so-called particle tracking)

In this study, as a first step, unsized data was used for mass balancing total solid and mineral flowrates in bulk. The result from the bulk mass balancing was then used as a constraint when mass balancing the minerals in size fractions. This stepwise procedure minimizes the error propagation and ensures that bulk and sized mass balances are consistent.

The adjustment of mineral grades in mass balancing for most of the minerals was minor as shown in Figure 27, where the parity line indicates no adjustment. Adjustment of anhydrate and titano-magnetite was relatively higher compared to others, and therefore information on these trace minerals is less reliable. This was mainly due to precipitation of anhydrate in tailing buckets and false identification of titano-magnetite during automated mineralogy. Titanium-bearing minerals such as titanite and rutile exist as the lamellae in magnetite grains (Lund, 2013), causing the identification of
some of the magnetite grains falsely as titano-magnetite. To resolve this problem, titano-magnetite in each particle was lumped together with the magnetite, and the anhydrate phase was removed. Each particle composition was normalized after removing the anhydrate phase. Afterward, mass balancing was redone (Table 27).

![Figure 26. Comparison of mineral grades between measured and balanced data. Values on the graph are showing corresponding R² value for each mineral.](image)

**Table 27. Bulk balanced values for WLIMS (mineral grades in wt%). For mineral abbreviations, see Table 11.**

<table>
<thead>
<tr>
<th>Streams</th>
<th>Solids Bal. t/h</th>
<th>Mgt Bal. %</th>
<th>Qtz Bal. %</th>
<th>Ap Bal. %</th>
<th>Bt Bal. %</th>
<th>Ab Bal. %</th>
<th>Act Bal. %</th>
<th>Cal Bal. %</th>
<th>Ttn Bal. %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed</td>
<td>454</td>
<td>83.8</td>
<td>0.83</td>
<td>3.16</td>
<td>3.50</td>
<td>2.85</td>
<td>3.86</td>
<td>1.76</td>
<td>0.28</td>
</tr>
<tr>
<td>Conc.</td>
<td>387</td>
<td>98.0</td>
<td>0.05</td>
<td>0.48</td>
<td>0.56</td>
<td>0.13</td>
<td>0.55</td>
<td>0.11</td>
<td>0.08</td>
</tr>
<tr>
<td>Tail.</td>
<td>68</td>
<td>2.20</td>
<td>5.25</td>
<td>18.48</td>
<td>20.33</td>
<td>18.34</td>
<td>22.76</td>
<td>11.21</td>
<td>1.44</td>
</tr>
</tbody>
</table>

The particle tracking technique (Lamberg and Vianna, 2007) aims at adjusting liberation data to match with mass balance results in bulk and size fractions. It is followed by the basic binning, which involves the classification of particles by size and composition into narrow liberation classes (bins). In principal, the number of bins can be as many as the possible combination of phases in particles and grade classes. Practically, in the basic binning stage the population of various particles in the stream defines how narrow the size classes should be and which combinations of phases in particles have to be considered. Population and mass distribution of particles in the studied samples showed that liberated and binary particles account for over 99% of the population (Table 28).

In some streams, some bins may have no or very few particles making the mass balancing result unreliable. In the following stage, the advanced binning, the bins with low numbers of particles are globally combined (i.e. in all the streams in a similar way) in order to reach a sound number of particles in each bin. In this work, the advanced binning was first done for the feed stream, and the minimum number of particles in each bin was set to 25. This equals to a maximum of 20% relative standard deviation for the mass proportion of the particle type (bin) in question. The other streams were binned in the same way by using the feed stream as a reference. In the final stage, the mass
The proportion of each bin (particle type) was adjusted to reach the mass balance in the whole circuit by keeping the total solids flowrate as constraints. Additionally, the particle flowrate of each bin was balanced among feed, concentrate and tailing by considering a weighting factor calculated from the number of particles observed in each bin. In this study, the particle tracking resulted in the mass balancing of 702 different kinds of particles around the WLIMS. Once the particle types were mass-balanced in streams, it was possible to calculate the recovery of each particle type.

Table 28. Population and mass distribution of particles in streams.

<table>
<thead>
<tr>
<th>Stream</th>
<th>Particle</th>
<th>Population (number of particles)</th>
<th>Mass distribution (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed</td>
<td>Liberated</td>
<td>69,056</td>
<td>69.55</td>
</tr>
<tr>
<td></td>
<td>Binary</td>
<td>22,240</td>
<td>30.10</td>
</tr>
<tr>
<td></td>
<td>Ternary</td>
<td>280</td>
<td>0.32</td>
</tr>
<tr>
<td></td>
<td>Complex</td>
<td>27</td>
<td>0.06</td>
</tr>
<tr>
<td>Concentrate</td>
<td>Liberated</td>
<td>81,068</td>
<td>72.46</td>
</tr>
<tr>
<td></td>
<td>Binary</td>
<td>20,846</td>
<td>27.41</td>
</tr>
<tr>
<td></td>
<td>Ternary</td>
<td>210</td>
<td>0.14</td>
</tr>
<tr>
<td></td>
<td>Complex</td>
<td>15</td>
<td>0.00</td>
</tr>
<tr>
<td>Tailing</td>
<td>Liberated</td>
<td>81,277</td>
<td>67.46</td>
</tr>
<tr>
<td></td>
<td>Binary</td>
<td>20,755</td>
<td>30.70</td>
</tr>
<tr>
<td></td>
<td>Ternary</td>
<td>881</td>
<td>1.41</td>
</tr>
<tr>
<td></td>
<td>Complex</td>
<td>327</td>
<td>0.55</td>
</tr>
</tbody>
</table>

Figure 27. Parity chart showing measured particle type (bin) masses in the feed, concentrate and tailing streams after advanced binning against mass-balanced particle types (bin) after the particle tracking.

6.4 Developing a process model for WLIMS

In the WLIMS, the rotating drum with the magnet is partially submerged into a slurry tank where it lifts out the magnetic particles. Based on the tank design and the feed slurry flow three types of setups can be distinguished: concurrent, counter-current and counter-rotation. Selection of the type of magnetic separator for treating an ore is governed by feed particle size, throughput, and concentrate grade and recovery (Stener, 2015).
Based on the type of the magnetic separator, slurry tank, and magnetic arc, several different zones can be defined. For example, the counter-current magnetic separator can be divided into three zones. The pick-up zone is where the fresh slurry feed encounters the drum. The scavenger zone is a shallow zone close to the tailings outlet where the drum’s rotation is opposite to the slurry flow. The dewatering zone or cleaning zone is where the drum pushes the concentrate up to the discharge, and the concentrate water flows back to the tank (Figure 28).

When a ferromagnetic material is exposed to the magnetic field, magnetic ordering occurs based on an intrinsic property of the material which defines spontaneous magnetization (Svoboda, 2004). The other phenomenon happening is the growth of magnetic domains. Depending on the size of the particle and the strength of the magnetic field, the magnetic particle can consist of single or multiple magnetic domains. If the external field is strong enough or the particle is small enough (less than 0.1 µm) particle magnetization becomes homogenous; this is called magnetic saturation. Even when the saturated particle is outside of the magnetic field, the particle will not become completely demagnetized.

Magnetized particles in the slurry tend to gradually gather into groups and form flocs or aggregates. This is called magnetic flocculation. Before magnetic saturation is reached, the strength of the flocs increases with the growth in field strength and efficient permeability. The magnetic content of the particles, the fineness and as well as the nature of the non-magnetic material affect the effective permeability (Lantto, 1977). It is believed that the magnetic flocculation plays a crucial role in the recovery of fine magnetic particles.

6.4.1 Physical explanations for observations

Recovery of binary magnetite-bearing particles

The major mass population of particles in the concentrate is formed by liberated and magnetite-rich binary particles, as expected. For modeling purposes, the aim is to find an equation for the recovery of particles into the magnetic concentrate when its composition and size is known. Therefore, in Figure 29 the recovery of particles is plotted against composition. Firstly, recovery is directly related to the magnetite content in the particle. For liberated magnetite particles, no matter the size, recovery is 100%. Secondly, it can be seen that the recovery of magnetite-bearing particles in coarse size fractions is higher than those in fine size fractions (Figure 29). This is mainly due to higher magnetic force on
coarse magnetite particles and their important contribution to increasing the effective permeability of flocs. For example, in the case of apatite, particles with around 10% magnetite have a recovery of around 22% in the fine size fraction (<37 µm), but the same particles in coarse size fraction (>125 µm) have more than 70% recovery to the concentrate. Similar behavior can be seen with other binary particles with magnetite.

Figure 29. Recovery of different binary particles with magnetite, error bar shows two standard deviations. Error in recovery was calculated by Monte Carlo simulation. High errors in some particle bins are due to a low number of particles in the bin.

The arbitrary trend curve shows magnetite content in particle and recovery relationship.

Recovery of liberated gangue particles
Liberation measurements revealed that there are liberated non-magnetic particles in the concentrate and the mass balancing confirms that there is a positive relation between the liberated gangue particle size and the recovery into the concentrate (Figure 30). For apatite, fully liberated particles contribute with around 30% of the total apatite in the concentrate. For other minerals, this value varies. Recovery of fully liberated gangue minerals in the concentrate can be artificial due to stereological bias, or true due to entrainment or entrapment.
Figure 30. Recovery of liberated gangue particles in various sizes. Error bars show twice the standard deviation.

**Stereological bias**

A stereological bias in two-dimensional particle image analysis means that particles that are regarded as liberated in sections can be composite particles in three dimensions. If this is the case, then the recovery should show a decrease by increasing particle size. Relatively speaking in a similar texture a fine-grained particle in coarse size fraction changes to the coarse-grained particle in fine size fraction, as depicted in Figure 31. This is analogous to that in fine textures the stereological bias is smaller (Leigh et al., 1996; Spencer and Sutherland, 2000). Therefore, stereological bias, as a possible reason for this observation can be excluded.

Figure 31. The stereological effect on recovery of particles in coarse and fine size fractions. With similar texture, stereological bias is higher in small particles than in coarse ones.

**Entrainment phenomena**

Entrainment means that particles are dragged into the concentrate with water. This effect is stronger for fine particles than for coarse ones (Neethling and Cilliers, 2009), i.e. opposite to the observation. Therefore, also this explanation is rejected.

**Entrapment**

As discussed earlier, in a flocculation process magnetite particles attach to each other. During this process, liberated gangue minerals can be trapped between magnetic particles. The entrapment of non-magnetic particles has been previously reported as enclosures in the flocs (Lantto, 1977). In the dewatering step (Figure 28) when the drum pushes the flocs up towards the concentrate discharge, water inside the flocs drains back to the tank and takes some of the fine liberated gangue particles with (drainage). Madai (1998) has shown that for fine particles the drag force is stronger than its counter force, the magnetic force. Therefore, fine particles have a higher probability to escape from
the flocs than coarser particles. On the other hand, the small porosity size in the flocs hinders the coarse gangue particles to be drained out from the flocs. Therefore, the coarse liberated gangue particles have higher chance to be trapped in the flocs and to end up in the concentrate (Figure 32).

![Figure 32. The effect of drainage water in dewatering zone to wash out fine gangue particles. Gray particles are magnetic particles, and bright ones are gangue particles. Drainage flow is shown by the straight arrow toward the bottom of the tank.](image)

6.4.2 Semi-empirical model of WLIMS

Even though observations show a clear correlation between the recovery of different particle types and the physical processes, it is not possible to develop a purely physical model. This is mainly due to numerous and complex sub-processes involved in the separation. Further, the data available from the plant survey describes only one operational point. Therefore, the model developed here is semi-empirical in nature and tries to reproduce recovery curves at mineral liberation level. Requirements to be formulated for such a model are that (i) it should be flexible to adapt to linear or curve shaped recoveries, (ii) should have a reasonably low number of parameters, and (iii) should reflect physical sub-processes in the system. At a later stage, the model can be further developed to consider operational variables.

A flexible and relatively simple way to model the recovery patterns of binary particles is to use the incomplete beta function $I_\alpha(a,b)$ (Abramowitz and Stegun, 1965). The incomplete beta function is defined as follows:

$$I_\alpha(a,b)=\int_0^t t^{a-1}(1-t)^{b-1} \, dt$$

(45)

If for the sake of simplicity, the $a$ parameter is fixed at 1, various curve shapes can be generated by changing only the $b$ variable alone.

For the entrapment, the observation shown in Figure 30 suggests that the probability of entrapment increases by size and nature of gangue mineral. A simple linear relationship based on the particle size can be applied for each mineral as follows:

$$R_e = E_1d + E_2$$

(46)

where $R_e$ is the recovery due to entrapment, $d$ is the particle size, and $E_1$ and $E_2$ are the constants. This linear model is applied to predict the entrapment of different sizes of liberated gangue particles.
To model the recovery of various magnetite binary particles in the WLIMS concentrate, the following function is used:

$$R_s = l_s(1,b)$$  \hspace{2cm} (47)

where $x$ is the grade of magnetite in the particle and $b$ is a spread value. Depending on the mineral type that is binary with magnetite, the $b$ can vary from 0.01 to 30. Finer size fractions generally have smaller $b$ value than coarser size fractions. The trend of increasing $b$ values from fine size fractions to coarse size fractions shows the spread of recovery curves. Therefore, the spread value in equation (47) is dependent on the particle size, the susceptibility of non-magnetic portion of the particle, shape of the particle, and specific gravity of the particle. Finally, the recovery model by considering entrapment becomes as follows:

$$R = R_s + (1-R_s)R_e$$  \hspace{2cm} (48)

Fitting the equation (48) with the experimental points gives various $b$ values for compositionally different binary particles in different size fractions. During the data fitting, each particle type recovery was assigned a weight factor calculated from the number of particles falling into the particle bin type. In addition, the highest and lowest $b$ values at 95% confidence level were calculated for the particles in each size fraction. In general, a linear regression describes the increase of $b$ values respect to the particles size. A similar approach was perused for calculating $R_e$. The results of the regression models for $b$ and $R_e$ are listed in Table 29.

<table>
<thead>
<tr>
<th>Regression model</th>
<th>Mgt-Qtz</th>
<th>Mgt-Ap</th>
<th>Mgt-Bt</th>
<th>Mgt-Ab</th>
<th>Mgt-Act</th>
<th>Mgt-Cal</th>
<th>Mgt-Ttn</th>
</tr>
</thead>
<tbody>
<tr>
<td>$b$</td>
<td>0.0408x</td>
<td>0.1174x + 1</td>
<td>0.1190x + 1</td>
<td>0.0261x</td>
<td>0.1040x + 1</td>
<td>0.0057x</td>
<td>0.0180x</td>
</tr>
<tr>
<td>$R_e$</td>
<td>6E-06x</td>
<td>0.10x</td>
<td>0.11x</td>
<td>6E-03x</td>
<td>0.11x</td>
<td>8E-03x</td>
<td>3E-03x</td>
</tr>
</tbody>
</table>

The results indicate that binary pairs of magnetite with gangue can be divided into two groups. The first group is magnetite binary particles with apatite, biotite, and actinolite and the second group is magnetite binaries with quartz, albite, calcite and titanite. For each group an average regression model for $b$ and $R_e$ can be selected and applied to the model as follows:

First group:

$$R = l_s(1,1+0.12 \times d)(1-l_s(1,1+0.12 \times d)) \times 0.11 \times d$$  \hspace{2cm} (49)

Second group:

$$R = l_s(1,1.02 \times d)$$  \hspace{2cm} (50)

where $x$ is the magnetite grade of the particle and $d$ is the particle size.

6.5 Verification of the model

To verify the developed model, the model was compared against observations at two levels. At the first level, the comparison was made against the bulk and sized mineral flowrates. At the second level, the comparison was made on liberation distribution in the concentrate.

6.5.1 Verification based on bulk and sized level

Comparison of solid flowrates and mineral grades from observations and model indicates that the model forecasts well the solid and mineral flowrates (Table 30). However, in the finest size fraction, the differences between model and observation are higher than in the other size fractions and in bulk.
This could be related to the unpredictable behavior of fine particles in the process. This can also be seen in the recovery of fine minerals in finest fraction (Figure 33).

Table 30. Solid and mineral flowrates in bulk and sized fractions from model and observations.

<table>
<thead>
<tr>
<th>Conc.</th>
<th>Fraction</th>
<th>Solid t/h</th>
<th>Mgt %</th>
<th>Qtz %</th>
<th>Ap %</th>
<th>Bt %</th>
<th>Ab %</th>
<th>Act %</th>
<th>Cal %</th>
<th>Ttn %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Obs.</td>
<td>Bulk</td>
<td>387</td>
<td>98.0</td>
<td>0.06</td>
<td>0.48</td>
<td>0.57</td>
<td>0.14</td>
<td>0.55</td>
<td>0.11</td>
<td>0.08</td>
</tr>
<tr>
<td>0-37 um</td>
<td>116.9</td>
<td>98.8</td>
<td>0.06</td>
<td>0.13</td>
<td>0.39</td>
<td>0.03</td>
<td>0.21</td>
<td>0.34</td>
<td>0.00</td>
<td>0.03</td>
</tr>
<tr>
<td>37-63 um</td>
<td>68.5</td>
<td>98.2</td>
<td>0.03</td>
<td>0.56</td>
<td>0.47</td>
<td>0.19</td>
<td>0.48</td>
<td>0.00</td>
<td>0.00</td>
<td>0.03</td>
</tr>
<tr>
<td>63-125 um</td>
<td>109.5</td>
<td>97.7</td>
<td>0.05</td>
<td>0.66</td>
<td>0.68</td>
<td>0.16</td>
<td>0.60</td>
<td>0.01</td>
<td>0.11</td>
<td></td>
</tr>
<tr>
<td>+125 um</td>
<td>91.7</td>
<td>97.1</td>
<td>0.09</td>
<td>0.67</td>
<td>0.73</td>
<td>0.19</td>
<td>0.99</td>
<td>0.02</td>
<td>0.18</td>
<td></td>
</tr>
<tr>
<td>Model</td>
<td>Bulk</td>
<td>385</td>
<td>98.0</td>
<td>0.06</td>
<td>0.47</td>
<td>0.51</td>
<td>0.07</td>
<td>0.50</td>
<td>0.05</td>
<td>0.09</td>
</tr>
<tr>
<td>0-37 um</td>
<td>115.5</td>
<td>98.0</td>
<td>0.01</td>
<td>0.19</td>
<td>0.31</td>
<td>0.02</td>
<td>0.20</td>
<td>0.03</td>
<td>0.02</td>
<td></td>
</tr>
<tr>
<td>37-63 um</td>
<td>68.5</td>
<td>98.6</td>
<td>0.04</td>
<td>0.49</td>
<td>0.39</td>
<td>0.04</td>
<td>0.37</td>
<td>0.03</td>
<td>0.07</td>
<td></td>
</tr>
<tr>
<td>63-125 um</td>
<td>109.4</td>
<td>98.0</td>
<td>0.05</td>
<td>0.59</td>
<td>0.55</td>
<td>0.05</td>
<td>0.50</td>
<td>0.04</td>
<td>0.11</td>
<td></td>
</tr>
<tr>
<td>+125 um</td>
<td>92.2</td>
<td>97.4</td>
<td>0.15</td>
<td>0.68</td>
<td>0.80</td>
<td>0.20</td>
<td>1.00</td>
<td>0.09</td>
<td>0.18</td>
<td></td>
</tr>
</tbody>
</table>

Figure 33. Recovery of minerals in size fraction from observations (left) and model (right).

6.5.2 Verification based on mineral liberation level

Evaluation of the model at particle level was done first by comparing the liberation curves for magnetite particles in the concentrate; thus comparing measured concentrate against modeled concentrate from the feed stream and developed equations (45)-(50). As shown in Figure 34, the model well describes the liberation of magnetite particles. However, the mode of occurrence of minerals in particles is not well described for certain minerals (Table 31 and Table 32). The differences for quartz, albite, calcite, and titanite are higher than for the other minerals. This is arising from using simple linear regression model for $b$ values in the model for this group of minerals. However, more observations of particles are required to form a better model.
Table 31. Mode of occurrence of minerals in the concentrate from observations. Each row describes the association of named mineral with the minerals stated on columns in percentages; each row sums up to 100%. Diagonal values give the mass proportion (wt%) of liberated particles.

<table>
<thead>
<tr>
<th>OBS</th>
<th>Mgt</th>
<th>Qtz</th>
<th>Ap</th>
<th>Bt</th>
<th>Ab</th>
<th>Act</th>
<th>Cal</th>
<th>Ttn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mgt</td>
<td>98.14</td>
<td>0.10</td>
<td>0.55</td>
<td>0.52</td>
<td>0.07</td>
<td>0.35</td>
<td>0.07</td>
<td>0.12</td>
</tr>
<tr>
<td>Qtz</td>
<td>75.79</td>
<td>9.42</td>
<td>1.23</td>
<td>3.37</td>
<td>0.40</td>
<td>3.55</td>
<td>0.70</td>
<td>0.60</td>
</tr>
<tr>
<td>Ap</td>
<td>59.88</td>
<td>0.07</td>
<td>32.62</td>
<td>0.71</td>
<td>0.49</td>
<td>0.97</td>
<td>0.25</td>
<td>0.01</td>
</tr>
<tr>
<td>Bt</td>
<td>66.33</td>
<td>0.33</td>
<td>0.50</td>
<td>27.99</td>
<td>0.60</td>
<td>0.78</td>
<td>0.16</td>
<td>0.32</td>
</tr>
<tr>
<td>Ab</td>
<td>41.75</td>
<td>0.96</td>
<td>0.95</td>
<td>1.09</td>
<td>45.63</td>
<td>2.15</td>
<td>1.44</td>
<td>0.22</td>
</tr>
<tr>
<td>Act</td>
<td>54.10</td>
<td>0.43</td>
<td>0.67</td>
<td>0.86</td>
<td>0.82</td>
<td>36.52</td>
<td>0.22</td>
<td>0.18</td>
</tr>
<tr>
<td>Cal</td>
<td>49.72</td>
<td>0.79</td>
<td>1.29</td>
<td>3.40</td>
<td>1.22</td>
<td>0.71</td>
<td>40.62</td>
<td>0.27</td>
</tr>
<tr>
<td>Ttn</td>
<td>91.32</td>
<td>0.46</td>
<td>0.05</td>
<td>1.47</td>
<td>0.96</td>
<td>0.95</td>
<td>0.51</td>
<td>1.50</td>
</tr>
</tbody>
</table>

Table 32. Mode of occurrence of minerals in the concentrate based on the model and the feed. Diagonal values give the mass proportion (wt%) of liberated particles.

<table>
<thead>
<tr>
<th>Model</th>
<th>Mgt</th>
<th>Qtz</th>
<th>Ap</th>
<th>Bt</th>
<th>Ab</th>
<th>Act</th>
<th>Cal</th>
<th>Ttn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mgt</td>
<td>97.93</td>
<td>0.10</td>
<td>0.59</td>
<td>0.53</td>
<td>0.11</td>
<td>0.39</td>
<td>0.10</td>
<td>0.12</td>
</tr>
<tr>
<td>Qtz</td>
<td>88.00</td>
<td>5.92</td>
<td>0.13</td>
<td>0.15</td>
<td>0.02</td>
<td>0.39</td>
<td>0.01</td>
<td>0.02</td>
</tr>
<tr>
<td>Ap</td>
<td>63.12</td>
<td>0.03</td>
<td>32.21</td>
<td>0.04</td>
<td>0.02</td>
<td>0.06</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td>Bt</td>
<td>72.19</td>
<td>0.02</td>
<td>0.09</td>
<td>23.52</td>
<td>0.08</td>
<td>0.22</td>
<td>0.05</td>
<td>0.01</td>
</tr>
<tr>
<td>Ab</td>
<td>71.34</td>
<td>0.02</td>
<td>0.10</td>
<td>0.59</td>
<td>17.25</td>
<td>1.31</td>
<td>0.02</td>
<td>0.03</td>
</tr>
<tr>
<td>Act</td>
<td>61.43</td>
<td>0.05</td>
<td>0.06</td>
<td>0.13</td>
<td>0.12</td>
<td>33.19</td>
<td>0.03</td>
<td>0.01</td>
</tr>
<tr>
<td>Cal</td>
<td>88.90</td>
<td>0.05</td>
<td>0.12</td>
<td>0.21</td>
<td>0.11</td>
<td>0.34</td>
<td>7.84</td>
<td>0.11</td>
</tr>
<tr>
<td>Ttn</td>
<td>95.15</td>
<td>0.02</td>
<td>0.02</td>
<td>0.12</td>
<td>0.07</td>
<td>0.38</td>
<td>0.03</td>
<td>0.00</td>
</tr>
</tbody>
</table>

6.6 Discussion on developing WLIMS process model

The developed particle-based WLIMS model can forecast recovery and product quality of any new feed stream if the particle level information is available. Generally speaking, process simulators and unit operation models that operate at particle level are developing and becoming more common. In addition, simulation of a process where the model level is at particle level stays straightforward, i.e. input and output stream of the model can be directly used by any other unit model.

The developed model can be used in optimization for example by testing the effect of grinding fineness and detaching of flocs before sending the concentrate to the cleaning stage. From the curve shapes, coarser grinding gives higher recovery but lower grade compared to fine grinding. A detachment of the flocs could potentially decrease the entrainment. Further development is needed to relate the model parameters to the operational parameters or include certain sub-processes of
magnetic separation if the model is intended to be used for process control or to investigate the effect of operational conditions.

Observations at particle level as well as physical theory imply that magnetic separation is a complex process that is controlled by both operational conditions and the feed stream properties. Studying and characterizing the feed stream at particle level provides insight into the performance of a magnetic separator that previously was not possible to reach accurately. The developed semi-empirical model of WLIMS describes the recovery of individual particles based on two mechanisms; recovery of particles due to magnetic volume and entrapment. This was achieved through applying the particle tracking technique. However, there are several other factors that need to be addressed.

6.6.1 The effect of mineral nature, grain size, and shape
The relationship between particle size and recovery of fully liberated gangue particles can be explained by the entrapment phenomenon. As seen in Figure 30, there are slight differences between the gangue minerals, i.e. apatite, actinolite, and biotite show higher entrapment than the rest. In the case of apatite, fine magnetite inclusion (<1 μm) were observed in the apatite in the concentrate, which was not possible to detect under normal condition of automated mineralogy. On the other hand, apatite in the tailings seems not to have magnetite inclusion as those found in the concentrate. This also can be true for actinolite and biotite since such an observation has been reported previously (Niiranen, 2015). Detection of fine magnetite inclusion can be easily missed in the measurements and data processing of automated mineralogy, hence magnetic susceptibility measurement of present minerals and individual particles, if possible, would be needed to verify whether the liberated gangue particles end up to concentrate because of their magnetic susceptibility rather than entrapment. While higher susceptibility due to magnetite inclusion probably plays a major role, the effect of grain shape should not be neglected. Actinolite and biotite, can vary in shape and are often elongated that makes their release from flocs harder. In addition, angular particles have naturally stronger magnetic forces at the corners and edges.

The spread factor $b$ in equation (47) is closely correlated to particle size, the susceptibility of a non-magnetic portion of the particle, shape of the particle, and specific gravity of the particle. The smaller the grain size is, the lower the magnetic force on the material becomes, resulting in weakening and shortening of the flocs (Lantto, 1977). On the other hand, coarse magnetic particles increase the strength of the flocs and the length of the chains, thus resulting in an increase of total recovery. The nature of gangue minerals, the magnetic susceptibility of grains, shape and total susceptibility of particles affect the flocs’ effective permeability. For particles with sharp corners, porosity in the flocs increases and the total effective permeability becomes smaller compared to when flocs are packed with rounded particles. The specific gravity of particles may have a high impact during the cleaning stage. Particles with lower specific gravity tend to follow drainage water more easily than others.

6.6.2 The effect of feed quality
As seen in observations, the entrapped liberated gangue particles in the concentrate are one of the sources of impurities in the products. While the formation of the flocs is stronger in high-grade magnetite ore and is crucial for the recovery of fine particles, releasing gangue particles from these flocs is highly unlikely. Unless the flocs become demagnetized or detached, entrapped gangue particles inside the flocs find their way to the concentrate. A mechanical detachment of the flocs can be momentarily but may be enough to let gangue particles escape from the flocs.
The studied ore is such a high grade and shows strong recovery not only in the first magnetic separation but also in the whole process. This raises the question whether liberation information is needed for the process simulation. However, in producing high-quality products, the recovery is not the main concern, but the impurities are. Thus the grade of gangue minerals in the concentrate is necessary. For a high-quality iron product, the requirements for certain impurities are tight and must be met (LKAB, 2014). For example, phosphorus and silicon contents of the product are the determinative criteria meaning that relatively high liberation is needed to reach a pure product. In some iron deposits, even sulfur exist mainly in the form of sulfides which is problematic. Especially when monoclinic (thus magnetic) pyrrhotite is present (Arvidson et al., 2013).

Conversely, in the processing of low-grade ore, the mineral liberation can cause a recovery issue as well. It is expected that the strength of formed flocs in the low-grade feed will be weaker and the loss of binary particles with magnetite and fine magnetite particles accordingly be higher.

6.6.3 The effect of stereological bias

As it is known, two-dimensional measurement of liberation which inherently is defined in three dimensions is a biased estimate of the liberation. The liberation is always overestimated, and the magnitude of the overestimation depends on ore texture. The bias exists for liberation estimation. However, the bias affects the model parameters in less degree. In the calculation of modal parameters, instead of using the absolute value of liberation, the recovery was used. This means the overestimation of liberation presents itself in feed and concentrate which to some extent cancel each other as the recovery is calculated by dividing the particle flowrate in the concentrate by corresponding value in the feed. In this way, the model can take the uncorrected liberation data as well as corrected liberation data as an input and gives the same quality of the liberation.
Chapter 7 - Demonstrating the process plant simulation based on particles

7.1 Plant circuit

A flowsheet used here consist of comminution and concentration circuits and is based on LKAB Kiruna concentration plant (Samskog et al., 1997; Söderman et al., 1996). A circuit is a general form of the process that LKAB uses in Kiruna for the beneficiation of magnetite ore. The feed to the plant is the product of crushing and cobbing plant. The beneficiation process consists of three major steps including comminution, magnetic separation and apatite flotation. The comminution circuits include autogenous grinding followed by the spiral classifier and pebble milling coupled with hydrocyclone (Figure 35).

Figure 35. Flowsheet of magnetite beneficiation plant for the demonstration of different levels of modeling and simulation.

7.2 Process units

The process unit models used in the simulation at different modeling levels are gathered in Table 33. The results from the mass balancing of the plant data were used for calibrating and defining the model parameter values of different models.
Table 33. The models that are used in the simulation of flowsheet at different levels.

<table>
<thead>
<tr>
<th>Unit</th>
<th>Bulk model</th>
<th>Mineral by size model</th>
<th>Particle level model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Autogenous Mill</td>
<td>Perfect mixer</td>
<td>(Fixed) PSD</td>
<td>HSC comminution model with decoupled size reduction and liberation models</td>
</tr>
<tr>
<td>Trommel</td>
<td>Mineral splitter/mass splitter</td>
<td>Efficiency curve / Efficiency curve by mineral</td>
<td>Efficiency curve/efficiency curve by mineral</td>
</tr>
<tr>
<td>Mixer</td>
<td>Perfect mixer</td>
<td>Perfect mixer</td>
<td>Perfect mixer</td>
</tr>
<tr>
<td>Pebble Mill</td>
<td>Perfect mixer</td>
<td>(Fixed) PSD</td>
<td>HSC comminution model with decoupled size reduction and liberation models</td>
</tr>
<tr>
<td>WLIMS</td>
<td>Mineral splitter</td>
<td>Mineral by size splitter</td>
<td>Developed WLIMS model (Parian et al. 2016)</td>
</tr>
<tr>
<td>Spiral classifier</td>
<td>Mineral splitter</td>
<td>Efficiency curve/efficiency curve by mineral</td>
<td>Efficiency curve/efficiency curve by mineral</td>
</tr>
<tr>
<td>Hydrocyclone</td>
<td>Mineral splitter</td>
<td>Efficiency curve/efficiency curve by mineral</td>
<td>Efficiency curve/efficiency curve by mineral</td>
</tr>
<tr>
<td>Flotation</td>
<td>Flotation kinetics by mineral</td>
<td>Flotation kinetics by mineral by size</td>
<td>Particle-based kinetic flotation model</td>
</tr>
</tbody>
</table>

7.3 Plant feeds

Two different magnetite ores were selected to be used for simulation. The first ore is the actual feed to the plant during the survey (Ore A). The second ore is D1 drill core sample which was studied in ore texture characterization (Ore B). The procedure for forecasting particle population from D1 sample was described earlier in chapter 5. The two ores are texturally different thus have different mineral grades and liberation distribution (Table 34, Figure 36). The assumptions that are used here are that mineral compositions and particle size distribution after crushing for both ores are same.

The ore B was selected because it represents an ore which is significantly lower in the magnetite head grade and texture is much more fine-grained giving lower liberation degree at given particle size (Figure 36). Also, the Ore B would represent the plant feed in a case where cobbing is not used. In the ore B the degree of liberation is high in the size fractions lower than 75 microns. This is important to note because the final grinding size is fine. Thus, even the difference is significant in the degree of liberation; the final metallurgical result in simulations may not be significantly different in such a fine grinding.

Table 34. Modal composition of plant feed samples. Ab = albite, Act = actinolite, Ap = apatite, Bt = biotite, Cal = calcite, Mgt = magnetite, Qtz = quartz.

<table>
<thead>
<tr>
<th></th>
<th>Ab (wt%)</th>
<th>Act (wt%)</th>
<th>Ap (wt%)</th>
<th>Bt (wt%)</th>
<th>Cal (wt%)</th>
<th>Mgt (wt%)</th>
<th>Qtz (wt%)</th>
<th>Ttn (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ore A</td>
<td>3.01</td>
<td>3.43</td>
<td>2.48</td>
<td>3.50</td>
<td>0.91</td>
<td>85.57</td>
<td>0.96</td>
<td>0.14</td>
</tr>
<tr>
<td>Ore B</td>
<td>12.88</td>
<td>0.00</td>
<td>7.24</td>
<td>10.27</td>
<td>0.00</td>
<td>64.09</td>
<td>5.52</td>
<td>0.00</td>
</tr>
</tbody>
</table>
7.4 Simulation for Ore A

Mass balancing results were used for calibrating models in bulk mineral and mineral by size levels. For simulation at particle level, models described in Table 33 were used and adjusted to match experimental and mass balancing results. In overall, for Ore A, three levels of simulation give the same grade and recovery for all minerals for the final concentrate of the plant with the calibrated parameters. The effect of coarse grinding was investigated by increasing product particle size in grinding circuit (pebble mill and hydrocyclone). The simulation reveals that even in coarse product magnetite recovery and grade is still preserved.

Table 35. Results of the simulations for Ore A at different levels: composition of the magnetite concentrate (Grade wt%) and mineral recoveries. For mineral symbols, see Table 34.

<table>
<thead>
<tr>
<th>Grinding</th>
<th>Level</th>
<th>Ab</th>
<th>Act</th>
<th>Ap</th>
<th>Bt</th>
<th>Cal</th>
<th>Mgt</th>
<th>Qtz</th>
<th>Ttn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine</td>
<td>Bulk</td>
<td>13.86</td>
<td>17.25</td>
<td>22.99</td>
<td>13.23</td>
<td>17.80</td>
<td>95.60</td>
<td>0.00</td>
<td>99.79</td>
</tr>
<tr>
<td></td>
<td>Grade (wt%)</td>
<td>0.50</td>
<td>0.70</td>
<td>0.68</td>
<td>0.55</td>
<td>0.19</td>
<td>97.21</td>
<td>0.00</td>
<td>0.17</td>
</tr>
<tr>
<td></td>
<td>Size</td>
<td>13.86</td>
<td>17.25</td>
<td>22.99</td>
<td>13.23</td>
<td>17.80</td>
<td>95.60</td>
<td>0.00</td>
<td>99.79</td>
</tr>
<tr>
<td></td>
<td>Grade (wt%)</td>
<td>0.50</td>
<td>0.70</td>
<td>0.68</td>
<td>0.55</td>
<td>0.19</td>
<td>97.21</td>
<td>0.00</td>
<td>0.17</td>
</tr>
<tr>
<td></td>
<td>Particle</td>
<td>13.87</td>
<td>17.17</td>
<td>23.02</td>
<td>13.19</td>
<td>17.80</td>
<td>95.62</td>
<td>0.00</td>
<td>99.70</td>
</tr>
<tr>
<td></td>
<td>Grade (wt%)</td>
<td>0.50</td>
<td>0.70</td>
<td>0.68</td>
<td>0.55</td>
<td>0.19</td>
<td>97.22</td>
<td>0.00</td>
<td>0.17</td>
</tr>
<tr>
<td>Coarse</td>
<td>Bulk</td>
<td>13.86</td>
<td>17.25</td>
<td>22.99</td>
<td>13.23</td>
<td>17.80</td>
<td>95.60</td>
<td>0.00</td>
<td>99.79</td>
</tr>
<tr>
<td></td>
<td>Grade (wt%)</td>
<td>0.50</td>
<td>0.70</td>
<td>0.68</td>
<td>0.55</td>
<td>0.19</td>
<td>97.21</td>
<td>0.00</td>
<td>0.17</td>
</tr>
<tr>
<td></td>
<td>Size</td>
<td>18.84</td>
<td>24.21</td>
<td>20.41</td>
<td>16.38</td>
<td>17.47</td>
<td>95.59</td>
<td>0.00</td>
<td>99.79</td>
</tr>
<tr>
<td></td>
<td>Grade (wt%)</td>
<td>0.67</td>
<td>0.98</td>
<td>0.68</td>
<td>0.68</td>
<td>0.19</td>
<td>96.71</td>
<td>0.00</td>
<td>0.17</td>
</tr>
<tr>
<td></td>
<td>Particle</td>
<td>10.17</td>
<td>22.33</td>
<td>23.23</td>
<td>16.24</td>
<td>26.54</td>
<td>95.81</td>
<td>0.00</td>
<td>99.74</td>
</tr>
<tr>
<td></td>
<td>Grade (wt%)</td>
<td>0.36</td>
<td>0.91</td>
<td>0.68</td>
<td>0.67</td>
<td>0.29</td>
<td>96.92</td>
<td>0.00</td>
<td>0.17</td>
</tr>
</tbody>
</table>

7.5 Simulation for Ore B

For the simulation of Ore B, the calibrated parameters that were used at bulk mineral, mineral by size and particle levels for Ore A, were used. The results show that at bulk mineral and mineral by size levels, the mineral recoveries are similar as for the Ore A in fine grinding (Table 36). This is a property of models which define the behavior of minerals on unsized or size-based: regardless of the plant feed the mineral recoveries (and distribution in the full process) is similar, but the grades change. When the head grade lowers, the concentrate grade drops as well.
At the liberation level, the result is, however, different. Similar particles behave in the same way as in
the base case, but because the mass proportion of particles (thus liberation distribution) is different in
the plant feed for the Ore A and Ore B, the final result will differ for both grades and recoveries. The
particle level simulation forecasts slightly lower grade and recovery for the Ore B as for the Ore A.
Compared to bulk and mineral by size level, the particle level simulation forecast lower gangue
recovery thus higher magnetite grade.

Table 36. Results of the simulations for Ore B at different levels for the ore B: composition of the magnetite concentrate
(Grade wt%) and mineral recoveries. For mineral symbols, see Table 4.

<table>
<thead>
<tr>
<th>Grinding Level</th>
<th>Ab</th>
<th>Act</th>
<th>Ap</th>
<th>Bt</th>
<th>Cal</th>
<th>Mgt</th>
<th>Qtz</th>
<th>Ttn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine (P_80 = 38 μm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bulk Recovery (%)</td>
<td>14.28</td>
<td>0.00</td>
<td>21.16</td>
<td>15.72</td>
<td>0.00</td>
<td>95.60</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Bulk Grade (wt%)</td>
<td>5.29</td>
<td>0.00</td>
<td>2.21</td>
<td>1.39</td>
<td>0.00</td>
<td>91.12</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Size Recovery (%)</td>
<td>14.28</td>
<td>0.00</td>
<td>21.16</td>
<td>15.72</td>
<td>0.00</td>
<td>95.60</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Size Grade (wt%)</td>
<td>5.29</td>
<td>0.00</td>
<td>2.21</td>
<td>1.39</td>
<td>0.00</td>
<td>91.12</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Particle Recovery (%)</td>
<td>7.68</td>
<td>0.00</td>
<td>17.60</td>
<td>9.28</td>
<td>0.00</td>
<td>89.29</td>
<td>3.21</td>
<td>0.00</td>
</tr>
<tr>
<td>Particle Grade (wt%)</td>
<td>3.13</td>
<td>0.00</td>
<td>2.02</td>
<td>0.90</td>
<td>0.00</td>
<td>93.58</td>
<td>0.37</td>
<td>0.00</td>
</tr>
<tr>
<td>Coarse (P_80 = 72 μm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bulk Recovery (%)</td>
<td>14.28</td>
<td>0.00</td>
<td>21.16</td>
<td>15.72</td>
<td>0.00</td>
<td>95.60</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Bulk Grade (wt%)</td>
<td>5.29</td>
<td>0.00</td>
<td>2.21</td>
<td>1.39</td>
<td>0.00</td>
<td>91.12</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Size Recovery (%)</td>
<td>19.80</td>
<td>0.00</td>
<td>18.85</td>
<td>19.66</td>
<td>0.00</td>
<td>95.58</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Size Grade (wt%)</td>
<td>7.18</td>
<td>0.00</td>
<td>1.92</td>
<td>1.70</td>
<td>0.00</td>
<td>89.20</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Particle Recovery (%)</td>
<td>6.79</td>
<td>0.00</td>
<td>15.22</td>
<td>13.89</td>
<td>0.00</td>
<td>89.62</td>
<td>7.26</td>
<td>0.00</td>
</tr>
<tr>
<td>Particle Grade (wt%)</td>
<td>2.75</td>
<td>0.00</td>
<td>1.73</td>
<td>1.34</td>
<td>0.00</td>
<td>93.34</td>
<td>0.83</td>
<td>0.00</td>
</tr>
</tbody>
</table>

7.6 Discussion on results of simulations

Comparison of simulations for Ore A and Ore B demonstrates the difference between mineral and
particle level modeling and simulation. In the Ore B, the results from the particle level simulation give
more plausible result than the mineral and mineral by size level. This is due to the fact that the
parameters were calibrated based on the liberation of particles instead of general calibration to the
ore in bulk mineral and mineral by size level. At the particle level, the assumption is that similar
particles behave in the same way whereas at the mineral level the assumption is that mineral behaves
identically regardless of texture and particle composition. Although no verification and validation for
results of Ore B were provided, the simulation results at particle level comparatively to other levels is
more credible.

This simulation framework at particle level coupled with ore textural characterization enables the
mineralogical approach of geometallurgy to be the most comprehensive approach and only one that
can handle quantitative mineralogy in simulation routinely.
Chapter 8 - Conclusions and recommendations

The main findings of the research study are divided into scientific and practical results. The major scientific results and novelties of this research are as follows:

1. A new Combined method for modal analysis.
2. A new magnetic separator model operating at particle and mineral liberation level.
3. A first published mass balancing an industrial-scale process at mineral liberation level (multiphase particles).
5. A new concept of utilizing ore texture and breakage information to forecast liberation distribution.
6. Demonstration of a geometallurgical simulation framework for magnetite ore at particle level.

Moreover, the practical outcomes of the study that has been employed or has the potential for implementation in geometallurgy and mineral processing area are:

10. Toolbox of automated mineralogy including
    - MATLAB code for generating mineral map from BSD and optical images, measuring mineral association, mineral liberation and exporting particles to HSC Chemistry 9.
    - MATLAB code for forecasting particle population from mineral map of ore textures.

Conclusions from different parts of the study are drawn and summarized in below, and future directions and research lines are suggested.

Conclusions from the modal analysis study are:

- Three different methods for the analysis of mineral grades were compared firstly in terms of the closeness (cf. trueness) and precision but also with respect to their applicability in geometallurgy. A comprehensive evaluation was done including detection limit, sample preparation, analysis time, costs and additional information that they provide.
- A combined technique of quantitative X-ray diffraction and Element-to-Mineral Conversion has been developed and introduced to overcome the limitations of each of the techniques. Based on critical evaluation it is suggested to be suitable for geometallurgy for the analysis of mineral grades in bulk.
- In iron ores, the combined method gives an estimate on both magnetite and hematite grades and can replace tedious Satmagan and wet chemical Fe$^{3+}$ analysis.
- A problem occurring with all modal analysis methods is that back-calculated chemical composition from mineral grades does not match perfectly with the elemental grades of commodities received from chemical assays. This can be partially solved by the combined
method. However, this can be fully avoided for certain elements by weighting, but this requires further study for developing a sound technique for determining weighting factors.

The conclusion from ore texture characterization and predicting particle population are:

- To the best of my knowledge, the Association Indicator was introduced for the first time and used for characterization of ore texture and breakage.
- In the studied Kiruna iron ore samples, the analysis of the Association Indicator values reveals that the breakage is preferential in the iron oxide phase and specifically in magnetite.
- The full particle population was generated artificially based on applying breakage frequency and superimposing particles on ore texture mineral map. The mass proportion of generated particles was adjusted to match the known modal composition of the samples. The outcome showed promising results.
- The developed technique for forecasting particle population from intact ore texture is not ore specific and can be used for any commodity and ore texture.

Conclusions from the WLIMS model development are:

- Using particle-tracking technique, in this study for the first time, demonstrated that the behavior of magnetite-gangue composite particles in magnetic separation is not only dependent on the magnetite grade and particle size but also on nature of the gangue mineral. Particles containing gangue minerals such as biotite, actinolite, and apatite are showing similar behavior in WLIMS where others such as albite, quartz, and calcite are having different behavior respect to the first group. The origin of differences in behavior seems to be tiny magnetite inclusions in the first group of minerals.
- The entrapment phenomenon in magnetic separation was pointed out, and a simple regression model was used for modeling the degree of entrapment for different particles.
- Even though the developed model lacks operating parameters, it can be used for any WLIMS. Entrapment parameters and spread values for each mineral by size must be calibrated. When calibrated for certain operational conditions the parameter value do not require changing as the feed composition changes.
- Benefits of the developed model are that it is portable and does not need continuous calibration according to fluctuation in feed mineralogy, particle size distribution, and liberation characteristics. The developed model requires that the feed be characterized at mineral liberation level.

Conclusions from the process plant simulation are:

- The benefits of different levels of modeling in process simulation were shown. The particle level simulation showed plausible results when feed liberation varied.
- Within this study, it has been demonstrated that simulations at bulk and mineral levels with calibrated parameters to the ore feed are only valid for ores of similar texture and thus having similar liberation characteristics. However, calibrated parameters at particle levels are based on the composition of particles and are capable of giving estimates that are more reliable. In iron ore, the forecasts for the iron grade and recovery do not differ significantly, but for the impurity levels, the particle level simulation gives results that are more reliable.
- The particle level simulation enables optimization, thus finding optimal processing conditions, e.g. in grinding fineness, for different textural ore types and geometallurgical domains.
The particle population forecasting has a wide potential to be used in mineralogical approach to geometallurgy as the forecasting the liberation distribution from texture is a critical issue and step between geology and mineral processing. Forecasted particle population from a studied ore texture was used to demonstrate the potential of simulation at particle level.

Based on this work and scope of the geometallurgical approach using mineralogy, following tasks are proposed for future development:

- Integration of *combined* method to be used in the mineral resource estimates.
- Development of texture model in meso-, macro-scale and possibly in three-dimensional space.
- Extension and development of the method for forecasting particle population from ore texture.
- Proper validation of particle forecast and process simulation.
- Development of particle-based process models for other unit operations important in iron ore processing (grinding, size classification, flotation, gravimetric separation).
- Development of the methods to evaluate the error in geometallurgical prediction.
- Practices to define adequate accuracy for geometallurgical predictions.
- Validation of developed low intensity magnetic separation model and further development to introduce operational parameters.
- Verification and validation of particle-based models for other ore deposits than iron ore.
- Developing the simulation framework in general form to be applied for any ore deposit.
- Applying forecasted particle population and simulation framework in the geometallurgical program and comparing results against processed products.
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Paper I
Analysis of mineral grades for geometallurgy: Combined element-to-mineral conversion and quantitative X-ray diffraction

Mehdi Parian a,⇑, Pertti Lamberg a, Robert Möckel b, Jan Rosenkranz a

a Minerals and Metallurgical Engineering, Luleå University of Technology, SE-971 87 Luleå, Sweden
b Helmholtz-Zentrum Dresden – Rossendorf, Helmholtz Institute Freiberg for Resource Technology, Halsbruecker Straße 34, 09599 Freiberg, Germany

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Abstract
Knowledge of the grade of valuable elements and its variation is not sufficient for geometallurgy. Minerals define not only the value of the deposit, but also the method of extraction and concentration. A number of methods for obtaining mineral grades were evaluated with a focus on geometallurgical applicability, precision and trueness. For a geometallurgical program, the number of samples to be analyzed is large, therefore a method for obtaining mineral grades needs to be cost-efficient, relatively fast, and reliable. Automated mineralogy based on scanning electron microscopy is generally regarded as the most reliable method for analyzing mineral grades. However, the method is time demanding and expensive. Quantitative X-ray diffraction has a relatively high detection limit, 0.5%, while the method is not suitable for some base and precious metal ores, it still provides significant details on gangue mineral grades. The application of the element-to-mineral conversion has been limited to the simple mineralogy because the number of elements analyzed limits the number of calculable mineral grades. This study investigates a new method for the estimation of mineral grades applicable for geometallurgy by combining both the element-to-mineral conversion method and quantitative X-ray diffraction with Rietveld refinement. The proposed method not only delivers the required turnover for geometallurgy, but also overcomes the shortcomings if quantitative X-ray diffraction or element-to-mineral is used alone.

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1. Introduction

Geometallurgy is a cross-disciplinary approach that connects information from geology, mineral processing and subsequent downstream processes into a model in order to describe variability in the ore deposit to be used in production planning and management (Dobby et al., 2004; Dunham and Vann, 2007; Jackson et al., 2011). Geometallurgy has gained attention in recent years and different approaches are used for implementation. It is natural to use mineralogy to some extent as a link between geology and mineral processing (Hoal, 2008; Lamberg, 2011). This is intuitive since minerals define the value of the deposit, the method of extraction, economic risk valuation and the concentration method (Hoal et al., 2013).

A geometallurgical program is an industrial application of geometallurgy. It provides a way to map the variation in the ore body, to handle the data and to give forecast on metallurgical performance on spatial level. The program also comprises a procedure to employ complex geological information and transfer them to geometallurgical domains to be used in process improvement, production planning and business decision-making. The program is an instrument, which should evolve and change to ensure that geometallurgical domains address properly the metallurgical performance.

Knowledge of the grades of valuable elements and their variation alone is not sufficient for geometallurgy. Firstly, in several ore types the distribution of the valuable elements is complex. For example in nickel sulfide ores, it is important to know the distribution of nickel between non-sulfides and the different sulfide minerals (Newcombe, 2011). Similarly, in the process design and optimization for porphyry copper ores it is critical to know how much of copper is hosted in different sulfide and oxide minerals (Gregory et al., 2013). Secondly, the gangue minerals also play a crucial role in processing. For example in lateritic nickel ores, the gangue minerals have a direct effect on the acid consumption and permeability of the heaps (David, 2008). In refractory and trace mineral ores, like gold and platinum group element ores, the gangue mineralogy defines the entire plant response. Therefore, elemental grades are not necessarily the best attribute to use for the estimation of recovery and ultimate value. Much of the sustainability and energy efficiency dimensions of geometallurgy are...
driven by mineralogy. Moreover, mineral grades are additive, which makes their geostatistical modeling relatively straightforward (Vann et al., 2011).

Different levels of mineralogical and chemical information as summarized in Table 1 are routinely used for ore characterization in geometallurgical programs. They can be divided into the following types with increasing complexity and details: (1) elemental composition, (2) qualitative mineralogy, (3) quantitative mineralogy, and (4) mineral textures (Jones, 1987; Lamberg et al., 2013). In addition, geometallurgical programs commonly use (5) geometallurgical and (6) metallurgical testing (Kojovic et al., 2010; Lamberg et al., 2013). To gather this information into a geometallurgical program, the most cost- and time-efficient analysis methods should be selected. Examples of the methods used in mineralogical characterization are (2) identification of minerals by X-ray diffraction (XRD), (3) analysis of mineral grades by quantitative X-ray diffraction (Monecke et al., 2001), and (4) deriving mineral liberation information by automated mineralogy based on scanning electron microscopy (SEM) (Fandrich et al., 2007). When considering different methods for obtaining the mineralogical information, the trueness and precision of the information must be known. Only then a selection of the most appropriate method can be done.

In a mineralogical approach of geometallurgy, information of the mineral grades is required for the entire ore body (Lamberg, 2011). Thus, the number of samples to be analyzed for mapping the ore variation in a geometallurgical project is normally large (>10,000; Richardson et al., 2004). When selecting a method, one must consider several factors such as the costs, required time, availability, reliability, trueness and precision. Particularly the information on the precision of the method is frequently not available for the material to be studied.

Mineral grades and textural information are commonly analyzed in polished sections. Automated mineralogy based on scanning electron microscopy (SEM) and optical image analyses (OIA) are the known techniques. SEM-based automated mineralogy is commonly regarded as the most reliable way of estimating mineral grades. However, the method requires careful and tedious sample preparation and the method itself is costly and time-consuming (Lastra and Petruk, 2014). On the other hand, OIA-based automated mineralogy has the lower cost and is less time demanding. CSIRO (Donskoi et al., 2013) has developed an OIA-based automated mineralogy which has been used for iron ore characterization. In high-grade samples, the OIA system results were close to the SEM-based automated mineralogy (QEMSCAN), but in lower grade samples and low resolutions the OIA results were drifting away from true values (i.e. results from QEMSCAN and XRD).

Alternative methods such as quantitative XRD by Rietveld analysis (Mandile and Johnson, 1998) and the element-to-mineral conversion method (Lamberg et al., 1997; Lund et al., 2013; Paktunc, 1998; Whiten, 2007) require simpler and faster sample preparation and can be non-destructive. Additionally, if the aim is the estimation of mineral grade, they may offer better value than automated mineralogical analysis system only if they can fulfill the requirements on trueness and precision.

The element-to-mineral conversion method is a traditional and simple way to estimate mineral grades by simultaneously solving a set of mass balance equations formulated between chemical elements and minerals. The method is restricted to relatively simple mineralogy where the number of minerals is not larger than the number of analyzed components and the chemical composition of the minerals (mineral matrix) is known. Mathematically this can be written in the following form:

$$ A \times x = b \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix} \quad (1) $$

where $A$ is the matrix of the chemical composition of minerals, $x$ is the vector including the unknown mass proportion of minerals (bulk mineralogy) in the sample and $b$ is the vector of analyzed chemical composition of the sample. The unknown $x$ can then be determined e.g. using the nonnegative least squares method (Lawson and Hanson, 1995). The element-to-mineral conversion can be improved by using additional mineral selective analysis methods such as bromine-methanol leaching for nickel ores (Penntinen et al., 1977), copper phase analysis for copper ores (Lamberg et al., 1997) and Satmagan analysis for iron ores (Stirling, 1991).

The element-to-mineral conversion should not be confused with normative mineralogy methods such as the CIPW Norm or the Cation Norm (Cross et al., 1902) which aims at allocating chemical compositions into minerals based on the order of mineral formation in rock. These techniques are frequently used in geochemistry and petrology for the classification of rocks. They suffer mainly from a preset mineral list with stoichiometric mineral compositions as well as from limitations when exotic minerals are present, which is common in ore deposit characterization. Hence, they are not suitable for geometallurgical purposes.

Quantitative XRD methods include Known Addition, Absorption-Diffraction, Mineral Intensity Factors (MIFs) and Full-pattern-fitting (Kahle et al., 2002). The Rietveld is a full-pattern-fitting method and is regarded as a standardless method. Moreover, sample preparation, measurement and data

<table>
<thead>
<tr>
<th>Level</th>
<th>Analysis result</th>
<th>Commonly used analysis methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Elemental composition</td>
<td>Chemical composition of samples</td>
<td>X-ray fluorescence spectroscopy (XRF); dissolution + Atomic absorption spectroscopy (AAS)/Inductively coupled plasma optical emission spectrometry (ICP-OES)/Inductively coupled plasma mass spectrometry (ICP-MS)</td>
</tr>
<tr>
<td>2. Qualitative mineralogy</td>
<td>List of minerals present in samples, lithology</td>
<td>X-ray diffraction (XRD); Optical microscopy</td>
</tr>
<tr>
<td>3. Quantitative mineralogy</td>
<td>Bulk mineralogy, i.e. mass proportion of minerals in samples (modal composition)</td>
<td>Quantitative XRD; Element-to-mineral conversion (EMC); SEM-based automated mineralogy (MLA, QEMSCAN, IncaMineral, etc.); Optical image analysis (OIA) (CSIRO Recognition1/Minerals13); Hyperspectral imaging (SisuRock)</td>
</tr>
<tr>
<td>4. Mineral textures</td>
<td>Chemical composition of minerals (as an extra measure to evaluate mineral grade against elemental grade)</td>
<td>Electron probe micro-analysis (EPMA) with energy-dispersive spectrometer (EDS); Wavelength-dispersive spectrometer (WDS)</td>
</tr>
<tr>
<td></td>
<td>Mineral grain sizes, grain shapes, associated minerals (rock samples), liberation distribution of minerals in samples (particulate samples)</td>
<td>SEM-based image analysis (MLA, QEMSCAN, TIMA, Mineralogic, IncaMineral, RockSCAN); Optical image analysis (CSIRO Recognition1/Minerals13); Electron backscatter diffraction (EBSD); Hyperspectral imaging (SisuRock)</td>
</tr>
</tbody>
</table>
analysis are considerably fast. Depending on the sample preparation, measurement conditions (X-ray source, data acquisition time) and crystallinity of the minerals, the detection limit can be as low as 0.5 wt.%. Spicer et al. (2008) have shown that it is possible to get reliable analysis on mineral grades for heavy mineral sands by the Rietveld method. Comparing with Mineral Liberation Analyzer (MLA) measurements, the Rietveld results were not significantly different for rutile, zircon, ilmenite, and total iron oxides but separately for magnetite and hematite the difference was significantly higher (König and Spicer, 2007; Spicer et al., 2008). The differences were originated from the way that the two techniques detect magnetite and hematite. MLA under normal analyzing condition cannot distinguish well between hematite and magnetite. Similarly, König et al. (2011) used the Rietveld analysis for phase quantification for sinter and slag from a steel plant.

Ramanidou and Wells (2011) studied the utilization of hyperspectral imaging for characterizing iron ores. The method is proposed for grade control in in-situ mapping and scanning of drill chips. The advantages of the method are that measurements are quick and samples of different volume can be processed. On the other hand, the method requires dry conditions for the imaging target (wall, drill core samples), and it fails in identifying certain phases such as sulphide minerals and magnetite.

To improve bulk mineralogy estimation, a combination of the Rietveld and chemical analysis has been used by Berry et al. (2011). They applied a nonnegative least square algorithm with weighted values to estimate mineral grades. Their combined method was partially successful in overcoming the limit of determination of the Rietveld analysis which initially posed by XRD measurement.

This study uses several types of iron ore samples to compare different methods of analyzing bulk mineralogy, i.e. mineral grades, to be applied in geometallurgy and process mineralogy. In the comparison of the methods, solely their potential to estimate bulk mineral grades is considered. Additional information that some methods offer are considered in the final evaluation of the methods. The element-to-mineral conversions, quantitative XRD by Rietveld analysis and SEM-based automated mineralogy are used in this study. An additional method called Combined EMC and XRD (or shorter: combined method) is developed in order to overcome some of the shortcomings in element-to-mineral conversion and quantitative XRD by Rietveld analysis. Practically, the algorithm that is used for combined method can be applied for any other method of modal mineralogy to adjust the mineral grades to match closely with chemical composition of given sample. In addition, this paper aims to develop a model for describing precision and trueness in analysis of mineral grades. The model should cover the whole grade range (0–100 wt.%), be easy to use and be informative.

2. Statistical terminology

Trueness is defined as “the closeness of agreement between the expectation of a test result or measurement result and a true value” whereas precision is the repeatability (or reproducibility) of the measurement method. Accuracy means “closeness of agreement between a measured quantity value and a true quantity value of a measured” (Reichenbächer and Einax, 2011). According to The International Vocabulary of Basic and General Terms in Metrology (VIM), accuracy is a qualitative concept and commonly regarded as a combination of trueness and precision.

The trueness of a measurement method is achievable when it is possible to conceive a true value. However, in chemical and mineralogical analysis it is quite common that the true value is unknown. This can be overcome by establishing a reference to another measurement method or by preparing a synthetic standard or reference sample (ISO 5725–4:1994). The trueness and precision are normally expressed in terms of bias and standard deviation, respectively (Menditto et al., 2007). To validate correctly a method result, both terms must be considered.

Commonly standards or artificially mixed samples are used for evaluating the trueness. For the analysis of mineral grades, standards are not commonly available. As this study aims to evaluate different analysis methods of mineral grades for practical geometallurgy, the usage of a synthetic sample was avoided. Synthetic samples would not represent the original textures, complexity and variation existing in natural samples. Moreover, using synthetic samples would lead to underestimating the error in the analysis of ore samples in practice.

The alternative way to evaluate the trueness is to compare against a valid reference. However, the references such as XRF analysis for chemical analysis or SEM-based automated mineralogy for mineral grades cannot be regarded as true values. Therefore, when using these references for the estimation of the trueness, which is now unknown, instead of the term trueness the term closeness was selected to evaluate how close the results are compared to the references.

Here, the precision of the methods is addressed by the standard deviation. The estimate of the standard deviation is done by replicate samples and replicate analyses. Repeating only the measurement gives the repeatability and repeating the sample preparation and measurement gives the reproducibility. In this study, the standard deviation calculated for XRF and quantitative XRD by Rietveld analysis is a measure of reproducibility, while for automated mineralogy it is a measure of repeatability.

Based on boot strapping technique Evans and Napier-Munn (2013) suggested that the standard deviation in an analysis of mineral grades is proportional to the square root of the total area of particles measured. Moreover, they conclude that the model reflects the relationship between standard deviation and number of particles measured. Similarly, the standard deviation of an estimated mineral grade can be calculated with the formula:

\[
\sigma = \sqrt{\frac{pq}{N}}
\]

where \(\sigma\) is the standard deviation, \(p\) is the measured mineral grade, \(q\) is the value of \((1-p)\) and \(N\) is the number of particles measured (Evans and Napier-Munn, 2013; Mann, 2010). Comparatively, the relationship between relative standard deviation and average mineral grade can be modeled as:

\[
RSD = ax^{-0.5}
\]

where \(x\) is the grade of mineral of interest, \(RSD\) is the relative standard deviation, and \(a\) is a coefficient. The formula suggests that the relative standard deviation is proportional to the square root of the grade. This model was used in the following to estimate the (relative) standard deviation of the measurements for any mineral grade.

The measurement of the closeness is more challenging. The paired \(t\)-test is often used for comparing two methods (e.g. Benvie et al., 2013). However, the \(t\)-test can be used to compare whether two methods give the same average value but it does not provide an easy way for estimating magnitude of the differences respect to a reference method. Nevertheless, the \(t\)-test was not completely rejected and it was used to validate the comparison of methods in two ways; by comparing mineral grades and back-calculated elemental grades against references. The selected references for evaluating mineral grades and chemical composition analyses were SEM-based automated mineralogy and XRF analysis, respectively.
For the measuring of closeness, a Root-Mean-Square-Deviation (RMSD) was used besides the t-test (Hyndman and Koehler, 2006). Principally, RMSD aggregates the magnitude of deviations from the reference value into a single value. Mathematically, it is a concept similar to the standard deviation, but the term is used to describe an average deviation from the reference. This is used as the degree of closeness and is expressed as follows:

\[ \text{RMSD} = \sqrt{\frac{\sum_{i=1}^{n} (\mu_i - x_i)^2}{n}} \]  
(4)

Relative RMSD = \( 100 \times \frac{\text{RMSD}}{\mu} \)  
(5)

where \( n \) is the number of measurements, \( \mu \) is the reference value, \( x_i \) is the measured value and \( \mu_i \) is average of the reference values. The Relative RMSD can be calculated for each mineral and element with different methods. The method showing smallest variation around the reference value (i.e. a lower RMSD) is regarded as the closest to the reference.

3. Materials and methods

3.1. Samples

Northern Sweden is a significant mining district in Europe and characterized by diverse styles of mineralization including Fe oxide, Cu ± Au and Au ores. More than 40 different iron ore deposits are known in the area and they all have a variation in character based on the ore type, main ore minerals and alteration features etc. (Bergman et al., 2001). The Fe content varies between 25–70% and the P content up to 5%. The main minerals are magnetite and hematite, and the gangue minerals are apatite, amphibole, feldspars, clinopyroxene and quartz. Garnet and calcite are present in some of the deposits. From textural point of view, there is a wide variation on grain size (100–1400 µm), shape and association of the main minerals. Different textures of iron oxides include homogenous magnetite, magnetite intergrowths of ilmenite and rutile, oxidation assemblage of hematite and rutile (Lund, 2013).

A total of 20 ore and process samples from different iron ore deposits in Northern Sweden were collected for this study. The iron grade in the ore samples (drill cores) varied from 21.3% to 63.0% Fe and the ore samples were classified as semi-massive hematite ore and massive magnetite ore (Niiranen, 2006).

The samples, for different analyses, went through multiple sample preparation steps. From crushed samples, a part was taken for a preparation of resin mounts. The remaining part was pulverized in the disc mill and split into two parts. The first part was used for X-ray fluorescence analysis, and the second was further ground with a swing mill. The fine powder was used for filling the back-loading holders with an opening of 26 mm in diameter for X-ray diffraction analysis. The \( \Phi_{80} \) of the powder was 20 µm.

3.2. Methods

3.2.1. Elemental assays

Chemical analyses of the samples (Table 2) were done at chemical laboratory of Luossavaara-Kiirunavaara AB (LKAB) using the company’s standardized methods. X-ray fluorescence spectrometry (MagiX FAST, PANalytical) was used for the 11 major and minor elements. Divalent iron was analyzed by the titrimetric method (ISO 9035:1989) and the mass proportion of magnetic material was measured with the Saturation Magnetic Analyzer (Satmagan) model 135 (Stradling, 1991). A calibration of the Satmagan analysis was done to give similar results as with the titrimetric Fe\(^{2+}\) method; i.e. for a pure magnetite sample, the Satmagan value was 24.3%.

3.2.2. Quantitative X-ray diffraction with Rietveld analysis

The first trial of the X-ray powder diffraction analyses were done at Luleå University of Technology (LTU) using a PANalytical Empyrean X-ray diffractometer equipped with a copper tube, Pixel3D detector and pyrolytic graphite monochromator. The 2θ range was from 5° to 75° with a step size of 0.02°. These conditions resulted in a total measurement time of 150 min for a single XRD scan. Mineral phases were identified using HighScore Plus Version 3 software package and the Crystallography Open Database (COD). In the Rietveld refinement, background correction, scale factors, unit cells, preferred orientations, and profile variables were included.

X-ray diffraction and Rietveld refinement with a copper tube and monochromator on the iron ore samples led to underestimation of iron mineral phases (Parian and Lamberg, 2013). This was mainly due to microabsorption (Pederson et al., 2004) and also fluorescence radiation of the iron ore samples by copper tube. Therefore, samples were reanalyzed at the Geological Survey of Finland (GTK) with PANalytical CubIX industrial XRD system equipped with Cobalt tube and X'Celerator detector. Phase identification and Rietveld refinement afterwards was same as described previously.

Additionaly, two of the samples were measured several times in Helmholtz-Institute for Resource Technology in Freiberg using PANalytical Empyrean, equipped with a Cobalt tube, monochromator and Xe proportional counter detector. The step width and 2θ range was same as previous measurements. The Rietveld refinement on these data was done by BGMN (BGMN by Bergmann et al., (1998)) and these data are used for estimating error for X-ray diffraction and Rietveld refinement.

3.2.3. Automated mineralogy

Automated mineralogy is commonly regarded as the most reliable method for the analysis of mineral grades. However, its capabilities are beyond reporting only mineral grades. It provides textural properties such as grain size and shape, mineral associations and mineral liberation numerically.

In ore projects, normally 0.3–2.0 m long drill core sections are collected for chemical assays and mineralogical study. However, crushed drill core has a wide size particle distribution, which is a problem in the analysis of mineral grades both in sample preparation and in measurement. In the preparation of resin mounts, crushed samples tend to segregate, i.e. large and dense particles are enriched in the lower part of the resin. This leads to a bias in particle size distribution as well as in the analysis of mineral grades (Kwitko-ribeiro, 2012). Therefore, the common procedure is to first size the samples into narrow size fractions, which is a measure used to minimize analysis error when the focus is on quantitative textural measurements, i.e. liberation etc.

When assaying a large number of samples (>10,000), sizing is not an option since it multiplies the number of samples to be analyzed. In analysis of polished sections, using unsized samples introduces segmentation and stereological errors. The stereological error is less significant than segmentation error and is more influential in the liberation analysis than bulk mineralogy analysis as shown by Lastra and Petruk (2014). To minimize the segregation, the samples were “double sectioned” also known as vertical sectioning. This technique is commonly used in several mineralogical laboratories and has been validated to reduce the sample segregation significantly (Kwitko-ribeiro, 2012). In double-sectioning samples were first mold in resin and after hardening sawed into slices. The slices were thereafter arranged in another mold in a way that
they show the sedimentation profile towards the side to be analyzed (Kwitko-Ribeiro, 2012).

A Merlin SEM – Zeiss Gemini (FESEM, Luleå University of Technology, Sweden) with Oxford Instrument EDS detector and IncaMineral software was used for automated mineralogy analyses. The IncaMineral system combines backscattered detector images with EDS information in the analysis of automated mineralogy (Lippo et al., 2012). Within the IncaMineral software, the raw analysis data is stored in a database and mineral identification and quantification can be done either during analysis or retrospectively. To obtain a reliable estimate, the number of particles analyzed for the mineral quantification was at least 10,000. In this study, mineral identification was done based on back-scattered information and EDS analysis. Developed software at Luleå university of Technology (by first author) was used for post-processing the data i.e. mineral identification, reporting mineral grades and chemical composition of a sample.

To confirm IncaMineral results quality, two resin mount samples were analyzed at the geometallurgy laboratory, Technical University of Freiberg by Mineral Liberation Analyzer (MLA) system, which was equipped with FEI Quanta 650F and two Bruker Quantax X-Flash 5030 energy-dispersive X-ray spectrometers.

The automated mineralogy analysis provided a mineral list, which includes more than 15 phases. In some of the samples, even several types of one mineral were found, e.g. several amphiboles. For geometallurgy, this is not practical and some simplification is necessary. The simplification is also required for comparing the samples. Therefore, the main phases in the samples were classified into groups of albite (Ab), actinolite (Act), apatite (Ap), biotite (Bt), diopside (Di), orthoclase (Or), quartz (Qtz), andradite (Adr), scapolite (Scp), calcite (Cal), magnetite (Mgt) and hematite (Hem). In the grouping of the minerals and the selection of group representer, the similar behavior of the minerals in the iron processing plant, similarity in their chemical compositions, and abundance of the mineral in the group were considered to streamline application and evaluation of the methods. For example, group of actinolite consists of various amphibole minerals such as tremolite, actinolite and hornblende. The chemical compositions of the minerals (Table 3) was provided by LKAB and partly taken from a previous study from LKAB’s mine in Malmberget (Lund, 2013). Analysis of mineral chemistry, in those studies, was carried out at the Geological Survey of Finland (GTK) using a Cameca SX100 electron microprobe equipped with five WDS. This information was also verified by automated mineralogy as the IncaMineral system provides the chemical composition of each analyzed grain and based on that an average composition of each phase can then be approximated calculated.

3.2.4. Element-to-mineral conversion (EMC) and combined method using EMC and XRD Rietveld analysis

EMC method is the fastest and the most practical method of obtaining mineral grades when the existing minerals and their chemical compositions are known. Principally, the EMC method solves a system of linear equations where mineral grades are the unknown variables. In cases where the linear system is not determined, the least-square method can be applied to find an approximate solution. Negative solutions are not acceptable for mineral grades, thus a nonnegative method is used. Several numerical methods exist for solving the system of equations with non-negativity constraints. These include the nonnegative least-square method (NNLS) (Lawson and Hanson, 1995), the Barzilai-Borwein gradient projection algorithm, the interior point Newton algorithm, the projected gradient algorithm, and the sequential coordinate-wise algorithm (Cichocki et al., 2009).

Based on the information available (elemental assays and chemical composition of minerals), mineral grades can be calculated by the nonnegative least-square method. However, here the system of linear equations is underdetermined by having 12 unknowns (mineral grades) and 9 equations (reliable elemental assays and Satmagan). Therefore, mathematically this system of linear equations does not have a unique solution not even when non-negativity constraint is added. Practically this means that mineral grades are calculated for nine phases and for other phases, the solution gives zero grades.

The calculation of mineral grades with the EMC method can be done sequentially, i.e. system of equations can be divided into two or more set of equations, and each set forms a calculation round of its own. The rounds are solved sequentially and the residual chemical composition of the round will be used in the following round. EMC with rounds enables to have a better control on important elements and to reach a solution where the back-calculated chemical composition matches perfectly with assays for selected elements. For example in iron ores, silicates are calculated first with non-negative least square solution and finally iron and titanium oxides are calculated from residual iron and titanium (Lund et al., 2013). This gives zero iron residual whereas elements in

<table>
<thead>
<tr>
<th>Sample</th>
<th>Na</th>
<th>Mg</th>
<th>Al</th>
<th>Si</th>
<th>P</th>
<th>K</th>
<th>Ca</th>
<th>Ti</th>
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<td>19.7</td>
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<td>0.69</td>
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<td>0.07</td>
<td>0.8</td>
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<td>0.070</td>
<td>70.0</td>
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<td>0.71</td>
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<td>0.240</td>
<td>0.097</td>
<td>0.077</td>
<td>62.3</td>
<td>20.1</td>
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</tbody>
</table>

* Margin of error (±σ) for XRF assays can be calculated by ±0.013 x √x, where x is the elemental assay.
several silicate minerals, like aluminum, magnesium and silica, may show non-zero residual. Therefore, the balance for iron, which is important element here, is good whereas for elements being less critical the balance is acceptable.

Generally, the combined EMC–XRD method originated to overcome limitations of EMC and XRD. It takes mineral grades by the Rietveld analysis as an initial estimate and changes mineral grades to minimize the following function:

$$f(x) = |b - A \times x|$$ (6)

where $b$ is the vector of chemical composition of the sample, $A$ is the matrix of chemical compositions of minerals, and $x$ is the vector of mineral grades, i.e. unknown to be solved. The absolute minimum of $f(x)$ would be the result of simple element-to-mineral conversion method by the methods described above (e.g. NNLS). However, finding a local minimum of $f(x)$ may show non-zero residual. Therefore, the balance for iron, which is important element here, is good whereas for elements being less critical the balance is acceptable.

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General...
±3.68 wt.% This can be regarded as acceptable in geometallurgy. On the other hand, for average ore grade of 1 wt.% such as apatite and biotite the coefficient of variation is between 4% and 22% (standard deviation 0.04–0.22 wt.%). The error is high for technical work like resource estimation or process mineralogy (Pitard, 1993) but the analysis quality is still good enough for geometallurgical purposes like domaining where acceptable error can be higher.

### 4.3. Closeness of the analyses

For quality control, two resin mounts analyzed by IncaMineral were also analyzed by Mineral Liberation Analyzer (MLA). Comparing analyzed minerals by IncaMineral against MLA analysis (Table 6), mineral grades by IncaMineral are close to MLA mineral grades, which suggest that the two methods are giving similar results.

Automated mineralogy analysis results were used as the reference values when comparing closeness of the methods. The paired t-test implies that generally XRD, combined EMC–XRD and EMC do not give significantly different results compared to automated mineralogy (Table 7). Meanwhile, relative RMSD shows that the difference between the automated mineralogy and EMC is relatively higher than that of the other methods (Fig. 2 and Table 7). Relative RMSD reveals that XRD results for iron oxide is closest to automated mineralogy while paired t-test suggests XRD results are slightly positively biased.

The alternative way of evaluating closeness was by regarding XRF analysis as the reference value and comparing back-calculated chemical compositions of the samples against it. Paired t-test results suggest that combined EMC–XRD and EMC methods give significantly different mean values for the chemical composition (Table 8). However, relative RMSD indicates all the methods in terms of deviations from XRF assays are in the same range.
such as geometallurgical domaining and ore block grading (Paine et al., 2011). This may work in high grade ores like iron, aluminum and industrial minerals. However, in the case of precious and most of the base metal ores the detection limit creates limitation, which restrict that the classification is capable to work only with main minerals, which may not be the most relevant for geometallurgical purposes like domaining.

A combined method using weighted values (Berry et al., 2011; Roine, 2009) provides an alternative to adjust mineral grades to match the Rietveld analysis results and chemical assays, but its problem is how to define the weighting factors in order to get reliable results. Weighting factors can be set based on the uncertainties of the elemental and mineral grade, but still this approach cannot overcome limitations such as XRD detection limit and high error in low mineral grades. Combined EMC–XRD method developed here, does not use weighting factors but can still find the closest solution to match both the Rietveld analysis results and chemical assays. Knowing the error model, more constraints can be established for estimating mineral grades by combined method.

Any technique for the analysis of mineral grades in a geometallurgical program requires careful mineralogical study before the method is routinely applied. In combined method, the mineralogical study must provide information on the list of all possible minerals, their crystal structure, and their chemical composition. Additionally, to be able to apply the combined method, the minerals need to be grouped in a sensible way, i.e. groups consist of minerals with similarity in chemical composition as well as process behavior. Therefore, nature of the ore body and the process define the grouping of minerals, acceptable error, and eventually the method to be used.

However, combined method is not a universal solution for every situation as it is. Principally, the algorithm for estimating mineral grades can take as many restrictive constraints as needed. Therefore, if several minor minerals are present in the sample but the information for calculating mineral grades is insufficient, the combined method requires additional constraints to converge to the optimal solution. In addition, the assumption used here is that the chemical composition of minerals is known and does not vary. Strictly speaking, this is not a realistic assumption, but it simplifies the complex situation for finding a bridge between elemental assays and mineral grades.

It is relatively rare to find error estimation for the analyses of mineral grades published in the literature and research reports. For quality control, back-calculated chemical composition is often plotted against the analyzed ones (e.g. Berry et al., 2011; Hestnes and Sørensen, 2012). As these illustrations visualize the quality, they do not quantify how big the difference really is. Paired t-test is used but as was shown in the results, it fails in measuring how close the results are. In addition, it requires that standard deviations are equal and not dependent on the grade, which is unrealistic assumption. Relative RMSE is an informative and effective way of measuring the closeness. The calculation is similar to the standard deviation, which makes it straightforward and portable for several purposes like mass balancing and modeling.

The precision and degree of trueness of an analysis for mineral grades are dependent on the abundance of a phase in a sample and the number of observations collected. In automated mineralogy, this depends on the number of particles and grains analyzed. In
X-ray techniques (X-ray diffraction and X-ray fluorescence), the ratio of signal to noise, thus analysis time, plays the role. Here a simple equation was used to describe the standard deviation and the RMSD in the wide grade range where analysis conditions are the same as commonly used in process mineralogy. This approach is practical when individual standard deviations are needed for measurements. Examples of such problems are circuit mass balancing and Monte Carlo simulations.

The methods available for obtaining mineral grades either directly (such as quantitative XRD by Rietveld analysis and automated mineralogy) or indirectly (EMC and combined EMC–XRD) have different advantages and disadvantages. Table 9 summarizes the different methods and their applicability in geometallurgy. To be used for metallic ores, the detection limit must be lower than 1 wt.%, which excludes XRD. In geometallurgical programs, the number of samples to be analyzed during developing a deposit model is high, several thousand in a year. Therefore, the requirements on sample preparation and analysis time and costs exclude the usage of automated mineralogy as a routine tool for the analysis of mineral grades in geometallurgy. Even though element-to-mineral conversion has good repeatability, it suffers from poor trueness in most of the real geometallurgical cases. This is due to a larger number of unknowns (minerals) than known quantities (chemical elements assayed) which makes the system mathematically underdetermined. Hence, the combined method fulfills the requirements to be used in ore characterization and deposit modeling for geometallurgy.

Table 7
Closeness of analysis methods for mineral grades by paired t-test and RMSD against automated mineralogy as the reference.

<table>
<thead>
<tr>
<th>Chemical Assays</th>
<th>XRD</th>
<th>CMB</th>
<th>EMC</th>
<th>RMSD</th>
<th>XRD</th>
<th>CMB</th>
<th>EMC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe oxides</td>
<td>-2.82&lt;sup&gt;a&lt;/sup&gt;</td>
<td>1.81</td>
<td>2.20</td>
<td>4.77</td>
<td>6.31</td>
<td>8.76</td>
<td></td>
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<tr>
<td>Apatite</td>
<td>-0.07</td>
<td>-0.52</td>
<td>-0.31</td>
<td>1.80</td>
<td>1.56</td>
<td>1.54</td>
<td></td>
</tr>
<tr>
<td>Biotite</td>
<td>0.56</td>
<td>1.53</td>
<td>1.49</td>
<td>0.79</td>
<td>1.59</td>
<td>1.74</td>
<td></td>
</tr>
<tr>
<td>Andradite</td>
<td>-1.38</td>
<td>-2.06</td>
<td>-2.21</td>
<td>1.74</td>
<td>2.12</td>
<td>9.64</td>
<td></td>
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<tr>
<td>Other silicate</td>
<td>-0.16</td>
<td>0.63</td>
<td>2.20</td>
<td>1.63</td>
<td>1.61</td>
<td>2.41</td>
<td></td>
</tr>
<tr>
<td>t critical</td>
<td>±2.26</td>
<td>±2.26</td>
<td>±2.26</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<sup>a</sup> Absolute value of t is greater than critical value indicating statistically significant difference in results between automated mineralogy and the method.

Fig. 2. Relative RMSD against mineral grades (EMC, XRD, CMB). Curves for different methods derived from fitting calculated RMSD for experimental data with Eq. (3). Relative RMSD values are calculated by Eqs. (4) and (5).

Table 8
Closeness of analysis methods for elemental grades by paired t-test and RMSD against XRF analysis as the reference.

<table>
<thead>
<tr>
<th>Chemical Assays</th>
<th>t Value by paired t-test</th>
<th>RMSD</th>
<th>XRD</th>
<th>CMB</th>
<th>EMC</th>
<th>AM</th>
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<tr>
<td>Na</td>
<td>1.39</td>
<td>-0.36</td>
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<td>0.13</td>
<td>0.03</td>
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<td>Mg</td>
<td>-2.75&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-2.07</td>
<td>-3.43&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-1.06</td>
<td>0.36</td>
<td>0.14</td>
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<tr>
<td>Al</td>
<td>0.86</td>
<td>-0.34</td>
<td>2.17&lt;sup&gt;a&lt;/sup&gt;</td>
<td>1.34</td>
<td>0.47</td>
<td>0.06</td>
</tr>
<tr>
<td>Si</td>
<td>2.40&lt;sup&gt;a&lt;/sup&gt;</td>
<td>2.03</td>
<td>1.48</td>
<td>0.42</td>
<td>0.92</td>
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<tr>
<td>P</td>
<td>-3.68&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-5.52&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-5.40&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.40</td>
<td>0.14</td>
<td>0.06</td>
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<tr>
<td>K</td>
<td>-0.06</td>
<td>4.35&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-0.23</td>
<td>0.25</td>
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<td>Ca</td>
<td>-0.94</td>
<td>2.72&lt;sup&gt;a&lt;/sup&gt;</td>
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<td>0.81</td>
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<tr>
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<td>5.18&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.18</td>
<td>0.13</td>
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<tr>
<td>V</td>
<td>-2.19&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-2.17&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-2.03</td>
<td>-1.52</td>
<td>0.06</td>
<td>0.06</td>
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<tr>
<td>Mn</td>
<td>-12.97&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-12.80&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-13.60&lt;sup&gt;a&lt;/sup&gt;</td>
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<td>0.08</td>
<td>0.08</td>
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<tr>
<td>Fe</td>
<td>-0.19</td>
<td>-1.17</td>
<td>2.57&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-1.42</td>
<td>1.91</td>
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<td>Satmagan</td>
<td>0.47</td>
<td>0.12</td>
<td>-2.67&lt;sup&gt;a&lt;/sup&gt;</td>
<td>1.12</td>
<td>1.09</td>
<td>0.47</td>
</tr>
<tr>
<td>t Critical</td>
<td>±2.09</td>
<td>±2.09</td>
<td>±2.09</td>
<td>±2.26</td>
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</table>

<sup>a</sup> Absolute value of t is greater than critical value indicating statistically significant difference between analyzed chemical composition (XRF) and back calculated composition from the mineral composition.

Fig. 3. Relative RMSD against elemental grades (AM, EMC, CMB, XRD). Curves for different methods derived from fitting calculated RMSD for experimental data with Eq. (3). Relative RMSD values are calculated by Eqs. (4) and (5).
The problem remaining is that with all methods the back-calculated chemical composition does not match perfectly with the chemical assays of the commodity elements. The challenge is that as resource geologists and metallurgists have a long tradition to work with chemical assays, they find it difficult to take parallel mineralogical information that is not fully consistent with chemical assays. Weighting can be a solution for that but more work is needed to establish solid grounds for defining the weighting factors and to control that weighing does not cause the mineral grades to drift too far away from the true mineral composition.

For a selection of the best possible option further information regarding practical considerations such as sample preparation, costs, detection limit, and the information that method offers are necessary (Table 9).

6. Conclusions

Conclusions from the work done are summarized below:

(1) Three different methods for the analysis of mineral grades were compared firstly in terms of the closeness (cf. trueness) and precision but also with respect to their applicability in geometallurgy. Detection limit, sample preparation, analysis time, costs and additional information that they provide were included in the evaluation.

(2) A combined technique of quantitative X-ray diffraction and element-to-mineral conversion has been introduced to overcome the limitations of each of the techniques. Thus, it is suggested to be suitable for geometallurgy for the analysis of mineral grades in bulk.

(3) The combined method gives an estimate on both magnetite and hematite grades and can replace tedious Satmagan and wet chemical Fe²⁺ analysis.

(4) A problem occurring with all methods is that back-calculated chemical composition from mineral grades does not match perfectly with the elemental grades of commodities received from chemical assays. This can be partially solved by combined method, however, this can be fully avoided in the evaluation, but this requires further development.

Acknowledgments

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References


Fredriksson from LKAB. Cecilia Lund (Luleå University of Technology) helped in automated mineralogy and finalizing the article. Megan Becker (University of Cape Town) gave comments and suggestions on the draft paper. They all are greatly appreciated. The authors are grateful to the ProMinNet research group for comments and advice provided during the meetings. The help of Jukka Laukkanen from Geological Survey of Finland (GTK) in XRD analysis is appreciated.


Paper II
Developing a particle-based process model for unit operations of mineral processing – WLIMS

Mehdi Parian *, Pertti Lamberg, Jan Rosenkranz

Minerals and Metallurgical Engineering, Luleå University of Technology, SE-971 87 Luleå, Sweden

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A B S T R A C T

Process models in mineral processing can be classified based on the level of information required from the ore, i.e. the feed stream to the processing plant. Mineral processing models usually require information on total solid flow rate, mineralogical composition and particle size information. The most comprehensive level of mineral processing models is the particle-based one (liberation level), which gives particle-by-particle information on their mineralogical composition, size, density, shape i.e. all necessary information on the processed material for simulating unit operations. In flowsheet simulation, the major benefit of a particle-based model over other models is that it can be directly linked to any other particle-based unit models in the process simulation. This study aims to develop a unit operation model for a wet low intensity magnetic separator on particle property level. The experimental data was gathered in a plant survey of the K3 iron ore concentrator of Luossavaara-Kiirunavaara AB in Kiruna. Corresponding feed, concentrate and tailings streams of the primary magnetic separator were sampled, assayed and mass balanced on mineral liberation level. The mass-balanced data showed that the behavior of individual particles in the magnetic separation is depending on their size and composition. The developed model involves a size and composition dependent entrapment parameter and a separation function that depends on the magnetic intensity of the particle and the nature of gangue mineral. The model is capable of forecasting the behavior of particles in magnetic separation with the necessary accuracy. This study highlights the benefits that particle-based models in simulation offer whereas lower level process models fail to provide.

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1. Introduction

Minerals and particles are the key elements in mineral processing operations and simulation. Both mineral properties and particle size define the selection of a process and particles govern the process performance. However, the full potential of using particles in mineral processing simulation has not been accomplished yet. This is partly due to lack of analyzing instruments to collect information on particle level as well as lack of mass balancing techniques and data reconciliation methods capable to work with the mineral liberation level. The development of automated mineralogy methods (Donskoi et al., 2010; Gu et al., 2014) has facilitated collecting particle level information. Additionally, data reconciliation and mass balancing techniques improved from the traditional approach of balancing solids and elements (Hodouin, 2010) to reconciling and adjusting particle populations (Lamberg and Vianna, 2007). These developments have built a foundation to take mineral processing unit models and simulation to a new level.

Taking a step back and looking at the bigger picture, where the feed has not reached the mineral processing plant yet, a holistic view of geology, mining and mineral processing exists. This approach is known as geometallurgy, a rapidly expanding area of geology and mineral processing to create spatially based models for production management (Lamberg, 2011). It requires geological and resource characterization information to be collected in a way to build predictive models for a mineral processing circuit.

As to the level of details, geometallurgical predictive models can be divided into three categories whether the smallest block in the simulation is an entire processing circuit (black box model), a section (e.g. comminution circuit) or a single unit operation (e.g. individual flotation cells). Another way of classifying geometallurgical models is based on the level to that the feed stream properties are described. A stream can have several attributes including flow rates and particle size classes. A bulk stream can be considered as a set of sub-streams each representing a particle size class. If there are no size classes available, then unsized or bulk information is used. The flow rates in a stream, from lowest to highest level of detailedness, are solids, elements, minerals and particles. Obviously, the study goal defines the selection of...
the level and size information. For instance, sized solids are often used to model and simulate comminution circuits whereas bulk-mineral information is common in flotation.

The selection of a modeling level comes with certain restrictions (Table 1) that limit its usability when expanding it outside the scope where the model is created and calibrated. For instance, while a model on solids flowrate level is enough for equipment sizing in the basic engineering stage of an ore project, it cannot be used for estimating the performance of a separator unit. In the grindability type criterion, material is divided into grindability types, e.g. hard and soft, and these types will behave differently in comminution circuit. Clearly, the feed stream that is defined only by grindability types cannot be adopted directly, for example, in a magnetic separator model, which at least requires elemental or mineral distribution. In minerals by behavioral types (in bulk or by size) level, each mineral is divided into behavioral types. For example in flotation modeling, the floatability component approach divides each mineral to fast and slow floating, slow floating and non-floating type (Runge and Franzidis, 2003). On particle level (or mineral liberation level), the assumption is that, similar particles (in terms of the particle’s attributes such as composition, size and shape) behave similarly regardless of from which part of the ore they originate. In a process or circuit simulation, the ideal situation is where all unit operation models work on a same level. If not, then transformation functions or models must be used where some of the required stream properties are generated based on existing information of the stream and additional information given in a model.

The purpose of this paper is to develop a particle-based unit operation model for geometallurgical purposes by using wet low intensity magnetic separation (WLIMS) as a case study. The aim is that a particle-based model can forecast composition and flow rates (i.e. recovery) of the magnetic concentrate and tailings for any new feed stream if the particle level information is available. This type of models can be coupled with any other particle-based unit models in mineral processing and recycling (Castro et al., 2005). This approach ensures that all necessary information is passed through the streams for each unit operation and all process streams including the final products carry particle level information (particle size distribution, mineral liberation distribution and etc.). This demands high level information for the plant feed since all required properties in any processing unit downstream must be generated mostly from that. The mineralogical approach to geometallurgy (Lanberg et al., 2013) aims to provide such a high level information to mineral processing simulation. Therefore, a particle-based model of mineral processing units can effectively work in the theme of geometallurgy to address variations in the ore body in order to provide a robust production forecast.

### 2. Models for wet magnetic separators

Literature on magnetic separators focuses on design and operation of the unit with recommendations for improving their performance (Cui and Forssberg, 2003; Dobbins et al., 2009; Oberteuffer, 1974; Svoboda and Fujita, 2003). Models suitable for flowsheet simulation are quite a few, mostly empirical, and rarely based on physical or chemical principles behind the process. In the following, various wet

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**Table 1**

Modeling levels and their limitations in minerals processing. The model is valid as long as the feed stream assumptions are met.

<table>
<thead>
<tr>
<th>Level</th>
<th>Feed stream assumptions</th>
<th>Example of application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk</td>
<td>Each particle will behave identically regardless of its size and composition</td>
<td>Solid splitter model, equipment scale-up, basic engineering</td>
</tr>
<tr>
<td>Solids</td>
<td>Particle size distribution and liberation distribution are unchanged</td>
<td>Mineral splitter model</td>
</tr>
<tr>
<td>Mineral</td>
<td>Particle size distribution is unchanged. Similar behavioral types will behave identically</td>
<td>Gravity separation model</td>
</tr>
<tr>
<td>Behavioral type</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sized</td>
<td>Each particle of given size will behave identically</td>
<td>Commination model, Size classification model, equipment scale-up</td>
</tr>
<tr>
<td>Solids</td>
<td></td>
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</tr>
<tr>
<td>Grindability type</td>
<td>Each particle type of given size will behave identically</td>
<td>Commination model</td>
</tr>
<tr>
<td>Element</td>
<td>Mineralogy and liberation distribution is unchanged</td>
<td>Recovery function model in size classes</td>
</tr>
<tr>
<td>Mineral</td>
<td>Liberation distribution is unchanged</td>
<td>Mineral splitter model in size classes</td>
</tr>
<tr>
<td>Behavioral type</td>
<td>Similar behavioral types will behave identically in narrow size fraction</td>
<td>Flotation model (fast and slow floating materials in size classes)</td>
</tr>
<tr>
<td>Particle</td>
<td>Similar behavior of particles of same composition and size</td>
<td>Gravity separation model in size classes</td>
</tr>
</tbody>
</table>

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**Table 2**

Magnetic separator models including model level and considered operational parameters.

<table>
<thead>
<tr>
<th>Model</th>
<th>Level</th>
<th>Feed properties used in model</th>
<th>Input parameters (given by user)</th>
<th>Output</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Davis tubes recovery functions</td>
<td>Elemental</td>
<td>Iron grade</td>
<td>Empirical functions for iron recovery</td>
<td>Iron recovery</td>
<td>Schulz (1963)</td>
</tr>
<tr>
<td>Dobby and Finch</td>
<td>Phase behavior type by size</td>
<td>Magnetic susceptibility and particle size distribution of the feed</td>
<td>$M_{50}$ and $R_{M}$</td>
<td>Recovery in size class</td>
<td>Dobby and Finch (1977)</td>
</tr>
<tr>
<td>Davis and Lyman</td>
<td>Mineral behavior type</td>
<td>Feed rate of magnetics (dry)</td>
<td>Drum speed, feed and squeeze pan clearances</td>
<td>Magnetite loss, Concentrate density</td>
<td>Davis and Lyman (1983)</td>
</tr>
<tr>
<td>USIM PAC</td>
<td>Mineral by size</td>
<td>Mineral composition of the feed by size fractions</td>
<td>Recovery of minerals in size fractions</td>
<td>Recovery of particles</td>
<td>Söderman et al. (1996)</td>
</tr>
<tr>
<td>King and Schneider</td>
<td>Particle</td>
<td>For each particle: magnetic volumetric grade, particle size</td>
<td>By-pass function</td>
<td>Recovery of particles</td>
<td>King and Schneider (1995)</td>
</tr>
<tr>
<td>Rayner and Napier-Munn</td>
<td>Mineral behavior type</td>
<td>Volumetric feed rate, gangue fraction, magnetic volume susceptibility, magnetic density, the volume of solids</td>
<td>Slurry viscosity in pickup zone</td>
<td>Magnetite loss in tailing</td>
<td>Rayner and Napier-Munn (2003b)</td>
</tr>
<tr>
<td>Metso</td>
<td>Particle</td>
<td>Not specified</td>
<td>Not specified</td>
<td>Not specified</td>
<td>Murarria (2013)</td>
</tr>
</tbody>
</table>
magnetic separator models are reviewed and compared against the modeling levels given in Table 1.

In magnetite ore processing, the Davis Tube test is traditionally used to develop recovery and grade models. Its development goes back to 1921 when a test previously performed manually mechanized (Schulz, 1963). Commonly, the models give the concentrate quality and iron recovery based on iron grade in the feed. The approach has proved to be practical for judging amenability of an ore to magnetic separation. However, the model is valid as long as mineralogy, ore texture, and distribution of particle size and liberation in the feed remain unchanged.

The empirical model of wet high intensity magnetic separator (WHIMS) by Dobby and Finch (1977) indicates that the recovery of particles into the magnetic concentrate is dependent on the magnetic susceptibility and size of particles. Their empirical model was defined as follows:

\[
R_d(x, d_p) = C + B \times \log_{10} \left( \frac{M_i}{M_{50}} \right)
\]

(1)

if \( M_i < M_{50} \times 10^{-45} \) then \( C = 0.05 \)

(2)

if \( M_{50} \times 10^{-45} \leq M_i \leq M_{50} \times 10^{45} \) then \( C = 0.5 \)

(3)

if \( M_i > M_{50} \times 10^{45} \) then \( C = 0.95 \)

(4)

where \( R_d \) is the recovery of particles having size \( d_p \) and volumetric magnetic susceptibility of \( x_i \); and \( M_{50} \) is the magnetic cut point at which the recovery is 50%. \( M_i \) and \( B \) are machine parameters and independent of the treated material. \( M_i \) is an empirical parameter calculated from a formula that is related to mass fraction of magnetic material in the feed, and magnetic and hydrodynamic force (King, 2012). Experimental test work is necessary to determine the distribution of particle size and magnetic susceptibility in the feed.

Davis and Lyman (1983) defined the feed stream using a binary system of magnetic and non-magnetic particles split into size classes and studied the effect of several operational variables like feed rate, drum speed and magnetite/non-magnetite particle size distribution on an Eriez full-scale high gradient wet magnetic separator. A two component model for the magnetite loss was described based on operational variables. The model lacks the ability to forecast the concentrate grade.

King and Schneider (1995) developed an empirical magnetic separator model that already uses particle properties. In the model, the distribution of particles between the concentrate and tailing is a function of the volumetric abundance of the magnetic phase in each particle. The fraction of particles that ends up in the tailings stream is described by the following formula:

\[
t(g_v, d) = \alpha(d) + (1-\alpha(d))r(g_v)
\]

(5)

where \( d \) is the particle size, \( \alpha(d) \) is the bypass fraction of particles in the feed that report directly to the tail. \( r(g_v) \) is the primary classification function based on volumetric grade of magnetic phase in the particle \( g_v \). The bypass function is modeled from experimental data using the reciprocal of natural exponential function with two coefficients. The primary classification function is modeled by a Rosin-Rammler distribution function and is only a function of particle composition, or more exactly the volumetric grade of the magnetic phase in a particle. The model was implemented in the MODSIMP simulation software. However, the size of a particle in classification function was not considered.

The magnetic separator model in the USIM PAC simulator is defined based on the recovery of minerals in size fractions. The user defines recoveries to the magnetic concentrate for each mineral by particle size fractions based on experimental results. An application example was given in the context of designing an iron ore beneficiation plant in Kiruna where a statistical model for a wet low intensity magnetic separator (WLIMS) was developed (Söderman et al., 1996). The authors simplified the model by assuming that recovery of magnetite per size class is not affected by minor changes in the head grade, feed rate or particle size distribution of the feed.

**Fig. 1.** Schematic view of approach for developing a unit model.

**Fig. 2.** Schematic procedure of preparing survey samples for analysis.
Rayner and Napier-Munn (2000) developed a model to predict the percentage loss of magnetic particles for a wet drum magnetic separator in a dense medium application. The model is represented by a flocculation rate and a residence time (Rayner and Napier-Munn, 2003a). The feed stream is described by the behavior type for magnetic particles and ferrosilicon as the dense medium. The size of the particles was not considered in this model.

A simplified approach called pseudo-liberation approach for simulating the effect of liberation in WLIMS was proposed by Ersayin (2004). The assumption behind the model was described as increasing grade of magnetite in the feed results in decreasing the degree of liberation of gangue minerals. For a given ore and plant, the pseudo-liberation model uses empirical data and cubic spline functions to generate a plant operating surface as a magnetic separator model.

Metso has developed a model for the LIMS that couples discrete element method (DEM), computational fluid dynamics (CFD) and finite element method (FEM) (Murariu, 2013). In the model, each particle is treated separately but details on how the model predicts the behavior of particles in the unit operation are not given. According to Murariu (2013) the model can be used to study the effect of operational parameters and geometry of LIMS on the separation efficiency. Although the model is not empirical, characterization of the feed in particle level is the requirement. The usage of the Metso model in flowsheet simulation has not been demonstrated in literature.

The models, as summarized in Table 2, are able to predict metallurgical performance to some extent. The majority of the models have been developed for optimization purposes with strict adoption to the feed type. Moreover, the available models are not able to make use of particle level information. The closest model among available models to provide such a feature is the King and Schneider (1995) model. However, the model considers particle size only for calculating the bypass to the tailings. Therefore, the development of a WLIMS particle-based model can be a starting point to generate more particle-based models for other processing units of mineral processing.

### Table 3

Average chemical composition of minerals (“the mineral matrix”) as wt.% and their specific gravity.

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Magnetite</th>
<th>Quartz</th>
<th>Apatite</th>
<th>Biotite</th>
<th>Albite</th>
<th>Actinolite</th>
<th>Calcite</th>
<th>Titanite</th>
<th>Titan-magnetite</th>
<th>Anhydrite</th>
<th>F (%)</th>
<th>S (%)</th>
<th>Na (%)</th>
<th>Mg (%)</th>
<th>Si (%)</th>
<th>P (%)</th>
<th>K (%)</th>
<th>Ca (%)</th>
<th>Ti (%)</th>
<th>V (%)</th>
<th>Mn (%)</th>
<th>Fe (%)</th>
<th>S.g.</th>
<th>Ash</th>
</tr>
</thead>
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<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
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<td>0.00</td>
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<tr>
<td>S %</td>
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<td>Na %</td>
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<td>Mg %</td>
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<td>10.26</td>
<td>10.09</td>
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<td>Si %</td>
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<td>0.00</td>
<td>0.00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* Specific gravity.

Fig. 3. Comparison of chemical composition between XRF assays against back calculated from IncaMineral modal measurements. Values on the graph are showing corresponding R² value for each element.
3. Methodical approach

Before starting to develop a process model, one needs to identify and decide on the level of detailedness needed for the purpose. A model can be established for the whole circuit, part of the circuit or a process unit. Once the smallest process entity is defined, model level based on achievable detail of feed stream (Table 1) and expectations from the model can be selected.

In mineral processing, developing and calibrating process models requires experimental work. The tests and corresponding analyses must be designed to meet the criteria of selected level; process/section/unit, element/mineral/particle, and bulk/sized. As the purpose of this study is to develop particle-based unit models for several mineral processing units in iron ore processing, the experimental work was based on a plant survey for an entire concentrator plant. However, at this stage only data around the primary magnetic separator was used here as the case study for developing particle-based unit models.

Before experimental data can be used in model development, the data must be mass-balanced. The mass balancing must be done on the same level the model is aiming to operate. For example, to address the liberation issues in the performance of a plant, the level of data collection and mass balancing needs to be on the particle composition level.

Once data reconciliation is done, the input and output of the unit is provided for model development. Principally, a mineral processing unit model is a set of mathematical functions representing the unit that uses the relevant input data such as feed properties and operating conditions for forecasting the performance of the unit. The modeling level and the model’s purpose usually specify the input and output parameters. The output of the model can be qualitative or a quantitative value. The unit models based on qualitative output are usually developed by unit manufacturers to reflect the effects of changes in the unit. On the other hand, a particle-based unit model is built to take particle properties as the input and provide the same level of output information. This ensures that the unit models can be coupled together and be used in flowsheet simulation.

The model should be developed in such way that unimportant details are neglected. The model can be developed based on empirical observations, or first principles behind the process, or by a combination of both. If the model uses a transfer function as the mathematical representation fitted to describe input and outputs, then a black box model is in use.

After development, the model needs to be compared against observations; this is called verification. The next step, the validation, is when the model is used to forecast the performance of the process based on observations not used in the modeling stage. Once a unit model has been verified and validated, it is ready to be used in simulation (Fig. 1). This paper focuses on model development and verification.

4. Experimental

4.1. Samples

The plant survey was done at one of the Luossavaara-Kiirunavaara AB (LKAB) iron ore processing plants in Kiruna, Northern Sweden. While the plant was operating at steady state, selected streams in the plant were sampled during a two hours period. The sampling protocol at LKAB was followed. Incremental sampling was performed around the circuit during the sampling period. Samples were taken at 10 minute intervals and added to the same bucket after each sampling interval. The cutter width was at least 3 times the diameter of the largest particles in the stream so as not to bias against their collection. Prior to sampling a dummy sample was taken and the sampler emptied out as it would be for the proper sample.

Additionally, all the information available from the control room was collected during the sampling campaign. For two of the streams, sampling was repeated three times in order to measure the experimental parameters.
error and to control the quality of the sampling. In this paper, samples around the primary WLIMS (feed, concentrate and tailings) are used to develop a particle-based model for the magnetic separator. The WLIMS feed comes from the overflow of a screw classifier and the concentrate is sent to a pebble mill for further grinding.

4.2. Sample preparation

The survey samples were prepared according to the procedure shown in Fig. 2. The sample preparation was started with weighting the samples in wet and dry state (steps 2–4), followed by deagglomeration and splitting on a rotary splitter to produce sub-samples for further sizing, ensuring there was 5–10 kg per sample to assure sufficient coarser particles per sample (step 5). The pulp samples were dried in room temperature (3). The first split was stored for later usage (8), the second for bulk chemical analysis by X-ray fluorescence (XRF) (6) and the third for wet sieving (7) followed by drying. Sieving provided four size fractions: +125, −125 + 63, −63 + 38, and −38 μm. Each size fraction from sieving (9) was split into two parts, one for a XRF analysis (11) and the other one for preparing resin mounts for optical and scanning electron microscopy.

4.3. Analytical methods

X-ray fluorescence analyses of the samples were done at the chemical laboratory of LKAB using the company’s standardized methods (MagiX FAST, PANalytical). Chemical analysis of the samples was used as a quick sanity check to evaluate the quality of modal mineralogy by automated mineralogy. Epoxy samples on size fractions were prepared at Kemi University of Applied Science. Scanning electron microscopy (SEM) and automated mineralogy analysis on epoxy samples were done by using a Merlin SEM (Zeiss Gemini - FESEM) with Oxford Instrument EDS detector at Luleå University of Technology, Sweden. The SEM system was coupled with the IncaMineral data acquisition system by Oxford Instruments in order to combine and store backscattered detector images with EDS information during automated mineralogy into a joint database (Lippo et al., 2012).

In average, >20,000 particles were measured in each size fraction, which sums up to around 300,000 particles in three studied streams. Identifying of minerals, reporting of mineral grades and back-calculation of chemical compositions were done by post-processing the raw data. The mineral list shown in Table 3 was used as the reference for the program and back calculation of chemical composition of samples. Chemical composition of minerals was taken from Lund et al. (2013) and verified by EDS analysis.

Mass balancing, data reconciliation, particle tracking, and LIMS modeling were done using the modeling and simulation software HSC Chemistry 8 by Outotec and MATLAB by Mathworks.

5. Results

5.1. Quality of data and measurements

Standard deviation for XRF and automated mineralogy measurements in repeated samples were calculated according to Parian et al. (2015). The standard deviation for XRF assays follows the equation

$$\text{STD}_{\text{XRF}} = \pm 0.007 \sqrt{x}$$

(6)

Table 5

<table>
<thead>
<tr>
<th>Stream</th>
<th>Particle</th>
<th>Population (number of particles)</th>
<th>Mass distribution %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed Liberated</td>
<td>69,056</td>
<td>69.55</td>
<td></td>
</tr>
<tr>
<td>Binary</td>
<td>22,240</td>
<td>20.10</td>
<td></td>
</tr>
<tr>
<td>Ternary</td>
<td>280</td>
<td>0.32</td>
<td></td>
</tr>
<tr>
<td>Complex</td>
<td>27</td>
<td>0.06</td>
<td></td>
</tr>
<tr>
<td>Concentrate Liberated</td>
<td>81,068</td>
<td>72.46</td>
<td></td>
</tr>
<tr>
<td>Binary</td>
<td>20,846</td>
<td>27.41</td>
<td></td>
</tr>
<tr>
<td>Ternary</td>
<td>210</td>
<td>0.14</td>
<td></td>
</tr>
<tr>
<td>Complex</td>
<td>15</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>Tailing Liberated</td>
<td>81,277</td>
<td>67.46</td>
<td></td>
</tr>
<tr>
<td>Binary</td>
<td>20,755</td>
<td>30.70</td>
<td></td>
</tr>
<tr>
<td>Ternary</td>
<td>881</td>
<td>1.41</td>
<td></td>
</tr>
<tr>
<td>Complex</td>
<td>327</td>
<td>0.55</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 5. Parity chart showing measured particle type (bin) mass in the feed, concentrate and tailing streams after advanced binning against mass balanced particle types (bin) after the particle tracking.

Fig. 5. Parity chart showing measured particle type (bin) mass in the feed, concentrate and tailing streams after advanced binning against mass balanced particle types (bin) after the particle tracking.
where \( x \) is the elemental grade in wt.%. Standard deviation for mineral grades measured by automated mineralogy follows the equation

\[
STD_{AM} = \frac{0.208}{\sqrt{x}}
\]  

Eq. (7) was used for setting standard deviations during mass balancing the data for minerals.

To evaluate the quality of automated mineralogy, back calculated chemical compositions were compared against chemical assays (Fig. 3). Generally, good overall correlation was observed. However, minor elements such as vanadium (V), manganese (Mn) and potassium (K) show weak correlation between chemical assays and back calculations. This could be due to either error in XRF analysis at low concentration or inaccuracy in the chemical composition of minerals (Table 3).

5.2. Mass balancing and data reconciliation

Mass balancing and data reconciliation improve the reliability of measurements and can under certain circumstances even enable the estimation of unmeasured streams and variables. It is a requirement for estimating the metallurgical performance of the circuit, for diagnosis of process bottlenecks, and for modeling the process. Well established methods exist for mass balancing and data reconciliation of mineral processing data and several software packages have been developed for performing these tasks (Hadjis, 2010).

Particle mass balancing is the state-of-the-art technique as developed by Lamberg and Vianna (2007) for mineralogical mass balancing. It transfers the mass balancing concepts of common chemical assays to the mineral level and finally to the mineral liberation level. The method requires delicate considerations to provide consistent results and to overcome missing liberation data. The following steps need to be included when extending the mass balancing to the particle level (i.e. mineral liberation level):

1) Bulk mass balance by minerals

\[
\text{Fig. 6. Schematic view of counter-current WLIMS. (Modified after Steiner (2014)).}
\]

\[
\text{Fig. 7. Recovery of various binary particles with magnetite, error bar shows two standard deviation. Error in recovery was calculated by Monte Carlo simulation. High errors in some particle bins are due to low number of particles in the bin. The arbitrary trend curve shows magnetite content in particle and recovery relationship.}
\]
2) Sized mass balance by minerals
3) Particle mass balance (by so-called particle tracking)

As a first step, unsized data was used for mass balancing total solid and mineral flowrates in bulk. The result from the bulk mass balancing was then used as a constraint when mass balancing the minerals in size fractions. This stepwise procedure minimizes the error propagation and ensures that bulk and sized mass balances are consistent.

The adjustment of mineral grades in mass balancing for most minerals was minor as shown in Fig. 4, where the parity line indicates no adjustment. Adjustment of anhydrate and titanomagnetite was relatively higher compared to others and therefore information on these trace minerals is less reliable. This was mainly due to precipitation of anhydrate in tailing buckets and false identification of titanomagnetite during automated mineralogy. Titanium bearing minerals such as titanite and rutile exist as the lamellae in magnetite grains (Lund, 2013), causing the identification of some of the magnetite grains falsely as titanomagnetite. To resolve this problem, titanomagnetite in each particle was lumped together with the magnetite and the anhydrate phase was removed. Each particle composition was normalized after removing the anhydrate phase. Afterwards, mass balancing was redone (Table 4).

The particle tracking technique (Lamberg and Vianna, 2007) aims at adjusting liberation data to match with mass balance results in bulk and size fractions. The particle tracking is a stepwise procedure that starts with adjusting the mass proportion of the particles in order to match modal composition received from bulk and sized mass balancing. It is followed by the basic binning, which involves the classification of particles by size and composition into narrow liberation classes (bins). In principal, the number of bins can be as many as the possible combination of phases in particles and grade classes. Practically, in the basic binning stage the population of various particles in the stream defines how narrow the size classes should be and which combinations of phases in particles have to be considered. Population and mass distribution of particles in the studied samples showed that liberated and binary particles account for over 99% of the population (Table 5).

In some streams, some bins may have no or very few particles making the mass balancing result unreliable. In the following stage, the advanced binning, the bins with low numbers of particles are globally combined (i.e. in all the streams in a similar way) in order to reach a sound number of particles in each bin. In this work, the advanced binning was first done for the feed stream and the minimum number of particles in each bin was set to 25. This equals to a maximum of 20% relative standard deviation for the mass proportion of the particle type (bin) in question. The other streams were binned in the same way by using the feed stream as a reference. In the final stage, the mass proportion of each bin (particle type) was adjusted to reach the mass balance in the whole circuit by keeping the total solids mass flow rates as constraints. Additionally, the particle flow rate of each bin was balanced among feed, concentrate and tailing by considering a weighting factor calculated from the number of particles observed in each bin. In this study, the particle tracking resulted in the mass balancing of 702 different kinds of particles around the WLIMS (Fig. 5). Once the particle types were mass balanced in streams, it was possible to calculate the recovery of each particle type.

5.3. Developing a process model for WLIMS

In the WLIMS, the rotating drum with the magnet is partially submerged into a slurry tank where it lifts out the magnetic particles. Based on the tank design and the feed slurry flow three types of setups can be distinguished: concurrent, counter-current and counter-rotation. Selection of the type of magnetic separator for treating an ore is governed by feed particle size, throughput, and concentrate grade and recovery (Stener, 2014).

Fig. 8. Recovery of liberated gangue particles in various sizes. Error bars show twice the standard deviation.

Based on the type of the magnetic separator, slurry tank and magnetic arc, several different zones can be defined. For example, the counter-current magnetic separator can be divided into three zones. The pick-up zone is where the fresh slurry feed encounters the drum. The scavenger zone is a shallow zone close to the tailings outlet where the drum's rotation is opposite to the slurry flow. The dewatering zone or cleaning zone is where the drum pushes the concentrate up to the discharge and the concentrate water flows back to the tank (Fig. 6).

When ferromagnetic material is exposed to the magnetic field, magnetic ordering occurs based on intrinsic property of the material which defines spontaneous magnetization (Svoboda, 2004). The other phenomenon happening is the growth of magnetic domains. Depending on the size of the particle and the strength of the magnetic field, the magnetic particle can consist of single or multiple magnetic domains. If the external field is strong enough or the particle is fine enough (<0.1 µm) particle magnetization becomes homogenous; this is called magnetic saturation. Even when the saturated particle is outside of the magnetic field, the particle will not become completely demagnetized.

Magnetized particles in the slurry tend to gradually gather into groups and form flocs or aggregates. This is called magnetic flocculation. Before magnetic saturation is reached, the strength of the flocs increases with the growth in field strength and effective permeability. The magnetic content of the particles, the fineness and as well as the nature of the non-magnetic material affect the effective permeability (Lantto, 1977). It is believed that the magnetic flocculation plays a crucial role in the recovery of fine magnetic particles.

5.3.1. Physical explanations for observations

5.3.1.1. Recovery of binary magnetite bearing particles. The major mass population of particles in the concentrate is formed by liberated and

Fig. 9. Stereological effect on recovery of particles in coarse and fine size fractions. With similar texture, stereological bias is higher in small particles than in coarse ones.
magnetite rich binary particles, as expected. For modeling purposes, the aim is to find an equation for the recovery of particles into the magnetic concentrate when its composition and size is known. Therefore, in Fig. 7 the recovery of particles is plotted against composition. Firstly, recovery is directly related to the magnetite content in the particle. For liberated magnetite particles, no matter of the size, recovery is 100%. Secondly, it can be seen that the recovery of magnetite particles in coarse size fractions is higher than those in fine size fractions (Fig. 7). This is mainly due to higher magnetic force on coarse magnetite particles and their important contribution to increase the effective permeability of flocs. For example, in the case of apatite, particles with around 10% magnetite have a recovery of around 22% in the fine size fraction (< 37 μm), but the same particles in coarse size fraction (> 125 μm) have > 70% recovery to the concentrate. Similar behavior can be seen with other binary particles with magnetite.

5.3.1.2. Recovery of liberated gangue particles. Liberation measurements revealed that there are liberated non-magnetic particles in the concentrate and the mass balancing confirms that there is a positive relation between the liberated gangue particle size and the recovery into the concentrate (Fig. 8). For apatite, fully liberated particles contribute with around 30% of the total apatite in the concentrate. For other minerals, this value varies. Recovery of fully liberated gangue minerals in the concentrate can be due to stereological bias, entrainment or entrapment.

a) Stereological bias
A stereological bias in 2-dimensional particle image analysis means that particles that are regarded as liberated in sections, can actually be composite particles in three dimensions. If this is the case then the recovery should show a decrease by increasing particle size. Relatively speaking in a similar texture a fine-grained particle in coarse size fraction changes to coarse-grained particle in fine size fraction, as depicted in Fig. 9. This is analogous to that in fine textures the stereological bias is smaller (Leigh et al., 1996; Spencer and Sutherland, 2000). Therefore, stereological bias as a possible reason for this observation can be excluded.

b) Entrainment phenomena
Entrainment means that particles are dragged into the concentrate with water. This effect is stronger for fine particles than for coarse ones (Neethling and Cilliers, 2009), i.e. opposite to the observation. Therefore, also this explanation is rejected.

c) Entrapment
As discussed earlier, in a flocculation process magnetite particles attach to each other. During this process, liberated gangue minerals can be trapped between magnetic particles. The entrapment of non-magnetic particles has been previously reported as enclosures in the flocs (Lantrit, 1977). In the dewatering step (Fig. 6) when the drum pushes the flocs up toward the concentrate discharge, water inside the flocs drains back to the tank and takes some of the fine liberated gangue particles with (drainage). Madai (1998) has shown that for fine particles the drag force is stronger than its counter force, the magnetic force. Therefore fine particles have higher probability to escape from the flocs than coarser particles. On the other hand, the small porosity size in the flocs hinders the coarse gangue particles to be drained out from the flocs. Therefore, the coarse liberated gangue particles have higher chance to be trapped in the flocs and to end up in the concentrate (Fig. 10).

5.3.2. Semi-empirical model of WULMS
Even though observations show a clear correlation between the recovery of particles and the physical processes, it is not possible to develop a pure physical model. This is mainly due to numerous and complex sub-processes involved in the separation. Further, the data available from the plant survey describes only one operational point. Therefore, the model developed here is semi-empirical in nature and tries to reproduce recovery curves at mineral liberation level. Requirements to be formulated for such a model are that (i) it should be flexible to adapt to linear or curve shaped recoveries, (ii) should have reasonably low number of parameters, and (iii) should reflect physical sub-processes in the system. At a later stage, the model can be further developed to consider operational variables.

A flexible and relatively simple way to model the recovery patterns of binary particles is to use the incomplete beta function $I(a,b)$ (Abramowitz and Stegun, 1965). The incomplete beta function is defined as follows:

$$I(a, b) = \int_{0}^{1} (1 - t)^{a-1} t^{b-1} dt$$

If for the sake of simplicity, the $a$ parameter is fixed at 1, various curve shapes can be generated by changing only the $b$ variable alone.

For the entrainment, the observation shown in Fig. 8 suggests that the probability of entrainment increases by size and nature of gangue mineral. A simple linear relationship based on the particle size can be applied for each mineral as follows:

$$R_E = E_1 d + E_2$$

where $R_E$ is the recovery due to entrainment, $d$ is the particle size, and $E_1$ and $E_2$ are the constants. This linear model is applied to predict the entrapment of different sizes of liberated gangue particles.

<table>
<thead>
<tr>
<th>Table 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear regression models for $b$ and $R_e$, $x$ in the function is the size of particle in microns.</td>
</tr>
<tr>
<td>Regression model for $b$</td>
</tr>
<tr>
<td>Regression model for $R_e$</td>
</tr>
</tbody>
</table>
To model the recovery of various magnetite binary particles in the WLIMS concentrate, the following function is used:

\[ R_x = I_x (1, b) \]  

where \( x \) is the grade of magnetite in the particle and \( b \) is a spread value. Depending on the mineral type that is binary with magnetite, the \( b \) can vary from 0.01 and 30. Finer size fractions generally have smaller \( b \) values than coarser size fractions. The trend of increasing \( b \) values from fine size fractions to coarse size fractions shows the spread of recovery curves. Therefore, the spread value in Eq. (10) is dependent on the particle size, the susceptibility of non-magnetic portion of the particle, shape of the particle, and specific gravity of the particle. Finally, the recovery model by considering entrapment becomes as follows:

\[ R = R_x + (1 - R_x) \times R_E \]

Fitting the Eq. (11) with the experimental points gives various \( b \) values for compositionally different binary particles in different size fractions. During the data fitting, each particle type recovery was assigned a weight factor calculated from the number of particles falling into the particle bin type. In addition, the highest and lowest \( b \) values at 95% confidence level were calculated for the particles in each size fraction. In general, a linear regression describes the increase of \( b \) values respect to the particle size. A similar approach was perused for calculating \( R_E \). The results of the regression models for \( b \) and \( R_E \) are listed in Table 6.

The results indicate that binary pairs of magnetite with gangue can be divided into two groups. The first group is magnetite binary particles with apatite, biotite, and actinolite and the second group is magnetite binaries with quartz, albite, calcite and titanite. For each group an average regression model for \( b \) and \( R_E \) can be selected and applied to the model as follows:

Firstgroup:  
\[ R = I_x (1.1 + 0.12d) + (1 - I_x (1.1 + 0.12d)) \times 0.11d \]  

Secondgroup:  
\[ R = I_x (1.02d) \]  

where \( x \) is the magnetite grade of the particle, \( d \) is the particle size.

6. Verification of the model

To verify the developed model, the model was compared against observations in two levels. In the first level the comparison was made against the bulk and sized mineral flow rates. In the second level the comparison was made on liberation distribution in the concentrate.

6.1. Verification based on bulk and sized level

Comparison of solid flow rates and mineral grades from observations and model indicates that the model forecasts well the solid and mineral flow rates (Table 7). However, in the finest size fraction, the differences between model and observation are higher than in the other size fractions and in the bulk. This could be related to the unpredictable behavior of fine particles in the process. This can also be seen in the recovery of fine minerals in finest fraction (Fig. 11).

6.2. Verification based on mineral liberation level

Evaluation of the model at particle level was started by comparing the liberation curves for magnetite particles. As shown in Fig.12, the model well describes the liberation of magnetite particles. However, the mode of occurrence of minerals in particles is not well described for certain minerals (Table 8 and Table 9). The differences for quartz, albite, calcite, and titanite are higher than for the other minerals. This is basically arising from using simple linear regression model for \( b \) values in model for this group of minerals. However, more observations of particles are required to form a better model for this group of minerals.

7. Discussion

Missing mineral liberation information and a lack of mass balancing techniques for multiphase particles has hindered the development of unit operation process models to be based on particle properties (Table 1). Particle level information provides an excellent opportunity to relate particle properties to physical sub-processes and to develop a model for forecasting the performance of any unit operation.
The developed particle-based WLIMS model can forecast recovery and product quality of any new feed stream if the particle level information is available. Process simulators and unit operation models that operate at particle level exist and are becoming more common. In addition, simulation of a process where the model level is at particle level stays straightforward, i.e. input and output stream of the model can be directly used by any other unit models. For example, the hydrocyclone model by Donskoi et al. (2005), which uses particle level information, can be coupled with the developed WLIMS model. In addition, development of more of such models is on-going for other unit operations such as flotation (Minz et al., 2013) and comminution (Mwanga et al., 2015). This approach ensures that all necessary information is passed between unit operations and is accessible for all process streams including the final product streams.

Notably for the purpose of geometallurgy, the liberation level model is suitable only if the geological model provides information on ore textures and if there is a mechanism to transfer this information to generate multiphase particles with compositional information in the comminution stage. The example of such a characterization was given by Lund (2013), who obtained detailed mineralogical data and combined it with a particle-based model.

The developed model can be used in optimization for example by testing the effect of grinding fineness and detaching of flocs before sending the concentrate to the cleaning stage. From the curve shapes coarser grinding gives higher recovery but lower grade compared to fine grinding. Detachment of the flocs could potentially decrease the entrainment. Further development is needed to relate the model parameters to the operational parameters or include certain sub-processes of magnetic separation if the model is intended to be used for process control or to investigate the effects of operational conditions.

Observations at particle level as well as physical theory imply that magnetic separation is a complex process that is controlled by both operational conditions and the feed stream properties. Studying and characterizing the feed stream at particle level provides insight about the performance of a magnetic separator that previously was not possible to reach accurately. The developed semi-empirical model of WLIMS describes the recovery of particles based on two mechanisms; recovery of particles due to magnetic volume and entrainment. This was achieved through applying the particle tracking technique. However, there are several other factors that need to be addressed.

7.1. The effect of mineral nature, grain size and shape

The relationship between particle size and recovery of fully liberated gangue particles can be explained by the entrainment phenomenon. As seen in Fig. 8, there are slight differences between the gangue minerals, i.e. apatite, actinolite, and biotite show entrainment higher than the rest. In the case of apatite, fine magnetite inclusion (<1 μm) were observed in the apatite in the concentrate, which under normal condition of automated mineralogy was not possible to detect. On the other hand, apatite in the tailings seems not to have magnetite inclusion as those found in the concentrate. This also can be true for actinolite and biotite since such an observation has been reported previously (Niiranen, 2015). Detection of fine magnetite inclusion can be easily missed in the measurements and data processing of automated mineralogy, hence magnetic susceptibility measurement of present minerals and individual particles, if possible, would be needed to verify whether the liberated gangue particles end up to concentrate because of their magnetic susceptibility rather than entrainment. While higher susceptibility due to magnetite inclusion probably plays a major role, the effect of grain shape should not be neglected. Actinolite and biotite, can vary in shape and are often elongated that makes their release from flocs harder. In addition, angular particles have naturally stronger magnetic forces at the corners and edges.

The spread factor b in Eq. (10), describing how close the recovery curves are for different size fraction, is closely correlated to particle size, the susceptibility of non-magnetic portion of the particle, to

<table>
<thead>
<tr>
<th>Table 8</th>
<th>Mode of occurrence of minerals in the concentrate from observations. Each row describes the association of named mineral with the minerals stated on columns in percentages.</th>
</tr>
</thead>
<tbody>
<tr>
<td>OBS</td>
<td>Mgt</td>
</tr>
<tr>
<td>Mgt</td>
<td>98.14</td>
</tr>
<tr>
<td>Qtz</td>
<td>75.79</td>
</tr>
<tr>
<td>Ap</td>
<td>59.88</td>
</tr>
<tr>
<td>Bt</td>
<td>66.33</td>
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<tr>
<td>Ab</td>
<td>47.75</td>
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<tr>
<td>Act</td>
<td>54.10</td>
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<tr>
<td>Cal</td>
<td>49.72</td>
</tr>
<tr>
<td>Tin</td>
<td>91.32</td>
</tr>
</tbody>
</table>

Shaded cells indicate the mass proportion of liberated particles.

<table>
<thead>
<tr>
<th>Table 9</th>
<th>Mode of occurrence of minerals in the concentrate from the model.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>Mgt</td>
</tr>
<tr>
<td>Mgt</td>
<td>97.93</td>
</tr>
<tr>
<td>Qtz</td>
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<tr>
<td>Ap</td>
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<tr>
<td>Bt</td>
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<tr>
<td>Ab</td>
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<tr>
<td>Act</td>
<td>61.43</td>
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<tr>
<td>Cal</td>
<td>88.90</td>
</tr>
<tr>
<td>Tin</td>
<td>95.15</td>
</tr>
</tbody>
</table>

Shaded cells indicate the mass proportion of liberated particles.

Fig. 12. Liberation curve for magnetite particles from observations (left) and model (right).
shape of the particle, and specific gravity of the particle. The smaller the grain size is, the lower the magnetic force on the material becomes, resulting in weakening and shortening of the flocs (Lantto, 1977). On the other hand, coarse magnetic particles increase the strength of the flocs and the length of the chains, thus resulting in an increase of total recovery. The nature of gangue minerals, magnetic susceptibility of grains, shape and total susceptibility of particles affect the flocs’ effective permeability. For particles with sharp corners, porosity in the flocs increases and the total effective permeability becomes smaller compared to when flocs are packed with rounded particles. Specific gravity of particles may have a high impact during the cleaning stage. Particles with lower specific gravity tend to follow drainage water more easily than others.

7.2. The effect of feed quality

As seen in observations, the entrapped liberated gangue particles in the concentrate are one of the sources of impurities in the products. While formation of the flocs is stronger in high grade magnetite ore and is crucial for the recovery of fine particles, releasing gangue particles from these flocs is highly unlikely. Unless the flocs become demagnetized or detached, entrapped gangue particles inside the flocs find their way to the concentrate. Mechanical detachment of the flocs can be momentarily but may be enough to let gangue particles escape from the flocs.

The studied ore is such a high grade and shows high recovery not only in the first magnetic separation but also in the whole process. This raises the question whether liberation information is really needed for the process simulation. However, in producing high quality products the recovery is not the main concern but the impurities are, thus the grade of gangue minerals in the concentrate. For a high quality iron product, the requirements for certain impurities are tight and must be met (LKAB, 2014). For example, phosphorus and silicon contents of the product are the determinative criteria meaning that relatively high product, the requirements for certain impurities are tight and must be met.

Conversely, in processing of low grade ore, the mineral liberation can cause a recovery issue as well. It is expected that the strength of formed flocs in low grade feed will be weaker and the loss of binary particles with magnetite and fine magnetite particles accordingly be higher.

7.3. The effect of stereological bias

As it is known, 2-dimensional measurement of liberation which inherently is defined in 3-dimension is biased estimate of the liberation. The liberation is always overestimated and the magnitude of the overestimation depends on ore texture. The bias exist for liberation estimation, however the bias affects the model parameters in less degree. In calculation of modal parameters, instead of using absolute value of liberation, the model can take the uncorrected liberation data as well as corrected liberation data as an input and gives the same quality of the liberation.

8. Conclusion

Using particle tracking technique for the first time demonstrated that the behavior of magnetic-gangue particles in magnetic separation is not only dependent on the particle size but also on nature of the gangue mineral. Particles containing gangue minerals such as biotite, actinolite, and apatite are showing similar behavior in WLIMS where others such as albite, quartz, and calcite are having different behavior with respect to the first group. The origin of differences in behavior seems to be tiny magnetite inclusions in the first group. Also the entrapment phenomenon is greater in the first group than in the second group.

The developed model requires that the feed stream is described at particle level and each particle must have information on its size and mineral composition. Even though the model lacks operating parameters it can be used for any WLIMS. Entrapment parameters and spread values for each mineral by size must be calibrated. When calibrated for certain operational conditions the parameter value should not change as the feed composition change.

Benefits of the developed model are that it is portable and does not need continuous calibration according to fluctuation in feed mineralogy, particle size distribution and liberation characteristics. The developed model requires that the feed is characterized on mineral liberation level. In geometallurgy, validated methods to provide such information through the whole ore body don’t exist and therefore fully utilization of the model requires that such a concept and model is developed.

Acknowledgment

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Paper III
Ore texture breakage characterization and fragmentation into multiphase particles
Mehdi Parian*, Abdul Mwanga, Pertti Lamberg and Jan Rosenkranz

* Corresponding author, Minerals and Metallurgical Engineering, Luleå University of Technology, SE-971 87 Luleå, Sweden; Tel. +46-920-492556; Fax +46-920-97364, e-mail: mehdi.parian@ltu.se.

Minerals and Metallurgical Engineering, Luleå University of Technology, SE-971 87 Luleå, Sweden

Keywords: Textural characterization, iron ore, mineral liberation, breakage, particle population

Abstract
The ore texture and the progeny particles after a breakage in the comminution are the missing link between geology and mineral processing in the concept of geometallurgy. A new method called Association Indicator Matrix based on co-occurrence matrix was introduced to analyze the mineral association of ore texture and particles. The Association Indicator Matrix can be used as a criterion to classify ore texture and analyze breakage behavior of ore texture. Within the study, the outcome of breakage analysis with Association Indicator Matrix was used to generate particle population of iron ore texture after crushing. The particle size of forecasted particles was taken from experimental and frequency of breakage in phases was defined based on Association Indicator and liberation of minerals. Comparison of liberation distribution of iron oxide minerals from experimental and forecasted population shows a good agreement.

1. Introduction
Ore texture characterization concept in geology focuses on the geological aspects of the texture such as ore formation and genesis (Craig, 2001; Nyström and Henriquez, 1994). For geometallurgical purposes, ore texture characterization should be quantitative and provide quantitative information regarding progeny particles formed in comminution and their composition, thus on liberation distribution (Petruk, 1988). The significance of ore texture on beneficiation and other downstream processes is recognized and has been evaluated in mineral processing (Bonifazi et al., 1990; Donskoi et al., 2008; Gaspar, 1991). Qualitative or categorical geological classification is not sufficient for mineral processing. The mineralogical approach to geometallurgy requires information on ore textures to enable quantitative evaluation of mineral liberation distribution and the required crushing and grinding energies for mineral liberation.

1.1 Terminology
The terminology used for describing mineral liberation and breakage has not been harmonized therefore the definitions of the key terms are given below (see Figure 1):

Particle: A unity consisting of single or multiple grains and single or multiple phases (particles 1, 2 and 3).
Grain: A unit composed of only one mineral that has a clear interfacial surface with other grains (A and B grains in particles 1 and 3).
Liberated particle: A particle consisting of only one phase (particles 2 and 3).
Degree of liberation: Mass proportion of mineral of interest occurring as liberated particles in
Mineral liberation:  
  a) An action where minerals are liberated (comminution).  
  b) A broad term which describes the mode of occurrence of mineral in particulate material.  

Liberation distribution: Mass distribution of mineral of interest in particle population.  

Preferential breakage: When breakage and cracking more frequently occurs in one phase (King, 2012).  

Random breakage: When breakage and cracking are not favored by any phase or boundary region.  

Figure 1. Composite particle and liberated particle.  

Definition of what encompasses ore texture varies among geologists and metallurgists (Leigh, 2008). A comprehensive review of the definitions for ore textures is given by Vink (1997) and Bonnici (2012). The common definition for ore texture refers to volume, grain size, shape, spatial distribution and association of each mineral in the ore, thus in intact, pristine stage, i.e. in the unbroken material. The other issue is in what scale textural information needs to be collected. Microtexture term is used for grain-scale features like mineral inclusions in another grain, mesotexture for hand specimen sizes, and macrotextures for scales larger than mesoscale (Richmond and Dimitrakopoulos, 2005). Ore texture is a generic term that refers to all scales.  

1.2 Ore texture measurement  
Ore texture measurement is commonly performed on thin sections, polished slabs, or drill cores depending on the required scale and details for intact ore or particulate samples. Optical microscopy, scanning electron microscopy (SEM), hyperspectral imaging, and x-ray diffraction mapping are common methods to acquire spatial distribution of phases in a sample. Generally, the mineral map is generated, and parameters of interest are calculated. Image analysis tools are commonly used to measure and quantify ore textural attributes (Nguyen, 2013; Pérez-Barnuevo et al., 2012; Zhang and Subasinghe, 2012).  

Ore texture and particle composition information is a critical part of the mineralogical approach to geometallurgy. The ore texture and the progeny particles after a breakage in the comminution are the missing link between geology and mineral processing in the concept of geometallurgy. Generally, ore texture is quantified in terms of descriptors (such as covariance function, proximity function and linear intercept length distribution (Zhang and Subasinghe, 2012)). However, these descriptors are mostly developed for binary systems, and there is no extension for three-dimensional ore texture volume. In this study, ore textures and particles are quantified by association indicator to show the trend of ore texture breakage in crushing.  

1.3 Mineral liberation modeling  
In the concept of liberation modeling, various approaches are known. The first approach is to model liberation independently from size reduction modeling and assuming that liberation process is related to the texture of the ore and the target size (Gaudin, 1939; Wiegel and Li, 1967). Usually, the main parameters in this liberation model are the average grade of phases and the size ratio between particles and grains. This approach is also called texture modeling and is achieved by superimposing
particles mesh over texture image. This approach further developed from simple textures to consider a variety of ore textures (Barbery, 1991) or transformation of textures to simple forms (Meloy and Gotoh, 1985). In this, the key parameters are the volumetric grade of the ore mineral and the interfacial surface area between phases which is related to the grain size.

The second approach was developed by extending the theory of liberation (Andrews and Mika, 1976; Wiegel, 1976). These authors have considered the problem of simultaneously accounting for liberation and breakage in a batch mill. Other approaches have been reported in the literature such as integration of liberation, size reduction and process modeling (Bax et al., 2016; Khalesi, 2010).

A fundamental part of liberation models is how the ore texture is defined or is characterized to be used for developing predictive liberation models. The second part of liberation model is how the mineral distribution in particles is defined. This can be described by distribution functions without measurement or measured on by images analysis techniques. A majority of liberation models are based on binary system (i.e. an ore mineral embedded in a gangue matrix), and they lack the capability of forecasting multiphase particles. A comprehensive review of liberation models and their development in 80’s and before was given by Barbery and Leroux (1988). Another important part of liberation modeling is how actually fragmentation (breakage) happens. As discussed earlier, a simple approach is to superimpose particle patterns over textures. A recent review of mineral liberation and liberation in comminution is given by Mariano et al. (2016).

Practical implementation of mineral liberation models in the mineral processing is rare. This is because the models are mainly for binary systems and taking models to the multiphase system is too complicated. However, in simplified ore textures (binary system) the models have been tested and compared against experimental data (Barbery and Leroux, 1988; Choi et al., 1986; Finch and Petruk, 1984; Hsih and Wen, 1994; Leigh et al., 1996; Schneider et al., 1991).

In simulation software in mineral processing, MODSIM has implemented complete Andrews-Mika liberation modeling. HSC Chemistry since version 7.1 (Outotec, 2012) has included liberation model as built-in comminution models. Traditional comminution models describe the product particle size distribution and internally the software forecast the liberation distribution of the product if the liberation information on the feed stream is given (Lamberg and Lund, 2012). This is done by keeping the liberation distribution within the size fractions unchanged, and the changes are applied only to mass proportions of different size fractions. As the mineral grades between the particle size fractions may be different, the shift in mass proportions of the particle size fractions would change the mineral grades in bulk. Therefore, there is extra reconciliation step to conserve the bulk mineral balance between the feed and product.

2. Materials and methods

2.1 Samples

Various AQ (core diameter 27 mm) and BQ drill cores (36.5 mm) of iron ore with variation in ore textures were selected from Kiruna and Malmberget ore bodies. The samples were cut along the core axis and were scanned by the flatbed scanner. Afterward, the drill cores were cut in intervals of two centimeters. Two pieces were used for preparing epoxy block; other pieces went through the crushing process. These pieces were crushed in laboratory jaw crusher with closed side setting opening of 3.35
The crushing product was sieved, and subsamples of each size fraction were selected to make epoxy samples for particle measurements (Figure 2).

Drill core sample

Axial cut

Cut in pieces (20 mm)

Two pieces for ore textural study

Crushing (-3.35 mm)

Sizing

Resin mounts for size fractions

Routine analysis of ore textural samples is affected by required details, image resolution, time and cost of analysis. Optical and SEM based automated mineralogy are the common methods of obtaining ore textural image. The image is treated by image processing tools to extract textural and mineralogical information.

Ore textural study was done in optical and scanning electron microscopy. The aim was to analysis particulate and intact rock samples to generate the mineral map. Afterward, the mineral map was used for retrieving textural attributes and liberation.

For eight drill cores, mineral maps were created for intact ore and particulates samples after crushing. Crushed sample sieved and sized in 1.68-3.35 mm, 0.85-1.68 mm, 0.43-0.85 mm and 0.30-0.43 mm size fractions. Measurement of -0.30 mm size fraction was skipped due to the high liberation of minerals in all samples.

2.2 Analysis

2.2.1 Image acquisition

Image acquisition of ore texture was performed by mosaic capturing of field images by automated stage optical microscopy (Zeiss Axio Imager) and SEM backscatter detector (AZtec - Zeiss Merlin). The whole image of the samples was generated by stitching field images by built-in programs. Minerals relating to specific gray level in backscatter image were identified by EDS analysis of the phases at that gray level. This data was used later in assigning phases in mineral maps.
2.2.2 Image processing

Image processing is a rapidly advancing area of retrieving information from images. The technique is used to classify objects in the image (such as grains, particles or phases) and retrieve a wide range of features. In an ore textural study, captured images are used for phase discrimination, calculation of object shape factors, mineral grades, and the association between phases. In this study, image processing sequences including phase discrimination, object separation, feature extractions were done by writing code in MATLAB. The code can analyze ore texture and particulate samples to give numeric ore textural features and liberation. The extension of the code can generate particle population from ore texture by defining breakage pattern and particle size distribution.

Phase separation

Phase separation began by assigning multiple threshold values according to a range of gray level of each phase in the sample. The image pixels corresponding to each threshold interval was assigned a new value representing a phase. In particulate samples, the epoxy region was assigned a zero value for simpler processing of objects during imaging processing.

Composition and liberation

Obtaining a mineral map of ore texture or particulate sample facilitates the calculation of mineral grades and liberation. Generally, the area of each phase (number of pixels occupied by the phase) in a particle or whole texture are calculated to obtain information on the composition of the particle. To convert this value to weight percentages, the density of minerals is used as weight factors in the calculation of composition.

The other important factor that can be useful in characterizing breakage and also interest in some aspect of mineral processing (such as flotation and leaching) is liberation by exposed surface area of particles. In each particle, this is calculated by normalizing measured shared boundary between phases and background (epoxy).

Mineral association

Association of minerals can be estimated based on the proportion of minerals in the particles. However, this approach for the intact ore texture only gives mineral grades of texture. Therefore, an alternative method is to calculate the interfacial surface area between minerals in the intact ore texture or particle as an indication of association.

An image can be considered as a matrix of pixel values. An easy and straightforward way of estimating association in the image is using co-occurrence matrix. A mineral map with \( n \) phases (\( n \) pixel values) will have \( n \times n \) size co-occurrence matrix. Each cell of the matrix, \( C(i,j) \), is correspondence to the number of times that the cell \( i \) is situated with cell \( j \) in the defined offset. Here, for calculation of association, the co-occurrence matrix is the sum of cell values for 0-360° in intervals of 45° (Figure 3).
For example, for a simple case with three-pixel values as below with one-pixel distance offset, the corresponding co-occurrence for various orientations is as Table 1.

```
Table 1. Table of co-occurrences, showing the abundance of co-occurrence cells in different orientations for Figure 4.

<table>
<thead>
<tr>
<th>Co-occurrence</th>
<th>0°</th>
<th>45°</th>
<th>90°</th>
<th>135°</th>
<th>180°</th>
<th>225°</th>
<th>270°</th>
<th>315°</th>
<th>Sum</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 – 1</td>
<td>2</td>
<td>1</td>
<td>3</td>
<td>0</td>
<td>2</td>
<td>1</td>
<td>3</td>
<td>0</td>
<td>12</td>
</tr>
<tr>
<td>1 – 2</td>
<td>2</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>1</td>
<td>4</td>
<td>4</td>
<td>22</td>
</tr>
<tr>
<td>1 – 3</td>
<td>3</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>13</td>
</tr>
<tr>
<td>2 – 1</td>
<td>2</td>
<td>1</td>
<td>4</td>
<td>4</td>
<td>2</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>13</td>
</tr>
<tr>
<td>2 – 2</td>
<td>4</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>4</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>16</td>
</tr>
<tr>
<td>2 – 3</td>
<td>2</td>
<td>4</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>14</td>
</tr>
<tr>
<td>3 – 1</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>3</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>13</td>
</tr>
<tr>
<td>3 – 2</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>2</td>
<td>1</td>
<td>14</td>
</tr>
<tr>
<td>3 – 3</td>
<td>2</td>
<td>1</td>
<td>4</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>4</td>
<td>2</td>
<td>18</td>
</tr>
</tbody>
</table>
```

Therefore, the co-occurrence matrix for Figure 4 is:

$$ C = \begin{bmatrix}
12 & 22 & 13 \\
22 & 16 & 14 \\
13 & 14 & 18 \\
\end{bmatrix} $$  \hspace{1cm} (1)

The co-occurrence matrix can be normalized to give an indication of association based on the abundance of a phase interfacial in the sample. This can be done by normalizing non-diagonal cells, row or column wise. This is called association indicator matrix (AIM). For example, for above example, AIM is:

$$ AIM = \begin{bmatrix}
- & 62.9 & 37.1 \\
61.1 & - & 38.9 \\
48.1 & 51.9 & - \\
\end{bmatrix} $$  \hspace{1cm} (2)
The non-diagonal values are the association indicators. For the above example, phase one has 62.9% association with phase two and 37.1% with phase three. In the particles, the exposed surface of particles may consider in the calculation. This can be done by including the background (epoxy) as another phase. This also makes the calculation of the surface exposure of minerals straightforward.

**Limitations**

The optical image was planned to be used for discrimination of hematite and magnetite in the samples. Even though hematite and magnetite could be distinguished easily in the optical image, imperfect image stitching by built-in programs lead to incorrect registration of image objects (Figure 5). Additionally, uncorrected uneven illumination in the image fields presented another obstacle in the image processing of the data (Figure 6). These problems could have been fixed by correcting uneven illumination in the field images as well as aligning field images in a proper way. However, AZtec system for capturing backscatter images does not provide an easy way to access field images.

![Figure 5. Imperfect image registration. The optical image (left), BSE image (middle), Blend of Optical and BSE images (right).](image1)

![Figure 6. The uneven illumination effect in the stitched images (left side optical image, right side BSE image).](image2)

### 3. Results

#### 3.1 Association indicator for ore texture characterization

The analysis of 8 drill cores of iron ore in terms of modal composition and association indicator shows variations in ore textures (Table 2). The average grain size of gangue phases was estimated in optical image microscopy while grain size of magnetite and iron oxide (magnetite and hematite) was measured by image processing technique.
Table 2. Phases, mineral grades, Association indicator matrix of ore textures and average grain size (80% passing size).

<table>
<thead>
<tr>
<th>Sample</th>
<th>Phase</th>
<th>Grades (wt%)</th>
<th>Association indicator matrix (%)</th>
<th>Average grain size (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>Biotite</td>
<td>3.17</td>
<td>[ - 47.11 21.44 31.45 ]</td>
<td>400</td>
</tr>
<tr>
<td></td>
<td>Amphibole</td>
<td>2.67</td>
<td>[ 34.64 - 24.43 40.92 ]</td>
<td>600</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>2.04</td>
<td>[ 17.82 27.77 - 54.41 ]</td>
<td>400</td>
</tr>
<tr>
<td></td>
<td>Magnetite</td>
<td>92.13</td>
<td>[ 20.87 36.86 42.28 - ]</td>
<td>881</td>
</tr>
<tr>
<td>F</td>
<td>Quartz</td>
<td>0.17</td>
<td>[ - 38.31 17.32 44.37 ]</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>Feldspar</td>
<td>1.10</td>
<td>[ 16.02 - 29.03 54.95 ]</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>1.35</td>
<td>[ 2.18 9.17 - 88.65 ]</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>Magnetite</td>
<td>97.38</td>
<td>[ 5.17 15.49 79.34 - ]</td>
<td>894</td>
</tr>
<tr>
<td>G</td>
<td>Quartz</td>
<td>0.92</td>
<td>[ - 59.82 3.89 36.28 ]</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>Feldspar</td>
<td>0.72</td>
<td>[ 51.18 - 6.86 41.96 ]</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>0.29</td>
<td>[ 15.48 31.67 - 52.85 ]</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>Magnetite</td>
<td>98.07</td>
<td>[ 36.87 48.68 13.45 - ]</td>
<td>1905</td>
</tr>
<tr>
<td>D1</td>
<td>Quartz</td>
<td>5.52</td>
<td>[ - 64.79 19.02 5.20 10.98 ]</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>Feldspar</td>
<td>12.88</td>
<td>[ 47.62 - 34.98 4.13 13.27 ]</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>7.24</td>
<td>[ 14.08 15.22 29.25 - 41.46 ]</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>Magnetite</td>
<td>64.09</td>
<td>[ 15.84 26.18 35.88 22.10 - ]</td>
<td>504</td>
</tr>
<tr>
<td>A2</td>
<td>Quartz</td>
<td>2.18</td>
<td>[ - 43.04 56.96 ]</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>1.87</td>
<td>[ 16.05 - 83.95 ]</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>Hematite</td>
<td>95.96</td>
<td>[ 20.10 79.90 - ]</td>
<td>1486</td>
</tr>
<tr>
<td>A1</td>
<td>Quartz</td>
<td>4.23</td>
<td>[ - 20.62 79.38 ]</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>3.86</td>
<td>[ 31.59 - 68.41 ]</td>
<td>500</td>
</tr>
<tr>
<td></td>
<td>Iron oxide</td>
<td>91.90</td>
<td>[ 64.35 35.65 - ]</td>
<td>1218</td>
</tr>
<tr>
<td>B2</td>
<td>Quartz</td>
<td>3.48</td>
<td>[ - 66.89 6.69 26.43 ]</td>
<td>400</td>
</tr>
<tr>
<td></td>
<td>Feldspar</td>
<td>2.32</td>
<td>[ 52.62 - 7.93 39.46 ]</td>
<td>400</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>1.88</td>
<td>[ 18.51 27.54 - 53.95 ]</td>
<td>600</td>
</tr>
<tr>
<td></td>
<td>Iron oxide</td>
<td>92.32</td>
<td>[ 27.45 52.18 20.38 - ]</td>
<td>1629</td>
</tr>
<tr>
<td>C1</td>
<td>Feldspar</td>
<td>1.28</td>
<td>[ - 40.06 59.94 ]</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>Apatite</td>
<td>6.90</td>
<td>[ 19.13 - 80.87 ]</td>
<td>700</td>
</tr>
<tr>
<td></td>
<td>Iron oxide</td>
<td>91.82</td>
<td>[ 26.44 73.56 - ]</td>
<td>1192</td>
</tr>
</tbody>
</table>

The association between magnetite and apatite in magnetite samples is in order of F > E > D1 > G while the association between apatite and magnetite is F > E > G > D1. Even though D1 has the highest apatite grade the association between magnetite and apatite is less than E and F samples with high-grade magnetite. Consideration of both modal composition and association indicator gives insight about the assemblage of phase in the texture. Approximately in all samples, apatite is highly
associated with magnetite and iron oxide phase regardless of apatite or magnetite grade. Also, considering grain size of phases, except in D1 sample that has roughly even grain size distribution, in the rest of the samples magnetite and hematite grains are coarser than the grains of other phases.

As many of the samples have high iron oxide grade and mineral liberation is expected to be very high in these, only four of the samples with a high amount of gangue phases namely E, D1, A1, and C1 were selected for further studies.

3.2 Association indicator for particle characterization

The AIM can be used for characterizing breakage behavior of particles and estimating the association of minerals based on the interfacial perimeter in the particle. The association indicator for particles is a unique way of assessing particle population. The AIM values for different type of particles are listed in Table 3. For example, particles P1 and P2 have a similar composition, but they have different AIM values. In the AIM of particles, surrounding area of particles (e.g. epoxy, free space) is considered as an additional phase. In this way, the exposed surface of particles is considered in the AIM. The first row of the AIM shows liberation by exposed surface.

![Figure 7. Particles with different composition and interfacial perimeter](image)

<table>
<thead>
<tr>
<th>Type</th>
<th>Composition</th>
<th>AIM</th>
<th>Type</th>
<th>Composition</th>
<th>AIM</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>60 40 0</td>
<td></td>
<td></td>
<td>60 20 20</td>
</tr>
<tr>
<td></td>
<td></td>
<td>12 44 44</td>
<td></td>
<td></td>
<td>50 33 17</td>
</tr>
<tr>
<td></td>
<td></td>
<td>56 0 44</td>
<td></td>
<td></td>
<td>50 33 17</td>
</tr>
<tr>
<td>P3</td>
<td>[65 10 25]</td>
<td>67 7 33</td>
<td>A</td>
<td>[100 0 0]</td>
<td>100 0 0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>61 24 15</td>
<td></td>
<td></td>
<td>100 0 0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>100 0 0</td>
<td></td>
<td></td>
<td>0 0 0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0 0 0</td>
<td></td>
<td></td>
<td>0 0 0</td>
</tr>
</tbody>
</table>

3.3 Ore texture and breakage characterization

Characterization of ore texture before and after breakage provides valuable insights about the fracture pattern in comminution, the population of particles for specific ore texture and their relation to parent ore texture. Characteristic of ore textures from simplest to more sophisticated way can be considered by analysis of particle size distribution after breakage, distribution of liberations and analysis of changes in associations. In the context of the mineralogical approach to geometallurgy, predicting the particle population from ore texture is a critical step to establish an interface between geology and mineral processing. This is also subject of interest in mineral processing for liberation analysis and comminution processes.
3.3.1 Particle size distribution after breakage

Particle size distribution of comminuted ore textures in one stage crushing, and 100% less than 3.35 mm are demonstrated in Figure 8. Generally, the crushed samples approximately have similar particle size distribution.

![Figure 8. Cumulative particle size distribution of particles after one stage crushing (left) and after 100% crushing less than 3.35 mm (right).](image)

Modeling of particle size distribution of the comminuted sample is a well-established area and not new. However, to compare the size distributions numerically and also enable generating the particle size distribution for further purposes, the particle size distributions were fitted with Rosin-Rammler distribution function as follows:

\[
f(D) = 100 \times \left( 1 - \exp \left( - \left( \frac{D}{D_{63.2}} \right)^n \right) \right)
\]

where

- \( f(D) \): Cumulative weight percentage of particles passing size \( D \)
- \( D \): The particle size
- \( D_{63.2} \): The particle size where the distribution value is 63.2%
- \( n \): A factor describing the spread of the distribution

The parameter values of particle size distributions (Table 4) suggests that more or less all the ore textures show similar particle size distribution after crushing. In general, textures with finer grain size have wider particle size distributions (lower \( n \) values) such as D1 and F samples. This data is used later for generating particle size distribution for forecasting particles.

### Table 4. Parameters for Rosin-Rammler equation.

<table>
<thead>
<tr>
<th>Texture</th>
<th>One stage crushing</th>
<th>crushing 100% less than 3.35 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( D_{63.2} )</td>
<td>( n )</td>
</tr>
<tr>
<td>E</td>
<td>1.90</td>
<td>1.31</td>
</tr>
<tr>
<td>D1</td>
<td>3.32</td>
<td>0.90</td>
</tr>
<tr>
<td>A1</td>
<td>2.47</td>
<td>1.09</td>
</tr>
<tr>
<td>C1</td>
<td>2.48</td>
<td>1.08</td>
</tr>
</tbody>
</table>
3.3.2 Distribution of particle types after breakage

The distribution of particle types (by composition) in the samples shows that most of the samples have very high liberation even in the coarsest size fractions, > 1 mm (Figure 9). Major liberation contribution is from iron oxide minerals. Even in the multiphase particles, iron oxide is the major contributor. Among the samples, D1 sample has the highest amount of locked particles.

![Figure 9](image-url) Distribution of particles by liberated, binary and complex particles in weight percent in size fractions. Liberated particle counted as >95 wt% of the phase of interest.

3.3.3 Association indicator distribution for binary and complex particles

Distribution of particle association indicator has significance in defining the breakage behavior of particles. By comparing the association indicator in the intact sample and in crushed one conclusion on randomness versus degree of preference in breakage can be made. This value is an estimation how the breakage separates one phase from another compared to original ore texture.

Before analyzing the Association Indicator for different phases, it is important to understand how the breakage pattern affects the Association Indicator values. In simple cases as demonstrated in Table 5, when breakage is a phase-boundary fracture, phases reach a liberated state in coarse particle sizes. This means the interfacial area between phases disappear and consequently, association indicator values become zero. On the other hand, the association with the background (exposed surface) reaches to its maximum i.e. 100% Association Indicator value.
In a case of preferential breakage in one phase, Association Indicator value for the phase where breakage occurs decreases for non-liberated particle compared to original particle while Association Indicator value of the phase with no breakage remains same. In the case of boundary-region breakage, Association Indicator values for the phases decrease respect to parent particle while due to generating free surface Association Indicator values between phases and background increases. An indication of this type of fracture is observing a significant number of non-liberated particles in fine size fractions.

Table 5. A simple demonstration of the effect of breakage type on variation in AI values for particles (A and B are phases and C is the free space). DOL is the degree of liberation.

<table>
<thead>
<tr>
<th>Parent particle</th>
<th>Breakage</th>
<th>Progeny particles</th>
<th>AI change</th>
<th>DOL A</th>
<th>DOL B</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Phase-boundary</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Preferential in B</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Boundary-region</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Looking at the distribution of Association Indicator values between phases, for example, magnetite and apatite in Figure 10, the Association Indicator value for apatite-magnetite after breakage compared to ore texture has not been changed significantly, however for magnetite-apatite the Association Indicator decreases in finer size fractions. These indicate that the breakage between magnetite and apatite (two major phase in D1 sample) is a combination of boundary-region and preferential in magnetite phase. The part that should not be neglected is the contribution of detachment breakage. Since the liberated particles are not considered in this graph, no conclusion can be made about this type of breakage. However, if the surface liberation of one phase increases dramatically simultaneously by decreasing particle size without leaving locked particles behind, that could be an indication of detachment process.
To investigate changes of Association Indicator values for different phases, the term AI\textsubscript{50} is introduced. The AI\textsubscript{50} is the value of the Association Indicator for 50% of the population of locked particles (median value). AIM\textsubscript{50} is the association indicator matrix filled for AI\textsubscript{50} values for each cell. AIM\textsubscript{50} can be generated for each size class of locked particles and compared against AIM of the original ore texture. This can be used to evaluate breakage and trend of separation of two specific phase from each other.

The graphs (Figure 11-14) show the changes in AI\textsubscript{50} values for different paired phases. AI\textsubscript{50} for a phase and background (epoxy) demonstrates the abundance of a phase free surface in locked particles. The trend along with the liberation of the phase show the generation of free surface for the specific phase in size fractions.

Figure 11. Changes in AI\textsubscript{50} from ore texture to size fractions for E sample.
Figure 12. Changes in Al<sub>50</sub> from ore texture to size fractions for D1 sample.

Figure 13. Changes in Al<sub>50</sub> from ore texture to size fractions for A1 sample.
A significant trend in all samples is the association between iron oxide minerals and gangue phases. The AI$_{50}$ value in size fractions decreases from ore texture while the iron oxide free surface in locked particles increases. This indicates that in these samples, the breakage is mostly preferential in iron oxide phase. Additionally, increased mass proportion of free particles (thus liberation degree) is another reason to support preferential breakage.

3.4 Forecasting the particle population from ore texture

Ore texture mapping and breakage behavior of ore are the critical steps for forecasting the particle population. Experimental work and analysis that has been done on the ore textures can be utilized for forecasting particle population. The particle size distribution of particles modeled by Rosin-Rammler equation along with the degree of breakage either preferential in phase or random estimated by breakage characterization are the main parameters for forecasting liberation distribution.

Simple assumptions can be made to reduce the complexity of forecasting particle population. For example, rectangular particle shapes are used, selectively or randomly positioned particles over ore textures is used to generate particles. The size of particles is taken from modeled particle size distribution. Schematically, the approach that is applied here is shown in Figure 15.
3.4.1 Assigning breakage frequency

To assign preferential breakage in a phase or entirely random breakage, breakage probability function was used for selecting pixels on the mineral map of ore texture. For example, if the breakage is known to be preferential in some specific phases, a probability function can be generated based on the degree of breakage to position random particles selectively over ore texture. To ensure that the particle has the surface exposure for that particular phase, the corner of the rectangle was selected for the anchor to position on the mineral map. For given ore texture D1, by random breakage and 100% preferential breakage in magnetite phase, the liberation distribution of magnetite in size fractions would be as Figure 16.
From the degree of liberation distribution and AIM values in size fractions, the degree of breakage can be roughly estimated as given in Table 6 for the studied samples. For example, the degree of liberation of D1 sample is around 74% for magnetite and 4% for apatite in the fine fractions while AIM50 for these phases indicates that surface exposure of the phases in the locked particles is increasing in the fine fractions as well. This is suggesting that for the liberation of magnetite and apatite, preferential breakage in these phases are the main contributor for liberation. If we assume that the main breakages in the sample are either preferential in phases or random (no preferences in any way), it is safe to use a degree of liberations as a rough estimate to position rectangle corner in phases. For the D1 sample, this would be 4% chance to place rectangular corner in apatite phase, 74% chance for magnetite phases and 21% chance to have no preferential positioning (random).

Table 6. The probability distribution for preferential breakage in a specific phase and random breakage established based on the degree of liberation.

<table>
<thead>
<tr>
<th>Breakage</th>
<th>E</th>
<th>D1</th>
<th>A1</th>
<th>C1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz</td>
<td>-</td>
<td>0.1</td>
<td>1.3</td>
<td>-</td>
</tr>
<tr>
<td>Feldspar</td>
<td>-</td>
<td>0.1</td>
<td>-</td>
<td>0.5</td>
</tr>
<tr>
<td>Biotite</td>
<td>0.3</td>
<td>0.8</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Amphibole</td>
<td>0.0</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Apatite</td>
<td>1.2</td>
<td>4.4</td>
<td>5.0</td>
<td>5.2</td>
</tr>
<tr>
<td>Iron oxide</td>
<td>88.1</td>
<td>73.5</td>
<td>83.3</td>
<td>83.2</td>
</tr>
<tr>
<td>Random</td>
<td>10.4</td>
<td>21.1</td>
<td>10.4</td>
<td>11.1</td>
</tr>
</tbody>
</table>

Applying preferential and random breakage over ore textures yields particle population. Approximately one million particles were generated for each sample.

3.4.2 Adjusting liberation to match modal mineralogy
Generating particles by this method does not necessary give the same modal composition as the experimental work for some size fractions specifically for finer fractions. However, the liberation distribution is still close to the experimental liberation. The differences in modal composition and degree of liberation of some minerals could be due to the way that the particles are generated. In realistic breakage with classification stage, when particle breaks preferentially in one phase, non-liberated progeny particles are generated as well. This means that non-liberated particle still has a chance to break to fully liberated particles in finer size fractions, but this cannot be considered in the particle generation approach. In current particle generation, grade of the phase with highest
preferential breakage increases in finer fractions. This specifically is true for the finest size fraction. Possible explanation is the resolution of the mineral map that in certain point particle size is reached. This means many fine particles are consist of only a few pixels or even one pixel. This can be fixed by the approach that was introduced by Lamberg & Vianna (2007) to adjust the mass proportion of particles to match the known bulk modal composition. This is not a perfect solution, but it solves the inconsistency between liberation distribution of particles and modal composition. The modal composition of selected samples from experimental and texture breakage with the adjusted composition are listed in Table 7-Table 10. In general, similar composition can be reached for all samples only by adjusting the mass proportion of particles.

Table 7. The modal composition of E sample from experimental (Exp.) and generated particles after adjusting liberation (Adj.).

<table>
<thead>
<tr>
<th>Fraction</th>
<th>Biotite (wt%)</th>
<th>Amphibole (wt%)</th>
<th>Apatite (wt%)</th>
<th>Magnetite (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;1680</td>
<td>1.64</td>
<td>1.57</td>
<td>1.51</td>
<td>1.52</td>
</tr>
<tr>
<td>850-1680</td>
<td>0.97</td>
<td>0.92</td>
<td>0.62</td>
<td>0.75</td>
</tr>
<tr>
<td>425-850</td>
<td>1.00</td>
<td>0.96</td>
<td>0.50</td>
<td>0.70</td>
</tr>
<tr>
<td>300-425</td>
<td>1.30</td>
<td>1.26</td>
<td>0.57</td>
<td>0.86</td>
</tr>
</tbody>
</table>

Table 8. The modal composition of D1 sample from experimental (Exp.) and generated particles after adjusting liberation (Adj.).

<table>
<thead>
<tr>
<th>Fraction</th>
<th>Quartz (wt%)</th>
<th>Feldspar (wt%)</th>
<th>Biotite (wt%)</th>
<th>Apatite (wt%)</th>
<th>Magnetite (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;1680</td>
<td>6.22</td>
<td>6.71</td>
<td>23.08</td>
<td>22.63</td>
<td>5.33</td>
</tr>
<tr>
<td>850-1680</td>
<td>3.63</td>
<td>4.08</td>
<td>13.02</td>
<td>12.49</td>
<td>5.64</td>
</tr>
<tr>
<td>425-850</td>
<td>1.50</td>
<td>1.51</td>
<td>2.07</td>
<td>2.58</td>
<td>7.15</td>
</tr>
<tr>
<td>300-425</td>
<td>1.50</td>
<td>1.76</td>
<td>2.78</td>
<td>3.22</td>
<td>7.28</td>
</tr>
</tbody>
</table>

Table 9. The modal composition of A1 sample from experimental (Exp.) and generated particles after adjusting liberation (Adj.).

<table>
<thead>
<tr>
<th>Fraction</th>
<th>Quartz (wt%)</th>
<th>Apatite (wt%)</th>
<th>Iron oxide (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;1680</td>
<td>6.67</td>
<td>6.46</td>
<td>3.90</td>
</tr>
<tr>
<td>850-1680</td>
<td>2.92</td>
<td>3.08</td>
<td>1.93</td>
</tr>
<tr>
<td>425-850</td>
<td>5.06</td>
<td>4.99</td>
<td>5.92</td>
</tr>
<tr>
<td>300-425</td>
<td>2.63</td>
<td>2.85</td>
<td>6.90</td>
</tr>
</tbody>
</table>

Table 10. The modal composition of C1 sample from experimental (Exp.) and generated particles after adjusting liberation (Adj.).

<table>
<thead>
<tr>
<th>Fraction</th>
<th>Feldspar (wt%)</th>
<th>Apatite (wt%)</th>
<th>Iron oxide (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;1680</td>
<td>1.52</td>
<td>1.49</td>
<td>3.26</td>
</tr>
<tr>
<td>850-1680</td>
<td>0.73</td>
<td>0.69</td>
<td>1.57</td>
</tr>
<tr>
<td>425-850</td>
<td>1.10</td>
<td>0.92</td>
<td>4.03</td>
</tr>
<tr>
<td>300-425</td>
<td>1.26</td>
<td>1.03</td>
<td>7.33</td>
</tr>
</tbody>
</table>
3.4.3 Comparison of liberation of iron oxide minerals

As the major phase in the samples is iron oxide mineral and its liberation is critical for mineral processing plant performance, the iron oxide liberation distribution comparison is made between experimental and forecasted particles. Generally speaking, in most of the samples, the trend of iron oxide liberation is predicted well (Figure 17). However, particle population of magnetite samples (E and D1) presents better liberation distribution than those where both magnetite and hematite are present. In overall, this suggests that the ore texture is a major factor controlling the liberation distribution in crushing.
4. Discussion

Image processing methods are widely used for ore texture and particle characterization, however, liberation by composition and exposed surface are still the dominated methods for liberation and particle characterization. One of the shortcomings of the existing methods for association and liberation distribution is the inability to compare the particle texture against the original ore texture numerically. Textural descriptors that are commonly used for particles (Pérez-Barnuevo et al., 2012) are to show the complexity of texture or identification, but they lack the capability to relate particles to the parent texture in a way that can be used for the breakage analysis and forecasting.

The association indicator matrix (AIM) can be regarded as an extension of pioneer work by Lund et al. (2015) to account for a grade of mineral in the particle in the assessment of association. The suggested method could not consider phase boundaries or exposed surface. Therefore, the applicability of association index was limited especially when there were disseminated grains or inclusion in the particle. Current method accompanied by particle composition can store valuable information about the distribution of interfacial areas between phases and liberation distribution by composition and exposed surface.

The merits of association indicator over absolute value of interfacial area or common co-occurrence matrix are not only that it is less sensitive to scale, for example, due to fractal effect, but also values can be compared to different textures as well as particles and can be used as criteria for textural classification.

The cell values in the AIM also gives relevant information about how the phases are occurring in the ore texture. For example, if the AI value goes near 100%, it is an indication that one phase is mainly accompanied by another phase, for instance as inclusions. Also, if the purpose is to identify or categorize new textures, the AIM can be used as a criterion.

The other potential strong point of AIM is the capability of evaluating the nature of breakage of given ore texture for further generation of full particle population. This was demonstrated by four drill core samples where liberation distribution of iron oxide minerals was compared. In general, results for magnetite samples were closer to experimental data. This could be because in iron oxide samples hematite and magnetite are lumped together, and same breakage frequency as magnetite was used for hematite.

Generated mineral map of ore texture from drill core mapping was used as an input for generating particles. The particle size distribution from crushing was used for generating various size of rectangles.
that were superimposed on the mineral map. For positioning the rectangles over the mineral map, breakage probability was used. The assumption was that the preferential breakage in the phase is the cause of the liberation of minerals and random breakage can yield both liberated and non- liberated particles. The obstacle in this approach is that grade of mineral with highest preferential in finer size fractions progressively increase. Therefore, liberation adjustment step was required to match modal composition in size fraction according to experimental.

The value of the developed method is that it links original texture and mineral liberation. The approach generates full particle population which can be directly used in particle-based process simulations.

5. Conclusions
To best of our knowledge, the association indicator was introduced for the first time and used for characterization of breakage. In addition, following points were introduced and applied in this work:

- In the studied samples, the analysis of the AI values indicates that the breakage is preferential in the iron oxide phases specifically in magnetite. This was further investigated by generating particles based on defined breakage. This can be done by establishing breakage probability function.
- The full particle population was generated based on applying breakage on ore texture mineral map. The mass proportion of generated particles was adjusted to match the known modal composition of the samples. The outcome was satisfactory.
- The particle population forecasting has a great potential use in mineralogical approach to geometallurgy as the forecasting the liberation distribution from texture is a critical issue there. This work is intended to be used for filling the gap between geology and mineral processing in the mineralogical approach to geometallurgy.

6. Acknowledgment
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References


Paper IV
Process simulation in mineralogy-based geometallurgy of iron ores
Mehdi Parian*, Pertti Lamberg, and Jan Rosenkranz

* Corresponding author, Minerals and Metallurgical Engineering, Luleå University of Technology, SE-971 87 Luleå, Sweden; Tel. +46-920-492556; Fax +46-920-97364, e-mail: mehdi.parian@ltu.se.

Keywords: Geometallurgy, mineral liberation, particles, process modeling, simulation

1. Abstract
The mineral processing simulation models can be classified based on the level that stream in plant and unit models is described. The levels of modeling in this context are: bulk, mineral or element by size, and particle. The particle level modeling and simulation utilizes liberation data in the feed stream and is more sensitive to the variations in ore quality. Within the paper, results of simulation for two texturally different magnetite ore are demonstrated at bulk, mineral by size and particle level. The models were calibrated for one ore and then in the simulation applied directly to the other ore. For the second ore the simulation results vary between the different levels. This is because, at the bulk level, the model assumes that magnetite, as well as other minerals, do not change their behavior if ore texture and grinding fineness are changed. At the mineral by size level, the assumption is that minerals behave identically in each size fraction even the ore texture changes. At the particle level, the assumption is that similar particles behave in the same way. The particle level approach gives more realistic results, and it can be used in optimization, thus finding the most optimal processing way for different geometallurgical domains. Even in the high grade iron ores where iron minerals are highly liberated the particle level shows its power in the prediction of impurity levels well.

2. Introduction
Variation in the quality of feed to a plant has been a challenge for mineral processing operations. A prior quantitative understanding of the characteristics of the feed over the lifespan of the mining operation is the solution to successful production planning, circuit design, optimization, and troubleshooting. Also, demands for effective utilization of ore bodies and proper risk management in the mining industry have emerged an interest in geometallurgy.

A mineralogy-based geometallurgical modeling employs quantitative mineralogical information, both on the deposit and in the process. The geological model must describe the minerals present, give their chemical composition, report their mass proportions (modal composition) in the ore body and describe the ore texture. The process model must be capable of using mineralogical information provided by the geological model to forecast the metallurgical performance of different geological volumes, such as samples, ore blocks, geometallurgical domains or blends prepared for the plant feed for different periods from hourly and daily scale to weekly, monthly and annual production.
As to the level of details, predictive models of mineral processing can be divided into three categories based on the size of the smallest block in the simulation. In the least detailed level, the entire processing circuit (black box model) is modeled in a single operation, sections (e.g. comminution circuit and flotation circuit) is used at a moderate level, and single unit operations (e.g. individual flotation cells) is used at the detailed level. In geometallurgy, it is common to use models which predict the full process with simple equations (black box models). For example in Hannukainen iron ore deposit, the iron recovery into the iron concentrate has been defined with a simple equation based on iron and sulfur head grade (Equation (1), SRK Consulting (2014)).

\[
R_{Fe} = 98.5 \times (1 - e^{0.065(Fe - 6)}) \times (-1.96 \times (\frac{S}{Fe}) + 1)
\]

Models describing the process section wise are also common especially in comminution circuits when throughput or comminution energy usage is being forecasted. Geometallurgical models going to unit operation level are rare. This is mainly due to the difficulty of obtaining quantitative results from geology to work at unit level as well as the lack of interface to connect geological data to mineral processing unit level.

Another way of classifying the models used in the mineral processing simulation is based on the level that the feed stream to the plant and unit operations is described. The flowrates information in a stream, from lowest to the highest level of detailedness, are total solids, chemical elements, minerals, and particles. Each of these properties can be further divided to be part of certain size class. Thus bulk stream is divided into different sub-streams each representing a particle size class. Obviously, the study goal defines the selection of the properties and size information. For instance, solids by size (i.e. total solids flowrate of narrow particle size class) are often used to model and simulate comminution circuits whereas bulk mineral information is common in froth flotation. The selection of a modeling level comes with certain restrictions (Table 1) that limit its usability when expanding it outside the scope where the model is created and calibrated.

Table 1. Modeling levels and their assumptions in minerals processing. The model is valid and can be extended outside the calibration point as long as the feed stream assumptions are met.

<table>
<thead>
<tr>
<th>Level</th>
<th>Feed stream assumptions</th>
<th>Example of application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk (B)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solids (BS)</td>
<td>Each particle will behave identically regardless of its size and composition</td>
<td>Solid splitter model, equipment scale-up, basic engineering</td>
</tr>
<tr>
<td>Element (BE)</td>
<td>Mineralogy, particle size distribution, and liberation distribution are fixed</td>
<td>Recovery function model for elements</td>
</tr>
<tr>
<td>Mineral (BM)</td>
<td>Particle size distribution and liberation distribution are unchanged</td>
<td>Mineral splitter model</td>
</tr>
<tr>
<td>Behavioral type (BB)</td>
<td>Particle size distribution is unchanged. Similar behavioral types will behave identically</td>
<td>Gravity separation model</td>
</tr>
<tr>
<td>Sized (S)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solids (SS)</td>
<td>Each particle of given size will behave identically</td>
<td>Comminution model, Size classification model, equipment scale-up</td>
</tr>
<tr>
<td>Grindability type (SG)</td>
<td>Each particle type of given size will behave identically</td>
<td>Comminution model</td>
</tr>
<tr>
<td>Element (SE)</td>
<td>Mineralogy and liberation distribution are unchanged</td>
<td>Recovery function model in size classes</td>
</tr>
</tbody>
</table>

2
Another critical dimension of a process model is what input parameters it takes, what are the limitations are and how it was developed. Empirical models are solely based on the data without any explanation of physical or chemical process governing the system. Phenomenological models are based on the data, but the theory of the process to some extent is used to define to correlate the equations and used parameters. Finally, the fundamental models are solely based on physical and chemical properties and sub-processes in the system without the need of experimental data. Fundamental models, which try to consider all involving elements in the process, have not yet found their place in flowsheet simulation. This is mainly due to many sub-processes has taken place even in simple mineral unit operation (e.g. pumping), a big number of particles in the system and huge demand on computational resources.

This study focuses on flowsheet simulation for geomeallurgy of iron ores. Process unit models to be studied are selected based on applicability at particle level for iron ore beneficiation and flowsheet simulation. The first purpose is to identify where appropriate models exist and where development is needed and second is to evaluate advantages and disadvantages of simulation at particle level compared to other levels.

### 3. Review of unit operation models for simulation of magnetite ore beneficiation plant at mineral and particle level

Minerals and particles are the fundamental elements in mineral processing operations and simulations. Both mineral and particle properties define the selection of a process and the process performance. However, the full potential of using particles in mineral processing simulation has not been accomplished yet. This has been partly due to lack of analyzing instruments to collect experimental information at particle level as well as the lack of mass balancing techniques and data reconciliation methods capable of working with the mineral liberation level when processing the experimental data to define model parameters of a unit process in question. Also, unit operation models which predict the behavior of individual (also multiphase) particles based on their properties are largely missing.

The development of automated mineralogy (Gu et al., 2014) has facilitated collecting particle level information. Additionally, data reconciliation and mass balancing techniques improved from the traditional approach of balancing solids and elements (Hodouin, 2010) to reconciling and adjusting particle populations (Lamberg and Vianna, 2007). These developments have built a foundation to take mineral processing unit models and simulation to a new level.

For the magnetic separation models reader is referred to a reviewed and model development of Parian et al. (2016). For other commonly used unit models, a review of existing models regarding modeling level (Table 1) is given in the following sub-chapters.

<table>
<thead>
<tr>
<th>Behavioral type (SB)</th>
<th>Particle (SP)</th>
</tr>
</thead>
<tbody>
<tr>
<td>liberation distribution is unchanged</td>
<td>Similar behavior of particles of same composition and size</td>
</tr>
<tr>
<td>Mineral splitter model in size classes</td>
<td>Principally applicable to all unit models</td>
</tr>
<tr>
<td>Flotation model (fast and slow floating materials in size classes), Gravity separation model in size classes</td>
<td></td>
</tr>
</tbody>
</table>
3.1 Size classification models

Particle size classification in mineral processing is mostly done by screening or hydrodynamic classifiers. In screening the separation of particles is affected by their sizes (as well as the size and the shape of the aperture in screen) while hydrodynamic classifiers use the motion of particles. Hydrocyclone and spiral classifier fall into the second category. For them the particle properties are fundamentally required to model classifiers however for screens, the size distribution of particles can be sufficient.

An extensive review of the hydrocyclone models and their applications are available in the literature (Barrientos and Concha, 1990; Chen et al., 2000; Frachon and Cilliers, 1999; Heiskanen, 1997; Kraipech et al., 2006; Svarovsky, 2000). In a context of flowsheet simulation in mineral processing, the number of suitable hydrocyclone models is limited. This is because solution from fundamental modeling of hydrocyclone is computationally intensive (Nageswararao et al., 2004). The remaining models are empirical or phenomenological models that require experimental work to obtain material specific constants. An example of a hydrocyclone model that used for considering particles and ore texture is a study by Donskoi et al. (2005). He used revised Plitt’s hydrocyclone model (Flintoff et al., 1987) in USIM PAC simulation package and defined a various class of particles (density based) in size fractions as a separate phase. This data was used to predict recovery of minerals, total iron, and masses in the hydrocyclone underflow.

A common method of representing separation efficiency by size is by efficiency curve (Napier-Munn et al., 2005). It relates mass proportion of each particle size in the feed which reports to the particle size. None of the above-listed models can truly treat particles individually and give different behavior for particles being similar in size but different in composition (density).

3.2 Comminution models

In iron ore beneficiation, the purpose of the comminution is mostly to liberate iron ore minerals from gangues. Further comminution to finer than liberation normally is unnecessary unless there is a particle size requirement for the product such as fine magnetite concentrate for pelletizing process. Comminution equipment in the mineral industry are many and differ in design and application. It is not possible nor is the objective of this study to cover all crushing and grinding models. Emphasize is made on models which are capable of delivering stream properties for flowsheet simulation instead power consumption, operating conditions or optimization. This means size distribution and liberation models which can be applied for size reduction processes. Considering modeling levels given in Table 1, only sized level models (S) are valid.

In the most simplified case, particle size distribution of discharge stream can be modeled by fitting particle size distribution functions such as Rosin-Rammler, lognormal or logistic distribution (see King 2012) for the product. Based on the experimental work and observations the best distribution function can be selected to model particle size distribution of the discharge stream. The distribution functions as such cannot forecast the size distribution if there are changes in federate, grinding conditions, residence time or material properties (like particle size distribution, mineralogy, ore texture). Some studies (Mwanga, 2016) have used an approach where P80 from Bond equation has been used to forecast the full particle size distribution by Rosin-Rammler equation by keeping the parameter describing the steepness of the cumulative distribution curve fixed. This kind of model can be described as a forecast of particle size distribution experimentally.
Population balance model (Austin et al., 1984) is versatile and has a wider range of forecasting capability than the one described above. Once the model is calibrated, it can forecast the particle size distribution even if the particle size distribution of the feed changes. It is based on the mass balances by particle size comprising a selection function \(S\) and the breakage function \(B\). The equation in cumulative form is defined as follows:

\[
\frac{\partial M(x, t)}{\partial t} = \int_x^\infty S(y)B(x, y) \frac{\partial M(y, t)}{\partial y} dy
\]

(2)

where:

- \(M(x, t)\): Cumulative mass of particles finer than size \(x\)
- \(S(y)\): The selection function which shows the mass fraction of size \(y\) which is going to be fragmented
- \(B(x, y)\): The cumulative breakage function which is the fraction of particles of size \(y\) which are fragmented to give particles of size less than \(x\)

The equation (2) in discrete form changes to

\[
\frac{dM_i}{dt} = -S_i M_i(t) + \sum_{j=1}^{i-1} b_{i,j} S_j M_j(t)
\]

(3)

The most popular of breakage function models are based on a mixture of two separate populations (Equation (4)). However, it can be even simplified as one population. A general and simplified representation of the selection function is in the form of equation (5).

\[
B(x, y) = K\left(\frac{x}{y}\right)^a + (1 - K)\left(\frac{x}{y}\right)^b
\]

(4)

\[
S(x) = Kx^a
\]

(5)

If one takes simplified forms of selection and breakage functions, the solution of equation (2) becomes well-known Rosin-Rammler distribution.

\[
M(x, t) = M(x, 0)e^{-Ax^t}
\]

(6)

Size-mass balance models can relatively well predict particle size distribution of a mill product even if the particle size distribution of the feed changes. However, the model is not capable of predicting neither mineral grade by size nor liberation distribution.

In the concept of liberation modeling, various approaches are known. The first approach is to model liberation independently from size reduction modeling and assuming that liberation process is related to the texture of the ore and the target size (Gaudin, 1939; Wiegel and Li, 1967). Usually, the main parameters in this liberation model are the average grade of phases and the size ratio between particles.
and grains. This approach is also called texture modeling and is achieved by superimposing particles mesh
over texture image. This approach further developed from simple textures to consider a variety of ore
textures (Barbery, 1991) or transformation of textures to simple forms (Meloy and Gotoh, 1985). In this,
the key parameters are the volumetric grade of the ore mineral and the interfacial surface area between
phases which is related to the grain size.

The second approach was developed by extending the theory of liberation (Andrews and Mika, 1976;
Wiegel, 1976). These authors have considered the problem of simultaneously accounting for liberation
and breakage in a batch mill. Other approaches have been reported in the literature such as integration of
liberation, size reduction and process modeling (Bax et al., 2016; Khalesi, 2010).

A fundamental part of liberation models is how the ore texture is defined or is characterized to be used
for developing predictive liberation models. The second part of liberation model is how the mineral
distribution in particles is defined. This can be described by distribution functions without measurement
or measured on by images analysis techniques. A majority of liberation models are based on binary system
(i.e. an ore mineral embedded in a gangue matrix), and they lack the capability of forecasting liberation
distribution for multiphase particles. A comprehensive review of liberation models and their development
in 80’s and before was given by Barbery and Leroux (1988).

Another important part of liberation modeling is how actually fragmentation (breakage) happens. As
discussed earlier, a simple approach is to superimpose particle patterns over textures. A recent review of
mineral liberation and liberation in comminution is given by Mariano et al. (2016).

Practical implementation of mineral liberation models in the mineral processing is rare. This is because the
models are mainly for binary systems and taking models to the multiphase system is too complicated.
However, in simplified ore textures (binary system) the models have been tested and compared against
experimental data (Barbery and Leroux, 1988; Choi et al., 1986; Finch and Petruk, 1984; Hsih and Wen,
1994; Leigh et al., 1996; Schneider et al., 1991). The results of these studies are encouraging, but the
application of the binary system is limited specifically nowadays that ore bodies grades are declining, and
deposits are becoming more complex.

In simulation software used in mineral processing, MODSIM includes complete Andrews-Mika liberation
modeling. HSC Chemistry since version 7.1 (Outotec, 2012) has included liberation model as built-in
comminution models. Traditional comminution models describe the product particle size distribution and
internally the software forecast the liberation distribution of the product if the liberation information on
the feed stream is given (Lamberg and Lund, 2012). This is done by keeping the liberation distribution
within the size fractions unchanged, and the changes are applied only to mass proportions of different
size fractions. As the mineral grades between the particle size fractions may be different, the change in
mass proportions of the particle size fractions would change the mineral grades in bulk. Therefore, there
is extra reconciliation step to conserve the bulk mineral balance between the feed and product.

### 3.3 Flotation models

It is known that kinetic model well describes the batch flotation results. In batch flotation modeling with
its specific assumptions, such as perfect mixing, full particle suspension and capture efficiency, the rate of
flotation is directly related to remaining floatable material in the cell (King, 2012). The flotation rate
equation in differential form is:
\[-\frac{dC}{dt} = kC^n\]  \hspace{1cm} (7)

where \( n \) denotes the order of the equation. In the simplest form, the first order kinetic, the equation (7) becomes:

\[C = C_0 e^{-kt}\]  \hspace{1cm} (8)

By the assumption that a fraction of each mineral is non-floatable and considering the ultimate recovery \( R_{\infty} \), the form of equation in terms of recovery of the mineral in batch flotation and perfect mixer (industrial single tank cell) becomes

\[R = R_x \left(1 - e^{-kt}\right)\]  \hspace{1cm} (9)

\[R = \frac{kt}{1 + kt}\]  \hspace{1cm} (10)

To find the constants, experimental data must be fitted with the equation (9). The extension of the first order kinetic model (Equation (9)) is the Klimpel model which has the rectangular rate distribution instead of uniform rate as the classic first order kinetic model (Dowling et al., 1985). The Klimpel (1980) kinetic model is defined as follow:

\[R = R_x \left(1 - \frac{1 - e^{-kt}}{kt}\right)\]  \hspace{1cm} (11)

The Klimpel model has been used for analysis of more than 300 flotation tests at WEMCO® and was found to fit experimental data reasonably well (Parekh and Miller, 1999).

Kelsall (1961) presented a kinetic based flotation model consisting slow and fast floating rate constant. Comparing to classic first order kinetic model, Kelsall’s model was considered to offer a better estimate. Later his model modified by Jowett (1974) to consider ultimate recovery as follow:

\[R = R_x \left((1 - \varphi) \left(1 - e^{-kt}\right) + \varphi \left(1 - e^{-kt}\right)\right)\]  \hspace{1cm} (12)

A comprehensive survey of flotation models exists in the literature (Dowling et al., 1985; Mavros and Matis, 1991; Runge and Franzidis, 2003; Wang et al., 2015). The other approach of flotation modeling are the models considering environment effects. These models remark the relation between metallurgical performance and environment variables (Gorain et al., 1999; Mathe et al., 1998; Tabosa et al., 2016; Vera et al., 2002; Wang et al., 2016). Compared to other unit processing models, flotation models are more mature in reaching to particle level modeling (Lamberg and Vianna, 2007; Savassi, 2006; Welsby et al., 2010).

### 3.4 Summary of the process unit models for particle-based simulation

In the concept of particle-based simulation, a minimum requirement for a unit model is the capability to work in particle size level and address relevant particle properties for the unit process. This means that
even some of the existing unit operation models are not designed to be used for mineral liberation data they can still be used in particle-based simulations with some considerations. For example, even though Efficiency Curve or Plitt’s hydrocyclone model is not particle-based in nature, the particle population can be used to generate the bulk information needed to calculate the cut size of a hydrocyclone. Mineral liberation information would be required in some areas, including magnetic separation and flotation. Regarding this study, magnetic separation model must perform simulations on liberation level. The applicability and limitation of existing unit operation models for the mineralogical approach are summarized in Table 2.

Table 2. Applicability of current unit models in particle-based simulation.

<table>
<thead>
<tr>
<th>Area</th>
<th>Model</th>
<th>Considerations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Magnetic separation</td>
<td>King and Schneider (1995), Parian et al. (2016)</td>
<td>-</td>
</tr>
<tr>
<td>Comminution</td>
<td>HSC Chemistry: combined fixed particle size distribution and liberation model</td>
<td>Assumes liberation in narrow size fractions remains unchanged</td>
</tr>
<tr>
<td>Particle size classifier</td>
<td>Fixed particle size distribution</td>
<td>The only size of particles is considered to affect separation</td>
</tr>
<tr>
<td>Hydrocyclone</td>
<td>Efficiency curve/Efficiency curve by mineral</td>
<td>Does not take into account particle/mineral densities</td>
</tr>
<tr>
<td>Flotation</td>
<td>HSC Chemistry, Lamberg &amp; Vienna</td>
<td>Kinetic constants for multiphase particles deviates from linear behavior</td>
</tr>
</tbody>
</table>

4. Materials and methods

4.1 Samples

The data that is used for plant simulation falls into two categories. The first set of data is from plant survey that has been done at one of the LKAB’s iron ore processing plants in Kiruna, Northern Sweden. Sample preparation and mass balancing of plant data in a mineral by size level are as described at Parian et al. (2016). The second set of data is the result of ore texture mapping and fragmentation to generate particle population as a feed stream to the flowsheet. Two magnetite drill core samples with variation in ore texture are used to generate two different liberation distribution. The procedure for generating particles from drill core ore texture was explained at Parian et al. (submitted to Journal).

4.2 Analysis

Chemical analyses of the survey samples were done at the chemical laboratory of LKAB. The data was used to achieve mineral grades in the stream by Element-to-Mineral conversion method described in Parian et al. (2015). Afterward, the plant data was mass balanced in a mineral by size levels. Mass balancing and data reconciliation was done using the modeling and simulation software HSC Chemistry 9 by Outotec and MATLAB by Mathworks. In the mass balancing of liberation data Particle Tracking technique (Lamberg and Vienna, 2007) was used.

The flowsheet was drawn in HSC Chemistry 9.1 Sim module and is used to demonstrate different levels of modeling according to Table 1. The newly made particle based WLIMS model (Parian et al., 2016) was also adopted in HSC Chemistry 9.1 Sim to be used for the simulation.
5. Results and discussion

5.1 Plant Circuit

A flowsheet used here consist of comminution and concentration circuits and is based on LKAB Kiruna concentration plant (Samskog et al., 1997; Söderman et al., 1996). A circuit is a general form of the process that LKAB uses in Kiruna for the beneficiation of magnetite ore. The feed to the plant is the product of crushing and cobbing plant. The beneficiation process consists of three major steps including comminution, magnetic separation and apatite flotation. The comminution circuits include autogenous grinding followed by the spiral classifier and pebble milling coupled with hydrocyclone (Figure 1).

![Diagram of Magnetite beneficiation plant flowsheet for demonstration of different levels of modeling and simulation](image)

5.2 Process units

The process unit models used in the simulation in different modeling levels are gathered in Table 3. The results from the mass-balancing of the plant data were used for defining the model parameter values of different models.

Table 3. The model that is used in the simulation of flowsheet at different levels.

<table>
<thead>
<tr>
<th>Unit</th>
<th>Bulk model</th>
<th>Mineral by size model</th>
<th>Particle level model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Autogenous Mill</td>
<td>Perfect mixer</td>
<td>(Fixed) PSD</td>
<td>HSC comminution model with decoupled size reduction and liberation models</td>
</tr>
<tr>
<td>Trommel</td>
<td>Mineral splitter/mass splitter</td>
<td>Efficiency curve / Efficiency curve by mineral</td>
<td>Efficiency curve/efficiency curve by mineral</td>
</tr>
<tr>
<td>Mixer</td>
<td>Perfect mixer</td>
<td>Perfect mixer</td>
<td>Perfect mixer</td>
</tr>
<tr>
<td>Pebble Mill</td>
<td>Perfect mixer</td>
<td>(Fixed) PSD</td>
<td>HSC comminution model with decoupled size reduction and liberation models</td>
</tr>
<tr>
<td>WLIMS</td>
<td>Mineral splitter</td>
<td>Mineral by size splitter</td>
<td>Developed WLIMS model</td>
</tr>
</tbody>
</table>
Spiral classifier | Mineral splitter | Efficiency curve/efficiency curve by mineral (Parian et al. 2016)
Hydrocyclone | Mineral splitter | Efficiency curve/efficiency curve by mineral
Flotation | Flotation kinetics by mineral by size | Flotation kinetics by mineral by size

5.3 Plant feeds
Two different magnetite ore were selected to be used for simulation. The first ore is the actual feed to the plant during the survey (Ore A). The second ore is one of the studied drill cores samples which was studied by Parian et al. (submitted) (Ore B). The procedure for generation of particle population from second ore is described in Parian et al. (submitted). The two ores are texturally different thus have different mineral grades and liberation distribution (Table 4, Figure 2). The assumptions that are used here are that mineral compositions and particle size distribution after crushing for both ores are same.

The ore B was selected because it represents an ore which is significantly lower in the head grade and texture is much more fine-grained giving lower liberation degree at given particle size (Figure 2). Also, the Ore B would represent the plant feed in a case where cobbing is not used.

Table 4. Modal composition of plant feed samples. Ab = albite, Act = actinolite, Ap = apatite, Bt = biotite, Cal = calcite, Mgt = magnetite, Qtz = quartz.

<table>
<thead>
<tr>
<th></th>
<th>Ab</th>
<th>Act</th>
<th>Ap</th>
<th>Bt</th>
<th>Cal</th>
<th>Mgt</th>
<th>Qtz</th>
<th>Ttn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ore A</td>
<td>3.01</td>
<td>3.43</td>
<td>2.48</td>
<td>3.50</td>
<td>0.91</td>
<td>85.57</td>
<td>0.96</td>
<td>0.14</td>
</tr>
<tr>
<td>Ore B</td>
<td>12.88</td>
<td>0.00</td>
<td>7.24</td>
<td>10.27</td>
<td>0.00</td>
<td>64.09</td>
<td>5.52</td>
<td>0.00</td>
</tr>
</tbody>
</table>

![Figure 2](image-url). Liberation curves of magnetite in the Ore A (left) and Ore B (right).
5.4 Simulation for Ore A

Mass balancing results were used for calibrating models at bulk mineral and mineral by size levels. For simulation at particle level, models described in Table 3 were used and adjusted to match experimental and mass balancing results. In overall, for Ore A, three levels of simulation give the same grade and recovery for all minerals for the final concentrate of the plant with the calibrated parameters. The effect of coarse grinding was investigated by increasing product particle size in grinding circuit (pebble mill and hydrocyclone). The simulation reveals that even in coarse product magnetite recovery and grade is still preserved.

Table 5. Results of the simulations at different levels: composition of the magnetite concentrate (Grade wt%) and mineral recoveries. For mineral symbols, see Table 4.

<table>
<thead>
<tr>
<th>Grinding Level</th>
<th>Level</th>
<th>Ab</th>
<th>Act</th>
<th>Ap</th>
<th>Bt</th>
<th>Cal</th>
<th>Mgt</th>
<th>Qtz</th>
<th>Ttn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine (P80 = 38 µm)</td>
<td>Bulk Recovery (%)</td>
<td>13.86</td>
<td>17.25</td>
<td>22.99</td>
<td>13.23</td>
<td>17.80</td>
<td>95.60</td>
<td>0.00</td>
<td>99.79</td>
</tr>
<tr>
<td>Size</td>
<td>Recovery (%)</td>
<td>13.86</td>
<td>17.25</td>
<td>22.99</td>
<td>13.23</td>
<td>17.80</td>
<td>95.60</td>
<td>0.00</td>
<td>99.79</td>
</tr>
<tr>
<td>Grade (wt%)</td>
<td>0.50</td>
<td>0.70</td>
<td>0.68</td>
<td>0.55</td>
<td>0.19</td>
<td>97.21</td>
<td>0.00</td>
<td>0.17</td>
<td></td>
</tr>
<tr>
<td>Particle</td>
<td>Recovery (%)</td>
<td>13.87</td>
<td>17.17</td>
<td>23.02</td>
<td>13.19</td>
<td>17.80</td>
<td>95.62</td>
<td>0.00</td>
<td>99.70</td>
</tr>
<tr>
<td>Grade (wt%)</td>
<td>0.50</td>
<td>0.70</td>
<td>0.68</td>
<td>0.55</td>
<td>0.19</td>
<td>97.22</td>
<td>0.00</td>
<td>0.17</td>
<td></td>
</tr>
<tr>
<td>Coarse (P80 = 72 µm)</td>
<td>Bulk Recovery (%)</td>
<td>18.84</td>
<td>24.21</td>
<td>20.41</td>
<td>16.38</td>
<td>17.47</td>
<td>95.59</td>
<td>0.00</td>
<td>99.79</td>
</tr>
<tr>
<td>Size</td>
<td>Recovery (%)</td>
<td>18.84</td>
<td>24.21</td>
<td>20.41</td>
<td>16.38</td>
<td>17.47</td>
<td>95.59</td>
<td>0.00</td>
<td>99.79</td>
</tr>
<tr>
<td>Grade (wt%)</td>
<td>0.67</td>
<td>0.98</td>
<td>0.60</td>
<td>0.68</td>
<td>0.19</td>
<td>96.71</td>
<td>0.00</td>
<td>0.17</td>
<td></td>
</tr>
<tr>
<td>Particle</td>
<td>Recovery (%)</td>
<td>10.17</td>
<td>22.33</td>
<td>23.23</td>
<td>16.24</td>
<td>26.54</td>
<td>95.81</td>
<td>0.00</td>
<td>99.74</td>
</tr>
<tr>
<td>Grade (wt%)</td>
<td>0.36</td>
<td>0.91</td>
<td>0.68</td>
<td>0.67</td>
<td>0.29</td>
<td>96.92</td>
<td>0.00</td>
<td>0.17</td>
<td></td>
</tr>
</tbody>
</table>

5.5 Simulation for Ore B

For the simulation of Ore B, the calibrated parameters that were used at bulk mineral, mineral by size and particle levels for Ore A, were used. The results show that at bulk mineral and mineral by size levels, the mineral recoveries are similar as for the Ore A in fine grinding (Table 6). This is a property of models which define the behavior of minerals on unsized or size based: regardless of the plant feed the mineral recoveries (and distribution in the full process) is similar, but the grades change. When the head grade lowers, the concentrate grade drops as well.

At the liberation level, the result is, however, different. Similar particles behave in the same way as in the base case, but because the mass proportion of particles (thus liberation distribution) is different in the plant feed for the Ore A and Ore B, the final result will differ for both grades and recoveries. The particle level simulation forecasts slightly lower grade and recovery for the Ore B as for the Ore A. Compared to bulk and mineral by size level the particle level simulation forecast lower gangue recovery thus higher magnetite grade.
Table 6. Results of the simulations at different levels for the ore B: composition of the magnetite concentrate (Grade wt%) and mineral recoveries. For mineral symbols see Table 4.

<table>
<thead>
<tr>
<th>Grinding Level</th>
<th>Level</th>
<th>Ab</th>
<th>Act</th>
<th>Ap</th>
<th>Bt</th>
<th>Cal</th>
<th>Mgt</th>
<th>Qtz</th>
<th>Ttn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine (P80 = 38 µm)</td>
<td>Bulk Recovery (%)</td>
<td>14.28</td>
<td>0.00</td>
<td>21.16</td>
<td>15.72</td>
<td>0.00</td>
<td>95.60</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>Grade (wt%)</td>
<td>5.29</td>
<td>0.00</td>
<td>2.21</td>
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<td>Size Recovery (%)</td>
<td>14.28</td>
<td>0.00</td>
<td>21.16</td>
<td>15.72</td>
<td>0.00</td>
<td>95.60</td>
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<td></td>
<td>Grade (wt%)</td>
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<td>0.00</td>
<td>2.21</td>
<td>1.39</td>
<td>0.00</td>
<td>91.12</td>
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<td>17.60</td>
<td>9.28</td>
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<td>89.29</td>
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<td>Bulk Recovery (%)</td>
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<td>21.16</td>
<td>15.72</td>
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<tr>
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<td>Grade (wt%)</td>
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<td>0.00</td>
<td>2.21</td>
<td>1.39</td>
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<td>1.70</td>
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Comparison of simulations for ores A and B demonstrates the difference between mineral and particle level modeling and simulation. In the ore B, the results from the particle level simulation give more plausible result than the mineral and mineral by size level. This is due to the fact that the parameters are calibrated based on the liberation of particles instead of general calibration to the ore at bulk mineral and mineral by size level. At the particle level, the assumption is that similar particles behave in the same way whereas in the mineral level the assumption is that mineral behaves identically regardless of texture and particle composition. Although no verification and validation for results of ore B were provided, however the simulation results in particle level comparatively to other levels is more credible.

6. Conclusions
The mineralogical approach of geometallurgy requires quantitative mineralogical data from geology model to be able to perform in its best form. It is common that for estimation of plant metallurgical response black box models or simple equation is used. However, this approach is not sensitive to the material changes. In the best case, they can adopt the changes in the head grade but not in variation in textures. Within this study, it is shown that simulation at mineral levels with calibrated parameters to the ore feed is only valid for ore having similar liberation characteristics. However, calibrated parameters at particle levels are based on the liberation of particles and are capable of giving more reliable estimates. In iron ore, the forecasts for the iron grade and recovery do not differ significantly, but for the impurity levels, the particle level simulation gives more reliable results. Also, the particle level enables optimization, thus finding optimal processing conditions, e.g. grinding fineness, for different textural ore types and geometallurgical domains.

7. Acknowledgment
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8. References


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