ANALYZING THE HYDRO DYNAMICS AND THE CHEMICAL REACTIONS IN PULP DIGESTER SYSTEMS USING CFD MODELLING

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Abstract
The aim of this thesis is to use differential analysis and finite volume method (FVM) to model and analyze a continuous pulp digester in order to create a detailed picture of the flow behaviour and chemical reactions in the digester. This information will be used to optimize wood chip flow and reactions and to diagnose and avoid faults such as hang-ups and channelling.

As digesters increase in size, the importance of control of the liquor flow in the wood chip bed also increases. Pulping reactors are often faced with production disturbances that cause reduced fibre quality, non-uniform chemical reactions and damaging channelling phenomena.

The models that are proposed in this thesis aim to consider the fluid dynamics, thermodynamics and chemical reactions together in order to create a model with more detail than has been previously reported.

The digester is of the continuous type and has a circular cross-section, with a height of 60 m and a diameter that increases stepwise from 6 m at the top to 7 m at the bottom. The geometry of the digester, including an internal pipe with three different diameters, three inlet flows at three levels of the digester, inlets and outlets at the top and bottom, and a number of peripheral circulation pipes connected to the screens at three levels, is represented in simulations by a 2D axisymmetric model constructed in Gambit.

The interactions between the two phases - the wood chips and the alkaline liquor - are studied using the finite volume method (FVM). Eulerian and Mixture numerical methods are evaluated for solving a mass transfer multiphase model with a porous matrix, species transport and reaction system in FLUENT. Variable porosity is used to model channelling in the digester.

Comparisons of the results of simulations with real digester data indicate that the multiphase model, with the species transport and mass transfer modules accurately predict the pulping chemical reactions inside the digester and are able to evaluate pulp quality.

The species transport model with reaction scheme is able to predict the mass balance equation and stoichiometry of the pulping reaction. The porous media scheme complements this approach to give a more complete view of pulp production, including the effect of faults in the process.

The approaches to the FVM described in this thesis enable an accurate view of the pulping process which can contribute to improved control and optimization of the process.
The purpose of this thesis has been to develop a numerical model that can be used to simulate and control the pulp production process. A finite volume method has been applied using the CFD (Computational Fluid Dynamics) program FLUENT.

Although the continuous sulphate process is the dominant chemical pulping process, our knowledge of events inside a digester is relatively poor with respect to hydraulics and chemical reactions.

This is because it is very difficult to measure conditions and obtain samples from points inside the digester. Phenomena such as hang-ups and channelling, that cause significant production and quality losses are especially poorly characterized.

There is no clear explanation for hang-ups, nor is there a solution to the problem, and the same is true for channel formation. Through the CFD simulations developed in this thesis we are able to simulate events inside the digester when these faults occur, and suggest ways of detecting these phenomena by measuring temperatures, pressures and Kappa numbers at different positions.

These CFD models help to picture events inside the digester and create an image of the pulping process. The simulations will hopefully be useful for investigating ways of counteracting faults in the process. The size of digesters is continuously increasing along with the demand for higher production rates, but this also increases the potential for failures in the process and the importance of correct management when problems occur with the chemical processes inside the digester.

Digesters may be of the batch or continuous type, but most modern digesters are of the continuous type. These often have complex circulation loops to ensure that the correct conditions are maintained with respect to temperature and concentrations of chemicals in different parts of the digester.

Among the problems that affect digesters are uneven distribution of liquids flowing through the chip bed, pressure from the chip column leading to chip compression, heterogeneous chip size and geometry, washing efficiency, swings between different wood grades and hanging of chips at the walls.

In this thesis a mathematical model has been developed that can be used to investigate all these variables and phenomena in order to increase the understanding of the flows and chemical reactions so that it is possible to manage the problems and optimize production.

By simulating different types of disturbances in the process and comparing this to real process data, it is possible to analyze the chemical processes inside the digester, even in the absence of actual measurements.

One of the most important features of pulp production modelling is the use of screens to separate chips and fibres from the liquids inside the digester. The majority of the liquor collected at the screens is re-circulated back into the digester.
In the thesis two numerical methods have been used to model the hydraulic behaviour of the digester. These are the Eulerian and Mixture methods.

In principle, it is desirable to model the digester with the highest possible degree of detail and in 3D. In reality computational capacity is a limiting factor. Different mesh sizes for modelling the digester were evaluated. A compromise was reached between sufficient modelling accuracy and reasonable calculation times. The digester is modelled as an axisymmetric 2D structure that includes the full digester volume. The actual digester, including the screens and the central pipe has been modelled with axisymmetric geometry in the Gambit software environment. Gambit is a pre-processor and is used to meet the specific geometry, mesh creation and boundary zone assignment for computational fluid dynamics and other scientific applications.

The CFD model predicts the chemical interactions between the solid phase (wood chips and fibres) and cooking liquor, and the exchange between the phases throughout the digester.

The models addressed in the literature have mostly focused on either hydraulics or chemical reactions in 2D axisymmetric scale setups. The investigation of the gradients of both chemical and hydraulic variables of the pulp process inside a real digester is novel. Different solution methods have been combined and tested here. The Eulerian and Mixture methods have been tested and evaluated with respect to the hydrodynamic properties typical for pulp digesters.

A mass transfer multiphase model with a porous matrix, species transport and reaction system has been used to model the chemical reactions inside the chips and the interactions between the solid and liquid phases. This is a flexible system with a large capacity to model and describe the pulping processes.

The Kappa number is a measure of the amount of remaining lignin at the fibre surface. The species transport model including the reactions has been introduced to analyze and calculate the chemical composition of the wood chips and the stoichiometry as determined from theoretical calculations and production data from the plant.

An Arrhenius expression describes the reaction kinetics and is combined with the material balances. The combined expressions are solved numerically to develop a reaction model that can be used for further optimizations. The hang-up phenomenon is modelled with a porous multi-phase matrix with mass transfer between the phases. The Kappa number near the created channel is calculated in order to determine the development of the chemical reactions around the fault.
CFD modellering av hydrodynamiska och kemiska reaktioner i massakokare

Huvudsyftet med denna avhandling har varit att utveckla en numerisk modell som kan användas för att simulera och styra massatillverkningsprocessen. Finit volym metod har tillämpats, med hjälp av CFD (Computational Fluid Dynamics) programmet FLUENT.

Även den kontinuerliga sulfatprocessen är dominerande för kemisk massa processen, är vår kunskap om vad som händer i kokaren och avseende på hydraulisk och de kemiska reaktionerna på en relativt låg nivå. Anledningen är att det är mycket svårt att ta ett prov från vilken punkt som helst i kokaren för att göra vissa mätningar.

Speciellt, hängningar och kanalbildning i kokaren är inte väl förstått trots att dessa fenomen orsakar betydande produktion och kvalitet förluster. Det finns varken en entydig förklaring till eller lösning för hur man skall kunna undvika hängning och kanalbildningar ännu.

Genom CFD-simuleringar som utvecklats i denna avhandling kan vi simulera vad som kan antas hända, och hur dessa fenomen kan upptäckas genom att mäta temperaturer, trycker och Kappa talen i olika positioner.

CFD-modellerna kan figurera vad som kan hända i kokaren och indirekt skapar en bild av massaprocessten. Förhoppningsvis kan simuleringarna också användas för att undersöka hur man kan motverka störningarna.

Storleken på kokare ökar kontinuerligt för att tillgodose högre produktionstakt men störleksökningen gör det samtidigt ännu svårare att hantera kemiska processer inne i kokaren. Det finns både satsvis- och kontinuerliga kokare, men de modernaste är kontinuerliga kokare. Dessa har ofta komplicerade cirkulations loopar för att kunna hålla rätt förhållande med avseende på temperatur och kemikaliekoncentrationer i olika delar av kokaren.

Problemen med kokare är bland annat ojämn fördelning av vätskeflödet genom flisen, trycket från flispelaren, fliskomprimering, flisrörelse i olika riktningar, heterogena träflisformer (och storlek på bitarna), tvättningseffektivitet, swing mellan olika vedkvaliteter och hängningar av flis längs väggarna.

I denna avhandling har en matematisk modell utvecklats där alla dessa faktorer och fenomen undersöks för att förbättra kunskapen om flödet och de kemiska processerna som gör det möjligt för oss att hantera och optimera produktionen.

Genom att simulera olika driftproblem och jämföra simuleringarna med processdata kan vi försöka analysera kemiska processen inne i kokaren.

En av de viktigare funktionerna i massatillverkningen är separering av träflis/fibrer och vätskeflödet inuti kokaren med hjälp av silar för att kunna recirkulera vätskan till kokaren.

I avhandlingen har två olika numeriska metoder provats för att modellera hydrauliska beteendet (Eulerian och Mixture).

I princip vill man modellera kokaren med så hög detaljeringsgrad som möjligt och i 3-D. I praktiken begränsas vi dock av att datorkapaciteten inte räcker till. Olika MESH storlek har därför provats för att hitta en kompromiss mellan tillräcklig noggrannhet, men inte alltför lång beräkningstid. Kompromissen blev en lösning med en axisymmetrisk 2-D-struktur som tar hänsyn till totala volymen i kokare. Både själva kokaren med silarna och formen på det ringformiga centrala röret i kokaren har konfigurerats med en axisymmetrisk geometri i miljön av Gambit mjukvara packet. Gambit är en pre-
processor och används för att uppfylla de särskilda geometrier, skapa nätverk i geometrin, bestämning av randvillkor och koppla samman användarnas behov för CFD och andra vetenskapliga applikationer. CFD-modellen predikterar fastfas- (träflis/fibrer) och vätskeflödet kopplat till kemiska reaktioner och utbyte mellan faserna genom hela kokaren.

Modellerna som presenteras i litteraturen vanligen har mestadels fokuserat på antingen hydraulisk eller kemiska reaktioner på små skalar. Utredning av fördelning av kemiska och hydrauliska variabler av massa process i en riktig kokare är ny. Olika lösningsmetoder har kombinerats och provats.

Eulerian och Mixture metoder har testats och utvärderats med avseende på de hydrodynamiska egenskaperna för typiska massakokare.

För att modellera de kemiska reaktionerna i chipsen och interaktion mellan fast och flytande fas användes en massöverföring-flerfas-modell med en porös matris, material transport och reaktionssystem. Metoden är ett flexibelt sätt med hög potential för att modellera och beskriva massaprocesserna.

Kappa-talet är ett mått på hur mycket lignin som finns kvar på ytan av fibrerna. Det beräknas numeriskt som den ursprungliga mängden lignin minus det som reagerar och löses ut då träflisen rör sig ner genom kokaren.

En materialtransport-modell inkluderar reaktionerna och har införts för att analysera den beräknade kemiska formeln för träflis och stökiometri som erhållits från de teoretiska beräkningar och produktionsdata i massabruk.

Ett Arrhenius-uttryck beskriver kinetiken och kombineras med massbalanserna. Kombinationen har lösats numeriskt för att skaffa en reaktionsmodell för ytterligare optimeringsändamål.

Hängningsfenomen har också modellerats med hjälp av en porös, flerfas metod med massöverföring mellan faserna. Kappa-talet har beräknats i närheten av den skapade kanalen för att undersöka utvecklingen av de kemiska reaktionerna här.
List of papers


II- Bijan Pourian, Erik Dahlquist, CFD modelling the continuous chemical interaction between the multiphase flows of the pulp and paper digester using the mass transfer scheme accepted by World Journal of Modelling and Simulation WJMS, 2011

III- Bijan Pourian, Erik Dahlquist, Modelling of the channelling phenomenon of the pulping digester using porous Media, (published by Scandinavian Modelling and Simulation Society, SIMS 50, conference in Fredrice, Denmark, October 7-8 (2009)

IV- Bijan Pourian, Erik Dahlquist, Continuous modelling of the Chemical reactions in the presence of the channelling using mass transfer and porous media, (Published in the International Review of Chemical Engineering Journal, September issue (2009)

V- Bijan Pourian, Erik Dahlquist, Modelling and simulation of chemical reactions between wood chips and white liquor in a continuous pulping digester Accepted by International Conference on Modelling, Simulation and Control (ICMSC 2010), Cairo, Egypt, 2-4 November (2010).

Contribution to the papers

I did all coding, numerical simulations and chemical and fluid dynamic computations were the main writer of all the papers.
**Licentiate title:** CFD Modelling and experimental study on the fluid flow and heat transfer in copper heat sink design

The licentiate thesis is not included in the PhD thesis.

The publications listed below are included in my Licentiate degree (2007) and are not included in this PhD thesis as they are more related to the product development area.


3. Numerical modelling of two proposed mechanically fabricated free-fins heat sinks


5. 3-Dimensional numerical and analytical study of thermal behaviour of proposed mechanical fabrication copper heat sink, Bijan Pourian, Mark Irwin, and Erik Dahlquist, (Published: International Scientific Conference on "Energy systems with IT" in connection with the Energiting March 11-12, 2009, Älvsjö fair, Stockholm, ISBN: 978-91-977493-4-3

**Note**

The author has his family name from Karimpourian to Pourian during the course of this work
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## Nomenclature

<table>
<thead>
<tr>
<th>Nomenclature</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>Molar concentration kmol/m³</td>
</tr>
<tr>
<td>d</td>
<td>Diameter (m)</td>
</tr>
<tr>
<td>(d_p)</td>
<td>Particle diameter (m)</td>
</tr>
<tr>
<td>(d_{im})</td>
<td>Diffusion coefficient for species i in the mixture.</td>
</tr>
<tr>
<td>D</td>
<td>Mass diffusivity m²/s</td>
</tr>
<tr>
<td>(e_{ss})</td>
<td>Coefficient of restitution for particle collisions</td>
</tr>
<tr>
<td>(\vec{F})</td>
<td>Body force (N)</td>
</tr>
<tr>
<td>(\vec{F}_D)</td>
<td>Drag force (N)</td>
</tr>
<tr>
<td>(\vec{F}_{Vm,q})</td>
<td>Virtual mass force (N)</td>
</tr>
<tr>
<td>(\vec{F}_q)</td>
<td>External body force (N)</td>
</tr>
<tr>
<td>(\vec{F}_{lift,q})</td>
<td>Lift force</td>
</tr>
<tr>
<td>G</td>
<td>Elasticity modulus</td>
</tr>
<tr>
<td>(G_k)</td>
<td>Generation of turbulent kinetic energy due to mean velocity gradient</td>
</tr>
<tr>
<td>(G_b)</td>
<td>Generation of turbulent kinetic energy due to buoyancy</td>
</tr>
<tr>
<td>g</td>
<td>Gravitational acceleration (m/s²)</td>
</tr>
<tr>
<td>(g_{ro})</td>
<td>Radial distribution function</td>
</tr>
<tr>
<td>(g_{\alpha,ss})</td>
<td>Radial distribution function</td>
</tr>
<tr>
<td>(h_q)</td>
<td>Specific enthalpy of phase q\textsuperscript{th}</td>
</tr>
<tr>
<td>(h_{qp})</td>
<td>Inter-phase enthalpy</td>
</tr>
</tbody>
</table>
\textbf{Nomenclature}

- \textit{I}_{2d}: Second invariant of the deviatory stress tensor
- \hat{J}_i: Diffusion flux of species i
- J: Diffusive mass transfer (kg/m\(^2\).s)
- k: Turbulent kinetic energy (m\(^2\)/s\(^2\))
- \textit{k}_{ls}: Momentum exchange coefficient between fluid and solid (kg/s-m\(^3\))
- L: Distance between particles
- \hat{m}: Mass flow rate (kg/s)
- \hat{m}_{pq}: Mass transfer from \(p^{th}\) to \(q^{th}\) phase (kg/s-m\(^3\))
- \hat{m}_{qp}: Mass transfer from phase \(q\) to phase \(p\) (kg/s-m\(^3\))
- \(M_{w,i}\): Molar mass of species \(i\)
- \(\dot{N}_A\): Volumetric production rate (kmol/m\(^3\) s)
- n: Number of phases, index for previous time step
- \(p_s\): Solid pressure (Pa)
- \(\dot{q}_q\): Heat flux
- Q_{pq}: Intensity of the heat exchange between \(p^{th}\) and \(q^{th}\) phases
- R: Heterogeneous reaction rate
- \(\hat{r}\): Constant rate of particle shrinking or swelling
- \(R_i\): Net rate of production of species \(i\) by chemical reaction
- \(R_{i^q}\): Net rate of production of homogeneous species \(i\) by chemical reaction for phase \(q\)
- \(\hat{R}_{ir}\): Arrhenius molar rate of Creation / destruction of species \(i\) in reaction \(r\)
- s: Distance between grains
- \(S_{t}\): Momentum sink, Rate of creation by addition from the dispersed phase plus any user-defined sources
$S_k$  Source term

$S_e$  Source term

$S_q$  Source term

$t$  Time (s)

$U_i$  Volume flux through the face

$V$  Volume of cell

$\vec{v}_m$  Mass-averaged velocity

$\vec{v}_{pq}$  Slip velocity (m/s)

$\vec{v}_q$  Velocity of phase q (m/s)

$\vec{v}_p$  Velocity of secondary phase (m/s)

$\vec{v}_r$  Radial velocity (m/s)

$\vec{v}_s$  Solid particle velocity (m/s)

$\vec{v}^T$  Transpose operation on velocity vector

$Y_M$  Contribution of the fluctuating dilatation incompressible turbulence to the overall dissipation rate

$\gamma_{pi}$  Mass fraction of species i in phase p

$\gamma$  Material density ratio

$\gamma_i$  Mass fraction of species i

$\alpha$  Packing limit

$\alpha_k$  Volume fraction of k

$\alpha_q$  Volume fraction of fluid q

$\alpha_s$  Volume fraction of solid phase

$p_m$  Mixture density (kg/m$^3$)

$p_q$  Density of fluid q (kg/m$^3$)
\( \bar{\tau}_s \) Solids stress strain tensor (Pa)

\( \bar{\tau}_q \) q\textsuperscript{th} phase stress-strain tensor (Pa)

\( \mu \) Viscosity (kg/m-s)

\( \mu_s \) Solid viscosity (kg/m-s)

\( \mu_{s,\text{col}} \) Collisional viscosity (kg/m-s)

\( \mu_{s,\text{kin}} \) Kinetic viscosity (kg/m-s)

\( \mu_{s,\text{fr}} \) Frictional viscosity (kg/m-s)

\( \mu_m \) Mixture viscosity

\( \lambda_s \) Solids bulk viscosity

\( \phi \) Angle of internal friction

\( \Phi_{fs} \) The energy exchange between the fluid or solid phase

\( \Theta_s \) Granular temperature (Kinetic energy of the fluctuating particle motion) (J/kg)

\( \alpha_k \) Volume fraction of phase k

\( \varepsilon \) Turbulent dissipation rate (m\(^2\)/s\(^3\))

**Abbreviations**

MCC: Modified Continuous Cooking  
C8: Circulation  
ITC: Isothermal Cooling

**Note:** In some cases non-SI units are commonly used in pulp and paper industry. To make the results understandable for mill staff I have kept their non-SI units for a number of flows, concentrations and similar but calculations are performed to convert them to SI units.
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Chapter 1: Introduction

1.1. Background
Dissolution of lignin from the wood chips in a digester results in pulp production. This is called the pulping process. The process is complex and the reactions are difficult to control. Defects in the process often occur and increase the costs considerably. The first step towards resolving the problem of defects is understanding and managing of the chemical reactions in the digester. At present the reactions can be partially directed. The process under consideration in this thesis is a continuous pulp process, which means that the chemical reactions are influenced by the flow regimes inside the digester. We have attempted to model the chemical reactions affected by the flow systems. This thesis describes the steps made in the attempt to overcome the complications of the flow influenced reactions.

1.2. Research task
This thesis addresses the spatial modelling of large reactors, specifically pulp digesters, in order to gain an understanding of the processes that occur inside them in spite of the practical impossibility of monitoring inside the reactor. The second task of this research is modelling of faults or undesirable phenomena.

By simulating different faults and monitoring the outcomes in simulations and in the output of the reactor, intelligent guesses can be made about the nature of the fault. Faults such as channelling and hang-ups in the digester are of particular interest. The intended outcome of this research is to make it possible to apply a simulation model, or a simplified version of one on-line, with input values from the process database, and to compare actual measurements from inside the reactor and at the outlet to the simulated values of the same variables. The on-line implementation lies outside of the scope of the thesis work. By fitting simulations of normal operations and those of different types of faults, the process performance can be evaluated. A good understanding of these phenomena may be achieved by considering different aspects such as fluid dynamics, mass transfer, chemical reactions, etc.

This thesis describes the development of the basis for a dynamic model, where both chemical reactions and fluid dynamics, including factors such as chip compression and mass transfer between the phases, are considered. This has not been done before, although other researchers have modelled individual areas. In addition, the model is tuned with real process data in order to verify the results.

The simultaneous modelling of hydraulics, including compression of wood chips due to dissolution of lignin and the impact of the weight of the chip pile, chemical transfer between liquid phase and solids phase, and the chemical reactions inside the wood chips, is new and has not previously been done at the level of detail described in this thesis. Modelling of channelling is also done at a greater level of detail than previously described. These high levels of detail are important for determining the impact of different types of fault in the digester, which is the motivation behind this thesis. This can be summarized by the following main research tasks:
**Question 1:** Is it possible to develop a new spatial model to increase understanding of the process, that unlike existing models pictures the pulping process and handles fluid dynamics and chemical reactions at every point inside the digester in 3D or 2D?

**Question 2:** Is it possible to model the failures in operation or undesirable phenomena (channelling) that take place in the digester in order to understand and control them?

**Question 3:** Can CFD models be used for future treatments and optimization of the process? Can the consequences of changing boundary conditions or chemical substances be observed in the established model?

**Question 4:** Can a numerical model provide a foundation for on-line applications?

### 1.3. Research method

A new solution technique (using differential analysis and FVM) is proposed for modelling the pulp production process, as opposed to the traditional methods (CSTR - Continuous Stirred Tank Reactors or PFR - Plug Flow Reactor). This method is expected to be more realistic and detailed at all points throughout the digester. In other words, this method is able to produce a spatial model.

The potential of the new approach to identify faults in the process is also investigated. This is novel in investigation of the pulping process.

My response to Question 1 about a 3D spatial model is affirmative. Such a model is possible but is dependent on the available resources, because 3D modelling of this type of digester requires a mesh of 1.8 billion cells. Assuming that computer can model one million cells, one thousand eight hundred computer units in a parallel network would be required to represent the digester in 3D. For this reason, a 2D model is established instead.

This thesis work is based on modelling and simulations which are conducted using the FVM and CFD code in FLUENT.

The work began with an investigation of research in this area over the last few decades. There have been studies of fluid dynamics, but these have seldom been done in much detail. Similarly, chemical reactions have also been studied, but seldom in any detail in combination with fluid dynamics. In this thesis, fluid dynamics and chemical reactions are combined to gather information about both properties simultaneously, in order to obtain information about faults such as hang-ups and channelling.

By using the different available functions I have tried to model the complexities of both chemical reactions and fluid dynamics in these huge vessels in a reasonably detailed way, to make it possible to observe the effects of different faults. The inputs and boundary conditions were obtained from operation conditions and physical properties of the Kraft pulping digesters at the Korsnäs and Vallvik plants. A number of theoretical calculations and studies were performed, including assignment of the reaction kinetics, physical and chemical assumptions to approximate wood chip dimensions and chemical formulae of the reactants in the pulping digester. During these studies I referred to handbooks and text books on the wood and pulping process, journal papers and scientific websites. I have also held discussions with the engineers and operators of the pulping digesters, observed the process directly, attended meetings at the Korsnäs and Vallvik plants, conducted laboratory studies at Kvaerner, and participated in several conferences.
The CFD model has been used to improve understanding of events inside the digester. These events cannot be measured directly, but it is possible to measure the results of the events. Simulations based on assumptions of the type of events that occur inside the digester, such as channelling and hang ups, should be able to predict the results at the blow line with respect to the Kappa number, and the free alkali and dissolved lignin concentrations in the extraction line.

In this thesis I present a detailed model that describes the normal operations of the digester and discuss different methods for the formulation of process problems such as channelling as well as numerical solution methods. The driving force behind this study is the prediction of the hydraulic behaviour and the chemical reactions within the digester.

### 1.3.1. CFD analysis method: Differential analysis, Discretization, Finite control volume

The contents of the pulping digester consist of two phases which make up the flow of solid and liquid material. These phases interact both hydraulically and chemically, but the exact nature of the interactions is unknown. Three analysis approaches are available to examine the pulping processes.

The first approach is the finite control volume formulas using the Reynolds transport theorem. This method is not able to analyze these interactions due to its restricted abilities in surface analysis.

The second approach is similitude or dimensional analysis, which is based on laboratory measurements. Empirical formulations can be developed from studies of these models. Due to the large scale of real digesters in the pulp production it is difficult to achieve any similarity between the small scale laboratory models and the real process. Moreover, the costs of establishing representative laboratory-scale processes are likely to be high.

The third approach is referred to as differential analysis and involves developing the conservation equations in an infinitesimal control volume. Detailed analysis such as differential analysis is needed to describe the flow behaviour and chemical processes in the digester, making use of our knowledge of the flow dynamics, the gradients of variables in the flow and the chemical reactions in the digester.

We can develop a differential analysis of a problem, but solution of the differential equations using analytical methods is not an easy task. CFD is therefore used as a tool to solve the differential equations.

In order to visualize the progress of the reactions and dynamic interactions of the phases in the digester we need to develop the conservation equations of mass, energy and momentum in an infinitesimal control volume within the flow field. The resulting governing equations are partial differential equations (PDE) that include unknown functions with several independent variables and their partial derivatives. Ordinary differential equations (ODE) contain functions with only one independent variable, and one or more of their derivatives with respect to that variable.

### 1.4. The research tasks in relation to state of the art in digester modelling

Several researchers, such as Christensen (1983), and others have modelled the fluid dynamics of digesters, concentrating more on the chemical reactions taking place non-spatially in the digester. Control of digesters has also been addressed where a statistical model was developed, such as by Funkqvist (1998) and Doyle (1996) who have been testing MPC (Model Predictive Control).
However, detailed descriptions of the fluid dynamics combined with chemical reactions, positions and with varying porosity in the digester have not been published, particularly with respect to problems such as channelling and hang-ups.

Research on digesters has focused mostly on chemical reactions or fluid dynamics. Researchers have had different goals when modelling digesters. Some have modelled for better design, others for better control, etc. None thus far has really focused on modelling to determine the effect of hang-ups, probably because of the difficulty in doing so. The problem is very complex. No single method can be used, and several approaches have to be combined. In the review below I describe the work of other researchers in this area.

A survey of the literature shows that modelling of the hydraulics and chemical reactions in the entire digester has not been widely performed using FLUENT or similar advanced CFD programs. Simpler models have been developed with other modelling tools. In the following sections, I discuss how other researchers have attempted to model the digester with other modelling tools.

Vroom (1957) modelled the H-factor and Smith (1974) approximated the digester as a series of continuous stirred-tank reactors (CSTRs) in which the solid phase consists of five species that react with the white liquor. Other researchers followed with improvements and modifications.

Johansson (1971) used a combination of the mass transfer and reaction kinetics in a wood chip to solve differential equations to describe the cooking process. He assumed that the diffusivity in wood was a function of temperature. However, Hartler (1962) showed that the diffusivity in wood was also dependent on the pH. Johansson used a single equation for three reaction stages.

A few researchers such as Gustafsson (1983) assumed that wood was composed of two main compounds. Gustafson improved Johansson’s model by using three kinetic equations for the chemical reactions. He expressed the diffusivity as a function of temperature, pH, and yield.

In the three stage models, the cooking process is divided into three phases: initial, bulk and residual. This means that three different kinetic reactions are defined for the dissolution of the lignin and carbohydrates.

Techniques used to measure cooking components include conductivity measurements, near infrared spectroscopy (NIR), Fourier transform infrared (FTIR) spectroscopy, gas-liquid chromatography, ion chromatography, refractive index measurement, UV-light absorption measurement, and titration.

These measurements only provide indirect information about the range of the cooking reactions of a digester.

The Anderson model is based on the three parallel kinetic equations for lignin. The first kinetic equation considers the initial reaction of the lignin, the second equation is adopted for the bulk reaction and the third kinetic equation attempts to satisfy the residual lignin reactions. The major difference between the Gustafson and Andersson models is that the Gustafson model is based on three cooking stages instead of three kinetic reactions for lignin, Rantanen (2006).

Christensen (1983) used the Purdue model as a base for modifications but also made a number of simplifications. He developed the kinetic model for several different samples of soft woods and hard woods. Plug flow was assumed for both wood chips and the liquor.

Harkonen (1987) also extended the earlier work and developed models for the Kamyr continuous digester. Harkonen derived a multiphase flow model that could describe the internal pressures, temperatures and velocities for phases using the mass, momentum, and energy differential equations. In his model he considered the use of the porous model to describe the solid phase.
Michelsen (1994) proceeded by combining the work of Harkonen and Christensen to make a more detailed digester model. He modelled the mass flow together with the reaction kinetics for a continuous steam-liquor digester. By solving for the compaction and the velocity of the chip plug, he attempted to provide a tool to control delignification. Further extensions of this work were also proposed by the authors such as consideration of the chip quality, varying the concentrations of the active ions, use of the energy balance to describe the temperature distribution in the digester, and tuning the model against the real plant in order to consider the effect of the solid reactor geometry such as conical side walls on the flow fields and reaction kinetics.

Michelsen (1996) attempted to create a model that could explain the complex behaviour of the digester in his later work, particularly the interaction between the reaction kinetics and the residence time.

The numerical solution of the model is based on a non-uniform discretization procedure for better handling of the geometry. Natercia (2000) ran a steady state operation of a continuous digester with ITC cooking and simulated two phases of a heterogeneous digester by means of a model that adopted 15 state variables at each axial position of the digester. This model was able to account for the solid content including both organic and inorganic materials. This model adopted an isothermal condition for the reaction.

Wisnewski (1997) also employed the CSTRs in his model, but with different equations and assumptions. Wisnewski’s work was an extension of the Purdue model in which the digester was approximated by a series of CSTRs, with each CSTR consisting of three phases. This model attempted to remove many of the previous assumptions by defining the solid concentrations on a mass per chip volume basis, by defining the compaction as the volume fraction of the CTSRs, and the porosity as volume fractions of the wood chips. Chip porosity and liquor density were also defined for this model.

Kayhan (1996) modelled a two-zone digester, i.e. impregnation as a mixing zone and a reaction zone. Partial differential equations were solved for each zone. They considered the solid and liquid phases to be in thermal equilibrium. The adopted kinetic model was the same as the Christensen model. Kayhan attempted to improve previous models by removing the limiting assumptions on the solid phase behaviour.

He defined the solid phase as a number of small distinct plug flows moving downward through the digester. For chip size distribution he considered different mass fractions for each plug flow. Three phases were defined in his model - solid, trapped liquor and free liquor. The reaction takes place between the solid and the trapped liquor. The solid compaction was computed dynamically for each plug flow depending on the chemical and hydrodynamic conditions of the plug.

Pougatch (2006) implemented a solid tangential stress sub-model which was developed for the digester. The advantage of this sub-model was that the solid phase behaviour reproduced the plug flow of the chips and eliminated the adopted non-physical assumptions of the Newtonian approach.

Pu (1991) continued the Gustafson project and proposed equations for the degradation of cellulose and hemicellulose.

Lee (2004) modelled a single phase liquor flow in a batch laboratory digester using CFD.

A number of researchers have attempted to simulate the movement of the fibres. Olson (2001) studied the movements of fibres in turbulent flows. He used a probability distribution function for fibre orientation and position throughout the suspending fluid.
Dong (2003) studied the fibre movement by solving the LES (Large Eddy Simulation) in turbulent flows. Stockie (2002) simulated the fibres in suspension using numerical simulation and the immersed boundary method.

In brief, three approaches to the delignification have been proposed. These are the Purdue model (in the 1970s), the Gustafson model (in the 1980s) and the Andersson model (developed in 2003). All three models base the kinetics of lignin and the other chemical species on the Arrhenius equation, with different activation energies defined for each species in the reaction.

In relation to my research questions, some researchers have covered fluid dynamics aspects and others have concentrated on chemical reactions, but nobody has covered the full spectrum by integrating these aspects, particularly for channelling, spatial treatment, axisymmetry, chemical reactions and where porosity is included.

1.4.1. CSTR and CFD approach from the flow patterns point of view

Assessment of the flow patterns which represent the motions of liquor and wood chips in the digester is crucial when designing the prediction of the hydraulic behaviour of the boiler. Different flow patterns have been adopted when modelling pulp digesters. The Purdue model is based on the CSTR whereas Gustafson assumed the plug flow pattern for the chip bed.

When small fluid bubbles, droplets or particles are dispersed in the reactor, the flow is dispersed, but when these small droplets combine together to make larger bullet –shaped bubbles the flow is called plug flow, Schmidt (1998 ).

In plug flow the velocity profile is uniform and the velocity of the fluid is assumed to be constant across any cross section. Another assumption in plug flow is that no boundary layer adjacent to the inner wall of the reactor is considered. The plugs travel axially through the digester. The fluid is mixed in the radial direction but no mixing occurs in the axial direction.

When using the CSTR model for the digesters, thorough mixing is assumed, i.e. the feed has a uniform composition throughout the reactor. The variables in CSTR are not a function of position, i.e. all the special derivatives go to zero. The exit stream has the same composition as the entire tank volume. The disadvantage of the CSTR in practice is low conversion per unit volume.

The Eulerian scheme of FVM considers the liquid and solid materials as continuous phases that are mixed together. The behaviour of the phases is largely dependent on the physical and chemical variables such as diffusivity, mass transfer rate, gravitational forces, and the size of the particles. The phases are characterized by definition of these variables in the CFD.

The advantage of the FVM is that it enables prediction of the gradients of the chemical and hydraulic variables of the pulping digester. Unlike in plug flow, the velocity profile is neither uniform nor constant at any direction. The chemical composition depends on the position at any point in the digester. This means that FVM represents the real process. In contrast to the CSTR model or the Plug flow model, FVM makes it possible to predict the channelling phenomenon where phases are not mixed together.

The simulations are performed in FLUENT code under the assumptions that the two phases mix at the interfaces and the reaction is affected by controlling factors such as specified mass diffusivity and mass transfer rate. The influence of the flow conditions on the reaction rate and Kappa number distribution are also considered in the simulations.
In the continuous stirred tank reactor (CSTR) of the Purdue model, mixing is complete and instantaneous. The plug flow reactor (PFR) considers a plug flow without back mixing.
Chapter 2: Overview of the work

2.1. Overview of the thesis

This section provides an overview of the thesis work. Chapter 3 introduces pulping processes for those who are not familiar with them. Chapter 4 includes definitions and important concepts for describing the pulping process. Chapter 5 summarizes structures of the basic chemical components and the important reactions of the pulping process. Chapter 6 describes applied schemes and the solution of the PDE (Partial Differential Equations) using FVM (Finite Volume Method) and Chapter 7 describes the governing equations. Chapter 8 describes the theoretical setup with chemical calculations and assumptions for Paper 5. Chapter 9 describes the modelling setup, boundary conditions and implementation for all five papers. Chapter 10 presents the results from the simulations in all five papers. Chapter 11 discusses the accuracy and reliability of the simulations. Chapter 12 discusses the results and Chapter 13 presents the conclusions of this work.

2.2. Overview of the papers

Paper 1 describes basic CFD modelling of solid-liquid multiphase flow, and tests a mathematical approach to modelling separation of the solid phase from the liquid phase at the screens in a continuous pulp digester. This paper forms the basis for the subsequent modelling work.

Paper 2 uses the mass transfer and species transport models to model the chemical reactions in the digester. This model includes consideration of diffusion of chemicals from the liquor (OH) into the liquid trapped inside the porous wood chips. The reaction rate is determined by the concentration of chemicals and the temperature of the liquid.

Paper 3 provides a study of channelling and models this phenomenon from a fluid dynamics perspective. This is achieved by varying the porosity in adjacent cells in the model. The flow resistance in cells that are identified as channels is reduced resulting in higher liquid flow through these cells.

Paper 4 considers channelling using a combination of fluid dynamics and kinetics of the chemical reactions, in order to identify the impact of the changed flow pattern on the concentrations of lignin and other chemicals in the liquid streams.

Paper 5 models the actual chemical reactions taking place in the digester based on a different approach to chemical modelling. The kinetics of the chemical reactions are computed based on operational data, yield and concentration of the reactants and products. The rate constants and pre-exponent factors of the Arrhenius equation are computed based on the reaction conditions in the pulping digester. The complete kinetic equation is then modelled numerically to investigate the distribution of the reactions within the digester environment using a porous media scheme. This approach complements the mass
transfer strategy presented in Paper 2. A more detailed illustration of applied equations, and modelling approaches for different purposes is given in chapters 7, 9, 10 and 12.

The following section summarizes the themes of the different papers and the applied governing equations.

Table 1: Papers and summary of applied governing equations

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Chapter 3: An introduction to pulping process digesters

3.1. General concepts of pulp and paper

Paper is a thin material, produced by dewatering of a suspension of fibres, (Biermann, 1993). The suspension of fibres is known as the grains and the fibres are generally designated as pulp or paper pulp.

Plant fibres containing cellulose may be treated chemically and/or mechanically. The fibres that remain after dewatering are linked by hydrogen bonds, which develop during pressing and drying, forming the paper, Kassberg (1998).

As well as cellulose, which is the main ingredient in paper, several other components are present in wood. The composition varies with the species of wood. For example, dry spruce contains 42% cellulose, 25% hemicellulose and 28% lignin. The remainder of the dry mass contains resins, proteins and minerals. The main metals in wood are calcium, magnesium and manganese.

Cellulose and most of the other substances in wood originate from photosynthesis, which occurs in leaves and needles. Chlorophyll absorbs solar energy and converts carbon dioxide and water to energy-rich substances such as glucose and free oxygen, Heathcock (1981).

\[6\text{CO}_2 + 6\text{H}_2\text{O} + \text{light energy} \rightarrow \text{C}_6\text{H}_{12}\text{O}_6 + 6\text{O}_2\]

Cellulose molecules are made up of glucose residues that are attached together to form long, linear chains. These straight molecular chains attach to each other to form fibres between 1 and 4 mm long with a diameter of 0.01 mm. Cellulose molecules bind to each other in the fibres through numerous hydrogen bonds. These hydrogen bonds give strength to the fibres.

Hemicellulose is related to cellulose, but also contains pentose residues. Hemicellulose lacks the strength of cellulose.

Lignin has a very important function in the wood, as it links the cellulose fibres and increases the strength of the overall fibre structure.

Lignin allows plants to form heavy and large organisms like trees. The aromatic component of lignin molecules gives them a bright yellow colour. In pulp production, the cellulose fibres must be as intact as possible, so that their strength is retained. The fibres must also be as clean as possible to maximize brightness.

Pulp is the raw material used in paper production. The predominant raw material for pulp manufacture is wood, but non-woody plants such as straw, flax and cotton can also be used. Synthetic fibres such as polyethylene and polypropylene can be used to confer specific properties to the paper.

There are several methods for manufacturing paper pulp. Recycled paper plays an increasing role as a raw material for papermaking, but there is a clear distinction between the processes for producing fresh and recycled pulp.
Fresh pulp is required for many paper products and is also necessary to supply the market with enough fibre for use in recycled fibre recovery.

For some specialized applications, such as notepaper and teabag paper, other plant materials such as cotton and linen fibres are used and the processes for handling these materials are very different from those used for normal wood pulp. Pulp is produced industrially on a large scale in the pulp and paper industry. Pulp composition depends on manufacturing method, but it always consists of separate fibres or fibre elements, which can form hydrogen bonds with each other to form paper.

3.1.1. Steps of the pulping production

Wood consists mostly of cellulose fibres held together by lignin. The length of the fibres affects the paper quality and differs between tree species. The length of softwood fibres is 3 to 5 mm, while leaf cellulose fibres are around half this length. In order to make paper from wood, fibres must be freed from each other so that they can then be arranged systematically in the network that forms the paper.

Wood from both softwood and hardwood is used in the manufacture of pulp, which is sometimes referred to as cellulose. The aim of the pulping process is to release the natural fibres found in wood. The first step in the manufacturing process is debarking, Matsson (2007). In this process, raw timber pieces are fed into large drums where they roll and rub against each other and against the drum walls, loosening the bark.

Bark falls through holes in the drum walls and is burned in the bark boiler, where it is converted to heat to help power the rest of the process.

The wood pieces come out of the debarking drum and are transported along a conveyor belt to the chip maker.

The chip maker consists of a large rotating metal disc fitted with a steel chopper. The disc cuts the pieces of wood into chips. The chips are then transported to the chip silos where they are stored before the next step in the process - boiling.

Here, the chips are cooked in cooking liquor in large digesters. The cooking liquor, which is called white liquor at this stage, consists mainly of a mixture of sodium hydroxide and sodium sulphide. The temperature in the middle of the digester is about 160 °C. This high temperature enables the cooking liquor to dissolve the lignin that holds the wood fibres together.

After boiling, the pulp is washed with water to remove residual chemicals. The washing water and the remaining cooking chemicals are collectively called black liquor.

The pulp is brown at this stage due to residual lignin. It can be used directly to manufacture unbleached paper or it can be bleached. Bleaching removes the residual lignin from the pulp to produce white or archival paper.

The pulp is bleached by treatment with various chemicals such as oxygen, hydrogen peroxide, chlorine dioxide or ozone.

Different fibre contents give the pulp different properties and are used to produce different end products. For example, conifer wood provides long fibre pulp, which is characterized by high strength and durability, and wood from deciduous trees provides short fibre pulp, which is used extensively for fine paper and high quality printing paper.
3.1.2. Chemical pulping methods

There is a clear distinction between mechanical pulp, semi-chemical pulp, and chemical pulp. Chemical pulp is produced through chemical processes where certain components of wood, particularly lignin, are broken down and dissolved out of the wood, and the fibres are released from each other with minimal mechanical input. This process dissolves the lignin that is bound to the cellulose fibres without breaking the fibres. The lignin and other dissolved wood components are separated from the pulp and sent to the chemical recovery system. The liquor with the dissolved wood components is called black liquor due to its dark colour.

A digester for chemical pulping is essentially a large vertical tank in which wood chips move downward. There are two main types of cooking process, batch cooking and continuous cooking. In batch cooking, the vessel is filled with wood chips and all other processes are performed by circulating different liquids through the pile of wood. The vessel is then emptied. In continuous cooking, wood chips and chemicals are fed continuously into the top of the digester and pulp is continuously removed from the bottom. The digester is divided into zones where the different stages of the cooking process occur. There is usually an initial impregnation step where the wood chips are impregnated with chemicals. This is followed by a cooking step where the chips are heated to 145-165 °C, depending on the type of wood. Finally, the fibres are washed with water to remove dissolved lignin and chemicals from the surface as far as possible. If a very clean surface is required, oxygen delignification and bleaching with different oxidizing chemicals may follow.

There are at least two different processes for the production of chemical pulp: the sulphite process and the sulphate processes. The sulphite process was the dominant method of pulp production from the late 1800s to the 1940s, whereas the sulphate process has dominated since the 1940s.

In the sulphite process, wood chips are boiled in solutions of sulphur dioxide (SO₂), (sulphur dioxide dissolved in alkali until the pH is 7 or lower). This process provides a relatively bright pulp, which is not as strong as pulp from the sulphate process.

The sulphate process has dominated since the 1940s and produces stronger paper than other methods. In the sulphate process, the wood chips are cooked in white liquor, a strongly alkaline solution of sodium sulphide and sodium hydroxide. Chemical pulp is stronger and cleaner than mechanical pulp, especially sulphate pulp which is used for fine papers and Kraft papers which are used to make paper bags.

The sulphide process is used mainly for production of daily newspapers, fine papers and tight papers such as butter and baking paper, but the process has been almost completely replaced by the sulphate process. Chemical pulp can also be mixed with mechanical pulp in different proportions, making it possible to produce paper with a range of properties.

Pulp can also be manufactured from recycled paper and paperboard, as well as from CTMP pulp or other types of mechanical pulp. Pulp that has a large proportion of recycled fibres is generally used for cartons, newspapers and sanitary paper. Recycled fibres can never fully replace fresh fibres from raw wood because the fibres get damaged and their quality deteriorates in each recovery cycle.

After dissolution of lignin, the pulp can be bleached to produce white paper. Chlorine was used for bleaching in the past, but more environmentally friendly alternatives such as oxygen, ozone, hydrogen peroxide and chlorine dioxide are more common nowadays.

After bleaching, the pulp can be pumped directly to a paper machine, which moulds and dries the pulp into different types of papers.
3.1.3. Mechanical pulping processes

Mechanical pulp manufacturing methods have been used since the 1840. The mechanical pulp produced by mechanical separation of the fibres with the help of refiners (and still to some extent by means of grinding stones) can be re-suspended in water.

Mechanical pulp obtained in this way is useful for paper products such as newspapers that do not require high strength.

There are several variations of mechanical pulp. In one process, water vapour, high temperature and pressure are used to produce thermo-mechanical pulp (TMP), while another process uses sodium sulphide in combination with heat, resulting in chemical-thermal-mechanical pulp (CTMP). The main product of mechanical pulp is TMP, which is used for newspaper production. Mechanical pulp contains in principle all the wood components (with minor chemical modifications). The yield of chemical manufacturing methods is between 45% and 55%. For mechanical methods the corresponding value is around 90%.

Papers made from mechanical pulp have a tendency to turn yellow over time because the lignin is not separated from the pulp, and is included as a binding material in the finished paper. In general, CTMP is stronger than TMP, which in turn is stronger than ordinary mechanical pulp. Chemical pre-treatment of wood may produce other desirable non-mechanical properties. Paper from pulp that has been treated in this way also comes under the CTMP category.

Part of the work described in this thesis may also be applicable to mechanical pulping, but these applications are only considered briefly.

3.2. The pulping Digester

Our typical digester is 60 m high and has a diameter of 6 m at the entrance at the top which increases stepwise to 7 m at the bottom. There are two pressure adjustment dischargers of 0.2 m diameter at the top end near the inlet. The diameter of the uppermost circulating pipe, which is called the transference pipe, is 0.35 m. Two other inlets at the bottom and near the bottom include a number of pipes that are not normally in service.

A large annular pipe hangs inside the digester. This pipe connects to the outlet pipes of the circulation loops, referred to as C8 (wash zone circulation) in the lower section, MCC (in the middle section) and ITC (isothermal cook circulation) in the upper section. The flows re-circulate into the digester separately at three different levels. The central pipe consists of three concentric pipes. The innermost pipe is the longest and flows from C8 into the digester. The diameters of the C8, ITC and MCC inlets are 0.21, 0.3 and 0.425 m respectively.

The MCC is connected to the middle pipe while the ITC is connected to the outermost pipe and drains the flow at the top section. The mixture passes through circular screens in the periphery of the digester before flowing into the collection pipes. The screens at the inlet to the pipes are 1 to 2 m high with 1 to 2 cm slots, and provide a large open area and thus a relatively small pressure drop compared to the pressure drop in the chip bed, as long as the surface remains unclogged. The flow is in a radial direction before it enters the outlet pipes.

The diameters of the C8, MCC and ITC outlet pipes are 0.15, 0.2 and 0.25 m respectively.

The digester is therefore designed in two dimensions, but the model in FLUENT accounts for the three dimensional volume of around 1800 m³.
As the chips are passed down through the digester and meet the circulating liquors, chemicals first impregnate the wood chips and then dissolve the lignin from the fibres. Subsequently, lignin is washed away from the fibres further down in the digester, before the fibres leave the digester at the bottom.

The inlet at the top, the wash liquor at the bottom and the extraction of black liquor in the middle of the digester are the main boundaries for the digester liquors. The liquors are extracted through screens into the extra circulation loops (C8, MCC and ITC). Wood chips are retained in the screens and are therefore prevented from entering the recirculation loops. The top and bottom of the digester define the boundaries for the wood chips.

Figure 1: A typical digester

Typical flows in the different loops are presented in paper 1, and paper 2 describes these flows in relation to flows and Kappa numbers. The controllable variable in the digester is the chemical addition of white liquor at the top. The temperature at the ITC loop is also controlled.

The Kappa number and the chemical reactions have been modelled in the FLUENT equation generator (the custom field function).
Chapter 4: Definitions and Concepts

4.1. Dry solids concentration and pulp consistency

The pulp consistency is the weight of the dried pulp divided by the weight of (pulp and liquid). The dry solids concentration is the percentage weight of dry solids in the liquid - the volume of the solids is ignored.

4.2. Chemical and technical concept of Kappa number

It is necessary to quantify the undissolved lignin that remains after pulp production in order to determine the final colour of the pulp. Determination of lignin content is complex and takes a long time. The amount of residual lignin between the fibres is calculated and formulated as the Kappa number.

The standard method for determination of Kappa number is titration. The Kappa number is determined in the laboratory as the volume in ml of 0.02 M potassium permanganate consumed by 1 g of pulp over a certain time and temperature. The Kappa number represents the degree of cooking and is often measured on-line with indirect methods that determine the absorption of UV light at the surface of the fibres. Kappa number actually measures all oxidizable components, and makes no distinction between lignin, hemicelluloses or even cellulose. From this perspective the Kappa number measured by the optical methods may even be better than the standard method. This poses a problem because commercially the true Kappa number is regarded as that determined by chemical oxidation in the laboratory. Considerable effort is expended toward predicting and managing the chemical reactions of the digester in order to minimize the Kappa number while maintaining the mechanical properties of the pulp. As the pulp quality depends on the lignin content, then from a technical point of view the Kappa number is a dimensionless quantity that is a measure of the pulp quality. When the mass fraction of the lignin is available then Kappa number is equal to the mass fraction of the lignin in the pulp multiplied by 100 and divided by 0.15. Kappa number is predicted in Papers 2 and 4.

4.3. Extractives

Extractives of cellulose pulp are the compounds that are soluble in petroleum ether, diethyl ether, dichloromethane, acetone, ethanol and water. Extractives are a heterogeneous group that includes lipids, terpenoids, phenolic components, glycosides, small carbohydrates, pectin, starch and protein
4.4. Lignin

Lignin is present mostly in the lamellae between the fibres and is also present to a lesser degree inside the cells. Pulp production involves separating the fibres from each other by dissolving the lignin from between the lamellae in the cooking solution. However residual lignin remains on the fibre surface.

4.5. Cooking

The purpose of cooking in the manufacture of chemical pulp is to remove the lignin that holds the cells together using heat and chemicals, so that the chips are easily defibrated. It is desirable to preserve the length and strength of cellulose fibres as much as possible. Cooking also removes extractives in the wood, as they can cause foaming and deposition later in the process. Sulphate cooking is currently the most common pulp production method. The cooking temperature in sulphate cooking is generally between 145 and 170 °C.

Sulphate cooking uses a mixture of sodium hydroxide (NaOH) and sodium sulphide (Na₂S) called white liquor. Sodium sulphide promotes the cooking reaction. Sulphides also reduce the dissolution of cellulose by sodium hydroxide. For bleached pulp, a typical Kappa number is 14 to 20 for hardwood pulp, and 20 to 30 for softwood pulp. If the pulp is not bleached then the Kappa number after cooking can be much higher, between 40 and 100. Paper 5 considers the chemical reactions in more detail and models the consumption of OH, but not the sulphide reaction, as it was considered too complex."

4.6. H-Factor

The H-factor indicates the relative rate at which lignin is dissolved. The rate depends on the cooking time and temperature. Lignin solubility is highly temperature dependent, and a temperature difference of a few degrees can cause major quality differences in the pulp. Temperature control is therefore of vital importance. The H-factor is defined so that its value is 1 with 1 hour of cooking at 100 °C.

4.7. Hardwood □ Softwood

Woods are classified into two main classes - hardwoods and softwoods, Dietenberger (1999). Hardwood trees generally have broad leaves, are deciduous and porous (i.e. they contain vessel elements) and grow in temperate regions. The vessels form an efficient system for transporting water and dissolved minerals from the roots to the leaves and other parts of the plant.

Softwood trees - with a few exceptions - are evergreens and are nonporous, i.e. they do not contain any vessels. The terms hardwood and softwood do not bear any relation to the hardness or softness of the wood.

The chemical composition of wood varies with the wood type, and may also vary within a particular wood type. In general the wood species cannot be determined by chemical analysis because the composition varies with geographical location, soil and weather conditions, and with the location of the analyzed piece of wood within the tree.
Chapter 5: Chemical elements of the pulping reaction

5.1. Mass percentage of components of the woods
On average, wood is made up of cellulose (40% to 50%), hemicellulose (20% to 30%), lignin (20% to 30%) and other compounds (10%). The other compounds are organic substances such as pinosylvin, fat, resin, starch, and protein. Table 2 shows percentages by mass of the constituents of three types of woods.

Table 2: Constituents of three common woods, Kassberg (1997)

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Spruce</th>
<th>Pine</th>
<th>Birch</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cellulose</td>
<td>42%</td>
<td>41%</td>
<td>41%</td>
</tr>
<tr>
<td>Hemicellulose</td>
<td>28%</td>
<td>28%</td>
<td>34%</td>
</tr>
<tr>
<td>Lignin</td>
<td>27%</td>
<td>27%</td>
<td>21%</td>
</tr>
<tr>
<td>Extractives</td>
<td>3%</td>
<td>4%</td>
<td>4%</td>
</tr>
</tbody>
</table>

In the pulping process, the wood chips are cooked at around 160 °C in order to dissolve the lignin that binds the cellulose and hemicellulose together, and release the fibres for use in downstream applications. Overcooking the chips until all the lignin has dissolved can reduce both the yield and the strength of pulp. Therefore, in practice, cooking does not proceed to complete lignin removal, Kassberg (1997). The solution is heated by screens and heat exchangers in one or more of the circulation stages.

The dominant chemical pulping process at the Korsnäs plant is the sulphate or Kraft process and the cooking liquor is alkaline with a pH of around 14. The solution is made up of sodium hydroxide (NaOH), sodium sulphide (Na₂S), sodium carbonate (Na₂CO₃), and sodium sulphate (Na₂SO₄). The composition of the solution may vary depending on the operation conditions or the properties of the wood chips.

Wood is a porous material, meaning that between 60% and 70% of its volume is occupied by air which explains its low density. The permeability of wood is variable and is defined as the flow of liquids under pressure into its pores. According to the Wood Handbook of the Forest Products Laboratory and the literature, Durbak (1998), this is due to the highly anisotropic shape and arrangement of the component cells and the variable condition of the microscopic channels between cells.

In the longitudinal direction, the permeability is 50 to 100 times greater than in the transverse direction. It is difficult to determine how the wood chips are arranged in the reactor and whether individual wood chips move down the reactor in the longitudinal or transverse orientation.
5.2. Monomers of lignin

Lignin is an amorphous, insoluble organic polymer and is very difficult if not impossible to isolate in a natural state. The molar mass of isolated lignin ranges from the low thousands to up to 50,000. Lignin is the natural glue that holds the fibres of wood together and is therefore a major component of all types of wood.

Lignin polymers are not composed of a single monomer but contain a number of different monomers with different molar mass. Figure 2 shows the lignin monomers and their molecular structure. Several lignin monomers are listed in Table 3.

Figure 2: A lignin molecule showing the molecular structure of the monomers. Adler (1966)

From the molecular structure of lignin monomers we can see that a lignin polymer is made up of the molecules listed in Table 3.
5.2. Monomers of lignin

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Figure 2: A lignin molecule showing the molecular structure of the monomers. Adler (1966)

![Lignin molecule](image)

<table>
<thead>
<tr>
<th>Lignin</th>
<th>Molecular formula</th>
<th>Molar mass (g/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>C_{11}O_{4}H_{12}</td>
<td>208</td>
</tr>
<tr>
<td>2</td>
<td>C_{9}O_{3}H_{10}</td>
<td>166</td>
</tr>
<tr>
<td>3</td>
<td>C_{10}O_{3}H_{10}</td>
<td>178</td>
</tr>
<tr>
<td>4</td>
<td>C_{10}O_{2}H_{11}</td>
<td>179</td>
</tr>
<tr>
<td>5</td>
<td>C_{10}O_{4}H_{12}</td>
<td>196</td>
</tr>
<tr>
<td>6</td>
<td>C_{11}O_{2}H_{10}</td>
<td>222</td>
</tr>
<tr>
<td>7</td>
<td>C_{10}O_{4}H_{12}</td>
<td>196</td>
</tr>
<tr>
<td>8</td>
<td>C_{10}O_{4}H_{11}</td>
<td>195</td>
</tr>
<tr>
<td>9</td>
<td>C_{10}O_{2}H_{10}</td>
<td>194</td>
</tr>
<tr>
<td>10</td>
<td>C_{10}O_{2}H_{10}</td>
<td>194</td>
</tr>
<tr>
<td>11</td>
<td>C_{10}H_{2}O_{11}</td>
<td>211</td>
</tr>
<tr>
<td>12</td>
<td>C_{11}O_{2}H_{14}</td>
<td>226</td>
</tr>
<tr>
<td>13</td>
<td>C_{10}O_{4}H_{12}</td>
<td>196</td>
</tr>
<tr>
<td>14</td>
<td>C_{10}O_{4}H_{11}</td>
<td>195</td>
</tr>
<tr>
<td>15</td>
<td>C_{7}O_{2}H_{7}</td>
<td>123</td>
</tr>
</tbody>
</table>

5.3. Cellulose

Cellulose is the main component of the wood cell wall, and typically makes up 40% to 50% of dry wood by weight. Pure cellulose is a polymer of glucose residues joined by 1, 4-β-glucosidic bonds. The degree of polymerization (DP) is variable and may range from 700 to 10,000 or more.

Figure 3: Molecular structure of cellulose
5.4. Monomers of hemicelluloses

Hemicellulose is a mixture of amorphous branched-chain polysaccharides consisting of a few hundred sugar residues. Hemicelluloses contain many different sugar monomers, including xylose, mannose, galactose, rhamnose, and arabinose. Hemicelluloses contain mostly D-pentose sugars, and occasionally small amounts of L-sugars.

Table 4: Monomers of hemicellulose, their molecular formulae and molar mass, Howard (1996)

<table>
<thead>
<tr>
<th>Hemi cellulose</th>
<th>Constituent</th>
<th>Molecular formula</th>
<th>Molar mass (g/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glucose</td>
<td>C₆H₁₂O₆</td>
<td></td>
<td>180</td>
</tr>
<tr>
<td>Galactose</td>
<td>C₆H₁₂O₆</td>
<td></td>
<td>180</td>
</tr>
<tr>
<td>Mannose</td>
<td>C₆H₁₂O₆</td>
<td></td>
<td>180</td>
</tr>
<tr>
<td>Xylose</td>
<td>C₅O₅H₁₀</td>
<td></td>
<td>150</td>
</tr>
<tr>
<td>Arabinose</td>
<td>C₅O₅H₁₀</td>
<td></td>
<td>150</td>
</tr>
<tr>
<td>Glucuronic acid</td>
<td>C₆O₇H₁₀</td>
<td></td>
<td>194</td>
</tr>
</tbody>
</table>

5.5. Molecular structure of Extractives and Ash

The amount of extractives in wood varies from 5% to 20% by weight and includes a wide variety of organic chemicals, Rowe (1989).

The ash content is between 0.2% and 0.5% by weight for temperate woods and 0.5% to 2.0% by weight for tropical woods.

Table 5: Extractive materials content in wood, Rowell (2005)

<table>
<thead>
<tr>
<th>Extractives</th>
<th>Constituent</th>
<th>Most occurrence</th>
<th>Molecular formula</th>
<th>Molar mass (g/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Starch</td>
<td>(C₆H₁₀O₅)n</td>
<td></td>
<td></td>
<td>162 (Monomer)</td>
</tr>
<tr>
<td>Fat</td>
<td>Glycerol</td>
<td>C₃H₅O₃</td>
<td></td>
<td>92</td>
</tr>
<tr>
<td></td>
<td>Plant oil</td>
<td>C₅₇O₆H₁₀₄</td>
<td></td>
<td>884</td>
</tr>
<tr>
<td>Rest</td>
<td>Pinosylvlin</td>
<td>C₁₄O₂H₁₂</td>
<td></td>
<td>212</td>
</tr>
</tbody>
</table>

In summary, wood consists of cellulose, hemicelluloses, lignin, and other materials. The objective of the pulping chemical reaction is to reduce the amount of lignin in the wood. A large Kappa number indicates high lignin content. Considerable effort is expended to predict and manage the chemical reactions of the digester in order to reduce the Kappa number.
Chapter 6: Applied schemes and solution of the PDE using FVM

6.1. Multiphase schemes

The main ingredients of the pulping digester from a physical point of view are the solid and liquid phases, irrespective of the wood species and constituents of the phases. The liquid flow participates in the circulations and discharges while the solid phase flows downward through the digester. Screens are mounted at the entrance of the circulation pipes to prevent wood chips from entering them.

Assigning a suitable multiphase mode in order to satisfy the modelling is a crucial issue. The material density ratio, Stokes number, volume fraction and particulate loading are all considered in the selection of a multiphase method.

As material density ratio approaching 1.0 indicates a liquid-solid flow. In our case the density of the fluid is about 1000 kg/m³ and the density of the solid varies from 1000 kg/m³ (moist chips) to 1200 kg/m³ (individual wood chips). Therefore, γ has a value of around 1.

The next convention in the description of a multiphase scenario is evaluation of the volume fractions of the phases. When the volume fraction of the dispersed phase is larger than 10% Mixture and Eulerian models are applicable. The Stokes number has a value of around 1, which specifies the different multiphase procedures to be used i.e. Mixture, Eulerian and Dispersed.

If the Stokes number is greater than 1 then the Eulerian model is the appropriate approach. As the particles have non-uniform shapes, estimating the distance between them is complex.

The particulate loading number β may be determined by estimating the void space between the chips. A rough estimate of β in the digester shows that it has an intermediate value which implies that there is mutual interaction between the liquid and solid flows. This means that the wood chips can decrease the turbulence and mean momentum of the liquid stream, while the liquid is able to stimulate the solid flow via turbulence and drag.

The performance of multiphase models in FLUENT has been studied and a primary comparison indicates that the most appropriate models for the dynamic behaviour of the digester are the Mixture and Eulerian models. It is essential to analyze the performance of the multiphase methods of FLUENT before using them in an application. The VOF (volume of fluid) multiphase method is excluded because it is primarily suited to stratified flows and immiscible fluids and when the position of the interface between the fluids is of interest.

The DPM (Discrete Phase Model) may be applicable if the volume fraction of the wood chips is below 10%.

As well as properly modelling the phases, an appropriate multiphase model should also be able to numerically simulate the separation of the phases at the inlets of the circulation pipes by the screens.
6.2. Porous media approach
This strategy can provide a clear view of the movement of the fluid phase through the solid bed when the chip bed is compressible.

The solid chip phase with a variable compressibility can be characterized using the Packing limit, which represents the resistance of the solid phase to expansion and compression.

The compressibility of the chip bed can be modelled with a variable porous media. Modelling these properties using other CFD strategies may be at the expense of increased computational cost.

As lignin dissolves, the wood chips soften and are compressed by the chip pile. This compression increases with depth within the digester. This is modelled by varying the porosity in the cells so that the porosity is highest at the top of the digester and diminishes as a function of distance from the top.

![Figure 4: The chip bed](image)

6.3. Physical modelling of the digester and chips — non porous-Granular

The digester is a continuous solid-liquid reactor and the flow inside it is therefore considered as a multiphase flow. The solid phase is made up of the wood chips and the liquid phase is white liquor. The flow regime inside the reactor is assumed to be turbulent when modelling the hydraulic behaviour of the digester due to the presence of the counter-current flow at the bottom of the digester. The wood particles that are fed into the digester are heterogeneous in shape and size. Modelling of billions of particles each with unique dimensions in Gambit would be very difficult. The solid phase is therefore modelled as a granular phase of constant diameter.

In order to simplify the dimensions of the chips, they are converted to spherical coordinates.

In order to select appropriate dimensions a number of randomly selected chips were measured. The average chip size was 2 cm × 2 cm × 0.5 cm. The smallest dimension of the chip is its thickness.
The granular multiphase model is limited to considering spherical solid particles. However it is possible to apply a user defined distribution of diameters. From the aspect ratio of a randomly selected chip among the solid feed we computed the ratio of the total surface area to volume of the chip. The computed value is applied to the surface area-volume ratio when using the spherical solid particles in FLUENT. The spherical chip with the computed diameter has approximately the same surface to volume ratio as the selected non-uniform chip.

The majority of chips in the real feed were found to have similar geometric parameters.

### 6.4. Solution strategy of FVM

As previously mentioned, the finite control volume using the Reynolds transport theorem (Equations 1 and 2) is not an appropriate method for analyzing the dynamic and chemical interactions inside the digester.

\[
\frac{dB_{sys}}{dt} = \frac{d(f_{sys}\rho bdv)}{dt} \quad \text{where } B \text{ is an extensive property} \tag{1}
\]

\[
\frac{dB_{sys}}{dt} = \frac{\partial}{\partial t} \int_{cv} \rho B d\mathbf{A} + \int_{cs} \rho B \mathbf{v} \mathbf{d}A \tag{2}
\]

The infinitesimal control volume method using PDE can be used to help analyze the chemical and dynamic interactions inside the digester. This section describes how the PDE are solved by CFD and other methods.

The linear second order PDE is of the following form: Polyanin (2003)

\[
A \frac{\partial^2 \phi}{\partial x^2} + B \frac{\partial^2 \phi}{\partial x \partial y} + C \frac{\partial^2 \phi}{\partial y^2} + D \frac{\partial \phi}{\partial x} + E \frac{\partial \phi}{\partial y} + F(\phi) + G(x, y) = 0 \tag{3}
\]

There are three different approaches to solving the PDE. The first approach and the one that results in an exact solution is the analytical approach. Analytical solution of the ODE is often much easier than solution of the PDE. Solution of the PDE is seldom possible, Arfken (1985).

\[
B^2 - 4AC < 0 \quad \text{Hyperbolic (wave equation)}
\]

\[
B^2 - 4AC = 0 \quad \text{Parabolic (heat conduction equation and diffusion equations)}
\]

\[
B^2 - 4AC > 0 \quad \text{Elliptic (Laplace equations, Poisson equations)}
\]

The graphical method is the second approach to solving the PDE. This approach gives an approximate solution.

The third approach is numerical solution using FVM (finite volume method), FDM (finite difference method), and FEM (finite element method). GFEM (generalized finite element method), SFEM (smoothed finite element method) and XFEM (extended finite element method) are methods related to FEM, Courant (1962).

Finite volume methods (FVM) are commonly used for numerical solution of conservation laws. A conservation law for a conserved quantity \( \Phi \) can be simply stated as:

Rate of change of \( \Phi \) in some region \( R = - (\text{Net flux of } \Phi \text{ across the boundary of } R) \)
Unlike the analytical solution, which solves the equations for all points in the domain, the numerical methods support only discrete points, and values are calculated at discrete locations on a meshed geometry.

These points are called nodes or nodal points. The collection of the nodes is termed the grid or mesh. This is known as grid generation. Each node represents a certain region and the value of a physical property at the node is the average of the same property in the region that it represents. The objects are subdivided into smaller regions by numerical methods and approximate results are obtained for discrete points.

In the finite volume approach the computational domain is divided into non-overlapping cells or small volumes and the partial differential equations apply to these volumes. Finite volume refers to the small volume surrounding each node point on a mesh.

These cells are usually polygonal (triangular or quadrilateral) in 2-D domains and polyhedral (tetrahedral, hexahedral, prism, etc.) in 3-D domains.

The FDM uses the differential form of the governing equations and applies the local Taylor series expansion to approximate the differential equations but the FVM and FEM use the integral form of governing equations, Peiro (2005). The main advantage of FVM over FDM is that the FVM does not require the use of structured mesh. In the FVM approach variables are placed at the cell centres rather than at nodal points. The values of field variables at vertices are obtained using interpolation.

Two approaches are used to discretize the PDEs. These are:

1- Taylor series discretization in FDM

2- Control volume discretization in FVM and FEM

The finite difference form of a function may be expressed by defining the derivative of the function:

$$\frac{\partial F}{\partial x} = \lim_{\Delta x \rightarrow 0} \frac{F(x_0, y_0) - F(x_0 + \Delta x, y_0)}{\Delta x}$$

Taylor series expansion is used to develop the finite difference form of the derivative to obtain an algebraic equation of the function.

Scalar quantity at any node is calculated based on FDM as follows, Incropera (2007).

If m is a node point between the nodes m+1 and m-1 then using the finite difference method:

$$\frac{\partial \psi}{\partial x} \bigg|_{m+\frac{1}{2}n} \approx \frac{\psi_{m+1,n} - \psi_{m,n}}{\Delta x}$$

$$\frac{\partial \psi}{\partial x} \bigg|_{m-\frac{1}{2}n} \approx \frac{\psi_{m,n} - \psi_{m-1,n}}{\Delta x}$$

$$\frac{\partial^2 \psi}{\partial x^2} \bigg|_{m,n} \approx \frac{\psi_{m+1,n} - 2\psi_{m,n} + \psi_{m-1,n}}{\Delta x^2}$$

The x and y locations in the nodal network are designated by the m and n indices, respectively. \(\psi_{m+1,n}\) is the value of \(\psi\) at the (m+1, n)th node. For example we can use the heat diffusion equation under the transient condition and constant thermal conductivity with no generation in Cartesian coordinates for a finite number of nodes as follows:

$$\frac{1}{\alpha} \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}$$

This partial differential equation reduces to a linear algebraic equation (in the transient condition).
Unlike the analytical solution, which solves the equations for all points in the domain, the numerical methods support only discrete points, and values are calculated at discrete locations on a meshed geometry. These points are called nodes or nodal points. The collection of the nodes is termed the grid or mesh. This is known as grid generation. Each node represents a certain region and the value of a physical property at the node is the average of the same property in the region that it represents. The objects are subdivided into smaller regions by numerical methods and approximate results are obtained for discrete points.

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Two approaches are used to discretize the PDEs. These are:
1- Taylor series discretization in FDM
2- Control volume discretization in FVM and FEM

The finite difference form of a function may be expressed by defining the derivative of the function:

\[
\frac{1}{\alpha} \frac{\partial P_{p+1,n}}{\partial t} = \frac{P_{p+1,n} + P_{p-1,n} - 2P_{p,n}}{(2\Delta x)^2} + \frac{P_{p+1,m} + P_{p-1,m} - 2P_{p,m}}{(2\Delta y)^2}
\]  

(9)

A system of algebraic equations will be provided through the solution of these equations at nodes of the grid.

\[ A_{11}T_1 + A_{12}T_2 + \ldots = C_1 \]

\[ A_{21}T_1 + A_{22}T_2 + \ldots = C_2 \]

\[ A_{m,n}T_1 + A_{m+1,n+1}T_2 + \ldots = C_n \]

The equations will be rearranged in the form of the matrices as follows:

\[ [A][T] = [C] \]  

(10)

Two approaches are available to solve these matrices: the direct approach, using the matrix inversion method

\[ [T] = [A]^{-1} [C] \]  

(11)

or the iteration technique using the Gauss-Seidel approach under the steady condition

\[ T_i^k = \frac{C_{ii}}{a_{ii}} - \sum_{j=1}^{i-1} \frac{a_{ij}}{a_{ii}} T_j^k - \sum_{j=i+1}^{N} \frac{a_{ij}}{a_{ii}} T_j^{(k-1)} \]  

(12)

Where \( k \) is the level of the iteration and \( a_{ii} \) and \( C_i \) are the members of matrices \( A \) and \( C \). The matrix inversion solution is recommended when the number of equations is small otherwise the Gauss Seidel iteration is applied. The iteration is terminated when the prescribed convergence criterion is satisfied.

\[ |T_i^k - T_i^{(k-1)}| \leq \varepsilon \]  

(13)

\( \varepsilon \) is the error in any approximated physical quantity.

The conservation form of the fluid flow equation for small control volumes (FVM) can be expressed as: Versteeg (2007)

\[ \frac{\partial (\rho \phi)}{\partial t} + \text{div}(\rho \phi u) = \text{div} (\Gamma \text{grad} \phi) + S_\phi \]  

(14)

The first term on the left-hand side of the conservation form of the fluid flow equation represents the rate of increase of \( \phi \) of the fluid element. The second term on the left-hand side accounts for the net rate of flow of \( \phi \) out of the fluid element. The first term on the right-hand side is the rate of increase of \( \phi \) due to diffusion. The last term on the right-hand side accounts for the rate of increase of \( \phi \) due to any source.

The conservation law is applied to each finite volume. This requires the computation of the flux across the boundary of each finite volume. Four algorithms are introduced to solve each of these terms by the FVM. Volume integrals of partial differential equations are converted to surface integrals, using the divergence theorem. The next step is to integrate the differential form of the governing equations over each control volume. Conservation equations for each volume may be solved simultaneously.

\[ \int_V \text{div}(F) \, dV = \int_S F \cdot n \, dS \quad \text{(Divergence theorem)} \]  

(15)

\[ \int_V \text{div}(\Gamma \text{grad}(\phi)) \, dV = \int_S \Gamma \text{grad}(\phi) \cdot n \, dS \quad \text{(Divergence theorem-Diffusion term)} \]  

(16)
\[ \oint_V \text{div}(\rho u \phi) \, dV = \int_S \rho (u \cdot n) \phi \, dS \]  
(Divergence theorem-convection term) \hspace{1cm} (17)

Any flux that enters a volume is equal to the exiting flux from the adjacent volume. This therefore describes a conservation of flux.

The integrals are transformed to the algebraic equations using the mean value theorem. If \( A \) is an element, \( P \) is the adjacent element to \( A \), and \( f \) is the any face of elements \( A \) and \( P \), then

\[ \sum_f \int_{\Gamma_\phi} \frac{\partial \phi}{\partial n} \, dS \] \hspace{1cm} (18)

The surface of any polyhedral control volume consists of a set of faces and therefore the sum of surface integrals over each face is used.

\[ \frac{\partial \phi}{\partial n} \approx \frac{\phi_A - \phi_P}{d_{AP}} \] \hspace{1cm} (Mean value theorem) \hspace{1cm} (19)

\[ \sum_f (\Gamma_\phi)_f A_f \left( \frac{\phi_A - \phi_P}{d_{AP}} \right) \] Diffusion term \hspace{1cm} (20)

\[ \sum_f \rho_f (u \cdot n)_f A_f \phi_f \] Convection term \hspace{1cm} (21)

\( A_f \) is the area of face \( f \). Typical implicit and explicit schemes for volume fraction in the VOF model:

Implicit:

\[ \frac{a^{n+1} + a^n q^n}{\Delta t} V + \sum_f (p^{n+1} u^{n+1} a^{n+1}_q) = \left[ S_{a_q} + \sum_{p=1}^{n} (\hat{m}_{pq} - \hat{m}_{qp}) \right] V \] \hspace{1cm} (22)

Explicit:

\[ \frac{a^{n+1} + a^n q^n}{\Delta t} V + \sum_f (p^n u^n a^n_q) = \left[ S_{a_q} + \sum_{p=1}^{n} (\hat{m}_{pq} - \hat{m}_{qp}) \right] V \] \hspace{1cm} (23)

These algebraic equations can be transformed into matrices, which can then be solved by iterative methods.

However, the accuracy of the solution must be examined, and depends on the type of applied discretization schemes. Round-off and truncation errors are the two main error types encountered when using FVM.

Truncation errors increase when \( \Delta x \) increases, and also increase the difference between the exact and approximate solution. This can affect the consistency of the solution. Cumulative error at every stage of the solution results in divergence and reduced stability in the solution process.
Chapter 7: Governing equations

The equations used in this thesis work are derived from the basic continuity equations, Navier-Stokes equations, the energy equations and the original equations provided in the FLUENT user guide. Some of the equations that are used in the different papers are reproduced in this chapter and are included in the heading of each subchapter. The FLUENT user guide is available at the FLUENT website: www.fluent.se, FLUENT (2009). The fluid motion and reactions are governed by the following equations:

7.1. Reduced form of incompressible/compressible Navier-Stokes equations: Continuity equation (steady state-Mixture model) (Paper 1)

The mixture model works in concert with the granular method and takes into account and computes the granular properties and variables. It is applicable for solid-liquid multiphase flows. The unsteady term from the original continuity equation is left out of equation because the simulations were run at steady state conditions. No mass transfer modelling is performed in this paper.

\[ \nabla \cdot (\rho_m \vec{v}_m) = 0 \]  
\[ \vec{v}_m \] : Mass-averaged velocity  
\[ \rho_m \] : Mixture density

This is the continuity equation for the mixture, but for any individual phase the \( \alpha_p, \vec{v}_p \) and \( \rho_p \) (\( p \) is the number of any phase and \( \alpha \) is the mass fraction of that phase) contribute to the Eulerian equations. The simulations were also run at constant density for any individual component but \( \rho_m \) is the mixture density. The effects of fluctuations are not considered in this equation. Mass average velocity is calculated by the following expression.

\[ \vec{v}_m = \frac{\sum_{k=1}^{n} \alpha_k \rho_k \vec{v}_k}{\rho_m} \]  
\[ \vec{v}_m \] : Mass-averaged velocity  
\[ \rho_m \] : Mixture density

For 2D axisymmetric geometries the reduced form of the continuity equation for a mixture at steady state conditions is given by

\[ \frac{\partial}{\partial x} (\rho_m \vec{v}_m) + \frac{\partial}{\partial r} (\rho_m \vec{v}_m) + \frac{\rho_m \vec{v}_m}{r} = 0 \]  
\[ \vec{v}_m \] : Mass-averaged velocity  
\[ \rho_m \] : Mixture density

Where, \( r \) is the radial coordinate and \( x \) is the axial coordinate, \( \vec{v}_m \) and \( \vec{v}_m \) are mass average velocities in \( x \) and \( r \) directions.
7.2. Reduced form of volume fraction (Mixture model- Paper 1)

The volume fraction of the secondary phase in a multiphase flow of the Mixture model in the Cartesian system is determined from the continuity equation. The volume fraction is the space occupied by each phase in the cell.

\[ \nabla \cdot (\alpha_p \rho_p \vec{v}_m) = -\nabla \cdot (\alpha_p \rho_p \vec{v}_{dr,p}) + \sum_{q=1}^{n} \dot{m}_{qp} - \dot{m}_{pq} \]  \hspace{1cm} (27)

Volume of phase p is defined by

\[ V_q = \int_{V} \alpha_p dV \]  \hspace{1cm} (28)

Where

\[ \sum_{p=1}^{n} \alpha_p = 1 \]  \hspace{1cm} (29)

\( \dot{m}_{qp} \) is the mass transfer from phase p to q. The mechanism of mass transfer in multiphase flows is different. In the mixture model simulation no mass transfer takes place between the phases and therefore the second term on the right hand side drops out of the equation. Therefore, the volume fraction equation was used in the following form:

\[ \nabla \cdot (\alpha_p \rho_p \vec{v}_m) = -\nabla \cdot (\alpha_p \rho_p \vec{v}_{dr,p}) \]  \hspace{1cm} (30)

7.3. The reduced form of conservation of momentum for a fluid phase q (Papers 2, 4)

The multiphase scheme was run in a porous environment. In this scheme, a superficial velocity is adopted which is related to physical velocity as follows:

\[ \vec{v}_{\text{superficial}} = \gamma \vec{v}_{\text{physical}} \]  \hspace{1cm} (31)

The momentum equation including mass transfer and momentum exchange in a Cartesian system is

\[ \nabla \cdot (\alpha_q \rho_q \vec{v}_q \vec{v}_q) = -\alpha_q \nabla p + \nabla \cdot \bar{\tau}_q + \alpha_q \rho_q \vec{g} + (K_{pq} (\vec{v}_p - \vec{v}_q) + \dot{m}_{pq} \vec{v}_{pq}) + (\bar{F}_q + \bar{F}_{lift,q} + \bar{F}_{vm,q}) \]  \hspace{1cm} (32)

In these simulations the inertial drag force is imposed by the pore walls on the fluid.

\[ -\frac{C_p}{2} |\vec{v}| \vec{v} \]

This force should be added to the right hand side of the momentum equation. The virtual mass force only occurs if wood chips accelerate relative to the liquor - it is therefore left out of the momentum equation. The lift force is not included in the model. This term is not appropriate for closely packed particles. \( K_{pq} \) is the momentum exchange coefficient between the phases.

The momentum equation for any phase with regard to porosity effects and mass transfer in a Cartesian system is therefore reduced to:

\[ \nabla \cdot (\alpha_q \rho_q \vec{v}_q \vec{v}_q) = -\alpha_q \nabla p + \nabla \cdot \bar{\tau}_q + \alpha_q \rho_q \vec{g} + (K_{pq} (\vec{v}_p - \vec{v}_q) + \dot{m}_{pq} \vec{v}_{pq}) - (\sum_{i=1}^{n} \alpha_q \sigma_{ij} \frac{1}{2} \rho |\vec{v}_q| |\vec{v}_{q,i}|) \]  \hspace{1cm} (33)

\( \bar{\tau}_q \): The q\textsuperscript{th} phase stress-strain tensor
7.2. Reduced form of volume fraction (Mixture model- Paper 1)

The volume fraction of the secondary phase in a multiphase flow of the Mixture model in the Cartesian system is determined from the continuity equation. The volume fraction is the space occupied by each phase in the cell.

\[ \text{(27)} \]

The volume of phase \( p \) is defined by

\[ \text{(28)} \]

Where \( \text{flux}_{pq} \) is the mass transfer from phase \( p \) to \( q \). The mechanism of mass transfer in multiphase flows is different. In the mixture model simulation no mass transfer takes place between the phases and therefore the second term on the right hand side drops out of the equation. Therefore, the volume fraction equation was used in the following form:

\[ \text{(30)} \]

7.3. The reduced form of conservation of momentum for a fluid phase \( q \) (Papers 2, 4)

The multiphase scheme was run in a porous environment. In this scheme, a superficial velocity is adopted which is related to physical velocity as follows:

\[ \text{(31)} \]

The momentum equation including mass transfer and momentum exchange in a Cartesian system is

\[ \text{(32)} \]

In these simulations the inertial drag force is imposed by the pore walls on the fluid. This force should be added to the right hand side of the momentum equation. The virtual mass force only occurs if wood chips accelerate relative to the liquor - it is therefore left out of the momentum equation. The lift force is not included in the model. This term is not appropriate for closely packed particles.

\[ \text{is the momentum exchange coefficient between the phases.} \]

The momentum equation for any phase with regard to porosity effects and mass transfer in a Cartesian system is therefore reduced to:

\[ \text{(33)} \]

\[ \text{The qth phase stress-strain tensor} \]

\[ \text{External body force} \]

\[ \text{Lift force} \]

\[ \text{Virtual mass force} \]

For 2D axisymmetric geometries the reduced form of the radial momentum equation in a Eulerian multiphase model including the porous source, momentum exchange and mass transfer can be expressed by

\[ \frac{1}{r} \frac{\partial}{\partial x} \left( r \alpha_q \rho_q v_{qx} v_{qx} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \alpha_q \rho_q v_{qr} v_{qr} \right) = -\alpha_q \frac{\partial \rho_q}{\partial r} + \left( \varepsilon_{pq} \left( v_{pq} - v_{qk} \right) \right) + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \mu \left( \frac{\partial v_{qr}}{\partial x} + \frac{\partial v_{qr}}{\partial r} \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \mu \left( 2 \frac{\partial v_{qr}}{\partial r} - \frac{2}{3} (\nabla \cdot \bar{v}_q) \right) \right] - 2 \mu v_{qr} + \frac{2}{3} \frac{\alpha_q}{r} (\nabla \cdot \bar{v}_q) - \left( \sum_{j=1}^{2} \alpha_q C_{ij} \frac{1}{2} \rho |\nabla \bar{v}_q| |\nabla \bar{v}_q| \right) \quad \text{(34)} \]

Where

\[ \nabla \cdot \bar{v}_q = \frac{\partial v_{qx}}{\partial x} + \frac{\partial v_{qr}}{\partial r} + \frac{v_{qr}}{r} \quad \text{(35)} \]

Where \( r \) is the radial coordinate and \( x \) is the axial coordinate, \( v_{qx} \) is axial velocity and \( v_{qr} \) is radial velocity of the component \( q \) of the multiphase system.

7.4. Species transport (Papers 2, 4)

When the species transport approach is selected and the individual species are defined in the model, the conservation equation, which includes convection and diffusion, is solved for each species. The mass fraction of the species is then predicted by FLUENT. The conservation equation for the species transport model is:

\[ \nabla \cdot (\rho \bar{Y}_i) = -\nabla \cdot \bar{j}_i + R_i + S_i \quad \text{(36)} \]

Where \( R_i \) is the net rate of production of species \( i \) by chemical reaction, and \( S_i \) is the rate of addition from the dispersed phase.

FLUENT uses the dilute approximation by default. The diffusion flux in the dilute approximation is

\[ \bar{j}_i = -\rho D_{lm} \nabla Y_i \quad \text{(37)} \]

\( D_{lm} \) is the diffusion coefficient of species \( i \) in the mixture. \( \bar{j}_i \) is the diffusion flux of species \( i \) which arises due to concentration gradients. \( Y_i \) is the local mass fraction of species \( i \).

The reaction rates in equation (36) are computed in FLUENT by one of three models:

Laminar finite rate model: The effects of turbulent fluctuations are ignored, and reaction rates are determined by Arrhenius expressions.

Eddy-dissipation model: Reaction rates are assumed to be controlled by the turbulence, so extensive Arrhenius chemical kinetic calculations can be avoided.

Eddy-dissipation-concept (EDC) model: Detailed Arrhenius chemical kinetics can be incorporated in turbulent flames.
7.5. Mass diffusion with homogeneous chemical reaction (Papers 2, 4)

Species transfer is influenced by homogeneous chemical reactions. If we are restricted to steady one dimensional transfer in the x direction, these conditions can be expressed in the following equation (Incropera, 2007).

\[
D_{AB} \frac{d^2 C_A}{dx^2} + \dot{N}_A = 0
\]  

(38)

Where \( \dot{N}_A \) is the volumetric reaction rate and for a zero order reaction \( N_A = K_0 \) and

\[
\frac{\rho_A}{M_A} = C_A
\]  

(39)

Therefore a homogeneous chemical reaction of zero order may be expressed as

\[
D_{AB} \frac{d^2 (\frac{\rho_A}{M_A})}{dx^2} = -k_0
\]  

(40)

Where \( M_A \) is the molar mass of the species A which is constant and \( k_0 \) is the rate of a zero order reaction. The reaction rate can therefore be expressed in terms of diffusivity and density.
Chapter 8: Theoretical set up (chemical calculations and assumptions of Paper 5)

As previously mentioned, the Kappa number is a measure of the amount of lignin remaining on the fibre surface. When modelling dissolution of lignin using species transport and reaction schemes a correlation must be made between the molar quantities and mass. In order to do this, the molar mass of lignin and the other compounds in the wood must be defined in some way.

8.1. Molar mass determination strategy
Definition of a molar mass for lignin and hemicellulose is performed as a conventional computation. Our strategy to assign the molar mass of lignin is based on a sample of one mole of lignin i.e. 6.02 \times 10^{23} molecules. It is reasonable to assume that this number of molecules contains a representative mixture of the lignin monomers. This enables us to calculate an average molecular mass for the lignin monomers.

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Average molar mass of monomers of constituents (g/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lignin</td>
<td>197</td>
</tr>
<tr>
<td>Cellulose</td>
<td>180</td>
</tr>
<tr>
<td>Hemi cellulose</td>
<td>172</td>
</tr>
</tbody>
</table>

8.2. Average molar mass of the fibres
As no distinction is made between the reaction rates of the cellulose and hemicellulose, and the operational data of the pulp production and its quality are known, it is possible to assign an average molar mass for the fibres using the average molar mass of the cellulose and hemicellulose.

<table>
<thead>
<tr>
<th>Element</th>
<th>Average molar mass (g/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fibres (Cellulose + Hemicellulose)</td>
<td>176</td>
</tr>
</tbody>
</table>
8.3. Mass percent of fibres in the wood

Pine wood contains around 33% hemicelluloses and 37% cellulose by mass. Total fibre content in pine is typically around 70%.

8.4. Molar mass of the wood chips

Additional assumptions are required to make it feasible to assign a molar mass for the wood chips. A number of strategies for determining the molar masses are presented. This task is made more complex by the presence of acetyl and extractives. If the chips only contained fibres (cellulose and hemicellulose) and lignin, the molar mass calculation would be much simpler. The different approaches differ in their treatment of the extractives. The calculation begins by applying the mass percentages shown in Table 8 to a base of 1000g of wood chips.

Table 8: Mass percentage of wood constituents from Table 2

<table>
<thead>
<tr>
<th>Mass % of wood contents</th>
<th>Mass %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fibres (cellulose + hemicellulose)</td>
<td>70</td>
</tr>
<tr>
<td>Lignin</td>
<td>20</td>
</tr>
<tr>
<td>Acetyl</td>
<td>4</td>
</tr>
<tr>
<td>Extractives</td>
<td>6</td>
</tr>
</tbody>
</table>

The first treatment assumes the contributions of phenolic components, lipids and pinosylvin to the extractives shown in Table 9.

Table 9: Determination of the molar percentage of the wood constituents for molar mass calculation using Table 8

<table>
<thead>
<tr>
<th>Wood molar mass Base: 1000 g wood</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constituent</td>
</tr>
<tr>
<td>Fibres (cellulose + hemicellulose)</td>
</tr>
<tr>
<td>Lignin</td>
</tr>
<tr>
<td>Acetyl</td>
</tr>
<tr>
<td>Fat (myristoleic acid)</td>
</tr>
<tr>
<td>Pinosylvin</td>
</tr>
</tbody>
</table>

As the kinetics of the reactions of the acetyl and extractives are not known, it is desirable to simplify Table 9 by using an average molar mass for the acetyl content and the extractives, as shown in Table 10, and considering them collectively for the purposes of the model.
3.8. Mass percent of fibres in the wood

Pine wood contains around 33% hemicelluloses and 37% cellulose by mass. Total fibre content in pine is typically around 70%.

3.9. Molar mass of the wood chips

Additional assumptions are required to make it feasible to assign a molar mass for the wood chips. A number of strategies for determining the molar masses are presented. This task is made more complex by the presence of acetyls and extractives. If the chips only contained fibres (cellulose and hemicellulose) and lignin, the molar mass calculation would be much simpler. The different approaches differ in their treatment of the extractives. The calculation begins by applying the mass percentages shown in Table 8 to a base of 1000g of wood chips.

Table 8: Mass percentage of wood constituents from Table 2

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Mass %</th>
<th>g/base</th>
<th>Molar mass g/mol</th>
<th>mol/1000g base</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fibres (cellulose + hemicellulose)</td>
<td>70</td>
<td>700</td>
<td>176</td>
<td>4</td>
</tr>
<tr>
<td>Lignin</td>
<td>20</td>
<td>200</td>
<td>197</td>
<td>1</td>
</tr>
<tr>
<td>Rest</td>
<td>10</td>
<td>100</td>
<td>78</td>
<td>1.3</td>
</tr>
</tbody>
</table>

Based on the following symbols representing the wood chip constituents: F = fibres, L = lignin and R = acetyls and extractives, we can write the molecular formula for the wood chips according to the molar ratios in Table 10 as:

\[ n \times (F^4 L^{1.3} R^{1.3}) \]

\( n = 1, 2, 3, 4, 5 \)

If \( n = 1 \) then the molar mass of the wood chips can then be calculated from the molecular formula:

Molar mass of \( F^4 L^{1.3} = 1002.4 \text{ g/mol} \)

In the second approach, the contributions of extractives to the reactions are considered small enough to ignore. If A represents acetyls, the molecular formula is

\( F^4 L^{1.3} A \)

Like the first method, the third method uses the mole fractions in Table 9, but uses the average molar mass for the combined extractive content of 6 %. The molecular formula of the chips therefore becomes:

\( F^{13} L^3 A_3 R \)

The molar mass calculated by this method is 3227 g/mol.
Chapter 9: Analyzing, modelling set up, boundary conditions and implementation

9.1. General setup

The work in this thesis primarily relates to continuous digesters. The principles are also valid for batch digesters. The difference between these is that in the continuous digester wood chips and liquors are both mobile, while in the batch digester only the liquors are mobile. The batch digester can therefore be seen as a sub-category of the continuous digester.

A pressure-based solver is adopted to solve the momentum, continuity and volume fraction equations for all simulations. The chip bed moves very slowly downward through the digester and therefore a pressure-based solver is appropriate for low velocity flows. In this approach the velocity field is obtained from the momentum equation and the pressure field is extracted by solving a pressure equation which is obtained by manipulating continuity and momentum equations. The pressure-based solver uses a solution algorithm where the individual governing equations are segregated from each other and solved separately. Governing equations are non-linear, hence the Gauss-Seidel iteration approach is used to obtain a converged solution. Conservation equations for laminar and turbulent flows are solved in an inertial (non-accelerating) reference frame because there are no rotating tools in the digester.

On the other hand, the density-based solver is more appropriate for high velocity flows. The current numerical equations are solved under the steady state condition through the implicit discretization scheme. Gravitational acceleration is specified under operating conditions in the positive x direction due to the axisymmetric geometry.

Under turbulent conditions the k-ε turbulent method is adopted due to the low Reynolds number and fluctuations in the digester.

From the flow velocities, it is not obvious that the flow is turbulent, but flow in the channels is likely to be turbulent because of the uneven shapes of the wood chips. A laminar flow is used in subsequent steps when predicting the chemical reactions. The capacity and performance of these methods when predicting the progress of the chemical reactions and the hydraulic properties of the digester are compared by simulating various scenarios. The procedure for setting up and solving the Mixture and Eulerian methods is outlined below. First and second order momentum equations can be applied.
Discretization set up:

Table 11: Discretization

<table>
<thead>
<tr>
<th>EQUATION</th>
<th>ORDER/solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Momentum</td>
<td>Second order</td>
</tr>
<tr>
<td>Volume fraction</td>
<td>First order</td>
</tr>
<tr>
<td>Energy</td>
<td>Second order</td>
</tr>
<tr>
<td>Phase 2</td>
<td>Second order</td>
</tr>
<tr>
<td>Pressure velocity coupling</td>
<td>Phase coupled SIMPLE:</td>
</tr>
<tr>
<td></td>
<td>Semi Implicit Method for Pressure Linked Equations</td>
</tr>
</tbody>
</table>

The liquid flow is selected as the primary phase and the wood chips as the secondary phase. The secondary phase is assumed to be granular, and its properties are defined primarily in the material panel where it is placed in the fluid materials category. The granular properties are then specified in the granular phase panel and the granular option is switched on. The density and viscosity of the solid is defined in the material window.

The bulk viscosity is set to zero. The granular properties, i.e. the diameter of the particles, granular viscosity, bulk viscosity, frictional viscosity, granular temperature, solids pressure, radial distribution and packing limit are then assigned in the secondary phase setup. As the diameter of the applied spheres is larger than the compressible values, the packing limit is set at 0.63. Granular viscosity is defined at 0.001 kg/m-s. An algebraic solution is adopted for granular temperature because we do not have enough information about the magnitude of random fluctuations of small solid particles to be able to use a constant granular temperature. For the radial distribution the Lun et al. formulation is adopted. A derived formulation is adopted for the elastic modulus.

No solid pressure or frictional viscosity is adopted for the solid phase and a constant value of 0.9 is adopted for solid phase collision. This is primarily to take into account the chip flows inside the reactor, where the velocity at the centre is higher than at the walls.

The Schiller-Naumann formulation is used to solve for the drag force in the Mixture mode. The Schiller-Naumann law is appropriate for use in most cases with spherical particles.
**SOLVER set up:**

Table 12: Solver, models and adopted solutions

<table>
<thead>
<tr>
<th>Solver and models</th>
<th>Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>Pressure based</td>
</tr>
<tr>
<td>Gradient option</td>
<td>Green Gauss cell based</td>
</tr>
<tr>
<td>Porous formulation</td>
<td>Superficial velocity</td>
</tr>
<tr>
<td>Velocity formulation</td>
<td>Absolute velocity</td>
</tr>
<tr>
<td>Formulation</td>
<td>Implicit</td>
</tr>
<tr>
<td>Species transport model</td>
<td>No reaction</td>
</tr>
<tr>
<td>Energy model</td>
<td>activated</td>
</tr>
<tr>
<td>Porous formulation</td>
<td>Superficial velocity</td>
</tr>
</tbody>
</table>

**Operating conditions:**

Gravitational acceleration = 9.8 m/s² in the x direction

Operating temperature: 430 K

**Inlet boundary:** Velocity inlet (paper 2, 4)

Mixture: no active option

Phase 1: Thermal: T = 430 K, velocity specification method: magnitude normal to boundary, 0.3 m/s, no other active option for species or multiphase

Phase 2: volume fraction: 0.5, T = 430 K, velocity specification method: magnitude normal to boundary, 0.3 m/s, Lignin species mass fraction in second phase = 0.3, multiphase: volume fraction: 0.5

Interaction: Mass transfer mechanism: mass transfer from phase 2 to phase: mechanism: constant rate: 1.7×10⁻¹²

**Outlet boundary:** Pressure outlet

Phase 1 (liquid): Thermal T = 430 K,

Phase 2 (solid): Lignin mass fraction in the outlet second phase = 0.03, multiphase: backflow volume fraction: 0.01

**9.2. Porous media modelling the chip bed set up**

A heterogeneous porous media is specified throughout the digester to represent the compressibility of the solids. Decomposition of the wood occurs when lignin is removed from the chips. The chemical dissolution process makes the chips soft and more compact. To model this, the digester is divided into 19 sections in which different porosities are defined. The prescribed porosity diminishes from the top to the bottom of the digester. This porosity range from 0.65 to 0.1 is used to investigate the behaviour
of the liquor between the solid particles. These values reflect the distribution of the fluid flow through the particles. The void space between the chips is called the free liquor and when the lignin dissolves into the liquid phase the chip bed is compressed and the free space between the chips decreases. When this occurs, the volume fraction of the chips in a cooking block increases and the volume occupied by the free liquor decreases. The inertial loss term of the momentum sink is activated and specified for each porous section of the digester in both x and y directions. Application of the porous scheme to the model contributes to increase the residence time of the chips in the digester although the inlet velocity in a continuous digester is constant in terms of flow rate. The flow velocity reduces appreciably in the digester and therefore the residence time increases to between 4 and 5 hours. This is also compatible with the compression of the wood chips. In a real pulping process the longer residence time of the chips is due to the compression of the wood chips, volume of the digester, and velocity reduction in the digester.

**Porous zone definitions:**

The porous zone is defined on the basis of the relative velocity resistance formulation and inertial resistance formulation in x and y directions which are defined for both phases.

Porosity is defined for the mixture zone. The solid material in the porous zone is wood.

Inertial resistance increases from top to bottom.

The values of inertial resistance increase from 29 at the top to 50 at the bottom of the digester.

### 9.3. Chemical modelling set up

The pulping production process is a continuous chemical interaction between a bulk phase (black/white liquor) and a dispersed phase (wood chips). There are two current approaches for numerical calculation of multiphase flows: the Euler-Lagrange approach and the Euler-Euler approach.

### 9.4. Euler-Lagrange approach

The Euler-Lagrange approach is a combination of the Euler approach, which solves the Navier Stokes equation for the continuous phase, and the Lagrangian formulation which tracks the motion of the individual particles of the dispersed phase in the continuous phase. The fluid phase is considered as a continuum. The dispersed phase material can be made up of solid particles, liquid droplets or bubbles. The Lagrangian formulation calculates the trajectory of the dispersed phase in the continuum at intervals.

This method is applicable in cases where the volume fraction of the dispersed phase is below 10%. It is permissible to use heavy particles with high densities which may lead to higher mass flow rates of the dispersed phase than the fluid phase. The Lagrangian dispersed phase approach ignores particle-particle interactions and the effect of the particle's volume fraction on the continuous phase. The volume fraction of the chips in the digester is greater than 20%. The DPM model is applicable under unsteady condition.
9.5. Euler–Euler approach

This method is not able to track individual particles of the solid phase because it treats the solid particles as a continuous phase. This is the main assumption in this model, which despite the physical states of the phases, treat them both as continua. Modelling objects in this way ignores the fact that matter is made of atoms, and is not continuous. Conservation laws may be applied to these models to drive the differential equations describing the behaviour of such objects.

Both the bulk flow and the dynamic properties of the dispersed particles in the multiphase flow are predicted by the Euler formulation. The phases are not totally separated but they transfuse into each other and the volume fraction therefore has a continuous characteristic.

This assumption of continuous phases makes the Euler-Euler approach suitable for modelling the transfusion of liquor into the wood chips. This approach has been used in all the papers.

There are three different Euler-Euler multiphase approaches: the volume of fluid (VOF) model, the Mixture model, and the Eulerian model.

9.5.1. The Eulerian model

Prediction of the multiphase flow behaviour using the Eulerian scheme is more complicated than with the other multiphase approaches. This is partly due to the additional equations applied in the model and the nature of the phases. The treatment of the phases depends on their physical states and can be more or less complex. The Eulerian model solves the conservation equations for each phase. Interactions between the phases are considered through the calculation of the pressure and inter-phase exchange coefficients $K_{pq}$ and $K_{lr}$. This scheme has been applied in all papers.

9.5.1.1. Limitation of Eulerian

Convergence is the major difficulty when using the Euler-Euler multiphase flow. The Eulerian model treats both phases as continua and therefore the solid particles or bubbles are not treated as dispersed particles even though the second phase is called the dispersed phase. The conservation equations are solved for each phase but a single pressure contributes for all phases.

9.5.1.2. Model comparisons

Applying the Mixture or Eulerian model essentially depends on the characteristics, application, requirements and our knowledge of the system of the multiphase problem. It is clear that the Eulerian model is more complicated than the Mixture model but some applications require the use of the Eulerian formulation. If we have knowledge of the inter-phase then the Eulerian model is recommended because it can make more accurate predictions. In other cases the Mixture method is adequate because it requires fewer equations for the phases and they are easier to converge. The Eulerian method is complicated and the calculations may not be stable, potentially reducing their accuracy. On the other hand the chip and liquor reactions are not exact, stable and repeatable either.

9.6. Species transport and reaction approach

The flow of species and the reactions are modelled in FLUENT by solving a convection-diffusion equation for each species. Prediction of the interactions between the chips and cooking liquor for
further investigations using the reaction option of species transport method is possible if data about the stoichiometry, kinetics, and the flow regime inside the reactor are available.

The extent of the reaction is quantified by the stoichiometry equation. The parameters of the Arrhenius equation are determined based on the kinetics of the reaction, the thermal conditions and the activation energy of the reaction. Experimental records show that the lignin and the fibres have different reaction rates with the hydroxide ions. At higher operation temperatures the lignin resolution increases but the pulp quality and yield decrease due to an increase in the transfer of fibres to the liquid phase.

9.7. Reaction kinetic (Paper 5)

For a chemical reaction such as

\[ aA + bB \rightarrow C \]

Where A and B are reactants and C is product, the lower case letters are the stoichiometry coefficients. The rate \( r \) of the reaction is

\[ r = k(T)[A]^n[B]^m \]  

\[ \frac{d[C]}{dt} = k(T)[A]^n[B]^m \]  

The instantaneous rate of reaction in derivative notation is given by:

\[ \text{rate} = \frac{d[C]}{dt} \]  

The rate of reaction is a positive quantity that tells us how the concentration of a reactant or product changes with time, Masterton (1977).

If the species is a reactant, the negative value of the slope is used, because the slope is negative and a positive rate is desired. In the example above \( k(T) \) is the rate constant of the reaction and \( n \) and \( m \) are the reaction orders, which depend on the reaction mechanism. These are sometimes, but not always the same as the stoichiometry coefficients of A and B, Levenspiel (1998).

The rate constant is an extremely useful quantitative characteristic of a chemical or physical process. It indicates the fraction of the molecules in the source compartment that undergo the process per unit time.

In the collision model of reaction rate the rate constant is defined according to the following expression:

\[ k = \rho Z e^{\left(\frac{-E_a}{RT}\right)} \]  

where \( Z \) is the collision rate, \( \rho \) is the steric factor, \( E_a \) is the activation energy, \( R \) is the gas constant and \( T \) is the temperature.

9.7.1. Arrhenius equation and pre exponential factor

It is a reasonable approximation to assume that the \( \rho Z \) term in the collision model of reaction rate is constant. This reduces the equation to

\[ k = A e^{\left(\frac{-E_a}{RT}\right)} \]
T is the absolute temperature of the reaction. $E_a$ is the activation energy that is needed to reach the temperature of the reaction. $A$ is the pre-exponential factor and $R$ is the gas constant ($R = 8.314 \text{ J/k mol}$). The units of the pre-exponential factor are identical to those of the rate constant and vary depending on the order of the reaction. If the reaction is first order it has the units $\text{s}^{-1}$, and for this reason it is often called the frequency factor or attempt frequency of the reaction.

The rate equation or rate of reaction equation is a mathematical expression of chemical kinetics that relates the rate of reaction to the concentration of each reactant. The rate constant $k$ quantifies the speed of the chemical reaction.

The Arrhenius equation defines the dependence of the rate constant $k$ of chemical reactions on the absolute temperature $T$ (in Kelvin) and activation energy $E_a$.

In chemical kinetics, the pre-exponential factor demonstrates an empirical relationship between the temperature and rate coefficient. It is usually designated by $A$ when determined experimentally, while $Z$ is the collision frequency. $k$ is the number of collisions per second that result in a reaction, $A$ is the total number of collisions per second (whether they lead to a reaction or not) and $e^{E_a/kT}$ is the probability that any given collision will result in a reaction. When the activation energy is given in molecular units, instead of molar units, e.g. Joules per molecule instead of J/mol, the Boltzmann constant is used instead of the gas constant. Increasing the temperature or decreasing the activation energy (for example through the use of catalysts) results in an increase in the reaction rate.

A homogenous reaction rate is used to account for the reactions in pulp production. The rate is determined based on the available operational data in the pulping process of Korsnäs. The fundamental values required to determine the reaction rate of the substances are conversion, residence time, mass fractions of the reactants and products, total volume of wood chips in the digester, and the reaction temperature. The reaction rate of lignin is

$$ r = \frac{d[L]}{dt} $$

$k$ is a reaction constant for dissolution of lignin that is dependent on the wood chip properties. It includes both chip-size (diffusion) as well as reactivity of the lignin components.

### 9.7.2. Stoichiometry

The activation energy is approximated for the wood chips based on the thermodynamic data from the real process.

The mass flow balance used in the species transport model is based on the available operational data provided from Korsnäs and the conventional theoretical calculations for determination of the chemical formula of the wood chips.

In summary, the following stoichiometry is computed for the chemical reaction between the wood chips and cooking liquor (OH): (OH" is represented by $V$ in the thesis.)

$$ F_{4.1} L R_{1.35} + V \rightarrow F_{1.35} V R_{1.3} L + F_{2.65} L^{0.087} $$

Wood chips + liquor → Black liquor + Pulp

In this equation the inlet wood chips contain 20% lignin, 10% extractives and the produced pulp contains only 3% lignin. The boundary conditions and set up of the model are defined as shown in Tables 13 and 14.
Table 13: Boundary conditions, Paper 5

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Definition</th>
<th>Other definitions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet boundary</td>
<td>Velocity inlet</td>
<td>T = 430 K</td>
</tr>
<tr>
<td>Species</td>
<td>Species mass fractions of wood chips 0.47, white liquor: 0.53</td>
<td></td>
</tr>
<tr>
<td>Pressure outlet</td>
<td></td>
<td>T = 430 K</td>
</tr>
<tr>
<td>Reaction</td>
<td>Finite rate</td>
<td></td>
</tr>
<tr>
<td>Activation energy</td>
<td>$1.7 \times 10^8 \text{ J/ kg-mol}$</td>
<td></td>
</tr>
<tr>
<td>Pre exponent factor (A)</td>
<td>0.14</td>
<td></td>
</tr>
<tr>
<td>Reaction mechanism</td>
<td>Volumetric</td>
<td></td>
</tr>
<tr>
<td>Density</td>
<td>Volume weighted mixing law</td>
<td></td>
</tr>
<tr>
<td>$C_p$</td>
<td>mixing law</td>
<td></td>
</tr>
<tr>
<td>Viscosity</td>
<td>Mass weighted mixing law</td>
<td></td>
</tr>
<tr>
<td>Mass diffusivity</td>
<td>Constant dilute appx: 0.01m²/s</td>
<td></td>
</tr>
</tbody>
</table>

Discretization set up:

Table 14: Discretization, Paper 5

<table>
<thead>
<tr>
<th>Equation / parameters</th>
<th>Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>Standard</td>
</tr>
<tr>
<td>Momentum</td>
<td>Second order</td>
</tr>
<tr>
<td>Volume fraction</td>
<td>First order</td>
</tr>
<tr>
<td>Energy</td>
<td>First order</td>
</tr>
<tr>
<td>$F_4 L R_{1.3}$</td>
<td>Second order</td>
</tr>
<tr>
<td>$F_{2.65} L_{0.087}$</td>
<td>Second order</td>
</tr>
<tr>
<td>$F_{1.35} V R_{1.3} L_{0.913}$</td>
<td>Second order</td>
</tr>
<tr>
<td>Pressure velocity coupling</td>
<td>SIMPLE</td>
</tr>
</tbody>
</table>

Due to the fact that the pulp reactions are irreversible the Include Backward Reaction button was disabled.

9.8. Mass transfer approach (Papers 2 and 4)

The mass transfer mechanism in the framework of the Eulerian multiphase model in FLUENT is adopted for the pulping process. The unidirectional mass transfer model which gives a positive mass flow rate per unit volume from phase p to phase q is solved to predict the quality of the pulp.
The FLUENT multiphase mass transfer code accommodates mass transfer between species belonging to different phases. Instead of a matrix type input, multiple mass transfer mechanisms must be input. Each mass transfer mechanism defines the mass transfer between entities. An entity is either a particular species in a phase, or the bulk phase itself if the phase does not have a mixture material associated with it. The mass transfer phenomenon can be specified either through the inbuilt unidirectional “constant-rate” mass transfer or through user-defined functions. The constant mass transfer rate is adopted for the simulations.

The interactions between groups of species are defined. The lignin starts off bound to the wood chips and transfers from the solid to the liquid phase during cooking. The mass transfer rate (which is homogeneous) and the diffusivity of the hydroxide ions contribute to the mass transfer rate, conversion rate, and quality of the pulp produced in the digester.

9.9. Mass transfer conjugated with Porous media (Papers 2 and 4)

The Eulerian mass transfer approach conjugated with the species transport scheme and porous media can be used to accurately predict the flow behaviour when modelling of both solid and liquid phases is intended. The compressibility of the chips means that the degree of compaction of the chip bed is variable and there is a void space between the solid chips. The void space is expressed as porosity which in turn represents the volume fraction of free liquor. There is an inverse relationship between the compressibility and the porosity, meaning that the porosity decreases as the compressibility increases.

Low porosity contributes to a steeper velocity sink in the momentum equation. In low porosity zones a laminar flow is generated and the reaction progresses more uniformly through the chip bed. The porous cells are completely open and the chip bed is only partially open to liquor flow. The contribution of compressibility to the loss factor increases down the digester.

The use of the porous media model can eliminate complications such as the model instability and divergence that arise from the granular method. It therefore used for the following simulations. A variable porosity is defined throughout the digester to represent the compressibility of the chips and pulp zones. Chip bed packing is computed using the chip softening model.

The solid chip phase with variable compressibility can be characterized as having a given bulk viscosity, which represents the resistance of the solids against expansion and compression. This can be modelled as a porous media. However the definition of these properties using other CFD strategies may result in more computational cost. The wood chips are considered as a phase which moves downward through a porous media.
Chapter 10: Results

10.1. Results with respect to hydraulics (Paper 1)

The results listed in Table 15 are obtained from the FLUENT mass balance at the "report of the fluxes" when the Eulerian method with phase separation is applied. The values of default interiors and walls are not incorporated in this table.

Table 15: Mass balance of phase 2, the wood chips at inlets and outlets-Eulerian approach

<table>
<thead>
<tr>
<th>Section</th>
<th>Mass flow rate: kg/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet</td>
<td>36</td>
</tr>
<tr>
<td>Extraction down</td>
<td>0</td>
</tr>
<tr>
<td>Extraction - top</td>
<td>0</td>
</tr>
<tr>
<td>Bottom outlet</td>
<td>-36</td>
</tr>
<tr>
<td>C8- inlet</td>
<td>0</td>
</tr>
<tr>
<td>C8 -Outlet</td>
<td>0</td>
</tr>
<tr>
<td>ITC-Inlet</td>
<td>0</td>
</tr>
<tr>
<td>ITC- Outlet</td>
<td>0</td>
</tr>
<tr>
<td>MCC- Inlet</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 15 shows that there is zero flow at all outlet positions except for the top inlet and bottom outlet. The names in the table represent different inlet and outlets in the digester according to the nomenclature developed by the supplier of the digester. The amount of fibres following the liquid streams is negligible. This table shows that it is possible to separate the fibres from the liquids well using the Eulerian approach.
The velocity distribution of the wood chips shown in Figure 5 indicates that the flow of wood chips passes out through the screens into the pipes when the Mixture model is used. In Figures 3-14 of Paper 1, the hydraulic variables of the solid and liquid phases are obtained from the Euler strategy. Figure 6 shows the absence of solid particles in the discharge pipe. The vectors are scaled up about 5 times. The wood chip flow velocity is higher along the central pipe, where the liquid flow supports the flow downwards.

Figure 6: Eulerian computation: Velocity vectors of the solid phase in the discharge pipe and digester, the digester is rotated through 90°.
Figure 5: MIXTURE MODEL: velocity vectors of wood chips in the discharge pipe. The velocity distribution of the wood chips shown in Figure 5 indicates that the flow of wood chips passes out through the screens into the pipes when the Mixture model is used. In Figures 3-14 of Paper 1, the hydraulic variables of the solid and liquid phases are obtained from the Euler strategy.

Figure 6: Eulerian computation: Velocity vectors of the solid phase in the discharge pipe and digester, the digester is rotated through 90°. The vectors are scaled up about 5 times. The wood chip flow velocity is higher along the central pipe, where the liquid flow supports the flow downwards.

Figure 7: Eulerian computation: velocity vectors of liquid phase in the digester and discharges. The digester is rotated through 90°.

Figure 7 shows the velocity distributions of the liquid phase in different zones inside the digester. Figure 8 shows the velocity distribution of the fibres in the reactor. These figure show that the solid flow (the chips) moves towards the outlet. This is one reason for the occurrence of hang-ups, as the chip particles have a tendency to move partly into the screens and form "hooks".

Figure 8: Eulerian computation: velocity distribution of the solid phase at the top of digester.

The solid phase is also pulled towards the circulation pipe due to suction. Figures 9 and 10 in Paper 1 show the velocity vectors of the liquid at the entrance of the MCC and ITC pipe. Chip velocity increases near the C8, MCC and ITC inlets due to momentum transfer from the liquid to the solid phase.
10.2. Porous modelling (Paper 1)

Figures 15-18 and Graph 1 of Paper 1 show the flows for the porous bed approach when a heterogeneous porosity is defined from the top to the bottom of the digester.

Figure 15 of Paper 1 shows the velocity of the liquid flow through the digester including the multiple inlets and outlets. The inlet velocity is high but the turbulence and momentum decrease as a result of interactions with the solid phase. Figure 9 shows the turbulence intensity (k) distribution from the C8 position to the bottom of the digester. The contours reveal that turbulence is generated at three inlet positions, the C8 inlet, and the bottom and vertical side inlets near the bottom of the digester. The turbulence and velocity increase again near the circulation inlets, for example MCC, ITC and C8.

Graph 1 plots the liquid velocity in all zones of the digester. The digester is divided into 19 sections and velocity increases at three or four positions and where the flow enters from the MCC, ITC and C8 inlets. Liquid velocity then decreases again due to interactions with the solid, generating a momentum sink in the fluid flow.
10.3. Multiphase mass transfer-species transport (porous) (Paper 2)

A number of simulations are performed to predict the chemical reactions in the pulping process. This section presents and discusses modelling of chemical concentrations and profiles of component mass fractions and Kappa number in a conventional continuous cooking process.

The Kappa number is defined in the Custom Field Functions using the values of the predicted lignin mass percentage. Lignin content is about 15% of the Kappa number.

The structure of the simulation model is presented in the modelling set up section. The input data for tuning and verifying the model is from Digester 3 at Korsnäs. In order to consider the effects of variables their values have been varied by between one and three orders of magnitude in each simulation.

10.3.1. Simulation 1

Figure 2 of Paper 2 shows the rate of delignification when the specified value for the isotropic mass diffusivity is 0.288. Diffusion is isotropic when it is the same in all directions. This option is only available if the species transport model is activated. The mass diffusivity does not describe the diffusion of the phases into each other but instead describes the surface diffusion and spreading of a species in a mixture due to its concentration gradient.

The substance transfer from one phase to another phase is managed by the mass transfer rate which is set in the ‘Phase Interaction’ panel. The contribution of the mass diffusivity in the reaction or species transport from one phase to another phase is related to the accessibility. A higher mass diffusivity implies a wider spatial distribution of the species in the medium which leads to increased availability of that species. When a species is more accessible it can react more quickly. If we suppose that the mass transfer occurs at the inter-phase between the phases, then once a species transfers from the inter-phase to the second phase, the higher mass diffusivity contributes to quicker movement and spreading away from the inter-phase into the continuous phase.

As shown in Figure 2 of Paper 2, the Kappa number drops dramatically when the wood chips have travelled 10 m through the digester. This drop in Kappa number from 200 to 130 occurs in about 22 minutes, out of a residence time of between 4 and 5 hours. This time is calculated based on the position of the wood chips in the digester and their average velocity. The reaction develops gradually downward towards the outlet of the digester. The reaction rate is not constant, but gradually decreases down the digester. Higher mass diffusivity leads to more even distribution of the species in the medium.

The mass fraction of the lignin is also calculated under the same conditions implemented for Figure 2 of Paper 2 and is shown in Figure 7 of Paper 2.

The mass fraction of the lignin is compatible with the computed Kappa number under the same conditions (Graph 1 of Paper 2). The mass percentage of the lignin is around 29% in the wood chips at the inlet and about 3 to 4% in the outlet pulp. The results agree with the real process data without significant deviation. The lignin content in the pulp is consistent with the Kappa number. The same distribution is predicted for the Kappa number and the lignin content of the pulp.

The mass fraction of the cellulose/fibres in the pulp is also computed under the same specified physical conditions as for Figure 2 and Graph 1 of Paper 2 (see Graph 5, Paper 2).
The mass fraction of the fibres increases abruptly after around 20 minutes. The mass fraction of cellulose/fibres in the pulp then increases gradually in a non-linear fashion due to dissolution of the lignin in the white liquor. The final mass fraction of the cellulose/fibres reaches 96-97 %, corresponding to a Kappa number of 24.

10.3.2. Simulation 2

Figure 10 and Graph 2 show the progress of the reaction in terms of the Kappa number when a lower diffusion and mass transfer rate (R12-D0.00288) are defined for the species in the mixture.

![Figure 10: Kappa number R12-D0.00288](image)

Delignification develops more evenly than in the previous case with a higher mass diffusivity. The slope of the curve varies stepwise rather than gradually diminishing as in the previous case.
The mass fraction of the fibres increases abruptly after around 20 minutes. The mass fraction of cellulose/fibres in the pulp then increases gradually in a non-linear fashion due to dissolution of the lignin in the white liquor. The final mass fraction of the cellulose/fibres reaches 96-97\%, corresponding to a Kappa number of 24.

10.3.2. Simulation 2

Figure 10 and Graph 2 show the progress of the reaction in terms of the Kappa number when a lower diffusion and mass transfer rate (R12-D0.00288) are defined for the species in the mixture.

Figure 10: Kappa number R12-D0.00288

Delignification develops more evenly than in the previous case with a higher mass diffusivity. The slope of the curve varies stepwise rather than gradually diminishing as in the previous case.

Graph 2: Kappa number R12-D0.00288

A porous media is defined for the chip bed and cooking develops evenly along the digester. The mass fraction of the fibres in the pulp is predicted under a porous discipline and a mass diffusivity of 1.7E-12 is defined for the mass transfer rate from the solid to liquid phase. A diffusion constant of 0.0028 is defined for the species. (see Figure 11 and Graph 3).

Although there are no abrupt changes in the slope of the graph the slope is still not linear. The fibre concentration is about 70\% at the entrance and then increases identically down through the digester.

Figure 11: Mass fraction of fibres in the pulp R12-D0.00288
10.3.3. Simulation 3

The mass diffusivity is further reduced to 0.00028m²/s and the simulation is used to predict the Kappa number.

Figure 4 and Graph 3 of Paper 2 show the results of this simulation. The Kappa number at the horizontal centre of the digester is higher for R5-D0.000288. This is due to a non-uniform horizontal velocity in the R5-D0.000288 simulation. The top inlet is positioned at the centre of the digester and velocity at the centre line of the digester is higher than at the walls.

The mass fraction of the lignin in the pulp is also shown when mass diffusivity is 0.000288 and the specified mass transfer rate is 8.2 E-05 (Figure 12).

The lignin content near the central pipe is higher than that away from the centre and near the walls at higher levels of the digester. The inlet flow is situated at the centre of the top inlet, the flow is laminar and the velocity of both phases is slightly higher in the bulk flow direction than at the corners or at the walls at the same horizontal level in the digester. This can result in a lower yield and mass fraction of fibres in the centre of the digester.
10.3.3. Simulation 3

The mass diffusivity is further reduced to 0.00028 m²/s and the simulation is used to predict the Kappa number. Figure 4 and Graph 3 of Paper 2 show the results of this simulation. The Kappa number at the horizontal centre of the digester is higher for R5-D0.000288. This is due to a non-uniform horizontal velocity in the R5-D0.000288 simulation. The top inlet is positioned at the centre of the digester and velocity at the centre line of the digester is higher than at the walls.

The mass fraction of the lignin in the pulp is also shown when mass diffusivity is 0.000288 and the specified mass transfer rate is 8.2×10⁻⁵ (Figure 12).

The lignin content near the central pipe is higher than that away from the centre and near the walls at higher levels of the digester. The inlet flow is situated at the centre of the top inlet, the flow is laminar and the velocity of both phases is slightly higher in the bulk flow direction than at the corners or at the walls at the same horizontal level in the digester. This can result in a lower yield and mass fraction of fibres in the centre of the digester.

10.3.4. Simulation 4

The mass fraction of the lignin is predicted when the specified diffusion is 0.00028 as in the previous simulation but the mass transfer rate is further reduced to 8.2 E⁻¹³. The results of this simulation diverge significantly from the previous simulations.

As the accessibility of the lignin to the liquor is poor, the Kappa number remains unchanged for a long time. The mass diffusivity is low as is the mass transfer rate. These conditions are unfavourable for delignification and are not consistent with the real reaction conditions in the digester.

The mass fraction of the cellulose/fibres is also computed with further reduction of the mass transfer rate and the results are shown in Graph 8 in Paper 2.

This diffusion rate is very low, given the expectation of a uniform cooking process. The low mass diffusivity and mass transfer rate lead to a significant delay in cooking up to the 25m position, as shown in Graph 8 in Paper 2. This may indicate the minimum mass transfer rate required for cooking.

10.4. Species transport & reaction (Paper 5)

The kinetic equations and stoichiometry of the reaction between the wood chips and the white liquor composed of hydroxide ions (OH) are modelled and details of the reaction are computed from the modelling. The pulp production in the digester is predicted. The mass fraction of the pulp is shown in Figure 13.
The distribution of pulp in the digester in terms of molar concentration is also calculated (Figure 14).

The predicted mass fraction of black liquor in the digester is shown in Figure 15.
The species transport and reaction model takes into account the delignification of the wood chips, dissolution of lignin, the generation of black liquor, and fibre pulp production with a quality index of 3 % lignin content. The total reaction is summarized in the mass balance equation.

Some researchers approach this problem by attempting to establish chemical and hydraulic models of the pulp production by understanding the essential principles of the process. Building a comprehensive theoretical model of the whole delignification process and the random behaviour of the digester is a very complex task.

The initial delignification rate is very high because of the high lignin concentration in the chips and the high solvent (OH-) concentration.

The flow velocity decreases downwards through the digester. The decrease in velocity is due to compaction of chips, which reduces the free space in the column. The compaction depends partly on the degree of delignification that has occurred and the hydraulic behaviour of the phases and digester.

10.4.1. Lignin reaction rate

The chemical reactions are dependent on flow regimes, phase interactions and kinetics of the reaction. As well as these parameters the lignin reaction rate depends on its concentration in the wood. Gustafson introduced three kinetic models at three different stages of the process. These models are based on the lignin content of the wood chips during the delignification process. The first kinetic model is applied for lignin content over 22.5 %, the second is applied for lignin content between 22.5 % and -2.2 % and the third equation is applied for lignin content below 2.2 %.

The most general treatment of the pulping process applies the Arrhenius kinetic equation to the lignin reaction. This equation takes into account the temperature dependency of the reaction. The Arrhenius
equation is used to calculate the effect of temperature on the rate of reaction between lignin and hydroxide ions.

The reactants must reach a threshold temperature in order for the reaction to proceed. If the reaction was exothermic it would proceed without external energy input. However, the lignin reaction appears to be endothermic because no energy is produced by the progress of the reaction. The following expression gives the reaction rate for lignin dissolution.

\[
\frac{-d[L]}{dt} = k \times [L]
\]  

(47)

\(d[L]/dt\) is the average lignin dissolution rate and \([L]\) is the initial lignin concentration.

Schmidt-Nielsen reviewed the Arrhenius equation for this reaction, Laakso (2008). His comments can be summarized as:

1- Cooking reactions are not monomolecular.
2- The cooking molecular concentration decreases during cooking.
3- Diffusion varies during cooking.

Two simulations are run using the species transport and reaction model for the digester. The mass balance and stoichiometry for the cooking of wood chips is applied and defined in the FLUENT species transport reaction panel for both simulations. (See Table 13)

The same activation energy is set up for both simulations in FLUENT. This value is similar to the value calculated from the theoretical consideration of the reaction.

The main difference between the two simulations is the value of the pre-exponent factor. In Simulation 1 the pre-exponent factor is high and is set based on the common reaction velocity values and convergence requirements such as consistency and stability. In Simulation 2 the applied pre-exponent factor is based on the theoretical calculations and operational data.

The cooking in the two simulations appears to have different reaction kinetics due to the difference between the pre-exponent factors.

The white liquor (OH-) dissolves the lignin and its concentration decreases as expected as we proceed through the digester. The dissolution of the wood chips in the digester is predicted according to the proposed stoichiometry. The reactants in the stoichiometry equation are wood chips and OH\(^-\), which react together to produce black liquor and pulp. The reaction is complete and non-reversible, meaning that the reactants are fully converted to the products.

Simulation 2, with the theoretically calculated pre-exponent factor, is more stable than Simulation 1, which has a high pre-exponent factor for normal volumetric reactions. This is due to the particular state of the pulp reaction and its long residence time.

The molar mass of the wood chips was estimated and a molecular formula was computed for the wood chips based on assumptions and operational data provided from pulp production.

The stoichiometry, based on the operational data and reaction kinetics calculations was set up in the reaction panel of the species transport model in FLUENT.

The two simulation methods can be compared directly - Figure 13 for Simulation 1 corresponds to Figure 16 for Simulation 2.
The reactants must reach a threshold temperature in order for the reaction to proceed. If the reaction was exothermic it would proceed without external energy input. However, the lignin reaction appears to be endothermic because no energy is produced by the progress of the reaction. The following expression gives the reaction rate for lignin dissolution.

\[
\frac{d[L]}{dt} \quad \text{is the average lignin dissolution rate and \([L]\) is the initial lignin concentration.}
\]

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The two simulation methods can be compared directly - Figure 13 for Simulation 1 corresponds to Figure 16 for Simulation 2.

Figure 16 shows a less uniform distribution and faster delignification kinetics overall throughout the digester.

In Simulation 2, there is moderate cooking in the first 20 m which slows down in the following 20 m, and increases again before finally slowing again in the bottom 10 m. In Simulation 1 however, cooking proceeds evenly through the first 50 m of the digester, and increases rapidly through the last 10 m. The different pre-exponent factors therefore result in very different predictions of reaction progress down the digester.

The result shows that the mass fraction of the black liquor increases evenly down the digester, and more rapidly in the bottom 10 m, as would be expected from the progress of the pulp reaction predicted by Simulation 1.

The mass fraction of the white liquor is determined by the second approach and the results are shown in Figure 9 of Paper 5.

Comparison of Figures 11 and 12 of Paper 5 indicates that the molar fraction of pulp only begins to increase when there is a rapid drop in the molar fraction of the wood chips. This is because the estimated molar mass of the wood chips is much larger than the molar mass of the pulp. Therefore, when the mole fraction of the wood chips drops to 1.2% the mole fraction of the pulp starts to increase.
10.5. Channelling (Paper 3)

Hydraulic characteristics of the channels are studied and introduced in Paper 3. The flow behaviour is investigated by calculating of flow velocity in the presence of channelling. Figure 17 shows the flow velocity and Figure 18 shows the velocity vectors inside and around the channel.

Channelling of the liquor flow in the chip bed occurs as a result of delignification and the transfer of lignin from the chips to the free liquor, as already described. Modelling of the channelling contributes to prediction of the thermodynamic and hydraulic behaviour of the digester in risky situations, which in turn can be used to indicate the likely occurrence of channelling in the digester.

Figure 17: Contours of distribution of the Velocity inside the digester from top to bottom (the figure is rotated through 90°)

Figure 18: Contours of distribution of the velocity in the channel (the figure is rotated through 90°)

Haas (1990) predicted the occurrence of channelling in the lowest level of the digester. In one experiment the washing screen temperature was studied before and after channelling, Toivonen (2004).
Channelling of the bottom washing liquor caused a very large temperature variation on one side of the screen. Hamilton (1961) also studied the delays in chip flow through the digester. He observed some chip rotation in the bottom of the digester but did not find any evidence of channelling of the chip flow because his study was based on an individual chip. Channelling may be associated with packing of the chip bed and it is therefore desirable to find optimal packing and flow conditions in order to avoid it. High temperature washing has also been implicated as contributing to channelling, Pageau (2002).

Some researchers consider channelling to be a result of flow direction in the digester. A change of flow direction from upward to downward leads to modified chip bed movement and a reduction in channelling, Lorincz (2001).

Temperature variations may explain the occurrence of channelling in specific zones of the digester. Making the digester smaller decreases the upward pressure exerted on the chip bed and improves the washing performance in the bottom zone, Wold (2001). This may reduce channelling.

Hydraulic modelling of channelling is described in Paper 3. Channelling is modelled by varying the porosity of the cells in the digester.

| Figure 19: Representing the channelling phenomenon in the digester |

The porosity in the top cells is the same as that of the wood chips, around 70%. Thereafter it decreases downwards as a function of lignin dissolution and compaction due to the weight of the chips pressing downwards. At the bottom the porosity is approximately 25%. The results are shown in the figures in Paper 3. An artificial channel is modelled in the digester using the porous media approach. The flow behaviour is studied around and inside the channel. The channel contains only liquid phase and the porosity outside the channel is low. From this starting point, a heterogeneous porosity is defined in the digester.

The channels are characterized as having a very high porosity in the digester in a special zone. Figures 17 and 18 show that the velocity of the liquor increases in the channels and the predicted velocity magnitudes and vectors of the velocity in the channels contribute to characterize the channel. When the liquor enters the channel its velocity increases due to the elimination of the momentum sink term and the low concentration of wood chips in the channel. This statement is supported by Figure 5 of Paper 3.

When the liquor leaves the channel the velocity decreases again because of obstruction by wood chips in the liquid path. This is shown in Figures 7 and 8 of Paper 3. Within the channel, the velocity is highest at the upstream end and decreases gradually toward the downstream end as shown in Figure 6.
10.6. Channelling and reaction (Paper 4)

The cooking of the pulp in the presence of channelling is also considered. When channelling occurs there are either no chips or a very small number of chips in the channel. As a result, the proportion of the pulping reaction supported by the channel is very small. Moreover, the chip velocity in the channel is higher than in the surroundings, due to the higher velocity of the liquid flow and momentum interactions between the phases, which in turn leads to shorter chip residence times, and therefore higher Kappa numbers in the channel.

The results show that the progress of the reaction inside the channel is very slow. The Kappa number is higher inside the channel than outside it. Un-reacted chips have higher Kappa numbers than reacted chips. This is because chip particles that pass through the channel descend much more quickly than the chips that descend outside the channel. Lignin dissolution is therefore reduced due to the lower residence time.

The Kappa number inside the channel is calculated and shown in Figure 20 and the corresponding molar concentrations of the produced fibres are shown in Figure 4 of Paper 4. The molar concentration of fibres inside the channel is about the same as at the entrance to the channel and is lower than outside the channel. The liquor velocity is also predicted in order to evaluate the flow behaviour inside the channel (Graph 4).

Figure 20: Kappa number in the channel
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Graph 4: Velocity of the liquor in the channel

Modelling the development of the cooking in the presence of channelling contributes to characterization of channel formation in the digester and troubleshooting.
Chapter 11: Numerical evaluation

11.1. Grid independence

The outlets, extractions and amounts of the circulation flows are obtained from simulation of the digester by adjusting the pressures. The results agree closely with the operation values from the Korsnäs process database.

The digester is about 60 m high and between 6 and 7 m in diameter. Three different types of meshes with different numbers of cells are used in the simulations. Models are constructed with meshes containing 16000 or 56000 triangular cells, or 21000 quadrilateral cells for each half of the digester, i.e. 60 m × 3 m. The other half of the digester is axisymmetric and is computed by FLUENT.

There are no differences between the results of the computations that use the 56000 triangles and the 21000 quadrilaterals. However, results using the intermediate mesh made up of 16000 triangular cells do not agree that well with the results from the other two meshes. This implies that the mesh with 16000 triangles is too coarse. Only minor differences are seen in results when using meshes with even larger numbers of cells.

A large aspect ratio, which is a measure of the cell stretching, in a triangular or tetrahedral cell invariably affects the skewness of the cell, which is undesirable as it may reduce accuracy and impede convergence. Meshes with high degrees of skewness may cause divergence or lack of robustness. No skewness is observed in our mesh building because of the symmetry and absence of small details in the geometry. The mesh quality influences the stability and accuracy of the numerical computation. The grid quality of the domain was checked and its structure was observed to have a high degree of quality.

11.2. Residuals

Several typical residuals of simulations related to calculations in Paper 2 and Paper 3 are shown in this section. The graphs show the difference value of a scalar quantity at the nodes at any stage of the solution process with respect to the previous stage. The explicit method (backward difference approximation) is applied to transform the differential equations into linear algebraic equations. In this method, evaluation of any scalar quantity at any node depends on the value of that quantity at its adjoining nodes, which are generally unknown. Hence, in order to determine the unknown nodal physical quantity, the corresponding nodal equations must be solved simultaneously.

The equations are solved using the Gauss-Seidel iteration method. In order to obtain a converged numerical solution the difference value should be < 0.001 for continuity and volume fraction. The convergence criterion for energy is < 0.00001. The implicit method is unconditionally stable. This means that the solution remains stable for all space and time intervals, in which there are no restrictions on Δx and Δt. Computational time may be reduced with little loss of accuracy when using larger values of Δt.
Graph 5: Residuals-Approach 1 - chemical reaction

Graph 6: Residuals of channeling
Chapter 12: Discussion

12.1. Mass Diffusion Coefficients

In the species transport and reaction procedure the diffusion of chemical species into each other is modelled by applying the Fick's law formulation. The Arrhenius expression is related to the production of species $i$ ($R_i$) in Equation 36.

The simulations are performed with softwoods and the appropriate density is specified in the calculations. The models are to be used for control and optimization. The chip bed and liquor flow are considered as the two phases in the model, and the species present in the phases are also prescribed in the models. As seen in the results increasing the mass transfer rate has a large initial impact, but further increases have less effect. The mass transfer rate is a limiting at first, but as it increases other factors become more important and act as bottlenecks.

12.2. Axisymmetric aspect

The digester cannot be modelled in 2D because FLUENT assumes that a 2D model is one length unit deep in the z direction. In this case this would mean the central pipe would have a uniform depth of 1 m. This geometry would affect the boundary conditions and velocity of the inlet and outlet flows.

The axisymmetric configuration - in which axisymmetric cell volumes are created by rotating the 2D cell volume around the x-axis - is appropriate for the cylindrical pulping digester.

The shape of the reactor and the dimensions of the components of the digester are significant in the simulation of delignification. The simulations show that this approach can be used to simulate both normal conditions and different types of faults.

12.3. Phase separation

Separation of phases in a multiphase stream is considered by defining the physical dimensions of the screens at the inlet of the extraction pipe in Gambit.

The Mixture and Eulerian multiphase models of FLUENT were analyzed. Traces of the solid phase were discovered in the extraction pipe when the Mixture approach was used.

The contours of the velocity vectors of phase 2 (the wood chips) in the discharge pipe (shown in Figure 5) indicate the contribution of the solid phase in the discharge pipe. This is in spite of the screens at the inlet of the discharge pipe whose gaps are smaller than the diameter of the solid particles.

It follows that the Mixture model is not appropriate for modelling separation of the phases.
The two phases are treated as interpenetrating continua in the Mixture model. The model solves the continuity, momentum and energy equations for the mixture, the volume fraction equation for the phases, and prescribes relative velocities to describe the dispersed phases.

The Eulerian approach for multiphase models solves a set of momentum and continuity equations for each phase. This is the key to effective separation of the phases. The Mixture method on the other hand, solves a single equation at the interface of the phases. Phase separation requires keeping track of the individual phases. The phases are characterized in the Eulerian scheme, which is found to separate the phases effectively at the entrance to the discharges pipes.

The report of the fluxes of the phases generated by FLUENT shows the ability of the Eulerian approach to mathematically separate the phases. This approach may have applications in other engineering areas. The solid phase moves down the reactor without contributing to the extraction or circulation streams. Figures 6 to 8 show the hydraulic variables of the solid and liquid phases calculated by the Eulerian approach. Figure 6, in which vectors are scaled up around 5-fold, shows the absence of the solid phase in the discharge pipe. Figure 7 shows the presence of the liquid phase alone in the discharge tube.

As the Eulerian approach is found to be more appropriate for phase separation, it is used in subsequent simulations.

Lagrangian trajectory computation of particles is available in FLUENT but is not analyzed in this paper, as it does not seem to be a feasible approach for solution of the dynamic characteristics of this digester.

### 12.4. Forces

The bed pressure influences the volume fractions of the chips and liquor in the digester, Laakso (2008). The chips pressure is the product of a number of forces acting on the solid phase. These forces act on the chip bed in different directions and an imbalance between the forces results in compaction in the chip bed. The gravitational force acts downwards and compresses the chips, increasing the degree of packing when a static chip is considered.

The combination of the chips and cooking liquor is called the chip column or chip bed. The direction of the chip flow and liquor can be concurrent or counter-current.

The digester walls may exert a frictional force on the chip bed as it moves downwards. There may also be a frictional force between the phases. The volumetric properties of the phases and the dynamic conditions of the packing bed are the direct results of these forces.

A high chip pressure contributes to a low porosity and high compression or packing grade. The difference in density between the chips and the free liquor can lead to an upward buoyancy effect. The non-uniform chip shape makes it difficult to model the details of frictional forces on individual chips. For this reason a volumetric frictional force against the chip bed is prescribed.

### 12.5. Porosity

Packing of the chip bed is simulated by using a non-uniform porosity throughout the digester. The chip bed packing is a result of delignification, chip softening, and the weight of the chips in the higher parts of the digester. This compressibility is modelled by using porosity that decreases from top to bottom through the chip bed. This diminishing porosity agrees with the trend for increasing lignin in
the liquor towards the bottom of the digester. The amount of liquor is accounted for in the form of a porous parameter.

Reduced porosity creates more restricted and uniform flow of the liquor inside the chip bed. The restriction of the liquor flow may lead to channelling or blockage of the apparent motion of the chip bed. As can be seen from the graphs obtained from the channelling simulations, the slope of the Kappa number is steeper in the lower zone of the digester where the porosity is lowest. This shows an inverse relationship between the porosity and packing of the bed. When the concentration of the lignin in the wood is higher the porosity is also higher and compressibility is lower.

The porosity influences the uniformity of the reaction because the velocity increases at higher porosities. The rate and progress of the reaction is also a function of the flow velocity and diffusivity.

The minimum porosity value specified for the simulation is 0.1 in the lower sections of the digester where the packing is densest. A heavy load of chips enters the digester. The weight and normal pressure of the upper chip beds on the lowest beds increases the risk of process disturbances because the flow at the bottom becomes restricted, which can lead to channelling of the liquor flow. An optimal bed packing is therefore needed at the entrance. The porous formulation is based on a nominal velocity which would be the velocity achieved by the fluid at the same volumetric flow if no porosity was defined. In addition to other specified hydraulic and chemical properties, designation of a porous scheme for the cooking process can contribute to better characterization of the wood chips and liquor flow. When the liquor flow enters the digester its velocity decreases as it flows through the chips bed. Porous media can reduce the momentum of the flow and it is therefore used to represent the chips bed.

12.6. Mass transfer model

A number of simulations are performed to evaluate the distribution of pulp production in the reactor. Three essential variables of simulation are considered - porosity, mass transfer rate and mass diffusivity. The values of these variables and the shortening expression for each simulation are shown in Table 16.

Table 16: Variables of simulation

<table>
<thead>
<tr>
<th>Mass diffusivity</th>
<th>Mass transfer rate between the phases</th>
<th>Porosity</th>
<th>Simulation shortening</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.288</td>
<td>2.0E-11</td>
<td>0.55-0.15</td>
<td>R11-D0.288</td>
</tr>
<tr>
<td>0.00288</td>
<td>1.7E-12</td>
<td>0.65-0.25</td>
<td>R12-D0.00288</td>
</tr>
<tr>
<td>0.000288</td>
<td>8.2E-05</td>
<td>0.5-0.1</td>
<td>R5-D0.000288</td>
</tr>
<tr>
<td>0.000288</td>
<td>8.2E-13</td>
<td>0.5-0.1</td>
<td>R13-D0.000288</td>
</tr>
</tbody>
</table>

12.6.1. Mass transfer rate

The change in the lignin content is modelled by a mathematical kinetic model. The diffusion of hydroxide ions into the pores of the wood is dependent on the lignin content and the hydroxide ion concentration. The cooking reaction slows when the lignin content decreases. The mass transfer rate from the chip bed into the liquor phase therefore decreases from the top to the bottom of the digester.
In the mass transfer model the lignin content of the chips decreases from 30% to about 3% to 4%, giving a yield of around 90%.

12.6.2. Kappa number and related components

The inlet chips contain around 20% lignin and 10% extractives. The pulp at the outlet of the reactor contains around 3% lignin. The Kappa number of the outlet pulp is around 24 when it contains 3.6% lignin. The simulations show how cooking develops at different levels of the digester.

The simulation approach is shown to be suitable for calculating the Kappa number as a function of chemical reactions, taking into consideration the chemical conditions, temperature, and mass transfer between the phases.

12.6.3. Validation and comparison of the Kappa number results from simulations

In order to compare the simulations, the Kappa numbers obtained from four simulations at different locations in the digester are shown in Graph 7.

The dissolution of lignin from the wood chips in the simulation with mass diffusivity of 0.288 m²/s and mass transfer rate of $2.0 \times 10^{-11}$ is faster at every point compared to the other simulations.

Additional statistical comparisons of the simulations are performed using the average value and absolute deviations of Kappa number at each point (Table 17).
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Graph 7: Kappa number obtained from four simulations

The dissolution of lignin from the wood chips in the simulation with mass diffusivity of 0.288 m²/s and mass transfer rate of 2.0 × 10⁻¹¹ is faster at every point compared to the other simulations. Additional statistical comparisons of the simulations are performed using the average value and absolute deviations of Kappa number at each point (Table 17).

Table 17: Average Kappa number and absolute deviation at 13 points

<table>
<thead>
<tr>
<th>Simulations →</th>
<th>R11-D0.288</th>
<th>R12-D0.00288</th>
<th>R5-D0.000288</th>
<th>R13-D0.00028</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kappa number at the bottom</td>
<td>27.52</td>
<td>29.27</td>
<td>25.65</td>
<td>26.04</td>
</tr>
<tr>
<td>Absolute deviation</td>
<td>3.52</td>
<td>5.27</td>
<td>1.65</td>
<td>2.04</td>
</tr>
</tbody>
</table>

The Kappa number from the real pulp process can only be measured at the top and bottom of the digester. The outlet pulp contains about 3.6% lignin, corresponding to a Kappa number of 24, which is the target value for the process. Table 18 shows the absolute deviations of the simulated values from experimental data.

Table 18: Absolute deviation of simulation results from experimental values

<table>
<thead>
<tr>
<th>Simulations →</th>
<th>R11-D0.288</th>
<th>R12-D0.00288</th>
<th>R5-D0.000288</th>
<th>R13-D0.00028</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kappa number at the bottom</td>
<td>27.52</td>
<td>29.27</td>
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</tr>
<tr>
<td>Absolute deviation</td>
<td>3.52</td>
<td>5.27</td>
<td>1.65</td>
<td>2.04</td>
</tr>
</tbody>
</table>

The simulated values reported in the table above are obtained from the bottom of the digester where the lignin content approaches its lowest value. The absolute deviation is calculated by the following equation:

\[ D_i = |x_i - \bar{x}| \]  

(48)

Where \( D_i \) is the standard deviation, \( x_i \) is the Kappa number at any location in the digester and \( \bar{x} \) is the average Kappa number at any specific location of the digester.

12.6.3.1. Comparison of the Finite volume method simulations with the Purdue, Gustafson and Andersson models

The lignin content at different heights in the digester as predicted by CFD simulations are compared to other models. Graph 8 shows the lignin contents of the wood chips at different times as predicted by the Andersson, Gustafson and Purdue models.
The simulations are run under steady state conditions and the Euler-Lagrange approach and batch operation are not used. In a batch operation concentration calculations can be performed at any point and at any instant. However, in a steady state continuous operation the particles move downwards continuously and operation conditions and concentrations at each location do not vary with time. It is therefore possible to calculate the average velocity of the chips inside the digester and therefore the average time that the wood chips take to reach any position in the digester. The average velocity is calculated using Area-Weighted Average Velocity. The velocity distribution inside the digester is also predicted.

Figure 21 shows the contours of wood chip velocity in the digester. The height of the modelled digester is about 60m.

The area weighted average velocities obtained from the FLUENT simulation are shown in Table 19.
The simulations are run under steady state conditions and the Euler-Lagrange approach and batch operation are not used. In a batch operation concentration calculations can be performed at any point and at any instant. However, in a steady state continuous operation the particles move downwards continuously and operation conditions and concentrations at each location do not vary with time. It is therefore possible to calculate the average velocity of the chips inside the digester and therefore the average time that the wood chips take to reach any position in the digester. The average velocity is calculated using Area-Weighted Average Velocity. The velocity distribution inside the digester is also predicted.

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The area weighted average velocities obtained from the FLUENT simulation are shown in Table 19.

<table>
<thead>
<tr>
<th>Phase 2</th>
<th>Zone</th>
<th>Area -Weighted Average Velocity magnitude (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Digester 1</td>
<td>0.0038920196</td>
</tr>
<tr>
<td></td>
<td>Digester 10-sil</td>
<td>0.0031701396</td>
</tr>
<tr>
<td></td>
<td>Digester 11-sil</td>
<td>0.0031581628</td>
</tr>
<tr>
<td></td>
<td>Digester 12</td>
<td>0.0031612692</td>
</tr>
<tr>
<td></td>
<td>Digester 13</td>
<td>0.0031616227</td>
</tr>
<tr>
<td></td>
<td>Digester 14-sil</td>
<td>0.0031660108</td>
</tr>
<tr>
<td></td>
<td>Digester 15-sil</td>
<td>0.003107436</td>
</tr>
<tr>
<td></td>
<td>Digester 16</td>
<td>0.0031210901</td>
</tr>
<tr>
<td></td>
<td>Digester 17</td>
<td>0.0031509299</td>
</tr>
<tr>
<td></td>
<td>Digester 18</td>
<td>0.0034289486</td>
</tr>
<tr>
<td></td>
<td>Digester 19-outlet_zon</td>
<td>0.007766922</td>
</tr>
<tr>
<td></td>
<td>Digester 2</td>
<td>0.0032264907</td>
</tr>
<tr>
<td></td>
<td>Digester 3</td>
<td>0.0032264199</td>
</tr>
<tr>
<td></td>
<td>Digester 4</td>
<td>0.0032263021</td>
</tr>
<tr>
<td></td>
<td>Digester 5-sil</td>
<td>0.0032233924</td>
</tr>
<tr>
<td></td>
<td>Digester 6</td>
<td>0.0032255405</td>
</tr>
<tr>
<td></td>
<td>Digester 7</td>
<td>0.0032265952</td>
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<tr>
<td></td>
<td>Digester 8</td>
<td>0.0032087076</td>
</tr>
<tr>
<td></td>
<td>Digester 9</td>
<td>0.0031842848</td>
</tr>
<tr>
<td></td>
<td>Net</td>
<td>0.0033872321</td>
</tr>
</tbody>
</table>

The average residence time of the wood chips in the digester is calculated based on the average velocity.

Average residence time = 60 m/0.0034m/s = 17647 s ≈ 4.9 h

The lignin content of the wood chips has already been predicted in terms of Kappa number at 13 points in the digester. It is therefore possible to compare the results of this simulation (Table 17) with the three previously reported models (Graph 9). The comparison is summarized in Table 20.

The lignin contents are stated in terms of the Kappa number and the time taken by the chips to reach particular points in the digester.
Table 20: Comparison of the FVM simulations with the Andersson, Gustafsson and Purdue models in terms of lignin contents and Kappa number

<table>
<thead>
<tr>
<th>Height (m)</th>
<th>1</th>
<th>5</th>
<th>10</th>
<th>15</th>
<th>20</th>
<th>25</th>
<th>30</th>
<th>35</th>
<th>40</th>
<th>45</th>
<th>50</th>
<th>55</th>
<th>60</th>
</tr>
</thead>
<tbody>
<tr>
<td>R11-D0.288</td>
<td>137,658</td>
<td>123,339</td>
<td>107,987</td>
<td>93,451</td>
<td>80,376</td>
<td>67,995</td>
<td>57,923</td>
<td>49,058</td>
<td>41,564</td>
<td>35,642</td>
<td>31,286</td>
<td>28,501</td>
<td>27,528</td>
</tr>
<tr>
<td>R12-D0.00288</td>
<td>194,287</td>
<td>184,341</td>
<td>178,787</td>
<td>164,754</td>
<td>144,246</td>
<td>123,458</td>
<td>100,258</td>
<td>83,406</td>
<td>58,686</td>
<td>55,711</td>
<td>44,900</td>
<td>39,931</td>
<td>35,655</td>
</tr>
<tr>
<td>R5-D0.000288</td>
<td>200</td>
<td>199.99</td>
<td>199.93</td>
<td>199.66</td>
<td>199.84</td>
<td>196.61</td>
<td>190.62</td>
<td>186.01</td>
<td>173.47</td>
<td>157.17</td>
<td>62.22</td>
<td>45.33</td>
<td>26.04</td>
</tr>
<tr>
<td>R13-D0.000288</td>
<td>185</td>
<td>160</td>
<td>128.7</td>
<td>98</td>
<td>63</td>
<td>43</td>
<td>34.7</td>
<td>30</td>
<td>25</td>
<td>20</td>
<td>18</td>
<td>16.7</td>
<td>13</td>
</tr>
<tr>
<td>lignin % - A</td>
<td>27.8</td>
<td>24</td>
<td>19</td>
<td>14</td>
<td>9.5</td>
<td>6.5</td>
<td>5.2</td>
<td>4.5</td>
<td>3.8</td>
<td>3</td>
<td>2.7</td>
<td>2.5</td>
<td>2</td>
</tr>
<tr>
<td>kappa-Andersson</td>
<td>185</td>
<td>160</td>
<td>128.7</td>
<td>98</td>
<td>63</td>
<td>43</td>
<td>34.7</td>
<td>30</td>
<td>25</td>
<td>20</td>
<td>18</td>
<td>16.7</td>
<td>13</td>
</tr>
<tr>
<td>lignin % - G</td>
<td>27.2</td>
<td>24.9</td>
<td>21.5</td>
<td>17.5</td>
<td>13.8</td>
<td>10.7</td>
<td>8.6</td>
<td>7.2</td>
<td>5.8</td>
<td>5.1</td>
<td>4.2</td>
<td>4</td>
<td>2.5</td>
</tr>
<tr>
<td>kappa-Gustafson</td>
<td>181</td>
<td>160</td>
<td>128.7</td>
<td>98</td>
<td>63</td>
<td>43</td>
<td>34.7</td>
<td>30</td>
<td>25</td>
<td>20</td>
<td>18</td>
<td>16.7</td>
<td>13</td>
</tr>
<tr>
<td>lignin % - P</td>
<td>21.5</td>
<td>22</td>
<td>20</td>
<td>18.8</td>
<td>17</td>
<td>13.8</td>
<td>10</td>
<td>7.2</td>
<td>6</td>
<td>4.9</td>
<td>4.2</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>kappa-Purdue</td>
<td>156.7</td>
<td>146.7</td>
<td>133</td>
<td>125</td>
<td>113</td>
<td>92</td>
<td>66.7</td>
<td>44</td>
<td>32.7</td>
<td>28</td>
<td>26.7</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>time (s)</td>
<td>294</td>
<td>1470</td>
<td>2941</td>
<td>4411</td>
<td>5882</td>
<td>7352</td>
<td>8823</td>
<td>10294</td>
<td>11764</td>
<td>13235</td>
<td>14705</td>
<td>16176</td>
<td>17746</td>
</tr>
<tr>
<td>time (min)</td>
<td>4.9</td>
<td>24.5</td>
<td>49</td>
<td>73.5</td>
<td>98</td>
<td>122.5</td>
<td>147</td>
<td>171.5</td>
<td>196</td>
<td>220.5</td>
<td>245</td>
<td>269.6</td>
<td>295.7</td>
</tr>
</tbody>
</table>

Graph 9: Comparison of mass transfer scheme simulations with the Purdue, Gustafson and Andersson models

It should be noted that the chemical reactions in laboratory Kraft cooking experiments are not identical to those in typical industrial pulp reactors. The kinetics of delignification in Gustafson’s model are widely considered to be more reliable than those in the Andersson and Purdue models, (Rantanen (2006). The cooking reactions are much more rapid in the Andersson model than in the other models. The lignin level in the Andersson model falls to 5% in a much shorter time than in the Gustafson and Purdue models. One of the FVM models (R11-D0.00288) agrees well with the Purdue and Gustafson models after 120 min of operation. It should be noted that the reaction rate may vary for different wood species.

According to Rantanen, a number of difficulties were encountered when the industrial cooking model was constructed using the Gustafson approach. Original parameters of the model were sensitive to factors such as temperature changes, unmeasurable variables and disturbances in process conditions. These problems were solved by optimizing the parameters and making adjustments to the model.

FVM has several advantages over current CSTR models. FVM is a physical model that provides the opportunity to model the industrial digester and develop the reactions inside the digester. Unlike the CSTR approach the post processing of FVM provides the opportunity to visualize the results and...
analyze the cooking process. It offers a wider space to analyze and picture physical phenomena, calculate the development of the reaction at any particular point in the digester (i.e. the gradient of the reaction), modify the dimensions of the digester, and optimize the cooking reaction. The influence of the dimensions of the digester and flow regimes on the local chemical reactions in the digester are also taken into account in the FVM.

Looking at the digester from a holistic perspective, from the analysis of the different sub-mechanisms it is apparent that if a channel forms, flow is redistributed towards the channel. This means that the liquid is not uniformly distributed to all chips. Lignin dissolution is therefore affected as the temperature may be too low or too high as the liquid flows and thus the chemicals are unevenly distributed. This means that less lignin is dissolved overall as the chemicals are consumed more rapidly. The diffusion of lignin is also limited as its concentration inside the wood chips increases as a result of limited flow of liquor. These effects lead to an increased Kappa number for the wood chips around the channel, while those very close to the channel have a much smaller Kappa number than intended, resulting in weaker cellulose fibres.

From the models we can predict how sizes and positions of channels affect the overall process, and the concentrations and temperatures that result at the circulation loops as a function of the channels. This is the practical application of the work presented in this thesis.

This possibility takes modelling significantly further than existing reports in the literature, and can be used as a tool to learn more about what goes on inside the huge reactor.

This approach can be used in design of digesters, but its primary intended application is for operational diagnostics. For example, a PLS model for the different screens from simulations using the CFD model in many different operational modes such as normal operating conditions, and with different channels, production rates etc. can be used for on-line process control.
Chapter 13: Conclusion

1. A new solution technique (Differential Analysis and FVM) is applied to pulping process modelling, as opposed to the conventional approaches (CSTR and PFR).

2. A new solution for pulping process reactions which is an alternative to Arrhenius and chemical balance methods is also introduced in the thesis. This approach should be applicable in other types of separations of multi-component solutions and combinations of chemical solutions. Progress of the pulping reaction is predicted without using variables such as the rate of reaction, activation energy, Arrhenius constants and reaction balance.

3. An undesirable process phenomenon called channelling is identified numerically. This is novel in modelling of the pulping digester. This occurs when using FVM solution of differential equations of the pulping process.

4. A new design of pulping digester is applied for modelling purposes. The screens are included in this design and the real volume of the digester is accounted for in the computations.

5. Phase separation which takes place in the screens of the digester is numerically developed. This is an outcome of using differential analysis and FVM and is novel in digester modelling.

**Question 1:** Is it possible to develop a new spatial model to increase understanding of the process, that unlike existing models pictures the pulping process and handles fluid dynamics and chemical reactions at every point inside the digester in 3D or 2D?

**Question 2:** Is it possible to model the failures in operation or undesirable phenomena (channelling) that take place in the digester in order to understand and control them?

**Question 3:** Can CFD models be used for future treatments and optimization of the process? Can the consequences of changing boundary conditions or chemical substances be observed in the established model?

**Question 4:** Can a numerical model provide a foundation for on-line applications?

**Response to Question 1:**

Such a model is possible. It is however dependent on the available resources, because 3D modelling of this type of digester requires a mesh of 1.8 billion cells. Assuming that computer can model one million cells, one thousand eight hundred computer units in a parallel network would be required to represent the digester in 3D. For this reason, a 2D model is established instead.

Furthermore I have shown how the reactions are influenced by flow velocity and position in the Results chapter.
Response to Question 2:

1- See point 3 above.

2- The simulations revealed that a higher Kappa number is reached in positions where the chip flow rate is higher than in the surroundings. This has serious consequences in cases where channelling occurs. Pressure at the circulation pipes is also likely to be affected. This area needs further investigation in order to characterize and control this fault.

Response to Question 3:

Yes, different results obtained from our simulations under four different conditions demonstrate the potential of the models for optimization purposes and their sensitivity to changes in the boundary conditions.

Response to Question 4:

This is possible but it depends on the type of information and the form (whether absolute or average value) in which it is needed for on-line applications.

The performances of a number of multiphase flow schemes were compared to examine whether these procedures could be extended for different applications.

Our results show that the Eulerian approach is capable of separating the phases. It is possible to define individual variables of the phases in the cell zones making it possible to manipulate the composition of the phases at specific locations. These conditions are not available when using the mixture model and therefore management of the critical variables of the individual phases in the specified cell zones is difficult when the mixture model is selected.

The porous model produces comparable results to the multiphase models and does so cost effectively. It can be used as a complementary computational tool when properties such as compression have to be defined.

The species transport with reaction scheme is able to model the mass balance equation and stoichiometry of the pulping reaction. It is thus able to compute the total pulp production, yield, and hydroxide consumption.

Species transport and reaction scheme conjugated with porous media can complement other approaches when modelling the pulp production. Application of this model can help the researcher and pulping mill to improve their knowledge of the pulping reactions and advance new strategies to control the pulping process.

In the thesis and the enclosed papers I have discussed how to model different aspects of the digester. The results show that it is not possible to use a single model for all tasks. Different setups are needed to analyse the different phenomena, and their applications are described. The thesis also describes formulation of boundary conditions with a special emphasis on modelling extraction of liquids through the screens without also letting the chips out. Also considered here is a solution that uses varying porosity between channels and the bulk flow to describe channelling.

CFD models for large reactors, and specifically for pulp digesters, have used the models to increase understanding of events inside the reactor given the practical impossibility of chemical monitoring inside the digester.

An extensive CFD code of a continuous pulp digester using the finite volume method has been constructed in FLUENT to deal with the physical and chemical characteristics of the delignification
process. The dynamic characteristics of the flow, delignification and channelling phenomena have been modelled with the aim of process control, management and optimization.

By simulating different faults and monitoring their outcomes, and monitoring the flow out of the reactor, informed guesses can be made about faults that may occur in the digester. Faults of special interest are channelling and hang-ups in the digester.

The designed numerical model demonstrates the potential of using the finite volume method to model large scale pulp production. Modelling of the pulping digester including flow behaviour, chemical reactions and pulp quality was performed mathematically under steady state conditions.

When combining a fluid dynamic and chemical reaction model, different disturbances such as hang ups and channelling can be studied.

Numerical modelling of reaction kinetics and elementary characteristics of the multiphase flows have been used to predict cooking of the wood chips.

Prediction of the characteristics of the critical parameters of the process such as Kappa number, distribution of the lignin dissolution, black liquor production, hydroxide degeneration, and pulp production have formed the bulk of this research.

Modelling of the delignification, and control and optimization of the chemical process enables prediction and reduction of destructive phenomena such as channelling of the liquor flow through the chip bed.

Furthermore, implementation of the FLUENT codes for the cooking of chips enables optimization of the digester geometry and informs new designs to reduce the risk of faults occurring.

The multiphase strategy along with the mass transfer, volumetric species transport and reaction kinetics is used to model the continuous pulping process reaction. Pulp quality is evaluated by predicting the Kappa number.

The mass transfer multiphase strategy enabled the construction of a code to model the pulping chemical reaction.

The results indicate that the multiphase model, the species transport and mass transfer models are able to accurately predict the pulping chemical reactions inside the digester. Moreover, these schemes can provide a good tool for evaluation of pulp quality.
Future work

The intention is to use the CFD model developed here as a reference to learn more about what is happening inside the digester. In the next phase we would like to use simpler on-line models for diagnostic purposes where the complex CFD model is used to identify expected results for the different type of up-sets and faults. It is also relevant to identify the flow behaviour at the entrance of the discharges and circulation pipes by implementing the operational pressure data in the CFD model to make a comparison it with the presence of channelling.

The presence of pressure measurement instruments at some locations in the digester in combination with prediction of the pressures at the MCC, ITC and other outlets with and without the channelling using CFD modelling can help the operators to manage and avoid undesirable events in the digester.
References


Appendix A: Other governing equations

Mixture density (Mixture model- Paper 1)
\[ \rho_m = \sum_{k=1}^{n} \alpha_k \rho_k \]  \hspace{1cm} (49)
\[ \alpha_k \] : Volume fraction of phase k

Reduced mixture momentum equation- steady state (Mixture model-Paper 1)
\[ \nabla \cdot (\rho_m \vec{v}_m \vec{v}_m) = -\vec{v}p + \nabla \cdot [\mu_m (\nabla \vec{v}_m)] \]
\[ + \rho_m \ddot{\vec{F}} + \nabla \cdot \left( \sum_{k=1}^{n} \alpha_k \rho_k \vec{v}_{dr,k} \cdot \vec{v}_{dr,k} \right) \]  \hspace{1cm} (50)
This equation is developed in the Cartesian coordinate system and is obtained for the mixture. Mass transfer and porous modelling were not conducted for the Mixture model simulation.
\[ \ddot{F} \] : Body force
\[ \mu_m \] : Viscosity of the mixture
\[ \mu_m = \sum_{k=1}^{n} \alpha_k \mu_k \]  \hspace{1cm} (51)
\[ \vec{v}_{dr,k} \] : drift velocity for secondary phase k
\[ \vec{v}_{dr,k} = \vec{v}_k - \vec{v}_m \]  \hspace{1cm} (52)

Slip velocity- steady state (Mixture model-Paper 1)
The slip velocity is the difference between the bulk flow and dispersed flow velocities or the difference between the velocities of two phases.
\[ \vec{v}_{pq} = \vec{v}_p - \vec{v}_q \]  \hspace{1cm} (53)

Solids shear viscosity (Granular viscosity) (Paper 1)
The viscosity of a suspension which is a mixture of solid and liquid phases depends largely on the concentration of the solid particles in the mixture.
The particle momentum is generated due to particle motion in the bulk flow. There is a momentum exchange between the moving particles and the bulk flow. The viscosity of the suspension is accounted for by the average weighted volume which consists of the viscosity of the solid and viscosity of the liquid.
The solid shear viscosity consists of three viscosities that arise from collisions of solid particles, kinetics of the particles and the friction between them. There is also friction between the solid particles and the liquid flow. The granular viscosity term is used to account for the viscosity of the suspension.

\[ \mu_s = \mu_{s,\text{col}} + \mu_{s,\text{kin}} + \mu_{s,\text{fr}} \]  

 Collisional viscosity (Paper 1)

\[ \mu_{s,\text{col}} = \frac{4}{5} \alpha_s \rho_s d_s g \sigma_{0,ss} (1 + e_{ss})\left(\frac{\theta}{\pi}\right)^{1/2} \]  

 Kinetic viscosity (Syamlal et al. Eq.) (Paper 1)

\[ \mu_{s,\text{kin}} = \frac{\alpha_s d_s \rho_s \sqrt{\nu \pi}}{6 (3 - e_{ss})} [1 + \frac{2}{5} (1 + e_{ss}) (3e_{ss} - 1) \alpha_s g \sigma_{0,ss}] \]

 Frictional Viscosity (Paper 1)

Friction between the particles is relevant in the mixture whenever the volume fraction of the solid phase approaches the packing limit. Stress is generated at this point due to friction between the particles.

The Schaeffer expression for frictional viscosity can be defined.

\[ \mu_{s,fr} = \frac{P_s \sin \theta}{2 \Sigma} \]

where \( P_s \) is the solids pressure, \( \theta \) is the angle of internal friction which is 30 by default. \( \Sigma \) is the second invariant of the deviatory stress tensor.

\[ \Sigma = \sigma_{xy}^2 + \sigma_{yz}^2 + \sigma_{xz}^2 - \sigma_{xx} \sigma_{yy} - \sigma_{yy} \sigma_{zz} - \sigma_{zz} \sigma_{xx} \]

 The value of the stress tensor can be calculated in a coordinate system that has been rotated or translated with respect to the original coordinate system. Several properties of the stress tensor remain unchanged by a change in coordinates. These properties are called invariants.

 Collisional dissipation of energy (Paper 1)

The collisional dissipation of energy \( \gamma \theta_s \) represents the rate of energy dissipation within the solid phase due to collisions between particles. This term is represented by the expression derived by Lun et al.

\[ \gamma \theta_m = \frac{12(1 - e_{ss}) g \sigma_{0,ss}}{d_s \sqrt{\pi}} \rho_s \alpha_s \sigma_s^2 \theta_s^{3/2} \]
Kinetic energy of random fluctuations in particle velocity (Paper 1)

The transfer of the kinetic energy from random fluctuations in particle velocity from the solid phase to the fluid or solid phase is calculated from:

$$\Phi_{is} = -3k_{is}\Theta_s$$  \hspace{1cm} (60)

$\Theta_s$ is the granular temperature

The following options are available in FLUENT to solve for the granular temperature:

1- The default option is an algebraic formulation which neglects the convection and diffusion terms in the transport equation.

2- Granular temperature is constant. This is a very good approximation when the volume fraction of the solid particles in the solution is high, as this leads to negligible random fluctuations.

3- Granular temperature is defined by a User Defined Function (UDF).

Solids pressure (Paper 1)

In suspension solutions or granular flows, the motion of the particles establishes a pressure gradient in the solution if the packing limit of the solid is less than 0.63, which is the maximum allowable value.

When the packing limit is less than 0.63, the solid phase is compressed and a pressure gradient of the solid particles ($\nabla p_s$) is produced independently. This term is omitted from momentum equation for solid phase if the specified packing limit is 0.63. The pressure gradient is included in the granular momentum term. The solid particles follow the Maxwell-Boltzmann probability distribution, and the kinetic energy of the particles represented by the granular temperature is included in the solids pressure equation and viscosity.

The solids pressure is composed of a kinetic term and a second term that accounts for particle collisions:

$$p_s = \alpha_s p_s \Theta_s + 2p_s(1 + e_{ss})\alpha_{ss}^{2}g_{0,ss}\Theta_s$$  \hspace{1cm} (61)

e_{ss} is the coefficient of restitution for particle collision. The default value for $e_{ss}$ is 0.9.

The transition from the compressible condition to the incompressible condition is managed by a distribution function. When the maximum packing limit of the solid (0.63) is reached, the solid flow is incompressible but when it is less than 0.63 the solid phase is compressible and the distance between the particles can be reduced. $g_{0,ss}$ is the radial distribution function.

Radial distribution (Paper 1)

When the volume fraction of the solid phase is at the maximum value, the probability of collision of the solid particles may need to be modified. This function assumes the particles have spherical forms:

$$g_0 = \frac{s+d_p}{s}$$  \hspace{1cm} (62)

$s$ here is the distance between the spherical particles.
Bulk Viscosity-(Paper 1)

The resistance of the solid particles to compression and expansion is expressed by the bulk viscosity. The expression for bulk viscosity is (Lun et al):

\[ \lambda_s = \frac{4}{3} \alpha_s \rho_s d_s \mathbf{g}_{0,ss} (1 + \varepsilon_{ss}) (\mathbf{g}_s / \pi)^{1/2} \] (63)

**The material density ratio**

\[ \gamma = \frac{\rho_{\text{Dispersed phase}}}{\rho_{\text{Carrier phase}}} \] (64)

This expression was used to evaluate the multiphase flow models.

Average distance between the individual particles and particle loading (Paper 1)

\[ \frac{L}{d_d} = \left( \frac{\pi + k}{\alpha_k} \right)^{1/3} \] (65)

\[ k = \frac{\theta}{\gamma} \] (66)

Elasticity modulus (Paper 1)

\[ G = \frac{\partial p_s}{\partial a_s} \quad G \geq 0 \] (67)

A derived elasticity modulus is set up in the model.

Reduced form of the granular temperature (Paper 1)

Granular temperature is the kinetic energy of random motion of particles which is produced as a result of fluctuation velocity. Velocity fluctuations of solids are much smaller than their mean velocity. The kinetic part of solids fluctuation is anisotropic. Velocity fluctuations of solids quickly dissipate as heat as a result of inter-particle collision.

\[ \frac{3}{2} \rho_s \left( \nabla \cdot (a_s \mathbf{v}_s \Theta_s) \right) = \left( -p_s \mathbf{l} + \mathbf{g}_s \right) \cdot \nabla \mathbf{v}_s + \nabla \cdot \left( k_{ss} \nabla \Theta_s \right) - \gamma \Theta_s + \Phi_{ts} \] (68)

1- Energy is generated due to the velocity distribution of the solid particles, which generates the solid normal stress and solid shear stress distribution in the momentum equation of the solid phase: \(-p_s \mathbf{l} + \mathbf{g}_s\) \cdot \nabla \mathbf{v}_s this term is sometimes called viscous dissipation heating. This quantity describes the degradation of mechanical energy into thermal energy which results in the temperature rise in the system. In isothermal systems no appreciable temperature change is expected to result from expansion, contraction or viscous dissipation, Byron Bird (2001).

Shear stress tensor formulation is defined as follows

\[ \mathbf{t} = \mu \left[ \left( \nabla \mathbf{v} + \nabla \mathbf{v}^T \right) - \frac{2}{3} \mathbf{v} \cdot \mathbf{l} \right] \] (69)

\( \mathbf{v}^T \) is the symmetric matrix of the velocity tensor or transpose of the velocity gradient tensor. \( \mathbf{l} \) is the first invariant of stress tensor or unit tensor. If we describe \( \mathbf{l} \) as \( \delta_{ij} \) then the Kronecker delta is zero if \( i \neq j \) and 1 if \( i = j \). Several properties of the stress tensor remain unchanged
following a change in coordinates. These properties are called invariants. \( \nabla \cdot \vec{v} \) is the divergence of velocity vector.

\[
I = \sigma_{xx} + \sigma_{yy} + \sigma_{zz} \tag{70}
\]

2- \( k_{\Theta_s} \) is the diffusion coefficient or granular temperature conductivity, and \( k_{\Theta_s} \nabla \Theta_s \) is the diffusion of energy.

3- Collisions between particles cause a dissipation of energy. This term is denoted by \( \gamma \Theta_s \), where \( \Theta_s \) is the granular temperature. \( \gamma \) is the heat capacity ratio.

4- The motion of the particles in the bulk flow leads to an energy exchange between them. The energy of the solids may be dissipated by physical interactions with the fluid. This term is denoted by \( \Phi_{ls} \) which is also related to the granular temperature.

The solid energy may also be dissipated to the fluid due to solid fluctuations.

**Eulerian equations**

The source terms added to mass and momentum equation due to mass transfer (Papers 2, 4)

If species \( i \) is transferred from a multi-component phase \( p \) to the bulk or any species such as \( j \) of phase \( q \) then

\[
m_q = -m_{piqj} \tag{71}
\]

\( m_{piqj} \) is the mass transfer rate per unit volume from species \( i \) of phase \( p \) to species \( j \) of phase \( q \).

For phase \( q \):

\[
m_q = m_{piqj} \tag{72}
\]

There is no momentum source in the cells for VOF and Mixture model but momentum source for Eulerian scheme for phase \( p \) is

\[
m_p \vec{u}_p = -m_{piqj} \vec{u}_p \tag{73}
\]

And for phase \( q \) is

\[
m_q \vec{u}_q = m_{piqj} \vec{u}_p \tag{74}
\]

Porous momentum sinks source term (Papers 1, 2, 3, 4, and 5)

Porous media contributes to reduced flow velocity due to generation of a pressure gradient in the cell zones. This is taken into account by an additional source term in the fluid flow equations. The source is a flow resistance and consists of two terms that are determined empirically. A viscous and an inertial loss term are included in the momentum equation in the porous cell zones.

\[
S_i = -\left( \sum_{j=1}^{2} D_{ij} \vec{V}_j + \sum_{j=1}^{3} C_{ij} \frac{1}{2} \rho |\vec{V}_j| \right) \tag{75}
\]
In our simulations this expression was reduced to the following form in the multiphase models:

\[ S_i = - \sum_{j=1}^{2} \alpha_i C_{ij} \rho_j |v_{ij}| \]  

(76)

Mass transfer and continuity (Papers 2, 4)

\[ \dot{m}_{pq} = \max \left[ 0, \lambda_{pq} \right] - \max \left[ 0, -\lambda_{pq} \right] \]  

(77)

\[ \lambda_{pq} = \dot{r} \alpha_p y_{pi} \rho_p \]  

(78)

Phase \( p \) is a mixture material and mass transfer is defined for species \( i \) of this phase. \( \dot{r} \) is a constant rate of particle shrinking or swelling such as the rate of burning of a liquid droplet. This is not available for VOF scheme. \( y_{pi} \) is the mass fraction of species \( i \) in phase \( p \).

The continuity in a Cartesian and 2D axisymmetric system under the steady state condition for multiphase flow involving mass transfer:

\[ \nabla \cdot (\alpha_q \rho_q v_q) = (\dot{m}_{pq}) \]  

(79)

\[ \frac{\partial}{\partial x} (\alpha_q \rho_q v_{qx}) + \frac{\partial}{\partial r} (\alpha_q \rho_q v_{qr}) + \frac{\alpha_q \rho_q \nu_{qr}}{r} = (\dot{m}_{pq}) \]  

(80)

The porous effect appears in the momentum equation. The N-ARY Summation is removed because there are only two phases in our system and mass transfer takes place between these two phases.

Conservation of momentum for the solid phase, general form (Eulerian model-Paper 1)

The hydrodynamic characteristics of the phases in the digester were investigated using the Eulerian model. The chemical reaction is not computed in this paper. Neither porous nor mass transfer is included.

\[ \rho_s \nabla \cdot (\alpha_s \tilde{v}_s \tilde{v}_s) = -\alpha_s \nabla p - \nabla p_s + \nabla \tilde{r}_s + \alpha_s \rho_s \tilde{g}_s + (\tilde{F}_s + \tilde{F}_{\text{lift},s} + \tilde{F}_{\text{vm},s}) \]  

(81)

\( p_s \) is the solids pressure and \( \tilde{r}_s \) is the solid phase stress. The intensity of the particle velocity fluctuations determines the stresses, viscosity, and pressure of the solid phase.

Conservation of energy, incompressible flow, Eulerian model (Papers 2, 4, 5)

An enthalpy equation is solved for each phase in the multiphase flow models, to express the conservation of energy in the model. However, the temperature is held constant through the simulations.

\[ \nabla \cdot (\alpha_q \rho_q u_q h_q) = -\alpha_q \frac{\partial p_q}{\partial t} + \tilde{r}_q : \nabla u_q - \nabla q_q + S_q + \sum_{p=1}^{n} (Q_{pq} + \dot{m}_{pq} h_{pq} - \dot{m}_{qp} h_{qp}) \]  

(82)
The Laminar Finite-Rate Model (Paper 5)

The laminar finite-rate model computes the chemical source terms using Arrhenius expressions, and ignores the effects of turbulent fluctuations. This formulation is accurate for laminar flows. The Arrhenius equation is non-linear and this non-linearity makes its application problematic for turbulent flows. In species transport models the reaction occurs in the continuous phase between the species.

The net source of any chemical species due to chemical reactions is computed as the sum of the Arrhenius reaction sources over the \( N_R \) reactions that the species participates in.

\[
R_i = M_{w,i} = \sum_{r=1}^{N_R} \hat{R}_{i,r} \tag{83}
\]

Where \( M_{w,i} \) is the molecular weight of species \( i \) and \( \hat{R}_{i,r} \) is the Arrhenius molar rate of creation/destruction of species \( i \) in reaction \( r \). \( N_R \) is the number of reactions. Reactions may occur in the continuous phase between continuous-phase species only, or at wall surfaces resulting in the surface deposition or evolution of a continuous-phase species.

Molecular diffusion (Paper 5)

For a multi component solution molecular diffusion of a species is the net transport of that species from a region of higher concentration to one of lower concentration by random molecular motion.

The diffusion results in a gradual mixing of material, complete mixing or equilibrium state in the absence of external forces on the species in the multi component solution. The diffusion may be expressed using Fick’s law, which expresses the relationship between the diffusive fluxes and the concentration. The flux of a species is from a region of high concentration to a region of low concentration.

\[
J = -D \frac{\partial \rho}{\partial x} \tag{84}
\]

\( J \) is defined as the diffusive mass flux of a species in the solution and is expressed in \( \text{kg/m}^2\cdot\text{s} \). \( J \) is a measure of the amount of a substance that moves by diffusion per unit time and area perpendicular to the direction of transfer.

\( D \) is the diffusion coefficient or mass diffusivity and is expressed in \( \text{m}^2/\text{s} \). At low solute concentrations, the diffusion increases with temperature. The mechanism of the diffusion of gases, liquids, and solids in solids is complicated and a general theory is not available. The diffusion is also dependent on the viscosity of the solution and is proportional to the squared velocity of the particles. The driving force for diffusion is the concentration gradient \( (\nabla \rho) \).

Species source (Paper 5)

The species source in a cell for species \( i \) of phase \( p \) is expressed as

\[
m_p^i = m_{pqi} \tag{85}
\]
Species transport incompressible multiphase-(Paper 5)

Only the laminar finite-rate, finite-rate/eddy-dissipation and eddy-dissipation/turbulence-chemistry models of homogeneous reactions are available for multiphase species transport.

For each phase $k$, the local mass fraction of each species $Y^k_i$ is predicted by solving a convection-diffusion equation for that species.

The generalized chemical species conservation equation when applied to multiple mixtures under the steady state condition is

$$\nabla \left( \rho^q C_q \nabla Y^q_i \right) = -\nabla \cdot \left( \rho^q \nabla Y^q_i \right) + \alpha^q R^q_i + \alpha^q S^q_i + \sum_{p=1}^{n} (\bar{m}_{p}^{q} Y^q_i - \bar{m}_{q}^{p} Y^q_j) + R$$  \hspace{1cm} (86)

$R$ is the heterogeneous rate of reaction and $R^q_i$ is the net rate of production of homogeneous species $i$ by chemical reaction for phase $q$. $\bar{m}_{p}^{q}$ is the mass transfer source between species $i$ and $j$ from phase $q$ to $p$. $S_i$ is the rate of creation by addition from the dispersed phase.

Turbulent equations

Turbulent kinetic energy of incompressible liquids (Paper 1)

No source terms are added for turbulence quantities due to mass transfer between the phases. However it is possible to do so using the user defined source terms but due to low flow velocity, zero or ignorable slip velocity, and the porous media effect these terms are neglected.

$$\rho \frac{\partial}{\partial t_k} (k \epsilon_k) = \frac{\partial}{\partial \xi_k} \left[ \left( \frac{\mu_k}{\sigma_k} \right) \frac{\partial k}{\partial \xi_k} \right] + G_k + G_b - \rho \epsilon - \gamma M + S_k$$  \hspace{1cm} (87)

Turbulent dissipation rate of incompressible liquids (Paper 1)

$$\rho \frac{\partial}{\partial t} \left( \epsilon \epsilon \right) = \frac{\partial}{\partial \xi} \left[ \left( \frac{\mu_k}{\sigma_k} \right) \frac{\partial \epsilon}{\partial \xi} \right] + C_1 \frac{\epsilon}{k} (G_k C_3 \epsilon G_b) - C_2 \rho \epsilon \frac{\epsilon^2}{k} + S_\epsilon$$  \hspace{1cm} (88)
Appendix B: Calculations of Paper 5

The following data are used for the tuning of the model:

**Pine chips**

**Inlet mass flow:**

\[ \dot{m}_W = 160 \text{ ton/h} \quad \text{Wet wood chips: [60 % dry concentration]} \]

\[ \dot{m}_D = 96 \text{ ton/h} \quad \text{Dry wood chips} \]

Wood chips (Dry) = 96000 kg/h  
Liquor flow: 1000 m³/h

Fibres = 70 %  
Lignin = 20 %  
Rest = 10 %

Fibre flow inlet \( \dot{F}_{\text{in}} = 67000 \text{ kg/h} \), Lignin flow inlet \( \dot{L}_{\text{in}} = 19000 \text{ kg/h} \), Rest flow \( \dot{r} = 10000 \text{ kg/h} \)

**Outlet Mass flow: Pulp**

Product = 51 ton/h  
pulp (90 % dry concentration)

0.9 \times 51 = 45.9  
ton dry pulp / h

**Outlet mass flow: Lignin & Fibres content of Pulp**

Kappa number = 24  
(Pulp): F-L  
F = Fibres (Cellulose + Hemicellulose)  
L = Lignin

\[ 24 \times 0.15 = 3.6 \% \text{ Lignin content in the pulp} \]

\[ \dot{L}_{O-P} = 45900 \times 3.6 \% = 1650 \text{ kg/h Lignin} \]

\[ \dot{F}_{O-P} = 45900 \times 1650 = 44250 \text{ kg/h Fiber} \]

**Outlet mass flow: Fibers & Lignin content of Black liquor**

\[ V F L r \quad V = \text{White liquor (OH-)} \quad F = \text{fibres (Cellulose + Hemicellulose)} \quad L = \text{Lignin} \]

\[ r = \text{Rest material} \]

\[ \dot{F}_{O-B} = 67000 \times 1650 = 22750 \text{ kg/h} \]

\[ \dot{L}_{O-B} = 19000 \times 1650 = 17350 \text{ kg/h} \]
Inlet mole flow: Fibers & Lignin content of wood chips

\[ \dot{F}_{\text{in}} = \frac{67000000 \text{g}}{176 \text{mol}} = 380682 \text{ mol/h} \]

\[ \dot{L}_{\text{in}} : \frac{19000000}{197} = 96446.7 \text{ mol/h} \]

Outlet mole flow: Fibers & Lignin content of pulp (F-L)

\[ \dot{F}_{\text{o-p}} = 44250000 \text{ g/h} \quad \dot{L}_{\text{o-p}} = 1650000 \text{ g/h} \quad \dot{F}_{\text{o-p}} = \frac{44250000}{176} = 251420.5 \text{ mol/h} \]

\[ \dot{L}_{\text{o-p}} = \frac{1650000}{197} = 8375.6 \text{ mol/h} \]

Outlet mole flow: Fibers and Lignin content of black liquor: F-L-V-r

\[ \dot{F}_{\text{o-b}} : \frac{22750000}{176} = 129261.4 \text{ mol/h} \quad \dot{L}_{\text{o-b}} = \frac{17350000}{197} = 88071 \text{ mol/h} \]

Mass flow balance

\[ \dot{F}_{\text{-r}} + V \longrightarrow \dot{F}_{\text{-l}} + \dot{F}_{\text{-l-v-r}} \]

67000- 19000-10000 kg/h + 1000000 \quad \longrightarrow \quad 44250-1650 \text{ kg/h} +22750-17350-1010000 \text{ kg/h} \]

Mole flow balance: F & L

\[ \dot{F}_{\text{-r}} + V \longrightarrow \dot{F}_{\text{-l}} + \dot{F}_{\text{-l-v-r}} \]

380682 - 96446.7 mol/h \quad \longrightarrow \quad 251420.5-8375.6 + 129261.4 -88071 mol/h

The accounted inlet and outlet flows and mole flow balance are used for mass transfer modelling. The following calculations are applied to kinetic reaction modelling and prediction of distribution of reactions.

Reaction kinetics

Residence time in the digester = 4-4.5 h

Initial | Cellulose + Hemicellulose| content: 380682 moles

Final Cellulose + Hemicellulose content: 251420.5 moles

Residence time = reaction time=4.5 h \quad \Delta T = 4.5 \times 3600 = 16200 s

\[ \frac{dF}{4.5 \times 3600} = 7.8 \text{ mol/s} : \text{Number of moles per second of reaction time} \]

Inlet lignin content at \( t_0 = 96 \text{ 446} \), 7 moles: lignin content of the wood before reaction

Outlet lignin content at \( t_f = 8375.6 \) moles: lignin content in the pulp (in the wood (pulp) after reaction)
Lignin content in the black liquor = 88071 moles

Residence time = reaction time = 4.5 h \[ \Delta T = 4.5 \times 3600 = 16200 \text{ s} \]

\[ \frac{d[L]}{dt} = \frac{88071}{16200} = 5.4 \text{ mol/s} \]

Number of moles per second of reaction time

Inlet dry chips = 96 ton/h

Density of the dry chips = 500 kg/m³

Inlet volume of the wood chips which is 192000 l/h (base was already accounted per hour and thus 192000 l is used = inlet volume)

\[ r = \frac{d[F]}{dt} = \frac{7.8}{192000} = 4.1 \times 10^{-5} \text{ mol/l.s} \]

Inlet conc. of (Cellulose + Hemicellulose): \[ [F] = 380682 \text{ mol/192000 l} = 1.983 \text{ mol/l} \]

\[ r = \frac{d[F]}{dt} = k(T)[F] \quad 4.1 \times 10^{-5} \text{ mol/l-s} = k(T) \quad 1.983 \quad k(T) = 2.07 \times 10^{-5} \text{ s}^{-1} \]

Concentration of lignin in the inlet wood flow:

\[ d[L] = 5.4 \text{ mol/s} \]

\[ r = \frac{d[L]}{dt} = \frac{5.4}{192000} = 2.8 \times 10^{-5} \text{ mol/l.s} \]

Nr of moles of L at t₀ at inlet flow = 96 446. 7 moles lignin content of the inlet wood flow

\[ [L]=96446.7\text{mol/192000l} = 0.5 \text{ mol/l} \]

\[ r = \frac{d[L]}{dt} = k(T)[L] \quad 2.8 \times 10^{-5} \text{ mol/l.s} = k(T) \quad 0.5 \quad k(T) = 5.6 \times 10^{-5} \text{ s}^{-1} \]

Activation energy

If \( T_1 = \) initial temperature of the chips is 30 °C \( T_2 = \) reaction temperature = 160 °C

Hard wood (OAK, MAPLE): \( C_p = 1255 \text{ J/kg. K} \)

Soft wood (FIR, PINE): \( C_p = 1380 \text{ J/kg. K} \)

\( m = 1 \text{ kg} \quad \text{Ea} = m \ C \ \Delta T \quad \text{Ea} = 1380 \times 130 = 180000 \text{ J/kg} \quad \text{Ea} = 180 \text{ J/g} \)

Pre exponent factor: Fibers

\[ \text{T} = 160 \text{ °C} = 433 \text{ K} \]

\[ k(T) = A \ e^{\frac{-E_a}{RT}} \]

\[ 2.07 \times 10^{-5} = A \ e^{\frac{-180 \times 176}{(8.31)(433)}} \quad A = 0.14 \text{ s}^{-1} \quad k(T) = 0.14 \ e^{\frac{-3812}{T}} \] Fibers
Pre-exponent factor: Lignin

\[ T = 160 \, ^\circ C = 433 \, K \quad E_a = 180 \, J/g \quad k(T) = A e^{-\frac{E_a}{RT}} \]

\[ 5.6 \times 10^{-5} = A e^{\frac{-180}{8.31(433)}} \]

\[ A = 1.1 \, s^{-1} \quad k(T) = 1.1 \, e^{-\frac{4267}{T}} \quad \text{Lignin} \]
Pre-exponent factor: Lignin

$T = 160 \, ^{\circ}C = 433 \, K$  
$E_a = 180 \, J/g$

$A = 1.1 \, s^{-1}$

Paper I
Abstract
This paper describes the use of a CFD multiphase model using finite volume method, FLUENT, to aid understanding of the physical behavior of solid and liquid flows in the digester of the pulping process. We take into consideration the mass balance of the multi-inlets, outlets and circulation flows in the digester. We also look at the application of a Porous media model to describe the dynamic behavior of the liquor flow through a bed of solid particles. The cylindrical Korsnas/vallvik pulping digester in Sweden is represented in the models as an axisymmetric two-dimensional model, which includes multiple feeds, outlets, pressure adjustment outflows and circulation pipes. The compaction of the wood chips is also considered in the modeling. In the Porous model, the digester is divided into sections of different porosity, and the behavior of individual suspension particles is not considered. The bulk of this paper concerns modeling mass balances and phases of the mixture in the digester using Eulerian and Mixture strategies.

Introduction
The aim of this paper is to develop a detailed CFD model of the digester in the pulping process that can be used as a reference for simpler models which will be used for on-line diagnostic purposes. The CFD model will also be used to better understand events inside the digester. These events cannot be observed directly, but the results of these events may be measured indirectly. If channeling, hang ups and other events occur, and are included in a
model we should be able to predict their effects at the blow line with respect to Kappa number, free alkali and dissolved lignin in the extraction line. In this paper we present a detailed model describing the normal operations of the digester. Different methods for the formulation of the problem and their solution are discussed.

Prediction of the hydraulic behavior of the pulp and paper digester is the driving force behind this paper. A survey of the literature reveals a shortage of data concerning hydraulic and chemical reaction modeling of the total digester using FLUENT. Simpler models have been developed using other modeling tools such as the Purdue model described by Smith and Williams (1974), where the digester is approximated by a series of continuous stirred-tank reactors (CSTRs) in which the solid phase consists of five species that react with the white liquor. Other researchers followed with improvements and modifications. Some, such as Gustafson et al (1983) assumed that wood was composed of two main compounds. Harkonen (1987) and Michelsen (1996) also extended the earlier work and developed models for the Kamyr continuous digester. The numerical solution of the Natercia (2000) model is based on a non uniform discretization procedure to improve handling of the geometry. Wisnewski et al (1997) also employed the CSTRs in his model, but used a different set of equations and assumptions. Pougatch et al (2006) implemented a solid tangential stress sub-model of the digester. Christensen et al (1983) developed a similar model for hardwood and softwood swings. A number of researchers have attempted to simulate the motion of fibers. Olson (2001) studied the motion of fibers in turbulent flows using a probability distribution function of fiber orientation and position throughout the suspending fluid. Yokogawa et al (1985) analyzed the pulp suspension in turbulent flow regime and studied the relationship between the turbulent intensity and fiber concentration.


The wood chips are treated as granular in our modeling. A few researchers such as Lanre et al (2002), Benington (1991) and Bhole (2009) used the granular multiphase scheme of the CFD codes exclusively in the stirred tank application to predict the pulp suspension behavior.
Forest et al (2003) investigated the wet granulation and Granule growth that may occurs when granules collide and stick together to form larger granules. In this study we are not going to deal with Granule growth.

Fu Pingle (1998) investigated the pulp suspension in the circular pipes. He considered the pulp slurries as a two-phase system and studied the slurries by the fibers behavior in the system.


The three phase state, i.e. gas, liquid and fiber, is significant in the pulping process following the digester when the lignin content of the wood chips is diminished to less than about 3 percent, and has been widely studied.

The ingredients of the pulping from a physical point of view are mainly solid and liquid phases irrespective the type of the wood species and constituents of the phases. The liquid flow takes part in the circulations and discharges while the solid phase only flows downward through the digester. Screens are mounted at the entrances all circulation pipes to prevent entry of wood chips.

It is important to assign a proper multiphase mode in order to satisfy the modeling. Knowledge of the material density ratio, stocks number, volume fraction and particulate loading is important when assigning a multiphase method.

A material density ratio ($\gamma$) of close to 1.0 indicates an increase in liquid-solid flow. In our case the density of the fluid phase is approximately 1000 kg/m$^3$ and the density of the solid phase varies from 1000 (moist chips) to 1200 kg/m$^3$ (individual wood chips). ($\gamma$) is therefore close to 1 in this case.

The next parameter to consider in the description of a multiphase scenario is the volume fraction of the phases. When the volume fraction of the dispersed phase is larger than 10% then the Mixture and Eulerian methods are the most suitable methods. Stocks number is approximated to a unit value which defines the different multiphase procedures i.e. Mixture, Eulerian and Dispersed.

The Eulerian model is the appropriate one to use when the stocks number is larger than 1. Estimation of the distances between particles is complicated by the fact that the particles have non-uniform shapes.

The particulate loading number ($\beta$) may be determined by estimating the void space between the chips. A rough estimate of $\beta$ shows that it has an intermediate value, indicative of mutual interactions between the liquid and solid flows. This means that the wood chips can decrease the turbulence and mean momentum of the liquid stream. Conversely, the liquid stimulates the solid flow through turbulence and drag.

The performance of multiphase models in FLUENT has been evaluated and a primary comparison
indicates that the most appropriate models for the dynamic behavior of the digester are the Mixture and Eulerian techniques. However, it is important to analyze the performance of the multiphase methods of FLUENT before using them in any application. The VOF (volume of fluid) multiphase method is excluded because it is primarily suited to stratified flows and immiscible fluids and when the position of the interface between the fluids is of interest.

The DPM (discrete phase model) may be applicable if the volume fraction of the wood chips is lower than 10%.

Our criterion for an appropriate multiphase model is one which in addition to properly modeling the phases also has the numerical ability to separate the phases through the screen into the circulation pipes.

**Porous media approach**

This strategy can produce a detailed view of the fluid phase through the solid bed when a non-constant porosity (packing limit) is used. The solid chip phase with variable compressibility can be characterized as having a given bulk viscosity, which represents the resistance of the solid phase to expansion and compression. This can be modeled as a porous medium. Defining these properties using other CFD strategies may be more computationally intensive.

Liquid mass balance and hydrodynamic behavior of the liquor is computed numerically by this procedure. As lignin dissolves, the wood chips soften and are compressed by the chips above them. This effect increases with depth in the digester.

**Problem set-up**

These models were developed for the Korsnas and Vallvik digester in Sweden. The digester has a height of 60 m and a diameter of 6 m at the entrance which increases stepwise to 7 m at the bottom. There are two pressure adjustment dischargers of 0.2 m diameter at the top end near the inlet. The diameter of the uppermost circulating pipe, called the transference pipe, is 0.35 m. Two other inlets at the bottom and near the bottom include a number of pipes which are normally not in service. The lay-out of the digester is shown in Figure 1.

Figure 1: Layout of the continuous digester

A large annular pipe hangs inside the digester. This pipe connects to the outlet pipes of the circulation loops, referred to as C8 (wash zone circulation) in the lower section, MCC (in the middle section) and ITC (isothermal cook circulation) in the upper section. The flows re-circulate into the digester separately at three different levels. The central pipe consists of three concentric pipes. The innermost pipe is the longest and flows from C8 into the digester. The diameters of the C8, ITC and MCC inlets are 0.21, 0.3 and 0.425 m respectively.
The MCC is connected to the middle pipe while the ITC is connected to the outermost pipe and drains the flow at the top section. The mixture passes through circular screens in the periphery of the digester before flowing into the collection pipes. These screens are 1 to 2 m high with 1 to 2 cm slots, and produce a large open area and thus a relatively small pressure drop, compared to the pressure drop in the chip bed, as long as the surface remains unclogged. The flow is in a radial direction before it enters the outlet pipes.

The diameters of the C8, MCC and ITC outlet pipes are 0.15, 0.2 and 0.25 m respectively.

This central pipe is modeled so that only the discharges to the digester are computed - the flow inside the pipe is not modeled. Therefore the inside of the pipes is not meshed, enabling us to manipulate the C8, ITC and MCC inlets. The C8, ITC and MCC circulations have different inlet and outlet mass flow rates because they mix with fresh liquor before they enter the digester.

The digester model is designed in Gambit in such a way that it is divided into two axisymmetric parts around the x-axis. The three dimensional shape of the digester is obtained by rotation of the two parts about the x-axis. The digester is therefore designed in two dimensions but FLUENT accounts for the total volume of around 1800 m$^3$. The cylindrical central pipe is designed exactly as it exists in the digester.

The outlets from the screen also rotate about the x-axis and therefore FLUENT treats them as circular outlets around the digester.

The mixture of wood chips and liquor enters at the top inlet. No other components are included in the model of the digester.

The input data values at the inlets are taken from Korsnas operating data. These values, the discharges, amount of circulating streams and outlet values are shown in Table 1.

The pumps are modeled by applying the pressures they exert at the outlet flows. These pressures may be negative during adjustment of the circulating flows. Wood chips of different diameters are excluded from the circulation pipes by varying the geometry of the gaps in the screens.

The physical modeling of the screens is ignored and the separation takes place numerically by manipulating the multiphase flow variables.

Circulation of the liquid streams takes place by employing the characteristics of the pumps mounted in the circulations.

The process of solving a multiphase system is inherently difficult, and stability or convergence problems often occur. Calculation of the mass balance and liquor behavior in the solid bed with a heterogeneous compressibility may be done using the Porous media code.
Physical properties of the model

As the digester is a continuous solid-liquid reactor, the flow inside it is considered as a multiphase flow. The solid phase is made up of the wood chips and the liquid phase is made up of the white liquor and water. The flow regime inside the reactor is assumed to be turbulent due to sharp edges on the non-uniform wood chips and high accounted Reynolds numbers. The solid phase is modeled as a granular phase with constant diameter. However, the wood particles which are fed into the digester are non-uniform in size and shape. Modeling of large numbers of particles with different dimensions in Gambit is not an easy task. We therefore measured a number of randomly selected chips. The measured chips had dimensions of approximately 2 × 2 × 0.5 cm.

The granular multiphase model is limited to spherical solid particles. However it is possible for the user to define a distribution of diameters. We used this ability to model compression.

By using the aspect ratios of randomly selected chips from the solid feed we computed the ratio of the total surface area to volume of the chips. FLUENT uses this computed value as the ratio for the spherical solid particles. The spherical chip used in the model has approximately the same surface to volume ratio as the selected irregular chips in the real reactor. Measurements of the feed wood chips indicate that the majority have similar dimensions to the modeled chips.

Governing equations

It is allowable to use the granular method when the mixture model applies for any prediction. The mixture model takes into account the granular properties and its variables. It is applicable for solid-liquid multiphase flows. The fluid motion is governed by incompressible Navier-Stokes equations: Fluent user guide (2009)

\[
\frac{\partial}{\partial t} (\rho_m \vec{v}_m) + \nabla \cdot (\rho_m \vec{v}_m \vec{v}_m) = -\nabla p + \nabla \cdot [\mu_m (\nabla \vec{v}_m + \nabla \vec{v}_m^T)] + \rho_m \vec{g} + \vec{F} + \nabla \cdot \left( \sum_{k=1}^{n} \alpha_k \rho_k \vec{v}_{dr,k} \vec{v}_{dr,k} \right)
\]
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\[
\nabla \cdot \mathbf{v} = 0
\]

Mass-averaged velocity,

\[

\bar{\rho} = \sum_{k=1}^{n} \bar{\rho}_k \mu_k
\]

\[

\mathbf{v}_{dr,k} = \mathbf{v}_k - \mathbf{v}_m
\]

Slip velocity

Slip velocity is the difference between the bulk flow and dispersed flow velocity or it is the difference between the velocities of two phases.

\[

\mathbf{v}_{pq} = \mathbf{v}_p - \mathbf{v}_q
\]

Volume fraction

The volume fraction of secondary phase in the multiphase flow is determined from the continuity equation for that phase.

\[
\frac{\partial}{\partial t}(\alpha \rho_p) + \nabla \cdot (\alpha \rho_p \mathbf{v}_m) = -\nabla \cdot (\alpha \rho_p \mathbf{v}_{dr,p}) + \sum_{q=1}^{n} (\bar{m}_{pq} - \bar{m}_{qp})
\]

Solids shear viscosity

Viscosity of a suspension which is a mixture of the solid and liquid depends largely to the concentration of the solid particles in the mixture. The particle momentum is generated due to particle motion in the bulk flow. There is a momentum exchange between the moving particles and bulk flow. The viscosity of the suspension is accounted by the average weighted volume which consists of the viscosity of the solid and viscosity of the liquid.

Solid shear viscosity consists of three viscosities that are arisen from collision of solid particles, kinetic of the particles and friction between them.

There is also a friction between the solid particles and the liquid flow. The granular viscosity term is used to account the viscosity of the suspension.

\[

\mu_s = \mu_{s, col} + \mu_{s, kin} + \mu_{s, fr}
\]

Collisional viscosity

\[

\mu_{s, col} = \frac{4}{5} \alpha \rho_s ds_{ss} \left[1 + e_{ss}\left(\frac{\Theta}{\pi}\right)^{\frac{1}{2}}\right]
\]

Kinetic viscosity:

\[

\mu_{s, kin} = \frac{\alpha d_s \rho_s \sqrt{\Theta \pi}}{6(3-e_{ss})} \left[1 + \frac{2}{5}(1 + e_{ss}) (3e_{ss} - 1) \alpha g_{o, ss}\right]
\]

Granular temperature

Granular temperature consists of three terms

\[

o = (-p_s \mathbf{I} + \tau_s)
\]

\[

\equiv \nabla \mathbf{v}_s - \gamma \Theta_s + \Phi_{ls}
\]

1- Energy is generate due to velocity distribution of the solid particles which generate the solid normal stress and solid shear stress distribution in the momentum equation of the solid (equation (16)):

\[
\nabla \mathbf{v}_s
\]
2- Particles lose energy when they collide to each other. The collisional energy is a dissipation of energy. This term is denoted by $\gamma_\Theta_s$.

3- The motion of the particles in the bulk flow leads to an energy exchange between them and energy of the solids may be dissipated by physical interaction with the fluid. This term is denoted by $\Phi_{ls}$.

The solid energy may also be dissipated to fluid due to solid fluctuations.

The collisional dissipation of energy

The collisional dissipation of energy, $\gamma_\Theta_s$, represents the rate of energy dissipation within the solids phase due to collisions between particles. This term is represented by the expression derived by Lun et al.

$$\gamma_{\Theta m} = \frac{12(1-e_s^2)g_{a,ss}}{d_s^2} \rho_s \alpha_s^2 \Theta_s^{1/2}$$  

Kinetic energy of random fluctuations in particle

The transfer of the kinetic energy of random fluctuations in particle velocity from the solids phase to the fluid or solid phase is calculated by

$$\Phi_{ls} = -3k_{ls} \Theta_s$$  

In the FLUENT the following options are available to solve the granular temperature:

1- The default option is an algebraic formulation which neglect the convection and diffusion terms in the transport equation (12).

2- Constant granular temperature. This is a very good approximation when the volume fraction of the solid particles is high in the solution which leads to ignorable random fluctuations condition.

3- UDF

Eulerian governing equations

The conservation of momentum for a fluid phase $q$ is given by:

$$\frac{\partial}{\partial t} (\rho_q \vec{v}_q) + \nabla \cdot (\rho_q \vec{v}_q \vec{v}_q) = \rho_q \nabla \cdot \vec{F}_{q} + \vec{F}_{\text{lift},q} + \vec{F}_{\text{vm},q}$$  

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$\tau_q$ Stress-strain tensor of phase $q$

$\vec{F}_q$ External body force,

$\vec{F}_{\text{lift},q}$ Lift force, and

$\vec{F}_{\text{vm},q}$ Virtual mass force
The conservation of momentum equation for the solid phase $s$ is
\[
\frac{\partial}{\partial t} \left( \alpha_s \rho_s \vec{v}_s \right) + \nabla \cdot \left( \alpha_s \rho_s \vec{v}_s \vec{v}_s \right) =
- \alpha_s \nabla p - \nabla \cdot \vec{\tau}_s + \alpha_s \rho_s \vec{g} + 
\sum_{j=1}^{N} \left( K_{st} (\vec{v}_j - \vec{v}_s) + 
\dot{\bar{m}}_{ls} \vec{v}_j - \dot{\bar{m}}_{sl} \vec{v}_s \right) +
(\vec{F}_s + \vec{F}_{lift,s} + \vec{F}_{visc,s})
\]  
(16)

**Solids pressure**

In the suspension solutions or granular flows, the motions of the particles establish a pressure gradient in the solution if the packing limit of the solid particular is less than 0.63 which is the maximum allowable value.

When the solids packing limit is less than the 0.63 then the solid phase is compressed and a pressure gradient of the solid particles is produced independently ($\nabla p_s$). The pressure gradient is introduced in the granular momentum. The solid particles follow the Maxwell-Boltzmann distribution which is a probability distribution and therefore the kinetic energy of the particles represented by the granular temperature is introduced in the solid pressure equation and viscosity.

The solids pressure is composed of a kinetic term and a second term due to particle collisions:
\[
p_s = \alpha_s \rho_s \Theta_s + 2 \rho_s (1 + e_{ss}) \alpha_s^2 g_{o,ss} \Theta_s
\]  
(17)

$e_{ss}$ is the coefficient of restitution for particle collision and the default value for $e_{ss}$ is 0.9.

The transition from compressible condition to incompressible is managed by a function known as distribution function. When the packing limit of the solid is maximum (0.63) then the solid flow is incompressible but when this value is less than 0.63 then the solid phase is compressible and spacing between the particles is possible to be diminished.

**Radial distribution**

When the volume fraction of the solid phase is Maximum then probability of the collision of the solid particles may need to be modified. This function assumes the particles have spherical forms.
\[
g_o = \frac{s + d_p}{s}
\]  
(18)

where $s$ is the distance between grains.

**Bulk Viscosity**

The resistance of the solid particles to compression and expansion is expressed by the bulk viscosity. Lun et al expression for Bulk viscosity is:
\[
\lambda_s = \frac{4}{3} \alpha_s \rho_s d_s \Theta_s (1 + e_{ss})(\Theta_s / \pi)^{1/2}
\]  
(19)

**Frictional Viscosity**

Friction between the particles is relevant in the mixture whenever the volume fraction of the solid phase approaches the packing limit. Then stress is generated due to friction between the particles.
The Schaeffer's expression is available to be defined.

\[
\mu_{s,f} = \frac{P_s \sin \phi}{2 \sum I_{2D}}
\]  

(20)

\(P_s\) is the solids pressure, \(\phi\) is the angle of internal friction, and \(I_{2D}\) is the second invariant of the deviatory stress tensor.

Material density ratio

\[
\gamma = \frac{\text{Dispersed phase}}{\text{carrier phase}}
\]  

(21)

Average distance between the individual particles and particle loading

\[
L = \left( \frac{\pi}{6} \frac{1 + k}{k} \right)^{\frac{1}{3}}
\]  

(22)

\[
k = \frac{\beta}{\gamma}
\]  

(23)

Porous momentum sink

A porous media contributes to lower velocity of the flow due to generation of a pressure gradient in the cell zones. The achievement is fulfilled by an additional source term in the fluid flow equations. The source is a flow resistance and consists of two terms that are empirically determined. A viscous and an inertial loss term is included in the momentum equation in the porous cell zones.

\[
S_i = \left( \sum_{j=1}^{3} D_{ij} \mu v_j + \sum_{j=1}^{3} C_{ij} \frac{1}{2} \rho v_j^2 \right)
\]  

(24)

Modeling set up

A pressure flow based solver is adopted for solving the momentum, continuity and volume fraction equations.

The current numerical equations are solved under the steady state condition through the implicit discretization scheme.

Gravitational acceleration is specified under the operating conditions in the positive direction of the x-axis due to the axisymmetric geometry.

A turbulent and the k-e method is adopted because of the high Reynolds number. The inlet flows have turbulent characteristic and the Reynolds number is between 40000 to 70000 but it does not mean that the turbulence is so high inside the reactor because of the momentum exchange with the wood chips.

The procedure for setting up and solving the Mixture and Eulerian models is outlined below.

Second order as well third order terms for the momentum equation can be applied.

The liquid flow is designated as the primary phase and the wood chips are the secondary phase, which is assumed to be granular. The properties of the primary phase are defined primarily in the material panel and should be placed in the fluid materials category. The granular properties are specified in the granular phase panel and the granular option is selected.

The density and viscosity of the solid is defined in the material window. The granular properties i.e. diameter of the particles, granular viscosity, bulk
viscosity, frictional viscosity, granular temperature, solids pressure, radial distribution and packing limit are prescribed in the secondary phase set up.

As the diameter of the applied spheres is larger than that for compressible values, a value of 0.63 is adopted for the packing limit.

The granular viscosity is set at 0.001 kg/m-s.

An algebraic solution is adopted for granular temperature because we do not have any knowledge of the size of random fluctuations of small solid particles in order to use the constant granular temperature.

The Lun et al formulation is adopted for radial distribution.

A derived formula is used to define the Elasticity modulus.

No solid pressure or frictional viscosity is assigned for the solid phase although a constant value of 0.9 is adopted for the solid phase collision parameter.

This is primarily to take the chip flows in the reactor into account, where the velocity at the center is higher than at the walls.

The Schiller-Naumann formulation is selected for solving the drag function in the Mixture model. In most cases with spherical particles, the Schiller-Naumann law is the most suitable.

**Porous set up**

A heterogeneous porous media is specified through the digester, representing the compressibility of the solid phase. Decomposition of the wood develops when lignin is removed from the chips. Loss of lignin from the chips makes them softer and more compact. To model this, the digester is divided into 19 sections, each with different assigned porosities. The prescribed porosities decrease downwards from the top of the digester. The distribution of the fluid flow through the particles is described by a porosity range of 0.65 to 0.25. The inertial loss term of the momentum sink is activated and specified for each porous section of the digester in both x and y directions.

**Results**

Table 1 shows results from the FLUENT mass balance at the report of the fluxes when an Eulerian method with phase separation is applied. The values of default interiors and walls are not incorporated into this table.

<table>
<thead>
<tr>
<th>Mass balance : Phase 2</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Section</strong></td>
</tr>
<tr>
<td>Inlet up</td>
</tr>
<tr>
<td>Circulation1-transport</td>
</tr>
<tr>
<td>Extraction down</td>
</tr>
<tr>
<td>Extraction top</td>
</tr>
<tr>
<td>Bottom inlet</td>
</tr>
<tr>
<td>Bottom outlet</td>
</tr>
<tr>
<td>C8- Inlet</td>
</tr>
<tr>
<td>C8-Outlet</td>
</tr>
<tr>
<td>ITC-Inlet</td>
</tr>
<tr>
<td>ITC-Outlet</td>
</tr>
<tr>
<td>MCC-Inlet</td>
</tr>
<tr>
<td>----------------</td>
</tr>
<tr>
<td>MCC-Outlet</td>
</tr>
<tr>
<td>Bottom side-inlet</td>
</tr>
</tbody>
</table>

Table 1: Mass balance of phase 2, the wood chips at the different inlets and outlets

Table 1 show that there is almost zero flow in every position except for the top inlet and bottom outlet flow. The amount of fibers that follows the liquid streams is negligible. Figure 2 shows how the wood chips flow out through the screens into the pipes, and the velocity distribution obtained using the Mixture model.

Figure 2: Mixture model - velocity distribution of the wood chips in the discharge pipe.

Figures 3 to 14 show the results of calculation of the hydraulic variables of the solid and liquid phases obtained from the Euler strategy. Figure 3 shows that the solid particles are absent from the discharge pipe. The vectors are scaled up approximately 5-fold in this figure.

The wood chip flow is faster along the central pipe where it is supported by the downward liquid flow.

Figure 3: Eulerian computation - velocity vectors of the solid phase in the discharge pipe and digester.

Figure (4) shows that the liquid phase is present in the discharge pipe.

Figure 4: Eulerian computation - velocity vectors of the liquid phase in the digester and discharge pipes.

Figures (5) and (6) show the velocity distribution of the liquid phase in different sections of the digester.

Figure 5: Eulerian computations - velocity distribution of the liquid phase in the middle of the digester.

The liquor velocity is increased near the discharge pipe which is due to the suction exerted by the pumps.

Figure (5) shows that the liquor velocity is greater at the centre of discharge pipe compared to near the walls of the pipe, which is likely due to contribution of the frictional losses at the walls.

Further in the horizontal direction from the outlet pipes toward the central pipe, the liquor velocity decreases because the two flows are completely mixed and porosity is lower in this region.

On the other hand the pressure field created by the pumps diminishes horizontally toward the center of digester.

The same trend can be seen in Figure 6 in which the liquor velocity increases near to and in the centre of the by-pass pipe in the result of the pressure exerted by pumps.

These figures show that the solid velocity is zero at the outlets but at the same time the solid flow is pulled towards them because of the contribution of the pumps in the outlets. These results exhibit a high concentration of the solid phase around the...
screens near any outlet. The flow is pulled upward under all three outlets (Figures 7 and 8), and this contributes to vortex flow under these outlets. A spiral motion is therefore expected to form under any horizontal outlet at the digester if any pump is employed to suck the flow into the pipe.

Figures (7) and (8) show the velocity distribution of the solid phase at the top and middle of the digester. Figures (9) and (10) show the velocity vector distribution of the liquid phase at the entrance of the MCC and ITC pipes.

The flow is downward but turbulence is observed in these regions which can be due to collision and momentum exchange with the downward bulk flow of the digester. The positions of the inlets of the by-pass flows are near the related outlets which can also contribute to formation of the turbulence in these regions.

Figure 6: Eulerian computations - velocity distribution of liquid phase at the top of the digester.
Figure 7: Eulerian computations - velocity distribution of the solid phase at the top of digester.
Figure 8: Eulerian computations - velocity distribution of solid phase in the middle of digester.

The chip velocity increases near the C8, MCC and ITC inlets due to momentum transfer from the liquid to the solid phase.

Figure 9 Eulerian computation - velocity vectors of the liquid phase at the MCC pipe inlet
Figure 10: Eulerian computation - velocity vectors of the liquid phase at the ITC pipe inlet
Figure 11: Eulerian computation - velocity vectors of the liquid phase at the C8 Pipe inlet. Colors represent the volume fraction.

Figure (11) shows the direction and magnitude of the liquid phase at the C8 Pipe inlet colored by volume fraction. The volume fraction of the liquid at the entrance is 100 percent and volume fraction is 1. A spiral motion is altered due to vicinity to the C8 outlet and momentum exchange with the bulk flow.

Figure 12: Eulerian computation - velocity vectors of the solid phase around the C8 Pipe. Colors represent the volume fraction

Figure (12) shows the size and direction of the solid phase volume fraction around the C8 Pipe. The volume fraction is zero near the opening, where turbulence is also created.

Figure 13 Eulerian computation - velocity vectors of liquid at the bottom outlet and near the bottom horizontal inlet
Figure (13) shows the magnitude and direction of the liquid flow as it enters horizontally from the side of the digester near the bottom, and also at the bottom outlet.

The flow from the side inlet is upward. However, the momentum exchange that results when it meets with the downward bulk flow results in a partially downward flow.

Figure 14: Eulerian computations - volume fraction of the solid phase at the bottom.

Figure (14) shows the volume fraction of the solid particles where it encounters the inlet liquid phase from the vertical side of the digester near the bottom. Collision of the phases in this region affects the direction of the chips motion. Figure (14) indicates that, the volume fraction of the wood chips is much lower at the centre than on either side. This is due to the entrance of liquor from the C8 inlet in the middle of this zone. A spiral motion is created, as shown by the distribution of the velocity vectors. Multiple inlets and outlets at the bottom of the digester therefore result in turbulence.

Figures 15 to 18 show the effects of the Porous model where decreasing porosity is assigned down the height of the digester.

Figure (15) shows the velocity of the liquid flow through the digester including the multiple inlets and outlets. The inlet velocity is high but due to interaction with the solid phase the turbulence and momentum decrease. Turbulence and velocity increase near the circulation inlets MCC, ITC and C8.

**Porous results**

Figure 15: Porous model - velocity distribution of the liquid from top to bottom of the digester, including circulation pipes C8, ITC and MCC.

The liquid velocities in all sections of the digester are plotted in Figure (16). The digester is divided into 19 sections. Velocities increase near the inlets to the circulation channels MCC, ITC and C8 and decrease away from the circulation channels due to interactions with the solid phase which generate a momentum sink in the fluid flow.

Figure 16: Porous model - plot of velocity through the digester.

Figure 17: Porous model - velocity vectors of the liquid at the bottom outlet and at the horizontal inlet near the bottom.

Figure (17) shows the velocity vectors of the liquid flow at the bottom outlet.

A spiral motion is created, as shown by the distribution of the velocity vectors. Multiple inlets and outlets at the bottom of the digester therefore result in turbulence.

Figure (18) shows the turbulence intensity (k) distribution from the C8 position to the bottom of the digester. The contours show high turbulence at
three inlet positions, C8, and the bottom and vertical side inlets near the bottom of digester, which dissipates away from the inlets.

Figure 18: Porous model: turbulence intensity at the horizontal inlet near the bottom, C8 inlet, and bottom inlet.

**Grid independence and validity**

The outlets, extractions and amounts of the circulation flows are obtained from simulation of the digester by adjustment of the pressures. The results of these computations agree with the operational values of the Korsnas process database. The actual digester is about 60 m in height and between 6 m and 7 m in diameter, as previously mentioned. The simulations are performed with three different types and numbers of meshes. Models were built with meshes of around 16000 or 56000 triangular cells, or 21000 quadrilateral cells for half of the digester, i.e. 60m×3m. The other half of the digester is computed by FLUENT from the symmetry. There is no difference between the results that use 56000 triangles and 21000 quadrilaterals, but the intermediate mesh that uses the 16000 triangular cells does not agree with these. The 16000 triangular cell model was assumed to be too coarse to accurately model the digester. Further increasing the number of cells above 56000 did not make a significant difference to the results.

All the circulation flows and discharges computed by the model agree with operational data of the Korsnas digester. This achieves one of the major aims creating this model.

There is no trace of the solid phase in the circulating pipes in the model, which is consistent with their function in the digester. The data shown in the Table 1 are taken directly from the FLUENT mass balance using the Euler-Euler approach. These data show that phase 2 (the solid phase) is not involved in any of the discharges or circulation processes, consistent with the functions of the digester. This supports the validity and quality of the applied modeling method. The absence of wood chips in the discharge flows is apparent in the Figures 3 and 7 and strengthens the case for the reliability of the finite volume method model.

**Discussion**

*Phase separation*

Separation of phases in a multiphase stream was considered by construction of the screens in the extraction geometry in Gambit. We tested the Mixture and Eulerian multiphase models of FLUENT.

The contour of velocity vectors of phase 2 - the wood chips - in the discharge shows the contribution of the grains in the discharge when most of the chips are separated.
In the Mixture model – the results of which are shown in Figure 1 - the phases are treated as interpenetrating continua. The Mixture model solves the continuity, momentum and energy equations for the mixture, and the volume fraction equation for the secondary phases.

The Mixture model solves the mixture momentum equation and prescribes relative velocities to describe the dispersed phases.

The Eulerian approach to the multiphase model solves a set of n momentum and continuity equations for each phase. This is the key to separation of the phases. The Mixture method solves one equation for both phases together while separation means the consideration of an individual phase.

Report of the fluxes of phase 2 from FLUENT indicates the suitability of the Eulerian approach for mathematical phase separation, which has potential applications in other engineering areas. The solid phase flowed down through the reactor and plays no part in the extraction or circulation streams. Figures 3 to 14 show results of calculations of the hydraulic variables of the solid and liquid phases using the Euler strategy. Figure 3 shows the absence of the solid particles from the discharge pipe. Figure 4 shows that the liquid phase is present in the discharge tube.

The Eulerian computation showed better performance in the separation of the phases than the Mixture method, and was therefore used in most of the simulations.

The Lagrangian trajectory computation of the particles is available in FLUENT but was not analyzed in this paper, as its use is not feasible for the solution of this digester problem.

**Conclusion**

The Eulerian model approach is capable of performing computational separation the phases in the model of the digester. Individual variables of the phases could be defined in the cell zones and it is therefore possible to manipulate the composition of the phases in particular locations. This is important in practice when using the FIXED VALUES option of the zone in the FLUENT and limits the variable parameters of any phase. This is not possible when using the Mixture model and management of the individual phases in the cell zones is therefore difficult using this model.

The Porous model can be cost effective compared to multiphase models and can also be a complementary computational tool when properties such as compression must be defined. We have established a complete CFD code of a continuous pulp digester using finite volume method, FLUENT, to deal with the physical behavior of the phases. It is also possible to model the reactions inside the pulp and paper digester. This will be presented in a follow-up paper. A combination of fluid dynamic and chemical reaction models can be
used to study different disturbances, such as hang ups and channeling.

Acknowledgments

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Nomenclature

\[ d \quad \text{Diameter (m)} \]

\[ d_p \quad \text{Particle diameter (m)} \]

\[ e_{ss} \quad \text{Coefficient of restitution for particle collisions} \]

\[ \vec{F} \quad \text{Body force (N)} \]

\[ F_D \quad \text{drag force (N)} \]

\[ \vec{F}_{vm,q} \quad \text{Virtual mass force (N)} \]
\begin{itemize}
\item \(\overrightarrow{F_q}\) External body force (N)
\item \(\overrightarrow{F_{\text{lift},q}}\) Lift force
\item \(g\) Gravitational acceleration (m/s\(^2\))
\item \(g(s)\) Radial distribution function
\item \(g(s,ss)\) Distribution function
\item \(\tau\) Second invariant of the deviatoric stress tensor
\item \(k_{fs}\) Momentum exchange coefficient between fluid and solid
\item \(\dot{m}\) Mass flow rate (kg/s)
\item \(n\) Number of phases
\item \(p_s\) Solid pressure (pa)
\item \(S_s\) Momentum sink
\item \(t\) Time (s)
\item \(\overrightarrow{v_m}\) Mass-averaged velocity
\item \(\overrightarrow{v_{pq}}\) Slip velocity (m/s)
\item \(\overrightarrow{v_q}\) Velocity of primary phase (m/s)
\item \(\overrightarrow{v_p}\) Velocity of secondary phase (m/s)
\item \(\overrightarrow{v_s}\) Solid particle velocity (m/s)
\item \(\alpha\) Packing limit
\item \(\alpha_k\) Volume fraction of phase k
\item \(\rho_m\) Mixture density (kg/m\(^3\))
\item \(\tau_s\) Solids stress strain tensor
\item \(\tau_q\) Stress-strain tensor of phase q
\item \(\mu\) Viscosity (kg/m-s)
\item \(\mu_s\) Solid viscosity (kg/m-s)
\item \(\mu_{s,\text{col}}\) Collisional viscosity (kg/m-s)
\item \(\mu_{s,\text{kin}}\) Kinetic viscosity (kg/m-s)
\item \(\mu_{s,\text{fr}}\) Frictional viscosity (kg/m-s)
\item \(\mu_m\) Mixture viscosity
\item \(\phi\) Angle of internal friction
\item \(\Phi_{fs}\) The energy exchange between the fluid or solid phase
\item \(\Theta_s\) Granular temperature (Kinetic energy of the fluctuating particle motion)
\item \(\alpha_k\) Volume fraction of phase k
\item \(\gamma\) Material density ratio
\end{itemize}
Figure 1: Layout of the continuous digester

Figure 2: Mixture model - velocity distribution of the wood chips in the discharge pipe.

Figure 3: Eulerian computation - velocity vectors of the solid phase in the discharge pipe and digester.
Figure 4: Eulerian computation - velocity vectors of the liquid phase in the digester and discharge pipes.

Figure 5: Eulerian computations - velocity distribution of the liquid phase in the middle of the digester.

Figure 6: Eulerian computations - velocity distribution of liquid phase at the top of the digester.
Figure 7: Eulerian computations - velocity distribution of the solid phase at the top of digester.

Figure 8: Eulerian computations - velocity distribution of solid phase in the middle of digester.

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Figure 10: Eulerian computation - velocity vectors of the liquid phase at the ITC pipe inlet. Colors represent the volume fraction.

Figure 11: Eulerian computation - velocity vectors of the liquid phase at the C8 Pipe inlet. Colors represent the volume fraction.

Figure 12: Eulerian computation - velocity vectors of the solid phase around the C8 Pipe. Colors represent the volume fraction.
Figure 13: Eulerian computation - velocity vectors of liquid at the bottom outlet and near the bottom horizontal inlet.

Figure 14: Eulerian computations - volume fraction of the solid phase at the bottom.

Figure 15: Porous model - velocity distribution of the liquid from top to bottom of the digester, including circulation pipes C8, ITC and MCC.
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Figure 18: Porous model: turbulence intensity at the horizontal inlet near the bottom, C8 inlet, and bottom inlet.
Paper II
CFD modeling of the continuous chemical interaction between the multiphase flows of the pulp and paper digester using the mass transfer scheme

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1. Abstract

This paper describes the construction of a CFD code for the physical structure of the pulping reactor and prediction of the continuous chemical reactions inside the digester. Models for chemical interactions between the wood chips and liquor flows in a pulping digester were designed using the FVM (Finite Volume Method), FLUENT software. The quality of the produced pulp was computed throughout the reactor from the top inlet to bottom outlet by modeling a dimensionless parameter, the Kappa number. A conjugated mass transfer and porous media model was tested to avoid the effect of granular instability and divergence on the chemical reaction model.

2. Introduction

One of the major chemical processes in the pulp mill develops in the digester. Two flows are fed into the digester. These are treated as phases according to their physical state, i.e. solid or liquid or as the chemical substances, depending on the application, i.e. either physical or chemical consideration. Researchers have investigated various aspects of the pulp production unit such as the structural design, flow regimes, chemical reactions, modeling, optimization and motion of fibers in the digester.

Chemical reactions in the digester are carried out either continuously or in batches. The Korsnas digester is a continuous digester, meaning that progress through it is regular and uninterrupted. The digester is essentially a large vertical tank in which wood chips move downward. Woods used in the digester are classified as either hardwoods or softwoods. Hardwoods generally come from broad-leaved deciduous trees from temperate regions, and are porous, meaning they contain vessel elements. These vessels form an efficient system for transporting water (and essential minerals) from the root to the leaves and other parts of the tree. Softwood trees, are mostly evergreens, nonporous and do not contain any vessels. The terms hardwood and softwood do not have any direct relation to the hardness or softness of the wood.

The constituents of wood vary with wood type, but may also vary within a particular wood type. The wood species cannot generally be determined by chemical analysis because its composition depends on factors such as geographical location, soil and weather conditions, and location of the wood within a given tree. Typically, wood is made up of 40 to 50% cellulose, 20 to 30% hemicellulose, 20 to 30% lignin and 10% other substances. These other substances include organic compounds such as Terpenes, lipids, resin, starch, and protein. Table 1 shows typical compositions of wood from three species of tree.

<table>
<thead>
<tr>
<th></th>
<th>Spruce</th>
<th>Pine</th>
<th>Birch</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cellulose</td>
<td>42</td>
<td>41</td>
<td>41</td>
</tr>
<tr>
<td>Hemicellulose</td>
<td>28</td>
<td>28</td>
<td>34</td>
</tr>
<tr>
<td>Lignin</td>
<td>27</td>
<td>27</td>
<td>21</td>
</tr>
<tr>
<td>Extractives</td>
<td>3</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

Table 1: Composition of wood from three tree (Kassberg, 1998)

In the digester, wood chips are cooked at around 160 °C. This process dissolves the lignin which binds the cellulose and hemicellulose together and releases the different fibers that have diverse industrial applications. The wood chips cannot be cooked until they are free of lignin without adversely affecting the yield and strength of the resulting pulp. (Kassberg, 1998)

The liquor is heated in one or more circulation stages by screens and heat exchangers. The dominant chemical pulping process in Korsnas is called the sulphate or Kraft process. This uses alkaline cooking liquor with a PH of around 14. This solution is composed of sodium hydroxide (NaOH), sodium sulfide (Na2S), sodium carbonate (Na2CO3), and sodium sulphate (Na2SO4). The composition of the solution is varied depending on
the operation conditions and the nature of the wood chips. Wood is a porous material. Between 60 and 70% of its volume is occupied by air, resulting in its characteristically low density. The permeability of wood is defined as the flow of liquids through the wood under an applied pressure. The permeability of wood varies due to the highly anisotropic shape and arrangement of the component cells and the variable microscopic channels between cells. (Durback et al., 1998)

The permeability longitudinal to the grain is 50 to 100 times greater than in the transverse direction. (Stamm, 1964)

It is difficult to determine the orientation of the wood chips with respect to their grain as they move down through the reactor. The essential constituents of the wood are lignin, cellulose, hemicellulose and less major content of wood is extractives. Lignin is an amorphous, insoluble organic polymer and is very difficult if not impossible to isolate in a natural state. Molecular weights of isolated lignin polymer range from the low thousands to around 50,000. Lignin is a polymer made up of different monomers of varying molecular weights.

**Cellulose** is the main component of the wood cell wall, and typically makes up 40 to 50% of the dry wood by weight. Pure cellulose is a polymer of glucose residues joined by 1, 4-β-glucosidic bonds. The degree of polymerization (DP) is variable and may range from 700 to 10,000 or more.

Hemicellulose is a mixture of amorphous branched-chain polysaccharides composed of several hundred sugar residues. Hemicelluloses contain many different sugar monomers. These monomers include Xylose, mannose, Galactose, Rhamnose, and Arabinose. Hemicelluloses contain most of the D-pentose sugars, and may occasionally contain small amounts of L-sugars.

**Extractives and Ash:** The amount of extractives in wood varies from 5 to 20% by weight and includes a wide variety of organic chemicals (Rowe, 1989). The ash content is 0.2 to 0.5% by weight for temperate woods and 0.5 to 2.0% by weight for tropical woods.

**Kappa number:** Kappa number is a dimensionless quantity that is a measure of the pulp quality. (Kappa number = mass fraction of lignin * 100 / 0.15).

Wood is made up of cellulose, hemicelluloses, lignin, and other materials. The objective of the pulping chemical reaction is to remove as much of the lignin as possible from the wood. The Kappa number is a measure of the lignin content of the wood pulp. A high Kappa number indicates high lignin content. Considerable effort has been expended to predict and manage the chemical reactions of the digester. Vroom (1957) modeled the H-factor, and Smith and Williams followed by producing the Purdue model, an approximated digester model consisting of a number of CSTRs (continuous stirred tank reactors) which accounted for the kinetics of the reaction (Smith et al., 1974). Since then, these models have been developed and modified by others. Johansson (1971) solved a combination of the mass transfer and reaction kinetics of the differential equations in a wood chip during the cooking process.

He assumed that the diffusivity in wood was a function of temperature. However, Hartler (Hartler and Onisko, 1962) showed that the diffusivity in wood also depended on the pH. Johansson used a single equation for three reaction stages.

Gustafson et al. (1983) improved Johansson’s model and used three kinematic equations for the three stages. He expressed the diffusivity as a function of temperature, pH and yield.

Christensen et al. (1983) began with a modified Purdue model but incorporated a number of simplifications. They developed the kinetic model for several soft and hard woods. The plug flow was assumed to occur for both wood chips and the liquor.

Harkonen (1987) derived a multiphase flow model to describe the internal pressure, temperature and velocities for phases using mass, momentum, and energy differential equations. This model applied the porous model to describe the solid phase.

Pu Q. (1991) continued the Gustafson project and proposed equations for the degradation of cellulose and hemicellulose.

Natercia et al. (2000) ran a steady state operation of a continuous digester with an ITC (isothermal cook circulation) and simulated two phases of a heterogeneous digester by means of a model that adopted 15 state variables at each axial position of the digester. This model had the capacity to account for the solid content including both organic and inorganic materials. This model adopted an isothermal condition for the reaction.

Michelsen and Foss (1994) combined the approaches of Harkonen and Christensen to make a more detailed digester model. He modeled the mass flow together with the reaction kinetics for a continuous steam-liquor digester. By solving the compaction and the velocity of the chip plug, he attempted to provide a control tool for delignification.
In subsequent work, Michelsen and Foss (1996) tried to create a model to explain the complex behavior of the digester, particularly the interaction between the reaction kinetics and the residence time.

Kayihan et al. (1996) modeled a two-zone digester, i.e., a mixing zone where impregnation takes place, and a reaction zone. Partial differential equations were solved in each zone. It was assumed that the solid and liquid phases were in thermal equilibrium. The adopted kinetic model was the same as the Christensen model.

Wisnewski et al. (1997) also extended the Purdue model, approximating the digester as a series of CSTRs, with each CSTR consisting of three phases. This extended model reduced the number of assumptions made in the Purdue model by defining the solid concentrations on a mass per chip volume basis, defining the compaction as the volume fraction of the CTSRs and the porosity as volume fractions of the wood chips. Chip porosity and liquor density were also defined in this model.

Pougatch and Salcudean (2006) implemented a solid tangential stress sub-model which was developed for the digester. The advantage of this sub-model was that the solid phase behavior reproduced the plug flow of the chips and eliminated the adopted non-physical assumptions of the Newtonian approach.

Quak and Benington (2004) modeled a single phase liquor flow in a batch laboratory digester using CFD.

Pingle et al. (1998) investigated the pulp suspension in the circular pipes. Xie et al. (2003) and Cui et al. (2007) studied three phases i.e., gas, liquid and solid to examine the pulp suspension.

We extend this work in this paper by considering factors such as the chip quality, variation in the concentration of active ions, and energy balance to describe the temperature distribution through the digester, and by tuning the model against data from the real plant. This could enable consideration of the effect of reactor geometry, such as the conical side walls on the flow fields and reaction kinetics.

3. Theoretical set up

Mass percentage of fibers in the wood

The pine wood contains about 41% hemicelluloses and 28% cellulose by weight. The total fiber content of pine wood is therefore about 70%.

Governing equations, FLUENT (2009)

Continuity: steady form:

\[ \nabla \cdot (\rho_m \bar{v}_m) = 0 \quad (1) \]

Drag Force

The drag force between the continuous and the dispersed phases is defined as

\[ F_{DC} = K_{DC} \left[ \bar{U}_d - \bar{U}_c - \left( \frac{\alpha_d \bar{U}_d}{\alpha_d} - \frac{\alpha_c \bar{U}_c}{\alpha_c} \right) \right] \quad (2) \]

However in these simulations the inertial drag force is imposed by the pore walls on the fluids.

Inertial resistance

\[ -\frac{c_p}{2} |\bar{v}| \bar{v} \quad (3) \]

This term is added to the right side of momentum conservation equation of the phases in the model. However C is not constant through the domain due to anisotropic characteristic of adopted porous media.

Superficial velocity

\[ \bar{v}_{\text{superficial}} = \gamma \bar{v}_{\text{physical}} \quad (4) \]

γ is defined as the volume occupied by the fluid to the total volume.

Volume fractions

The phases in the Euler-Euler multiphase are treated as interpenetrating continua. Transfusion of the phases into each other incorporates the concept of volume fractions, which represent the space occupied by each phase.

The volume fraction of phase q, \( V_q \), is defined by

\[ V_q = \int \alpha_q dV \quad \text{where} \sum_{q=1}^{n} \alpha_q = 1 \quad (5) \]

Conservation of mass (steady form):

The continuity equation for phase q:

Since the flows reside in a porous media therefore a superficial velocity may be considered for them and the conservation equation of mass for any phase is:

\[ \nabla \cdot (\alpha_q \rho_q \bar{v}_q) = \sum_{p=1}^{n} (\bar{m}_{pq} - \bar{m}_{qp}) + S_q \quad (6) \]

Conservation of energy (steady form)

To describe the conservation of energy in Eulerian multiphase applications, a separate enthalpy equation can be written for each phase.

\[ \nabla \cdot (\alpha_q \rho_q \bar{h}_q) = \alpha_q \frac{\partial \bar{h}_q}{\partial t} + \bar{F}_q \nabla \bar{u}_q - \nabla \bar{q}_q + S_q \quad (7) \]
Reduced conservation of momentum
(laminar & steady state) for a fluid phase q in a porous media is described thus:
\[ \nabla \cdot \left( \alpha_q \rho_q \vec{v}_q \right) = -\alpha_q \nabla p + \alpha_q \rho_q \vec{g} - \alpha_q \frac{C_p}{2} \left( \nabla \cdot \vec{v} \right) + \sum_{p=1}^{N} \left( K_{pq} \left( \nabla \cdot \vec{v}_p - \nabla \cdot \vec{v}_q \right) + m_{pq} \rho_p \vec{v}_p - m_{qp} \rho_q \vec{v}_q \right) \]  
(8)

The material density ratio is defined as
\[ \gamma = \frac{\rho_{\text{Dispersed phase}}}{\rho_{\text{Carrier phase}}} \]  
(9)

Average distance between the individual particles and particle loading
\[ \frac{1}{\delta_d} = \left( \frac{\pi^{1/3}}{6} \right)^{1/3} \]  
(10)

\[ k = \frac{\beta}{\gamma} \]  
(11)

Mass transfer
\[ \dot{m}_{pq} = \max \left[ \alpha \lambda_{pq} \right] - \max \left[ o \lambda_{pq} \right] \]  
(12)

Fick’s law
\[ J = -D \frac{\partial \rho_0}{\partial x} \]  
(13)

Diffusive mass flux (mass transfer rate)
\[ \dot{J}_i = -D \frac{\partial \rho_0}{\partial x} \nabla \gamma_i \]  
(14)

The continuity equation (steady form) for 2D axisymmetric geometries (mass conservation equation)
\[ \frac{\partial}{\partial x} \left( \rho v_x \right) + \frac{\partial}{\partial r} \left( \rho v_r \right) + \frac{\rho v_r}{r} = S_m \]  
(15)

Axial Momentum conservation equation for 2D axisymmetric geometries (steady form)
\[ \frac{1}{r} \frac{\partial}{\partial x} \left( rv_x v_x \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( rv_x v_r \right) = \]  
\[ -\frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} \left[ \mu \left( \frac{\partial v_x}{\partial x} + \frac{2}{3} \left( \nabla \cdot \vec{v} \right) \right) \right] + \]  
\[ \frac{1}{r} \frac{\partial}{\partial r} \left[ \mu \left( \frac{\partial v_r}{\partial r} \right) \right] \]  
(16)

Reduced radial Momentum equation (steady form)
\[ \frac{1}{r} \frac{\partial}{\partial x} \left( rv_x v_r \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( rv_r v_r \right) = \]  
\[ \frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} \left[ \mu \left( \frac{\partial v_r}{\partial r} + \frac{2}{3} \left( \nabla \cdot \vec{v} \right) \right) \right] + \]  
\[ \frac{1}{r} \frac{\partial}{\partial r} \left[ \mu \left( \frac{2}{3} \frac{\partial v_r}{\partial r} \right) \right] \]  
(17)

4. Modeling set up

The pulping production process is a continuous chemical interaction between a bulk phase (black/white liquor) and a dispersed phase (wood chips).

A number of simulations were performed to examine and compute the diffusivity and mass transfer rate of the pulping reaction.

The process of the pulping chemical reaction and production has many features and therefore several modeling approaches may be used to express different aspects of the production.

The mass diffusivity was used as the adjustment variable to attain a suitable Kappa number distribution when simulating the reaction.

There are two approaches for the numerical calculation of multiphase flows: the Euler-Lagrange approach and the Euler-Euler approach.

Euler-Lagrange approach

The Euler-Lagrange approach is a combination of Euler, which solves the Navier stokes equation for continuous phase and the Lagrange formulation which tracks the motion of the separate particles of the dispersed phase in the continuous phase. The fluid phase is considered as a continuum. The dispersed phase material can be of solid particles, liquid droplets or bubbles. The Lagrange formulation calculates the trajectory of the dispersed phase at intervals in the continuum.

This method is applicable in cases where the volume fraction of the dispersed phase is below 10%. It is permissible to use the heavy particles with high densities which may lead to higher mass flow rates of the dispersed phase than the fluid phase. The Lagrange dispersed phase approach ignores particle-particle interactions and the effect of the particle volume fraction on the fluid phase.

Euler-Euler approach

This method is not able to track individual particles of the solid phase because it treats the solid particles as a continuous phase. This is the major assumption of this model which despite the different physical states of the phases, treats them both as continua.

Both the bulk flow and the dynamic properties of the dispersed particles in the multiphase flow are predicted by the Euler formulation. The phases are not totally separated but transfuse to each other and
therefore the volume fraction has a continuous characteristic.
There are three different Euler-Euler multiphase approaches: the volume of fluid (VOF) model, the mixture model, and the Eulerian model.

The Eulerian model

Prediction of the multiphase flow behavior using the Eulerian scheme is more complicated than the other multiphase approaches. This is partly due to additional equations applied in the model and the type of the phases. The phases are treated according to their physical states and the treatment may be more or less complex. The Eulerian model solves the conservation equations for each phase. Interactions between phases are taken into account by calculation of the pressure and inter-phase exchange coefficients $K_{pq}$ and $K_p$.

Limitation of the Eulerian model

Convergence is the major disadvantage when using the Euler-Euler multiphase flow. The Eulerian model treats the phases as a continuum, meaning that solid particles or bubbles are not treated as dispersed particles. The conservation equations are solved for each phase but a single pressure applies for all the phases.

Comparison of models

Applying the mixture or Eulerian model essentially depends on the characteristics, application, requirements and our knowledge of the system of the multiphase problem. It is evident that the Eulerian model is more complicated than the mixture model. However, despite its computational advantages, the mixture model is not always preferred in place of the Eulerian model. For example, if the properties of the inter-phase are known, the Eulerian model is recommended because it can be much more accurate. In most other cases the mixture model is adequate and easier to converge. The Eulerian model is complicated and the calculations may not be stable, reducing the accuracy of the results.

Structural properties of the digester

The digester has a height of 60 m and a diameter of 6 m at the entrance which changes through several steps down the digester to 7 m at the bottom. A large annular pipe hangs inside the digester. This pipe is connected to the outlet pipes of the circulation loops C8 (wash zone circulation from the lower section), MCC (in the middle section) and ITC the upper section. The flows re-circulate back into the digester separately at three different levels.

The central pipe comprises of three concentric pipes. The innermost pipe is the longest and recirculates from C8 into the digester. The diameters of the C8, ITC and MCC inlets are 0.21 m, 0.3 m and 0.425 m respectively. However, the effective diameters of the two outer pipes are reduced because they include the smaller inner pipes. The effective diameters were therefore used in the construction of the digester model. The model was designed in Gambit as two axisymmetric sections around the x-axis. The final shape of the digester was obtained by rotation of these sections around the x-axis. The digester was therefore designed in 2D but FLUENT takes into account the total digester volume of around 1800 m$^3$ and that of the circular central pipe as it exists in the digester.

Figure 1: The pulping digester

The chemical reactions in the Kraft pulping process are highly complex and in some cases are unknown and therefore simplifying assumptions are unavoidable when designing a mathematical model.

Mixture variables

The physical properties in the digester were defined as follows: A constant value is defined for viscosity of the mixture. The volume weighted mixing law is used to compute the density of the mixture. For increased accuracy the double precision version of FLUENT was used for calculations.

Four simulations are performed and an Eulerian multiphase method of Euler- Euler approach was applied in order to design the phases, i.e. wood chips and liquor flow.

Modeling simplifications and assumptions
The hydraulic behavior of the digester, multiple circulations, multiple inlets and outlets, chemical processes, wood constituents and properties, chemical liquor composition, temperatures and pressures are neither persistent nor regular enough for us to define a fixed and global model for the hydraulic and chemical behavior of the pulping process. These conditions demand a number of assumptions and simplifications so that an approximate model of the pulp production process can be established. It is difficult to avoid making these assumptions and simplifications. In our model we have made simplifications and assumptions regarding the hydraulic behavior and chemical reactions, partly due to lack of knowledge of these processes and partly due to limitations and the capacity of the modeling tools. We neither modeled wood chips as the individual physical particles and nor used the Lagrange model to follow them. Such a model that takes the total volume of the digester including total individual particles and the associated reactions is simply beyond the reach. We have simplified the reaction of particles using mass transfer scheme and Eulerian approach. We treated the wood chips as a continuous phase. The recirculation flows are neglected but instead the total amount of these flows are accounted and added to the inlet flow. The circulation flows are heated out of the digester and then returned into the digester to keep the temperature constant. In order to take this influence into consideration, we have run the simulations at constant temperature. The calculations were performed for pulping of softwood.

**Mass transfer approach**

The mass transfer mechanism in the frame work of the Eulerian multiphase model in FLUENT was adopted for the pulping process. Pulp quality was predicted by solving the unidirectional mass transfer model, which describes a positive mass flow rate per unit volume from phase p to phase q.

The FLUENT multiphase mass transfer code accommodates mass transfer between species belonging to different phases. Instead of a matrix type input, multiple mass transfer mechanisms must be input. Each mass transfer mechanism describes the process of mass transfer from one entity to another. An entity is either a particular species in a phase, or the bulk phase itself if the phase does not have a particular species associated with it. The mass transfer process may be specified either through the built unidirectional "constant-rate" mass transfer or through user-defined functions.

The interaction between groups of species was also defined. The lignin is associated with the wood chips at the beginning of the process and moves from the solid to the liquid phase during exposure to the cooking liquor. The mass transfer rate is homogeneous. The diffusivity of the liquor is also significant in determining the mass transfer rate, conversion, and quality of the produced pulp through the digester.

**Mass transfer conjugated with Porous media**

A combination of the Eulerian mass transfer approach with the species transport scheme and porous media can be used to predict the flow behavior when modeling of both solid and liquid phases is required. Use of the porous media model can eliminate complications such as modeling instability and divergence that arise from the granular method. A non constant and variable porosity was defined throughout the digester to represent the compressibility of the chips and pulp zones. Two porous model is available the first is viscous resistance and the next one is inertial resistance. In these simulations the inertial resistance is used. Porous model contributes to decelerate the flows in the digester. when lignin dissolves and moves from phase1 to phase2 then phase 1 is soften and causes a momentum change in the flows. Therefore a decreasing porosity is defined in the model.

Mass transfer model were conducted to perform transition of the lignin from one phase to other phase. Diffusivity and mass flux (mass transfer rate) were two main parameters.

The resistance of the solid chip phase with variable compressibility to expansion and compression can be represented by assigning a bulk viscosity. This can be modeled as a porous media. However, defining these properties using other CFD strategies may be at the expense of higher computational cost.

**5. Grid independence and validity**

The outlets, extractions and amounts of the circulation flows were obtained from simulation of the digester by adjustment of the pressures. The results were compared with the operation values of the Korsnas process data base and agreed with the data from the mill. The actual digester is around 60 m in height and its diameter varies from 6 to 7 m, as previously mentioned. The simulations were performed with three different types of meshes with different numbers of cells. Models were built with meshes made up of 16000 and 55776 triangular cells, and with 21000 quadrilateral cell meshes for one half of the digester i.e. 60 m × 3 m. The other half of the digester is axisymmetric and was computed by FLUENT. There was no difference between the results with the 56000 triangles and 21000 quadrilaterals, but the intermediate mesh made up of 16000 triangular cells did not agree.
well with the results from the other two meshes. The lignin contents at outlets were higher compared to other simulations. We concluded that the mesh of 16000 triangles was unable to give sufficiently accurate results. Results of tests using even larger numbers of cells were little different to those carried out with the 56000 or 21000 cells. A homogeneous mesh is used which means that the mesh size is constant in all directions. The surfaces are meshed with the same size. The mesh size is 1 cell/5 cm of the digester at all directions.

6. Discretization, boundary conditions, set up

As the digester of the Korsnas/Vallvik pulping plant is a vertical cylinder, the geometry in the model was constructed from an axisymmetric two dimensional scale model of the digesters. In contrast to two-dimensional symmetric models, this can take the total volume of the reactor into account.

Discretization:

<table>
<thead>
<tr>
<th>Discretization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Momentum</td>
</tr>
<tr>
<td>Volume fraction</td>
</tr>
<tr>
<td>Energy</td>
</tr>
<tr>
<td>Phase 2</td>
</tr>
<tr>
<td>Pressure velocity</td>
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<tr>
<td>coupling</td>
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</table>

Table 2: Discretization formulations

Models set up:

<table>
<thead>
<tr>
<th>Models</th>
</tr>
</thead>
<tbody>
<tr>
<td>SOLVER</td>
</tr>
<tr>
<td>Gradient option</td>
</tr>
<tr>
<td>Porous formulation</td>
</tr>
<tr>
<td>Velocity formulation</td>
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<tr>
<td>Formulation</td>
</tr>
<tr>
<td>Species transport model</td>
</tr>
<tr>
<td>Energy</td>
</tr>
</tbody>
</table>

Table 3: The applied models

Inlet boundary:

Velocity inlet, Mixture: no active option
Phase 1: Thermal: T= 430 K, velocity specification method: magnitude normal to boundary, 0.3 m/s, no other active option for species or multiphase
Phase 2: 50 percent, T= 430 K, velocity specification method: magnitude normal to boundary, 0.1 m/s, species: lignin, species mass fraction= 0.3
The Schiller-Naumann formulation is adopted to solve for the drag force in the mixture mode.

Operating conditions

<table>
<thead>
<tr>
<th>Operating conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gravitational acceleration</td>
</tr>
<tr>
<td>Operating temperature</td>
</tr>
</tbody>
</table>

Table 4: Operating conditions

7. Results

A number of simulations were performed to evaluate the distribution of pulp produced in the reactor. The simulations were performed to examine the effect of the specified mass diffusivity, mass transfer rate and porosity.

Figure 2: Distribution of Kappa number in the digester from top to bottom –R11-D0.288
Figure 3: Contour plots of Kappa number R12-D0.00288

Figure 4: Contour plots of Kappa number-R5-D0.000288

Figure 5: Contour plots of Kappa number –R13-D0.000288

Graph 1: Kappa number – R11-D0.288

Graph 2: Kappa number – R12-D0.00288
Figure 3: Contour plots of Kappa number R12-D0.00288

Graph 3: Kappa number – R5-D0.000288

Figure 4: Contour plots of Kappa number R5-D0.000288

Graph 3: Kappa number R13-D0.000288

Figure 7: Mass fraction of lignin in the pulp R12-D0.00288

Figure 6: Distribution of the mass fraction of the lignin in the pulp R11-D0.288

Figure 8: Mass fraction of lignin in the pulp R5-D0.000288
8. Discussion

A number of simulations were performed to evaluate the pulp production rate in the reactor. For this purpose three essential variables were examined and other variables and boundary conditions are held constant.

<table>
<thead>
<tr>
<th>Diffusivity</th>
<th>Transfer Rate</th>
<th>Porosity</th>
<th>Abbreviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.288</td>
<td>2.0E-11</td>
<td>0.55-0.15</td>
<td>R-11-0.288</td>
</tr>
<tr>
<td>0.00288</td>
<td>1.7E-12</td>
<td>0.65-0.25</td>
<td>R12-0.00288</td>
</tr>
<tr>
<td>0.000288</td>
<td>8.2E-05</td>
<td>0.5-0.1</td>
<td>R5-0.000288</td>
</tr>
<tr>
<td>0.000288</td>
<td>8.2E-13</td>
<td>0.5-0.1</td>
<td>R13-0.000288</td>
</tr>
</tbody>
</table>

Table 5: Variables of simulations
The mass transfer rate is accounted analytically according to rate of pulp generation which is about $8 \times 10^{-3}$ kg/s.m$^2$. Many other values of these parameters were examined but they failed to reach a kappa number of 24 at the bottoms of the digester. The parameters are given in this paper are the “only” which gave us right product with right composition. The difference between these parameters is that they show different lignin distribution inside the digester.

Figures 2 to 5 and Graphs 1 to 4 display the Kappa number of the pulp through the digester under different simulation conditions. Graphs 1 to 4 reveal differences in the lignin dissolution process in terms of Kappa number. The inlet chips contain around 20% lignin and 10% extractive materials. The pulp at the outlet of the reactor contains around 3% lignin. The Kappa number corresponding to pulp containing 3-4% lignin at the outlet is about 24. The simulations show how cooking develops at different levels of the digester. The mass fraction of the lignin in the pulp is shown in figures 6 to 9, which show that lignin made up around 30% of the mass of wood chips at the top of the digester, and reduced to around 3% of the mass of the pulp at the outlet.

Figures 2, 6 and graph 1 show a large decrease in Kappa number and lignin content of the wood chips at the uppermost parts of the reactor, indicating an intensive cooking process at those levels.

Figure 5, 9 and graph 4 show feeble release of lignin from the wood pulp at uppermost levels of the digester, whereas the more abrupt change in gradient in graph 8 shows that lignin dissolved more rapidly in lower sections of the digester.

Figure 3, 7 and graph 2 show more even and temperate cooking throughout the reactor.

Figure 4, 8 and graph 3 show that there was lesser cooking around the centre pipe than away from the pipe walls at uppermost parts of the reactor. Graph 3 is thicker at upper sections which can be interpreted as different cooking rates horizontally at x-direction.

Graphs 5 to 8 show the mass fraction of fibers in the digester. The wood chips at the top of the digester contain around 70% fibers and 30% lignin and extractives by mass. The fiber content of the pulp was differently distributed in these figures, representing the differences in the cooking processes.

The lignin content drops faster when the chips travel 10m downward from the top of the digester according to the simulation results specified with the R11-D0.288 (figures 2, 6, and graphs 1, 5) compared to other 3 simulations. The lignin dissolution is slowest in the last 10 m of digester according to R11-D0.288 simulation. This simulation turns out 3 different reaction rates through the digester.

Results obtained from second simulation shows more reaction rates for lignin dissolution. The rate changes every 10-20m of the digester this means that the rates shift the trend after every 10-20m. The rate is diminishing in the last 10m of the digester. The results obtained from this simulation are figures 3, 7, and graphs 2, 6.

The third simulation shows also about 5 reaction rates but the progress of the reaction is heterogeneous horizontally at any height. Mass fraction of lignin increases as moving from the walls toward the center of the digester. Figures 4, 8, and graphs 3, 7 are gained from the third simulation.

The forth simulation is rather more homogeneous and variation of the lignin mass fraction at the X direction is lower. The resulted curves are thinner compared to former simulation. See figures 5, 9, and graphs 4 and 8.

The third and forth simulations are run with the same and low mass diffusivity but the later has rather a lower mass transfer rate. Now it is not surprising that the lignin dissolution delays in the forth simulation compared to others.

9. Validation and comparison of the Kappa number resulted from Mass transfer scheme simulations

The simulations were compared with experimental results. The experimental data are available at the top and bottom (product) of the digester. The product (at the bottom of the digester) has about 3% lignin and 97% fibers. When lignin content of the product (at the bottom of the digester) is 3% then Kappa number is about 24. The simulations showed very good agreement these values. Kappa number at the bottom of the digester is 23.6, 24.8, 24.6, and 23.7 for different simulation. (See figures 2,3,4,5 respectively)

Mass fraction of the pulp product is between 3-4% according to the experimental results which agree well with the simulations results. The following values of the lignin content of the product are gained from simulations: 3.54%, 3.72, 3.58, and 3.55 (See figures 6, 7, 8, 9). These values show
very good agreement with the experimental data of the pulp product.

The simulations reveal different gradients or distributions of the fibers and lignin in the digester. The lignin dissolution accounted by the Purdue, Gustafson, and Andersson models is shown in the next graph.

Graph 9: Lignin content calculated by different Kraft cooking models Laaksoo (2008)

In order to compare our FVM Mass transfer schemes simulations with 3 above models we computed the lignin content of the wood chips in terms of lignin percent in our simulations at 13 vertical points of the digester. The velocity distribution of the secondary phase is shown in the next figure.

Figure 10: Contours of Velocity of wood chips
The Area-Weighted Average Velocity through the digester is also accounted.

Area weighted average velocity = 0.0034 m/s

The residence time of the wood chips is estimated based on the Area-Weighted Average Velocity and total height of the digester.

Residence time:
60 m/0.0034 m/s = 17647 s ≈ 4.9 h

The time at which the chips spent to reach any of 13 selected vertical points in our models is calculated (based on the height and average velocity of wood chips) and the lignin percent is compared to corresponding time with the Purdue and Gustafson, and Andersson models. The next graph compares the Mass transfer scheme simulations with the Purdue, Gustafson, and Andersson models.

Graph 10: Comparison of mass transfer simulation models with Purdue, Gustafson and Andersson models

Lignin percents of graph 9 are expressed in terms of Kappa number in graph 10. Kappa numbers predicted from simulations are accounted at different height of digester but since the flow is continuous then the Kappa number at any height is expressed in terms of the time in which the chips have spent to reach any height of digester.

The cooking reactions are much faster in the Andersson model than the others. One of the mass transfer scheme simulations (R11-D0.288) fit the Purdue and Gustafson model after about 120 min.

Simulation graph of R5-D0.000288 is also very close to the Purdue and Gustafson models. Mass transfer rate for this simulation is accounted analytically.

The essence of the FVM is the solution of the conservation equations of mass, momentum and energy including the chemical reactions in every finite volume of the reactors. Furthermore, unlike the CSTR method, the FVM provides a powerful
meaningful graphics, animation and reports that make it easy to convey CFD results.

10. Conclusion

FVM was used to mathematically model the flow behaviour, chemical reactions and pulp quality in a pulping digester under steady state conditions.

The digester was represented as a two dimensional axisymmetric model which takes its total volume into account. We demonstrated that this approach was able to model the conditions in the pulping process. The performance of the mass transfer multiphase strategy indicates that it is useful code for simulation of the pulping chemical reaction.

Pulp quality was predicted by prediction of the Kappa number which was defined in the Custom Field Function panel.

The results indicate that a combination of the multiphase model, species transport, mass transfer and porous can predict the pulping chemical reactions inside the digester. This system can also provide a good prediction of the pulp quality. Application of this model is expected to help researchers and operators of the pulping mill to improve their knowledge of the pulping reactions and aid in devising new and improved strategies to control the pulping process.

11. Future work

Sometimes due to incidence of disturbances and happening of some degrading phenomena in the pulping process the quality of the product decreases. It is possible to simulate these errors and show what will take place inside the digester in the presence of these undesirable phenomena.

12. References


FLUENT USER GUIDE is available on the www.fluent.se


Hartler, N. and W. Onisko, ”Svensk Papperstidn,” 65, 905 (1962).


Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tr>
<td>d</td>
<td>Diameter (m)</td>
</tr>
<tr>
<td>d_p</td>
<td>Particle diameter (m)</td>
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<tr>
<td>C_2</td>
<td>Inertial factor</td>
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<td>D</td>
<td>Diffusion coefficient or mass diffusivity m^2/s</td>
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<td>D_{lm}</td>
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Paper III
Modelling of the channelling phenomenon of the pulping digester using porous media

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Abstract

This paper describes the development of a dynamic model of a continuous pulping digester to characterize the channeling phenomenon. The CFD codes in FLUENT are used to compute the hydraulic behavior of the digester under both normal and various specific operating conditions. Included in this model are all the circulation flows, extractions and multiple inlets and outlets.

The digester is designed in Gambit and an axisymmetric 2d model of the digester is applied. A porous scheme is implemented in the model in order to design the fluid flow and channeling phenomenon inside the digester. A heterogeneous porous media is specified in order to take into account the compression of the pulp. The simulation can be used as a prognostic model to predict risky situations and thereby reduce economic damage. The k-ε turbulent model contributes to computation of the flow “regimes” or eddie formation in turbulent zones of the digester.

Key words

CFD, channeling, porous media, turbulent, axisymmetric, pulping digester

Nomenclature

\begin{align*}
g & \quad \text{Gravitational acceleration} \\
G_k & \quad \text{Generation of turbulent kinetic energy due to mean velocity gradient} \\
G_b & \quad \text{Generation of turbulent kinetic energy due to buoyancy} \\
k & \quad \text{Turbulent kinetic energy} \\
r & \quad \text{Radial coordinate} \\
S_i & \quad \text{Momentum sink} \\
S_m & \quad \text{Mass added to continuous phase from dispersed phase} \\
x & \quad \text{Axial coordinate} \\
v_m & \quad \text{Mass-averaged velocity} \\
v_z & \quad \text{Swirl velocity} \\
|v| & \quad \text{Magnitude of velocity} \\
v_x & \quad \text{Axial velocity} \\
v_r & \quad \text{Radial velocity} \\
\rho & \quad \text{Density} \\
\epsilon & \quad \text{Turbulent dissipation rate} \\
\mu & \quad \text{Viscosity (kg/m-s)} \\
\mu_t & \quad \text{Turbulent viscosity (kg/m-s)} \\
\alpha_k & \quad \text{Volume fraction of phase k}
\end{align*}

Introduction

Modelling of the pulping digester has been of interest to many researchers from different areas. The digester is the major element of the pulping process. Pulp production develops in stages and different modes of cooking may occur in the digester.

The economic consequences of any disruption in the pulping process can be
The details of the pulping process are still largely unknown and many studies have been performed to understand what really happens inside the digester.

The studies initiate from those of Vroom [1], who modelled the H-factor. The Purdue model was later established by Smith et al. [2]. This was a new approach to modelling this process and many researchers followed with improvements. The model was modified by taking different aspects of pulp processing into account and implementing them into the Purdue model. Johansson [3] implemented a temperature dependent diffusivity into the model. Hartler applied a pH dependent diffusivity into the Purdue model. Gustafson [4] improved Johansson’s model by using three cooking kinetic reactions instead of a single equation. Christensen [5] developed kinetic models that took the wood used in the digester into account.


The study described in this paper is based on models applying commercial CFD codes within FLUENT.

The digester is a moving bed reactor where the wood chips are fed in from the top and the liquor has several inlets and outlets at the bottom, top, and around the digester. The wood chips consist of fibres, lignin and extractives. The lignin which holds the cells together reacts with the liquor chemicals and transfers to the liquid phase. The fibres within the wood chips are freed when the lignin is removed to the liquid phase. The free fibres are called pulp. In suspension solutions or granular flows, the motion of particles establishes a pressure gradient in the solution if the packing limit of the solid particles is less than the maximum allowable value of 0.63.

When the packing limit of the solid is less than the 0.63, the solid phase is compressed and a pressure gradient of the solid particles is produced independently \((\nabla p_s)\). The pressure gradient is introduced by the granular momentum. The solid particles follow the Maxwell-Boltzmann distribution which is a probability distribution.

The pulping digester, shown in Figure 1, has a height of around 65 m and a diameter of 6 m at the top and of around 7 m at the bottom. The diameter increases stepwise from top to bottom.

![Figure 1. The pulping digester.](image)
compressibility of the solids. Decomposition of the wood develops when lignin is removed from the chips. The chemical dissolution process makes the chips soft and more compact. In order to model the deformation of the wood chips, the digester is divided into small sections which contribute to define different porosities in these regions. In order to investigate the behaviour of the liquor as it moves down the chip bed, the prescribed porosities are highest at the top and reduce down the digester. The void volume between the chips is called the free liquor. As the lignin dissolves, the chip bed is compressed and the free space between the chips decreases. The volume fraction of the chips in the cooking blocks increases and the volume fraction occupied by the free liquor decreases.

**Governing equations**

The continuity equation for 2D axisymmetric geometries (mass conservation equation)

\[
\frac{1}{r} \frac{\partial (r \rho_v v_r)}{\partial x} + \frac{1}{r} \frac{\partial (r \rho_v v_z)}{\partial r} = \frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} \left( \mu \left( \frac{\partial v_r}{\partial r} + \frac{\partial v_z}{\partial x} \right) \right) = \frac{\partial}{\partial x} \left( \rho \frac{\partial v_r}{\partial x} \right) + \frac{\partial}{\partial r} \left( \rho \frac{\partial v_z}{\partial r} \right) = S_m \tag{1}
\]

Axial Momentum conservation equation for 2D axisymmetric geometries

\[
\frac{1}{r} \frac{\partial (r \rho_v v_r)}{\partial x} + \frac{1}{r} \frac{\partial (r \rho_v v_z)}{\partial y} = \frac{\partial p}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} \left( \mu \left( \frac{\partial v_r}{\partial x} + \frac{\partial v_z}{\partial y} \right) \right) = \frac{\partial}{\partial x} \left( \rho \frac{\partial v_r}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho \frac{\partial v_z}{\partial y} \right) = S_m \tag{2}
\]

Radial Momentum equation

\[
\frac{1}{r} \frac{\partial}{\partial x} \left( r \rho v_r v_r \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \rho v_r v_z \right) = \frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} \left( \mu \left( \frac{\partial v_r}{\partial r} + \frac{\partial v_z}{\partial x} \right) \right) + F_r \tag{3}
\]

Porous momentum sink

Increased porosity reduces flow velocity due to generation of a pressure gradient in the cell zones. This is accounted for in the model by including an additional source term in the fluid flow equations. The source is a flow resistance and consists of two terms that are empirically determined. A viscous loss term and an inertial loss term are included in the momentum equation in the porous cell zones.

\[
S_i = \sum_{i=1}^{3} \int_{y} D_{ij} \mu v_{ij} + \sum_{i=1}^{3} C_{ij} \frac{1}{2} \rho |v| v_i \tag{4}
\]

Turbulent kinetic energy

\[
\frac{\partial}{\partial t} \left( \rho k \right) + \frac{\partial}{\partial x_i} \left( \rho u_i k \right) = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \tag{5}
\]

Turbulent dissipation rate

\[
\frac{\partial}{\partial t} \left( \rho \varepsilon \right) + \frac{\partial}{\partial x_i} \left( \rho u_i \varepsilon \right) = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_{\varepsilon}} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + \frac{C_{1e} \varepsilon}{k} (G_k C_{3e} G_b) - C_{2e} \rho \frac{\varepsilon^2}{k} + S_\varepsilon \tag{6}
\]

Reynolds number
\[ \text{Re} = \frac{\rho ud}{\mu} \]  
\[ \text{Homogenous porous media} \]

\[ S_i = \left( \frac{\mu}{\alpha} v_i + C_2 \frac{1}{2} \rho |v_i| \right) \]  
\[ \text{Darcy's law in porous media} \]

\[ \nabla p = -\frac{\mu}{\alpha} \vec{v} \]  
\[ \text{Inertial loses in porous media} \]

\[ \nabla p = -\sum_{j=1}^{3} C_2 g \left( \frac{1}{2} \rho v_j |v_j| \right) \]  
\[ \text{Modeling set up} \]

A turbulent model and a heterogeneous porous media are defined for the digester. In the porous media the flow velocity decreases but generation of turbulence and the dissipation rate are still modelled through the media by the default approach in FLUENT. It is not necessary to restrict the turbulence in any zone in the porous media. In order to suppress the turbulence in any zone it is sufficient to activate the “laminar zone” in the fluid panel of that zone. In this way the turbulent viscosity (\( \mu_t \)) is considered zero in that section. The turbulence created in the porous media does not affect the momentum of the flow. The turbulent elements transport through the porous zones. The inertial loss term of the momentum sink is activated and specified for each porous section of the digester in both x and y directions. A porosity range is defined from 0.65 to 0.25, to account for the distribution of the fluid flow through the particles. Porosity value in the channels is 0.95. The length of top and lower channels is respectively about 10 and 7 m. Channels include smaller ducts in order to examine other channel size.

The effect of gravity is taken into account and a value of 9.8 m/s\(^2\) is specified for gravitational acceleration in the positive x direction.

![Results Channelling](image1)

Figure 2: Contours of distribution of the Velocity inside the digester from top to bottom

![Results Channelling](image2)

Figure 3: Contours of distribution of the Velocity at the top of the digester
Discussion

Due to the unique geometric design of the reactor, the heterogeneous reaction, the hydraulic characteristics of the zones, long residence time, and the multiple inlets and outlets it is not unreasonable to assume that different flow regimes are present in different zones within the digester. In some sections the flow is unidirectional and downward and in others the flow runs against this current. These unique characteristics contribute to the formation of a double flow regime in the digester.
Therefore, assigning an exclusive flow regime to characterize the digester is an ineffective approach. Multiple Reynolds numbers may be accounted for in the multiple inlets of the digester. The free liquor flow through the chips bed follows the laminar flow regime at the top and middle of the digester. Very low velocities are observed throughout the digester despite the high velocities at the inlets. This may be due to the solid phase, which is itself mobile, and leads to a momentum exchange with the fluid flow, and also behaves as a porous media for the liquid phase and considerably reduces its momentum. The Reynolds numbers at the inlets are defined at between 40000 and 70000. The inlet diameters are 0.35, 0.30, 0.20 and 0.16m. The viscosity is around 0.001 kg/m s. The mesh size is 0.13 and it is of type quad map type.

A k-ε turbulent model is defined due to the presence of the counter-current flow in the bottom of the digester which results in a turbulent regime. Applying a turbulent model contributes to the computation of small eddies in the lower zones of the digester.

The velocity of the liquor increases in the channels as shown by the “velocity magnitude” and “vectors of the velocity” in Figures 2 to 8.

When the liquor flow enters the channel its velocity increases due to the elimination of the momentum sink and the low amount of wood chips in the channels, as shown in Figures 2-4. When the liquor leaves the channel the velocity decreases again due to the presence of wood chips at its path, as shown in Figures 7 and 8. Inside the channel the velocity is higher at the beginning and decreases gradually as shown in Figure 6. The velocity inside the channel has a negative gradient in the vertical direction. The reaction of the lignin and liquor takes place at high temperatures of above 150 °C. One study where the temperature of the washing screen was measured showed a large variation in its temperature before and after the channelling [8].

The model of the channelling can be used to locate the channels by comparing the operating parameters before and after channelling. Channelling affects operating conditions such as the outlet flow rate, pressure and temperature.

Any deviation of these parameters from the normal operational conditions may indicate channelling. However, the magnitude of the deviation that indicates channelling must be determined because the normal operating conditions are unsteady and only deviations over a certain magnitude may indicate channelling.

**Conclusion**

A pulping digester has been modelled to examine the destructive phenomenon of channelling. An artificial channel is modelled in the digester using a porous media model. A heterogeneous porous media is defined to represent the solid phase and its compressibility. Compared to a homogenous solid phase, using the heterogeneous solid phase has the effect of increasing the volume fraction of the liquid phase in the channel while reducing the porosity outside of the channel. The channels are characterized by defining a very high porosity in the digester.
The flow behaviour is examined around and inside the channel. The results of the modelling show that the liquor velocity is higher inside the channel than outside it.

This effect can affect the circulation flow in the pipes which may be an indicator of dangerous conditions.

The liquor velocity around the channel decreases and the circulation flows which are located along the channel degenerate. However, the mass flow rate in the circulation pipes under the channel would be expected to increase under these conditions. This can lead to a pressure drop in the pipes along the channel and an increased pressure in the pipes that are located under the channel.

These pressure changes are important parameters for the operation of the digester, and calculation of their magnitudes is an important topic for future studies.

Channel modelling improves our knowledge of the hydraulic behaviour of the pulping digester which can assist in diagnosis of dangerous operating conditions and implementation of evasive action.

References


Paper IV
Modelling of the Chemical Reactions in a Continuous Pulping Digester in the Presence of the Channelling Phenomenon

Bijan Pourian, Erik Dahlquist

Abstract – The objective of this paper is to predict the chemical and hydraulic behaviour of the pulping digester under hazardous conditions which include the channelling phenomenon. The pulping digester was modelled using the CFD, finite volume method in FLUENT, including the channelling phenomenon and chemical reactions in the channel. A 2D geometry of the digester was built and symmetric planes were defined in Gambit. The mesh was then exported to the FLUENT and the geometry was treated with the axisymmetric function to establish a complete model of the digester. The Eulerian scheme was applied to represent the multiphase flows in the digester. A heterogeneous porous media was defined for the compressible bed. Species transport was applied to define a mixture template of the wood chips components. The Kappa number was predicted in and around the channel to characterize how cooking develops under hazardous conditions. Copyright © 2009 Praise Worthy Prize S.r.l. - All rights reserved.

Keywords: Pulping Digester, Channelling, Mass Transfer, Lignin, Chemical Reaction, Porous Media, Multiphase, Axisymmetric

Nomenclature

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<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<td>C, D</td>
<td>Prescribe material</td>
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<tr>
<td>d</td>
<td>Diameter</td>
</tr>
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<td>D_p</td>
<td>Particle diameter</td>
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<td>n</td>
<td>Number of phases</td>
</tr>
<tr>
<td>P_s</td>
<td>Solid pressure (Pa)</td>
</tr>
<tr>
<td>\tilde{q}_q</td>
<td>Heat flux</td>
</tr>
<tr>
<td>Q_{pq}</td>
<td>Intensity of the heat exchange between phase p and phase q phases</td>
</tr>
<tr>
<td>r</td>
<td>Radial coordinate</td>
</tr>
<tr>
<td>R</td>
<td>Heterogeneous reaction rate</td>
</tr>
<tr>
<td>R_i</td>
<td>Net rate of production of species i by chemical reaction</td>
</tr>
<tr>
<td>R_{g,q}</td>
<td>Net rate of production of homogeneous species i by chemical reaction for phase q</td>
</tr>
<tr>
<td>R_{f,r}</td>
<td>Arrhenius molar rate of Creation/destruction of species i in reaction r</td>
</tr>
<tr>
<td>s</td>
<td>Distance between grains</td>
</tr>
<tr>
<td>S_i</td>
<td>Rate of creation by addition from the dispersed phase plus any user-defined sources</td>
</tr>
<tr>
<td>S_q</td>
<td>Source term</td>
</tr>
<tr>
<td>S_i</td>
<td>Momentum sink</td>
</tr>
<tr>
<td>S_m</td>
<td>Mass added to continuous phase from dispersed phase</td>
</tr>
</tbody>
</table>
I. Introduction

Cooking process

The function of cooking in the manufacturing of pulp is to use heat and chemicals to remove the lignin that holds the cells in wood together. This makes it possible to extract the fibres from the wood pulp. It is important to preserve the quality of the fibres as far as possible, to maintain their length and strength for downstream applications. The cooking process is also aimed at removing extractives, which can cause foaming and deposition later in the process. Nowadays, Kraft or sulphate cooking is the most common pulp production process.

The cooking temperature in sulphate cooking is generally between 150 and 170 °C. The cooking liquor is formulated to remove as much lignin as possible from the wood chips while maximising the retention of cellulose.

Sulphate cooking uses a mixture of sodium hydroxide (NaOH) and sodium sulphide (Na2S) as the so-called white liquor. Sodium sulphide promotes the cooking reaction. Sulphides reduce the amount of cellulose that is dissolved by the sodium hydroxide. The lignin content in the fibres after boiling is expressed as the Kappa number. Mass percentage of components of the woods: On average, wood is composed of 40 to 50% cellulose, 20 to 30% hemicelluloses, 20 to 30% lignin, and 10% other materials. These remaining materials (the extractives) are organic substances such as Terpene, lipid, resin, starch and protein. Table I shows the chemical compositions of wood from three species.

### TABLE I

<table>
<thead>
<tr>
<th>Component (%)</th>
<th>Spruce</th>
<th>Pine</th>
<th>Birch</th>
</tr>
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<tbody>
<tr>
<td>Cellulose</td>
<td>42</td>
<td>41</td>
<td>41</td>
</tr>
<tr>
<td>Hemicellulose</td>
<td>28</td>
<td>28</td>
<td>21</td>
</tr>
<tr>
<td>Lignin</td>
<td>27</td>
<td>27</td>
<td>4</td>
</tr>
<tr>
<td>Extractives</td>
<td>3</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

Digestor: The digester under consideration at Korsnas/Vallvik is 60 m high and its diameter increases stepwise from 6 m at the entrance at the top to 7 m at the bottom.

There is a large annular pipe inside the digester which is connected to the outlet pipes of the circulation loops C8 (wash zone circulation at the lower section), MCC (in the middle) and ITC (isothermal cook circulation in the upper section). The flows re-circulate into the digester separately at three different levels.

The recirculation pipe consists of three concentric pipes. The innermost pipe is the longest and discharges C8 into the digester. The diameter of the C8, ITC and MCC inlets are 0.210 m, 0.300 m and 0.425 m respectively.

However, as these pipes are concentric, the effective diameters of the outer two pipes are smaller than their total diameters.

Therefore, only the effective diameters were used to construct the model of the digester.

The digester model is designed in Gambit so that it is divided into two axisymmetric sections around the x-axis. When one half is rotated around the x-axis the other half also rotates and the complete shape of the pipe is attained.

The digester is therefore initially designed in two dimensions but FLUENT is able to take into account its total volume of around 1800 m³ and the circular central pipe exactly as it exists in the digester (Fig. 1).
Application of the Eulerian formulation to represent particle flows is limited to spherical solid particles. However, it is possible to apply a user-defined distribution of diameters. This was used to model compression in the digester. We used the aspect ratio of a randomly selected chip among the solid feed to calculate the ratio of the total surface area to volume of the chip.

The computed value was applied to calculate the diameter of the spherical solid particles in FLUENT. The spherical chip in the model had approximately the same surface area to volume ratio as the randomly selected irregularly shaped chip. Measurements of chips from the feed confirmed that the majority had similar dimensions.

The chemical reactions of the Kraft pulping process are complex and some are still unknown. Simplifying assumptions are therefore unavoidable when designing mathematical models of the process.

Previous work: Work in this field was initiated by Vroom [2], who modelled the H-factor. The Purdue model was then established by Smith et al. [3], and many researchers followed with refinements to this new model. Several researchers implemented different aspects of pulp processing in the Purdue model. Johansson [4] implemented a temperature dependent diffusivity into the model and Hartler [5] applied a pH dependent diffusivity. Gustafson [6] improved Johansson’s model by using three kinetic equations for the cooking reaction instead of just one. Christensen [7] developed kinetic models for soft and hardwoods. Harkonen [8] derived a multiphase model in the Purdue model for the pulping digester. Michelsen [9] created a more detailed model by combining the Harkonen and Christiansen models. Natercia et al. [10] ran a steady state operation of a continuous digester with an ITC (isothermal cook circulation) and simulated two phases of a heterogeneous digester. Kayihan [11] modeled a two-zone digester, i.e., a mixing zone where impregnation takes place, and a reaction zone. Partial differential equations were solved in each zone. It was assumed that the solid and liquid phases were in thermal equilibrium. The adopted kinetic model was the same as the Christensen model.

Pougatch [12] implemented a solid tangential stress sub-model which was developed for the digester. The advantage of this sub-model was that the solid phase behavior reproduced the plug flow of the chips and eliminated the adopted non-physical assumptions of the Newtonian approach. Quad Foo et al. [13] modeled a single phase liquor flow in a batch laboratory digester using CFD. Fu Pingle [14] investigated the pulp suspension in the circular pipes. T. Xie et al. [15] and Heping Cui [16] studied three phases i.e., gas, liquid, and solid to examine the pulp suspension.

Channelling: Channelling of the liquor flow in the chip bed occurs as a result of delignification and the transfer of lignin from the chips to the free liquor. Modelling the channelling contributes to prediction of thermodynamic and hydraulic behaviour and can help predict areas in the digester where channelling is likely to occur. Haas [17] predicted channelling in the lowest level of the digester. Channelling of the bottom wash liquor caused large variations in temperature at the washing screen [18]. Hamilton [19] studied chip flow delays in the digester.

He observed that some chips were rotated in the bottom of the digester but he did not find any trace of channelling of the chip flow because his studies were based on individual chips. Paching of the chip bed may be contributed to the channelling. Finding and applying optimal packing and flow conditions may therefore help to avoid the channelling. The high temperature wash may also contribute to channelling. [20]

A number of researchers have examined channelling as a result of changes of the direction of flow in the digester. The flow direction is changed in some digesters from up-flow to down-flow. This has led to modification of chip bed movement and reduction of the channelling [21].

It was assumed that channelling in particular zones of the digester could be explained by variations in temperature.

Diminishing the size of the digester decreases the upward pressure exerted on the chips bed and at the same time improves the washing performance at the bottom zone [22].
II. Governing Equations [23]

The continuity equation for 2D axisymmetric geometries (mass conservation equation):

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial r}(\rho v_r) + \rho \frac{v_r}{r} = S_m
\]  

(1)

Axial Momentum conservation equation for 2D axisymmetric geometries:

\[
\frac{1}{r} \frac{\partial}{\partial x} (r \rho v_x v_x) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v_r v_r) = \frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial x} \left[ r \mu \left( \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial x} \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \mu \left( \frac{\partial v_r}{\partial r} + \frac{\partial v_r}{\partial r} \right) \right] + F_x
\]  

(2)

The Radial Momentum equation:

\[
\frac{1}{r} \frac{\partial}{\partial x} (r \rho v_x v_r) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v_r v_r) = \frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial x} \left[ r \mu \left( \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial x} \right) \right] \]  

\[- \frac{1}{r} \frac{\partial}{\partial r} \left[ r \mu \left( \frac{\partial v_r}{\partial r} + \frac{\partial v_r}{\partial r} \right) \right] - 2 \frac{\mu}{r^2} v_r + \frac{2}{3} \mu \left( \nabla \cdot \mathbf{v} \right) + \frac{\rho v_r^2}{r} + F_r
\]  

(3)

Porous momentum sink: A porous media contributes to lower velocity of the flow due to generation of a pressure gradient in the cell zones.

This is accounted for by an additional source term in the fluid flow equations.

The source is a flow resistance and consists of two terms that are empirically determined.

A viscous and an inertial loss term are included in the momentum equation in the porous cell zones:

\[
S_i = \left( \frac{3}{5} D_i \mu v_i + \frac{3}{5} C_i \rho \frac{v_i}{2} \right)
\]  

(4)

Homogenous porous media:

\[
S_i = \left( \frac{\mu}{\alpha} v_i + C_2 \frac{1}{2} \rho \frac{v_i}{2} \right)
\]  

(5)

Darcy’s law in porous media:

\[
\nabla p = -\frac{\mu}{\alpha} \mathbf{v}
\]  

(6)

Inertial loses in porous media:

\[
\nabla p = -\frac{3}{5} \sum_{j=1}^C \left[ \frac{1}{2} \rho \frac{v_j}{2} \right]
\]  

(7)

Volume fraction: The volume fraction of the secondary phase in the multiphase flow is determined from the continuity equation:

\[
\frac{\partial}{\partial t} (\alpha_p \rho_p \tilde{\mathbf{v}}_p) + \nabla (\alpha_p \rho_p \tilde{\mathbf{v}}_p \cdot \mathbf{v}_p) = 0
\]  

(8)

The conservation of momentum for a fluid phase q:

\[
\frac{\partial}{\partial t} (\alpha_q \rho_q \tilde{\mathbf{v}}_q) + \nabla (\alpha_q \rho_q \tilde{\mathbf{v}}_q \cdot \mathbf{v}_q) = \alpha_q \nabla p + \nabla (\tilde{\tau}_q) + \alpha_q \rho_q \tilde{\mathbf{g}} + \sum_{p=1}^n \left( K_{pq} \left( \tilde{\mathbf{v}}_p - \tilde{\mathbf{v}}_q \right) + m_{qp} \tilde{\mathbf{v}}_p - m_{pq} \tilde{\mathbf{v}}_q \right) + \left( \tilde{F}_{q} + \tilde{F}_{lift.q} + \tilde{F}_{vm.q} \right)
\]  

(9)

Where:

\[
\tilde{\tau}_q = \text{The stress-strain tensor in phase } q;
\]

\[
\tilde{F}_{q} = \text{The external body force};
\]

\[
\tilde{F}_{lift.q} = \text{The lift force};
\]

\[
\tilde{F}_{vm.q} = \text{The virtual mass force}.
\]

The conservation of momentum for the solid phase:

\[
\nabla (\alpha_s \rho_s \tilde{\mathbf{v}}_s) = \alpha_s \nabla p + \nabla (\tilde{\tau}_s) + \alpha_s \rho_s \tilde{\mathbf{g}} + \sum_{q=1}^N \left( K_{qs} \left( \tilde{\mathbf{v}}_q - \tilde{\mathbf{v}}_s \right) + m_{qs} \tilde{\mathbf{v}}_q - m_{qs} \tilde{\mathbf{v}}_s \right) + \left( \tilde{F}_s + \tilde{F}_{lift,s} + \tilde{F}_{vm,s} \right)
\]  

(10)

Conservation of energy: The enthalpy equation is solved for each phase in the multiphase flow models to express the conservation of energy in the model.

\[
\frac{\partial}{\partial t} (\alpha_q \rho_q \tilde{h}_q) + \nabla (\alpha_q \rho_q \tilde{h}_q \cdot \mathbf{v}_q) = -\alpha_q \nabla p + \nabla (\tilde{\tau}_q) + \sum_{q=1}^N \left( K_{pq} \left( \tilde{\mathbf{v}}_p - \tilde{\mathbf{v}}_q \right) + m_{pq} \tilde{\mathbf{v}}_p - m_{pq} \tilde{\mathbf{v}}_q \right) + \left( \tilde{F}_q + \tilde{F}_{lift,q} + \tilde{F}_{vm,q} \right)
\]  

(11)
Mass transfer:

\[ m_{pq} = \max(0, \lambda_{pq}) - \max(\alpha, \lambda_{pq}) \]  

(12)

For a multi-component solution, molecular diffusion of a species means the transport of that species from a region of higher concentration to one of lower concentration by random molecular motion.

The diffusion results in a gradual mixing of material, and complete mixing or equilibrium state in the absence of external forces on the species of the multi-component solution.

Fick’s law expresses the relationship between the diffusive fluxes and the concentration:

\[ J = -D \frac{\partial \phi}{\partial x} \]  

(13)

\(J\) is defined as the diffusive mass flux of any species in the solution and its SI unit is kg/m².s. \(J\) is a measure of the amount of a substance that moves by diffusion per unit time and per unit area perpendicular to the direction of transfer.

\(D\) is the diffusion coefficient or mass diffusivity and it is expressed in m²/s. When the concentration of the solute in the solvent is small the diffusion increases with temperature. The mechanism of the diffusion of the gases, liquids, and solids in solids is complicated and there is no general theory available to describe it. The diffusion is also dependent on the viscosity of the solution and is proportional to the squared velocity of the particles. The driving force for diffusion is concentration gradient \(\nabla \phi\).

III. Modelling Set Up

Axisymmetric: Modelling a two-dimensional structure of the digester, either symmetric or non-symmetric, would lead to wrong dimensions of the digester because FLUENT assumes one unit of length in the z direction for 2D geometry. In this case the depth of the central pipe in the z direction would be 1 m. This geometry would affect the boundary conditions and velocity of the inlet or outlet flow.

The axisymmetric configuration was selected in order to represent the cylindrical pulping digester more accurately.

The axisymmetric cell volumes were created by rotating the 2D cell volume about the x-axis.

The shape of the reactor and the dimensions of the components of digester are significant in the simulation of delignification.

Mass transfer

The mass transfer mechanism in the frame work of the Eulerian multiphase model was adopted for the pulping process.

The unidirectional mass transfer model which assigns a positive mass flow rate per unit volume from phase p to phase q was solved to predict the quality of the pulp.

The multiphase mass transfer code accommodates mass transfer between species belonging to different phases. Instead of a matrix-type input, multiple mass transfer mechanisms must be input. Each mass transfer mechanism defines the transfer of mass from one entity to another entity. An entity is either a particular species in a phase, or the bulk phase itself if the phase does not have a mixture material associated with it. The mass transfer can be specified either through the inbuilt unidirectional constant - rate mass transfer or through user-defined functions.

The interaction between groups of species was defined. The lignin is bound to the wood chips at the start but transfers from the solid to the liquid phase when it is exposed to the cooking liquor. The mass transfer rate is homogeneous and the diffusivity of the liquor is significant in determining the mass transfer rate, conversion, and quality of the pulp produced through the digester.

Mass transfer conjugated with Porous media: The Eulerian mass transfer approach conjugated with the species transport scheme and porous media can provide an appropriate prediction of the flow behaviour when modelling of both solid and liquid phases is required. Porous media can eliminate complications such as modelling instability and divergence that arise from the granular method. A non constant and variable porosity is defined throughout the digester, which represents the compressibility of the chips and pulp zones.

The solid chip phase with variable compressibility can be characterized as having a given bulk viscosity, which represent the solids resistance to expansion and compression. This can be modelled as a porous media. However the definition of these properties using other CFD strategies may result in higher computational cost.

Porous

A laminar model and a heterogeneous porous media were defined for the digester.

The inertial loss term of the momentum sink was activated and specified for each porous section of the digester in both x and y directions.

The porosity range was defined as ranging from 0.65 to 0.25, to express the distribution of the fluid flow through the particles.

The effect of gravity was taken into account and the gravitational acceleration was assigned a value of 9.8m/s² in the positive x direction.

Heterogeneous porous media was used to represent the compressibility of the solids. Decomposition of the wood develops when lignin is removed from the chips. The chemical dissolution process makes the chips soft and more compact. To model this, the digester was divided into 19 sections, each with different assigned porosity. The prescribed porosity was highest at the top and lowest at the bottom section. The void space between the chips is called the free space. When the lignin dissolves into the liquid phase the chip bed is compressed and free space between the chips (the free
liquor volume) decreases and the volume fraction of the chips increases.

**Multiphase:** In the species transport method the diffusion of chemical species is modelled by applying Fick’s law. The simulations were applied to softwoods and the density of this wood type was specified in the calculations.

The models were to be used for control and optimization. The chip bed and liquor flow were considered as the phases but the species of the phases were also prescribed in the models.

**Species transport:** To prescribe the constituents of the wood chips and create an environment for reaction between species a mixture template was defined for wood chips elements. The liquor was defined as the primary phase and the fibres and lignin were defined as the secondary phase.

IV. **Grid Independence and Validity**

The outlets, extractions and amounts of the circulation flows were obtained from simulation of the digester by adjustment of the pressures.

The results were compared with the operation values of the Korsnas process data base and agreed with the data from the mill.

The actual digester is about 60 m high and between 6 and 7 m in diameter, as mentioned previously. The simulations were performed with three different mesh and cell configurations. The models were built with 16000 or 55776 triangular cells or 21000 quadrilateral cells for each half of the digester. The other half of the digester was axisymmetric and was computed by FLUENT.

There was no difference between the results using the 55776 triangles and 21000 quadrilaterals but the intermediate mesh that used 16000 triangular cells did not agree well with the results from the other two meshes.

We conclude that the mesh that used 16000 triangles was too coarse. Using even larger number of cells made little difference to the results.

V. **Results and Discussion**

The cooking of the pulp in the channels in the pulp processor was considered.

The results show that the progress of the reaction inside the channels was very slow.

The Kappa number, which is a measure of the lignin concentration in the pulp, was higher inside the channels than on the outside.

Unreacted chips have higher Kappa number than the reacted wood chips. Two channels were considered in this simulation, one at the top and the other at the bottom of the digester.

The Kappa number inside the channels is shown in the Figs.3 and 4. The corresponding molar concentration of the produced fibres is also shown in Fig. 5.
that there is a defect in the reactor. Fig. 6 shows the velocity vectors in the channel which indicate increased velocity in the channel.

Fig. 6. Contours of distribution of the Velocity vectors inside the channel

Fig. 7 shows the velocity of the liquor through the channel and indicates that velocity increased at the beginning of the channel and decreased at the end of the channel. Fig. 8 shows the Kappa number in and around the upper channel. The dark and light blue curves represent the Kappa number in the channel and the other curves illustrate the Kappa number around the channel. The Kappa number was higher in the channel than in the immediate surroundings.

Fig. 7. Velocity of the liquor in the upper channel

Fig. 8. Kappa number in and around the upper channel

Fig. 9 shows that velocity was increased at the entrance of the channel, and Fig. 10 shows that velocity decreased as the flow reached the end of the channel. Fig. 11 shows the velocity vectors in the lower channel and at the top and bottom surrounding of the channel. The flow is directed in the channel and there is a lower velocity around the lower channel than the upper channel due to a lower flow rate around the channel.

Figs. 12 and 13 show the velocity of the liquor in the lower (Fig. 14) and upper channel.

Fig. 10. Velocity vectors of liquor flow in the channel

Fig. 11. Velocity vectors of liquor in the lower channel
It is evident that the velocity is higher in the upper channel than in the lower channel. This comparison is clearer in Fig. 15 which presents the velocities in both channels in the same scale. Figs. 4 and 16 show the development of the Kappa number in and around the lower channel.

The yellow, red and light pink represents three sections of the channel. The other colours indicate the Kappa number of different zones around the channel. The kappa number is higher in the channel than in the zones around it. This is consistent with the increased velocity in the channel, which slows the reaction down, thereby increasing the Kappa number.

VI. Conclusions

The channelling phenomenon of the pulping digester is considered in this simulation using the finite volume method in FLUENT software. The hydraulic characteristics of the channel were investigated. Two channels at two different levels of the reactor were examined to compare spatially the hydraulic behaviour of the channelling phenomenon. The development of the cooking in the digester was also considered in the context of channelling.

The results of the simulation indicate that there is less cooking and increased flow velocity in the channels. Furthermore, the velocity of the flow was higher in the upper channel than the lower. A two-dimensional symmetrical model of the digester was designed in Gambit and then rotated to create an axisymmetric model to properly represent the digester. The cooking materials have different physical states and therefore a multiphase flow was adopted to represent them. Among the multiphase schemes, the Eulerian model was adopted to examine the phases. A heterogeneous porous media was defined to represent the compressible chip bed. Species transport was applied to define a mixture template of the wood chip components. The Kappa number was predicted in the channels and in other zones of the digester to characterize the development of cooking under hazardous conditions.
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Paper V
Modelling and simulation of chemical reactions between wood chips and white liquor in a continuous pulping digester

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Abstract
Chemical interactions between the fibers of cellulose and liquor flow in a continuous pulping digester were modeled using CFD, and the finite volume method. A 2D geometric representation of the digester was constructed in Gambit. The total volume of the reactor was considered using the axisymmetric function of FLUENT. In order to avoid complications arising from instability and divergence, the circulation flows around the digester were ignored. The calculations were performed for the pulping of softwood chips.
In order to model the kinetics of the pulping reactions, the chemical reactions of the fibers were calculated theoretically and the Arrhenius constants for the reactions were computed. The activation energy was also calculated according to data provided for the cooking conditions.
The stoichiometry of the reaction equation was determined from the operational data of the cooking process. The stoichiometry and Arrhenius parameters were prescribed by CFD codes in order to characterize the pulping chemical reactions in the digester.
The reaction was modeled under isothermal conditions. The species transport and reaction scheme were incorporated with a homogeneous porous media to represent compaction of the fibers in the digester.
The progress of the reaction represents the quantitative development of the pulping process. However, the qualitative progress is controlled by the stoichiometry of the reaction. This means that a good model of the reaction stoichiometry can ensure continuous production of high quality pulp.

Key words
Pulp, digester, modeling, species transport, CFD, chemical reaction, wood chips, fibers, liquor, chemical formula

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>Prescribed material</td>
</tr>
<tr>
<td>D</td>
<td>Prescribed material</td>
</tr>
<tr>
<td>D_{i,m}</td>
<td>Diffusion coefficient for species i in the mixture</td>
</tr>
<tr>
<td>d</td>
<td>Diameter</td>
</tr>
<tr>
<td>E</td>
<td>Energy</td>
</tr>
<tr>
<td>F_{X}</td>
<td>External body force</td>
</tr>
<tr>
<td>F</td>
<td>Body force (N)</td>
</tr>
<tr>
<td>G</td>
<td>Elasticity modulus</td>
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<tr>
<td>g</td>
<td>Gravitational acceleration (m/s²)</td>
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<tr>
<td>h</td>
<td>Enthalpy</td>
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<tr>
<td>J_{i}</td>
<td>Diffusion flux of species i</td>
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<tr>
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<td>Effective conductivity</td>
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<td>r</td>
<td>Radial coordinate</td>
</tr>
<tr>
<td>R_{i}</td>
<td>Net rate of production of species i by chemical reaction</td>
</tr>
<tr>
<td>P</td>
<td>Pressure</td>
</tr>
<tr>
<td>S_m</td>
<td>Mass added to continuous phase from dispersed phase</td>
</tr>
<tr>
<td>S_h</td>
<td>Source of energy</td>
</tr>
<tr>
<td>T</td>
<td>Temperature</td>
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<td>Swirl velocity</td>
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<td>Local mass fraction of each species</td>
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<td>Density</td>
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<td>Turbulent dissipation rate</td>
</tr>
<tr>
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<td>Viscosity (kg/m-s)</td>
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<tr>
<td>μ_t</td>
<td>Turbulent viscosity (kg/m-s)</td>
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<tr>
<td>α_k</td>
<td>Volume fraction of phase k</td>
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<td>τ</td>
<td>Stress tensor</td>
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</table>

I. Introduction

The digester plays an important role in pulp production in the pulp and paper industry. The majority of the cooking process takes place in the digester. The size of digesters and the process in the digester is changing rapidly due to the growth in demand and intensive competition between producers. Increases in digester size increase the complexity of the reactions inside the digester. Managing these complex reactions is also increasingly difficult, particularly when not all the reaction data, such
as the kinetics of particular steps, is available. As well as the kinetics and chemical behaviour of the fibers, many physical parameters of the pulping process are influenced by the dimensions and geometry of the digester. In addition, constituents of different types of wood also vary, and these affect the kinetics and residence times of the pulping reaction. The cooking temperature in sulphate cooking is generally maintained between 150 and 170 °C. The outlet pulp from the digester contains lignin, whose content is measured by a dimensionless parameter called the Kappa number. The outlet Kappa number varies depending on whether the chips loaded into the reactor are made up of hard wood or soft wood. The Kappa number for soft wood has a value of around 24.

Mass percentage of wood components

Table 1 shows the constituents of three types of woods. Wood chips are cooked at around 160 °C in order to resolve the lignin which binds the cellulose and hemicellulose together, to release the fibres so that they can be used in downstream applications. Cooking is not allowed to proceed until all the lignin is removed, because long cooking times can worsen both the yield and the strength of the pulp [2].

<table>
<thead>
<tr>
<th>Constituent (%)</th>
<th>Spruce</th>
<th>Pine</th>
<th>Birch</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cellulose</td>
<td>42</td>
<td>41</td>
<td>41</td>
</tr>
<tr>
<td>Hemicellulose</td>
<td>28</td>
<td>28</td>
<td>34</td>
</tr>
<tr>
<td>Lignin</td>
<td>27</td>
<td>27</td>
<td>21</td>
</tr>
<tr>
<td>Extractives</td>
<td>3</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

Heating takes place in one or more circulation stages through screens and heat exchangers. Lignin is a binding agent in the wood. It is difficult to biodegrade. The molar mass of isolated lignin ranges from the low thousands to as high as 50,000. Lignin polymers consist of multiple monomers with different molecular weights. Figure 1 shows the molecular structure of lignin monomers.

Figure 1: Molecular structure of lignin monomers

Cellulose is the main component of the wood cell wall, and typically makes up between 40 and 50% of the dry wood by weight. Pure cellulose is a polymer of glucose residues joined by 1, 4 -β-Glucosidic bonds. The degree of polymerization (DP) is variable and may range from 700 to 10,000 or more.

Hemicellulose is a mixture of amorphous branched-chain polysaccharides consisting of several hundred sugar residues. Hemicelluloses contain many different sugar monomers, including Xylose, mannose, Galactose, Rhamnose, and Arabinose. Hemicelluloses contain mostly D-pentose sugars, and occasionally contain small amounts of L-sugars.

Table 2: Monomers of hemicellulose

<table>
<thead>
<tr>
<th>Hemicellulose</th>
<th>Monomer</th>
<th>Molecular formula</th>
<th>Molar mass (g/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Glucose</td>
<td>C_{6}H_{12}O_{6}</td>
<td>180</td>
</tr>
<tr>
<td></td>
<td>Galactose</td>
<td>C_{6}H_{12}O_{6}</td>
<td>180</td>
</tr>
<tr>
<td></td>
<td>Mannose</td>
<td>C_{6}H_{12}O_{6}</td>
<td>180</td>
</tr>
<tr>
<td></td>
<td>Xylose</td>
<td>C_{5}H_{10}O_{5}</td>
<td>150</td>
</tr>
<tr>
<td></td>
<td>Arabinose</td>
<td>C_{5}H_{10}O_{5}</td>
<td>150</td>
</tr>
<tr>
<td></td>
<td>Glucoronic acid</td>
<td>C_{6}H_{10}O_{5}</td>
<td>194</td>
</tr>
</tbody>
</table>

Extractives and Ash: The amount of extractives in wood varies from 5 to 20% by weight and includes a wide variety of organic compounds [5]. The ash content is 0.2 to 0.5% by weight in temperate woods and 0.5 to 2.0% by weight in tropical woods.

Table 3: Extractive content of wood

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Most abundant</th>
<th>Molecular formula</th>
<th>Molar mass (g/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Starch</td>
<td>(C_{6}H_{10}O_{5})n</td>
<td>162</td>
<td></td>
</tr>
<tr>
<td>Fat</td>
<td>Glycerol</td>
<td>C_{3}H_{8}O_{3}</td>
<td>92</td>
</tr>
<tr>
<td></td>
<td>Myristoleic Acid</td>
<td>C_{14}H_{26}O_{2}</td>
<td>226</td>
</tr>
<tr>
<td>Pinosylvain</td>
<td>C_{14}H_{20}O_{12}</td>
<td>212</td>
<td></td>
</tr>
</tbody>
</table>

Previous work in this field

Vroom [3] was the first to use a model of the pulping reaction to model the H-factor. A new approach to modelling - the Purdue model – was then established by Smith et al. [4]. Many researchers followed with refinements to this approach by taking into account different aspects of pulp processing. Johansson [5] implemented a temperature dependent diffusivity into the model. Hartler applied a pH dependent diffusivity in the Purdue model. Gustafson [6] improved the Johansson model by using three equations for the kinetics of the cooking reaction instead of a single equation for the reactions. Christensen [7] developed several additional kinetic models, and Harkonen [8] derived a multiphase model in the Purdue model for the pulping digester. Michelsen [9] combined the Harkonen and Christensen models to achieve a more detailed model. Kayihan [10] modeled the digester as two zones, i.e. a mixing zone where impregnation takes place and a reaction zone. Partial differential equations were solved for each zone. The solid and liquid phases were considered as being in thermal equilibrium. Kayihan used the kinetic model developed by Christensen. Wisnewski’s [11] work was an extension of the Purdue model. The digester was approximated by a series of CSTRs, with each CSTR consisting of three phases. Several of the assumptions of the Purdue model were removed by defining the concentration of the solids on a mass per chip volume basis, defining the compaction as the volume fraction of the CSTRs and defining porosity as the volume fraction of the wood chips. Chip porosity and liquor density were also defined in this model. Pougatch [12] implemented a
solid tangential stress sub-model which was developed for a digester. The advantage of this sub-model was that the solid phase behavior reproduced the plug flow of the chips and eliminated the need to make non-physical assumptions. Foo et al. [13] modeled a single phase liquor flow in a batch laboratory digester using CFD. Dong et al. [14] studied the motion of fibres, and solved the Large Eddy Simulation (LES) in turbulent flows. Stockie [15] simulated the fibres in suspension by numerical simulation and the immersed boundary method. Ein-Mozaffari [16] investigated two different pulp suspensions: a long-fibred softwood pulp and a shorter-fibered hardwood pulp.

Foo et al. [17] modeled a single phase liquor flow in a batch laboratory digester using CFD. Lanre et al. [18], Benington [19] and Bhale [20] have previously used the granular multiphase scheme of the CFD codes exclusively in the stirred tank application to predict the pulp suspension behaviour. Forest et al. [21] investigated wet granulation and granule growth that may occur when granules collide and stick together to form larger granules. The model we describe here does not take granule growth into consideration. Pingle [22] investigated the pulp suspension in the circular pipes. He considered the pulp slurries as a two-phase system and studied the slurries by considering the behavior of the fibers in the system.

II. Theoretical set up
Molar mass determination strategy

The molar mass of lignin and hemicellulose used in our model are assigned by conventional computation. Our strategy for estimating the molar mass of lignin is based on the assumption that a sample of one mole of lignin (i.e. $6.02 \times 10^{23}$ molecules) contains a representative mixture of lignin monomers. This procedure enables us to calculate the average molar mass of monomers. Table 4 shows the molar mass assigned to the various wood constituents.

Table 4: Molar mass of wood constituents

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Average MW of constituents</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lignin</td>
<td>197</td>
</tr>
<tr>
<td>Cellulose</td>
<td>180</td>
</tr>
<tr>
<td>Hemicellulose</td>
<td>172</td>
</tr>
</tbody>
</table>

Average molar mass of the fibres: As the operation data of the pulping process does not distinguish between the reaction rate of cellulose and hemicellulose, an average molar mass that accounts for both cellulose and hemicelluloses (collectively referred to as fibres) must be assigned. We assigned the average of the molar mass of cellulose and hemicelluloses as the molar mass of the fibres.

Table 5: Average molar mass of fibres

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Average molar mass g/mole</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fibres</td>
<td>176</td>
</tr>
</tbody>
</table>

Mass percent of fibres in the wood

Pine contains 28% hemicelluloses and 27% cellulose by weight. The total fibre content of pine is therefore set at 70%.

Molar mass of the wood chips

Additional assumptions have to be made to make it feasible to assign a molar mass for the wood chips. We present a number of strategies to determine the molar mass of the chips. These strategies differ in how they deal with the presence of the extractives.

The assignment of molar mass would be easier if the extractives were not considered at all, i.e. if the wood was assumed to consist only of fibres and lignin. Table 6 shows the percentage by weight of each constituent of the wood.

Table 6: Percentage of wood constituents by mass

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Mass %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fibres</td>
<td>70</td>
</tr>
<tr>
<td>Lignin</td>
<td>20</td>
</tr>
<tr>
<td>Acetyl</td>
<td>4</td>
</tr>
<tr>
<td>Extractives</td>
<td>6</td>
</tr>
</tbody>
</table>

The first step in calculating the molar mass of the wood is to calculate the molar ratios of the constituents.

Assigning molar mass of wood – approach I

In this method, we assume that the three classes of compounds are present in different proportions, i.e. acetyl, fat and Pinosylvilin. (Table 7)

Table 7: Determination of the molar amounts of the wood constituents

<table>
<thead>
<tr>
<th>Wood molar mass, Base: 1000 g wood</th>
<th>Mass %</th>
<th>g/ base</th>
<th>MW</th>
<th>Moles per 1000 g</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fibre</td>
<td>70</td>
<td>700</td>
<td>176</td>
<td>4</td>
</tr>
<tr>
<td>Lignin</td>
<td>20</td>
<td>200</td>
<td>197</td>
<td>1</td>
</tr>
<tr>
<td>Acetyl</td>
<td>4</td>
<td>40</td>
<td>43</td>
<td>1</td>
</tr>
<tr>
<td>Myristoleic Acid</td>
<td>1</td>
<td>10</td>
<td>226</td>
<td>0.044</td>
</tr>
<tr>
<td>Pinosylvilin</td>
<td>5</td>
<td>50</td>
<td>212</td>
<td>0.023</td>
</tr>
</tbody>
</table>

There is no accurate data on the kinetics of each constituent. Therefore, in order to avoid overcomplicating the molar mass calculation we consider the extractives as a whole and assign them an average molar mass based on their relative abundance.

Table 8: Determination of the chemical formula of the wood chips - approach I

<table>
<thead>
<tr>
<th>Wood molar mass Base: 1000 g wood</th>
<th>Mass %</th>
<th>g/ 1000g</th>
<th>Molar mass</th>
<th>moles</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fibre</td>
<td>70</td>
<td>700</td>
<td>176</td>
<td>4</td>
</tr>
<tr>
<td>Lignin</td>
<td>20</td>
<td>200</td>
<td>197</td>
<td>1</td>
</tr>
<tr>
<td>Rest</td>
<td>10</td>
<td>100</td>
<td>78</td>
<td>1.3</td>
</tr>
</tbody>
</table>

Based on the provided moles in Table 8, we can write a chemical formula for the wood where F represents the...
fibres, L represents lignin, and R represents remaining compounds (acetyl and extractives): F L R 1.3
The molar mass of wood, based on the molar mass of the constituents is therefore 1002.4 g/mole.

Assigning the molar mass of wood – approach II

This approach also involves a chemical formula for wood, but in this case the extractives are ignored, as they are far less abundant than the fibres and lignin. In this case the molecular formula would be F 4 L A. Where A represents the Acetyl and the molar mass of this compound is 1003.1 g/mol.

Assigning molar mass of wood – approach III

The average molar mass of the extractives is therefore 219 g/mol if it involves only Pinosylvin and Myristoleic Acid.

| Table 9: Determination of the chemical formula of the wood chips – approach III |
| Mass % | g/1000g base | Molar mass g/mol | moles |
| Fibres | 70 | 700 | 176 | 4 |
| Lignin | 20 | 200 | 197 | 1 |
| Acetyl | 4 | 40 | 43 | 1 |
| Rest (Pinosylvin + Myristoleic Acid) | 6 | 60 | 219 | 0.3 |

The chemical formula derived as a result of these assumptions is therefore F 13L3A3R The molar mass is 3227 g/mol in this case.

III. Governing equations

Energy Sources (steady form)

\[ \nabla \cdot (\rho E + p) = \nabla \left( k_{\text{eff}} \nabla T - \sum_j h_j \hat{J}_j + (\bar{\tau}_{\text{eff}} \cdot \hat{u}) \right) + S_h \]  

The energy equation includes terms for the heat of the chemical reactions (S_h) expressed in W/m^3, conduction - including the conductivity coefficient, species diffusion - including \( \hat{J}_j \), and viscous dissipation - including \( \bar{\tau}_{\text{eff}} \).

The energy term \( E \) includes terms for kinetic energy (\( \frac{v^2}{2} \)), pressure work (\( \frac{p}{\rho} \)) and heat of reaction (\( h \))

\[ E = h - \frac{p}{\rho} + \frac{v^2}{2} \]

For incompressible flows

\[ h = \sum_j Y_j h_j + \frac{p}{\rho} \]

Pressure work and kinetic energy terms are negligible in incompressible flows.

The continuity equation (steady form) for 2D axisymmetric geometries (mass conservation equation)

\[ \frac{\partial}{\partial x} (\rho v_x) + \frac{\partial}{\partial r} (\rho v_r) + \frac{\rho v_r}{r} = S_m \]

Axial Momentum conservation equation for 2D axisymmetric geometries

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \rho v_r \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( \rho v_v \right) = \frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \mu \left( \frac{\partial v_r}{\partial r} + \frac{\partial v_v}{\partial x} \right) \right] + F_x \]

Radial Momentum equation

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \rho v_v \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( \rho v_r \right) = \frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \mu \left( \frac{\partial v_r}{\partial r} + \frac{\partial v_v}{\partial x} \right) \right] + \frac{2 \mu v_r}{r} + \frac{\mu}{3} \left( \nabla v_r \right) + \rho \frac{v_r^2}{r} + F_r \]

Porous momentum sink

Porous media generates a pressure gradient in the cell zones, reducing the flow velocity. This effect is accounted for in the fluid flow equations by an additional source term. This source is a flow resistance and consists of two empirically determined terms. Viscous and inertial loss terms are included in the momentum equation in the porous cell zones.

\[ S_i = \sum_{j=1}^3 D_{ij} \mu v_j + \sum_{j=1}^3 C_{ij} \frac{1}{2} \rho |v_j|^2 \]

Homogenous porous media

\[ S_i = \left( \frac{\mu}{\alpha} v_i + C_2 \frac{1}{2} \rho |v_i|^2 \right) \]

Inertial losses in porous media

\[ \nabla p = -\sum_{j=1}^3 C_{2j} \left( \frac{1}{2} \rho v_j |v_j|^2 \right) \]
Species transport

In the species transport approach the individual species are defined in the model and conservation equations, including convection and diffusion are solved for each species. FLUENT predicts the mass fractions of the species. The conservation equation for the species transport model is:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i$$  \hspace{1cm} (10)

Where $R_i$ is the net rate of production of species i, and $S_i$ is the rate of creation by addition from the dispersed phase. FLUENT uses a dilute approximation for the diffusion flux by default:

$$\vec{J}_i = -\rho D_{i,m} \nabla Y_i$$  \hspace{1cm} (11)

$\vec{J}_i$ is the diffusion flux of species i, which arises as a result of concentration gradients. $D_{i,m}$ is the diffusion coefficient for species i in the mixture.

The Laminar Finite-Rate Model

The lamellar finite-rate model computes the chemical source terms using Arrhenius expressions, and ignores the effects of turbulent fluctuations. This formulation is accurate for laminar flows. The Arrhenius equation is non-linear, which makes it difficult to apply to turbulent flows. In species transport models the reaction occurs in the continuous phase between the species.

The net production of a chemical species as a result of chemical reactions is computed as the sum of the Arrhenius reaction sources over the NR reactions that the species participate in:

$$R_j = M_{w,j} = \sum_{r=1}^{N_R} \frac{\dot{X}_i}{X_i} R_{j,i,r}$$  \hspace{1cm} (12)

IV. Model Set Up

The models applied for pulping reactions including chemical species and related physical properties must be defined for the mixture.

The viscosity of the mixture is set at a constant value. The other thermodynamic properties are composition dependent. The mixture law is used to calculate the mixture density.

The double precision version of FLUENT is selected for the calculations for increased accuracy.

Modeling simplifications and assumptions

The hydraulic behavior of the digester, multiple circulations, multiple inlets and outlets, chemical process, woods constituents and properties, chemical liquor composition, temperatures and pressures are neither persistent nor regular enough to determine a fixed and global model for the hydraulic and chemical behavior of the pulping process. These conditions mean a number of assumptions and simplifications have to be made so that an approximate model of the pulp production process can be established. We have made some modeling simplifications and assumptions regarding the hydraulic behavior and chemical reactions, partially due to lack of knowledge of the reactions and flow behavior and also due to limitations and capacity of the modeling tools.

Species transport and reaction approach

An appropriate approach to model the chemical interaction and transport of a mixture of materials is the solution of the energy equation including the energy sources arising from chemical reactions, diffusion and convection. The chemical reaction between the wood chips and white liquor is predicted using the species transport and reaction method. Stoichiometry, the reaction equation, the reaction rate of the species, activation energy and Arrhenius constants are the primary data required to apply this method.

The Arrhenius constants are determined based on the kinetics, temperature and activation energy of the reaction.

The experimental records show that the lignin and the fibers have different rates of reaction with the cooking liquor. At higher operating temperatures the lignin dissolution increases but the pulp quality and quantity is simultaneously diminished due to the increase in fibers transferring to the liquid phase.

Reaction kinetics

We use a homogenous reaction rate for the model of the pulp production. The rate is determined based on the available pulping process data. The conversion, residence time, mass fractions of the reactants and products, total volume of wood chips in the digester, and the reaction temperature are the fundamental variables required to determine the reaction rate of the substances.

The reaction rate for lignin:

$$r = k(t) = \frac{dL}{dt} \hspace{1cm} \text{Reaction rate of fibers:}$$

$$r = K(T) = \frac{dF}{dt} \hspace{1cm} r = \frac{dF}{dt} = 4.1 \times 10^{-5} \text{mol} \cdot l^{-1} \cdot s^{-1}$$

Estimation of Arrhenius equation designed for pulp production

$$k(T) = 0.14 e^{\frac{-2502}{T}} \hspace{1cm} \text{Activation energy for the wood chips is estimated based on data from the process.}$$

Stoichiometry and mass balance equation
The mass balance for the species transport model is based on the available operational data provided from Korsnas and the conventional theoretical calculations for determination of the chemical formula of the wood chips. It is possible to consider all the methods described above for calculating the wood molar mass, but only Method 1 is considered here. The mass balance is computed for the chemical reaction between the wood chips and cooking liquor when using Method to assign the molecular formula.

\[ F_{4}L R_{1.3} + V \rightarrow F_{1.35} V R_{1.3} L_{0.913} + F_{2.65} L_{0.087} \]

Wood chips + liquor → Black liquor + Pulp

In this equation the inlet wood chips initially contain 20% lignin and 10% extractives and the pulp produced contains 3% lignin. The Kappa number is therefore defined by the stoichiometry of the reaction, and has a value of 24.

V. Results

Figure 2: Species transport model: mass fraction of pulp in the digester (Simulation 1)

Figure 3: Species transport: molar concentration of pulp in the mixture (Simulation 1)

Figure 4: Mass fraction of the black liquor (Simulation 1)

Figure 5: Mass fraction of wood chips (Simulation 1)

Graph 1: Mass fraction of pulp (Simulation 1)
The mass balance for the species transport model is based on the available operational data provided from Korsnas and the conventional theoretical calculations for determination of the chemical formula of the wood chips. It is possible to consider all the methods described above for calculating the wood molar mass, but only Method 1 is considered here. The mass balance is computed for the chemical reaction between the wood chips and cooking liquor when using Method to assign the molecular formula.

\[
\text{F}_{4L} \text{R}_{1.3} + \text{V} \rightarrow \text{F}_{1.35} \text{V} \text{R}_{1.3} \text{L}_{0.913} + \text{F}_{2.65} \text{L}_{0.087}
\]

Wood chips + liquor \rightarrow Black liquor + Pulp

In this equation the inlet wood chips initially contain 20% lignin and 10% extractives and the pulp produced contains 3% lignin. The Kappa number is therefore defined by the stoichiometry of the reaction, and has a value of 24.

V. Results

Graph 2: Mass fraction of black liquor (Simulation 1)

Graph 3: Mass fraction of wood chips (Simulation 1)

Figure 2: Species transport model: mass fraction of pulp in the digester (Simulation 1)

Figure 3: Species transport: molar concentration of pulp in the mixture (Simulation 1)

Figure 4: Mass fraction of the black liquor (Simulation 1)

Figure 5: Mass fraction of the un-reacted chips (Simulation 2)

Graph 4: Mass fraction of black liquor in the digester (Simulation 2)

Graph 5: Mass fraction of the un-reacted chips (Simulation 2)

Figure 6: Mass fraction of black liquor in the digester (Simulation 2)

Figure 7: Mass fraction of produced pulp (Simulation 2)
Graph 6: Mass fraction of produced pulp (Simulation 2)

Figure 9: Mass fraction of white liquor (Simulation 2)

Figure 10: Molar concentration of the pulp (Simulation 2)

Graph 7: Mass fraction of white liquor (Simulation 2)

Graph 8: Molar concentration of the pulp (Simulation 2)

Figure 11: Mole fraction of the chips (Simulation 2)
VI. Discussion

Two simulations were run using the species transport model in the digester. The mass balance and stoichiometry for the cooking of wood chips was applied and defined in the FLUENT species transport panel for both simulations. The same activation energy was set up for both cases in FLUENT and this value was similar to that calculated from the theoretical consideration of the reaction.

The main difference between the two simulations is the value of the pre-exponent factor. In Simulation 1 the pre-exponent factor was high and was set based on the convergence requirements such as consistency and stability. In Simulation 2 the applied pre-exponent factor was based on the Arrhenius kinetic reaction for lignin and pulp. The cooking in the two simulations appears to have different reaction kinetics due to the difference between the pre-exponent factors. Simulation 2, with the theoretically calculated pre-exponent factor, was more stable than Simulation 1, which had a high pre-exponent factor for normal volumetric reactions. This is due to the particular state of the pulp reaction and its long residence time. Figures 2 to 5 and Graphs 1 to 3 show the results of Simulation 1.

The molar mass of the wood chips is estimated based on Method 1 described above. The stoichiometry, based on the operational data and reaction kinetics calculations is set up in the reaction panel of the species transport model in FLUENT.

The two simulation methods can be compared directly - Figure 2 and Graph 1 for Simulation 1 correspond to Figure 8 and Graph 6 for Simulation 2. Figure 2 and Graph 1 show that the first 50 percent of the cooking process develops with roughly constant slope down the first 50 m through the digester, after which the reaction progresses more rapidly. Figure 2 and Graph 1 also show that the mass percentage of the pulp increases from zero at the top of the digester to around 50% at the bottom of the digester. The lignin content is incorporated in the chemical formula of the pulp (F_{2.65}L_{0.087}), equivalent to around 3%. However, Figure 8 and Graph 6 show that in Simulation 2 there is a less even progress of delignification down the digester. In Simulation 2, cooking occurs rapidly in the first 10 m and stops in the following 20 m, and increases again before slowing again in the bottom 10 m. In Simulation 1 however, cooking for the wood chips only approaches to 30 % after about 17.5m from the top inlet. The reaction is completed at the bottom of the digester. Figure 6 and Graph 4 show that production of black liquor follows the progress of the pulping reaction. Simulation 2 predicts a mass fraction of black liquor at the bottom of the digester to be around 50%. The transversal distribution of any physical quantity is represented in the wider and smaller graphs. Figure 7 and Graph 5 show that wood chips dissipate in the digester according to the proposed stoichiometry. According to the stoichiometry equation the wood chips react with the white liquor to produce black liquor and pulp. The reaction is complete at the bottom of the digester, and no un-reacted wood chips remain. Figure 9 and Graph 7 show that the white liquor is used up concomitantly with the conversion of wood chips as expected. The mass fraction of the white liquor is close to zero at the bottom of the digester, indicating that the reaction with the wood chips proceeds to completion. Molar concentration is also predicted by approach II. Figure 10 and graph 8 show the increasing trend of molar concentration of pulp using the second method.

Comparison of Figures 11 and 12 indicates that the molar fraction of pulp only begins to increase when there is a rapid drop in the molar fraction of the wood chips. This is because the estimated molar mass of the wood chips is much larger than the molar mass of the pulp. Therefore, when the mole fraction of the wood chips drops to 1.2% the mole fraction of the pulp starts to increase.

VII. Conclusion

The cooking of the wood chips is predicted numerically by modelling the reaction kinetics and stoichiometry equation using the finite volume method in FLUENT. The finite volume numerical method was applied to characterize the progress of chemical reactions and hydraulic behavior of the flows spatially through the digester. The species transport model with the reaction scheme is an appropriate approach to model the mass balance equation of the pulping reaction and is able to calculate the total pulp production, yield, and liquor consumption.
The species transport and reaction scheme conjugated with porous media can complement existing tools for modelling pulp production. Application of this model will enable the researcher and pulping mill to improve their knowledge of the pulping reactions and to advance new strategies to control the pulping process. Two different simulations were performed to model the cooking of the wood chips. The first simulation was based on a higher pre exponent factor which was set based on the common reaction velocity values and convergence requirements such as consistency and stability. In Simulation 2 the applied pre-exponent factor was based on the theoretical calculations and operational data.

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The species transport and reaction scheme conjugated with porous media can complement existing tools for modelling pulp production. Application of this model will enable the researcher and pulping mill to improve their knowledge of the pulping reactions and to advance new strategies to control the pulping process. Two different simulations were performed to model the cooking of the wood chips. The first simulation was based on a higher pre-exponent factor which was set based on the common reaction velocity values and convergence requirements such as consistency and stability. In Simulation 2 the applied pre-exponent factor was based on the theoretical calculations and operational data.

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