Modelling and simulation of gas stratification and mixing in a containment

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ABSTRACT

During a severe accident in a Nuclear Power Plant, large production of hydrogen and its combustion can lead to a serious damage on the safety-related equipment and undermine the integrity of the reactor containment. Current safety codes cannot always provide adequate prediction of the hydrogen behaviour in the containment due to complexity of the physical phenomena as well as computational limitations. Many national and international projects have been launched with purpose of increasing the knowledge of hydrogen phenomenology in order to improve its modelling and thus enhance severe safety management through safety assessment.

The aim of this thesis is to provide some modelling guidelines for gas stratification and mixing phenomena. Two tests were conducted in which low momentum vertical jet was used to erode a stagnant helium rich layer that was located at the top of a large vessel. A thermal-hydraulics software package GOTHIC was used for the investigation and the results were validated against experimental data that was provided from PANDA facility (PSI). Comparison has been carried out considering the helium volume fraction, temperature and velocity profiles at different time and locations inside the vessel.

GOTHIC was found to be reliable when dealing with stratification and mixing phenomena in large volumes. However, it is crucial to follow some modelling standards and guidelines in order to obtain reasonable results.

Before conducting a simulation it is recommended to perform a pre-test analysis and to determine parameters such as Reynolds number, Froude number and jet spreading, for better understanding of the test conditions. Also this should be considered when creating a computational model in GOTHIC:

- Domains in which large velocity, temperature and density gradients are expected should be addressed separately.
- The size of the jet volume should be adequate depending on the jet spreading.
- The cell size in the jet volume should be adequate and depend on the injection pipe diameter.
- Mesh around the density interface should be adequate and depend on the injection pipe diameter.
- Mesh in the remaining parts should be adequate to minimize computational costs.
- The author recommends to apply a turbulence model in the following order:
  - The STD k-ε turbulence model.
  - The Mixing-Length turbulence model.
  - The combination of the STD k-ε and the Mixing-Length turbulence model.
More detailed guidelines and further explanations are provided in the Results and Discussions section along with the analysis of the conducted simulations.

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LIST OF ACRONYMS

BWR               Boiling Water Reactor
CEA               French Alternative Energies and Atomic Energy Commission
CFD               Computational Fluid Dynamics
DCH               Direct Containment Heating
DW                Dry-well
EURATOM           European Atomic Energy Community
GDCS              Gravity Driven Core Cooling System
GTH               GOTHIC
HYMERES           Hydrogen Mitigation Experiments for Reactor Safety
IC                Isolation Condenser
LP                Lumped Parameter
LWR               Light Water Reactor
MCCCI             Molten Core Concrete Interaction
ML                Mixing Length
NL2               Second order approximation of Reynolds stress term
NPP               Nuclear Power Plant
NPS               Nuclear Power Safety Division
OECD/NEA          Organisation for Economic Co-operation and Development/The Nuclear Energy Agency
PAR               Passive Autocatalytic Recombiners
PCC               Passive Containment Cooler
PSI               Paul Scherrer Institut
PWR               Pressurized Water Reactor
RANS              Reynolds-Averaged Navier-Stokes
RG                Renormalized group
RMSE              Root mean square error
<table>
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<tr>
<td>ROSATOM</td>
<td>Russian Rosatom State Atomic Energy Corporation</td>
</tr>
<tr>
<td>RPV</td>
<td>Reactor Pressure Vessel</td>
</tr>
<tr>
<td>SBWR</td>
<td>Simplified Boiling Water Reactor</td>
</tr>
<tr>
<td>SETH</td>
<td>The SESAR Thermal-Hydraulics project</td>
</tr>
<tr>
<td>SC</td>
<td>Suppression Chamber</td>
</tr>
<tr>
<td>STD</td>
<td>Standard</td>
</tr>
<tr>
<td>TMI</td>
<td>Three Mile Island</td>
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<td>WW</td>
<td>Wet-well</td>
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NOMENCLATURE

\( U \) Velocity \([m/s]\)

\( L \) Characteristic Length \([m]\)

\( \nu \) Kinematic viscosity \([m^2/s]\)

\( Re \) Reynolds number

\( x_i \) Position vector \([m]\)

\( u_i \) Velocity vector \([m/s]\)

\( t \) Time \([s]\)

\( s_{ij} \) Strain-rate tensor \([s^{-1}]\)

\( p \) Pressure \([kg/(ms^2)]\)

\( \rho \) Density \([kg/m^3]\)

\( U_i \) Time averaged velocity vector \([m/s]\)

\( u'_i \) Fluctuating part of the velocity vector \([m/s]\)

\( \tau_{ij} \) Reynolds-stress tensor \([kg/(ms^2)]\)

\( \mu_T \) Eddy viscosity \([kg/(ms)]\)

\( l_{mix} \) Mixing-length \([m]\)

\( \alpha \) Closure coefficient which for jets is equal to 0.08

\( \delta \) Jet width \([m]\)

\( \kappa \) Kármán constant which is equal to 0.41

\( k \) Turbulent kinetic energy \([m^2/s^2]\)

\( \epsilon \) Dissipation rate \([m^2/s^3]\)

\( C_{\epsilon 1}, C_{\epsilon 2}, \sigma_k, \sigma_\epsilon \) Closure coefficients for RANS equation

\( Fr \) Froude number

\( g \) Gravitational acceleration \([m/s^2]\)

\( \overline{Re} \) Volume averaged Reynolds number

\( y^+ \) Dimensionless distance from surface

\( u_\tau \) Shear velocity \([m/s]\)

\( \tau \) Wall shear stress \([kg/(ms^2)]\)
$C_f$ Friction coefficient
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1 Introduction

1.1 Motivation

Almost 440 commercial nuclear power reactors are currently operating around the world with a total net installed capacity of 377 GWe [1]. Additional 69 NPPs are planned to be constructed in Asia and Eastern Europe. The history of nuclear energy and its use in NPPs is over 60 years old [2] that sums up to a great amount of experience and has throughout the years resulted in improvements in technique, engineering, and above all safety. The Three Mile Island Accident (TMI) in 1979 demonstrated the importance of understanding the process of hydrogen production and combustion. Since then safety measures concerning hydrogen have been developed and for new power plants these are already implemented in the design. However, the phenomenology of hydrogen is a complex process that depends on many parameters and not all safety computer programs are capable of accurate prediction of the hydrogen distribution in case of severe accident [3]. The recent accident at Fukushima in 2011 was unfortunate; however it highlighted once again the hydrogen issue. The reactor containment constitutes what is called the last barrier of defence against the radioactive release to the environment. During a severe accident chemical reaction between zirconium and steam can generate large amount of hydrogen within a relatively short period of time. The high local concentrations of hydrogen may lead to its detonation if the combustive conditions are achieved and the ignition source is present in the system. The magnitude of the detonation will determine if the integrity of the reactor containment may be threatened due to the associated static or dynamic pressure loads [4]. Furthermore damage of safety-related equipment is probable due to the increased pressure and temperature.

In 2013 OECD/NEA (Organisation for Economic Co-operation and Development/The Nuclear Energy Agency) initiated HYMERES (Hydrogen Mitigation Experiments for Reactor Safety). The main objective of the project is to increase knowledge of the hydrogen risk in nuclear reactor containment, address the issue and enhance the safety assessment [5]. The large-scale, multi-purpose facility PANDA at PSI serves as site for conducting thermal-hydraulic experiments for investigation of the containment integrity in response to accident conditions. The project includes twelve participating countries among which Sweden is present. Safety analysis includes the use of advanced computational codes to deal with complex three-dimensional and time-dependent issues. For this reason the demands on the efficiency and performance of the computers are very high. Thus what is needed is an efficient code that can generate accurate results at relatively low computational costs. The Nuclear Power Safety Division at KTH (KTH-NPS) has been contributing to the project by providing analytical support to the experimental program. The thermal-hydraulic code GOTHIC has been used to compute the hydrogen distribution. Preliminary simulations done at KTH against available experimental data from previous PANDA experiments have shown that GOTHIC has the potential to provide good results in an efficient
manner [6]. However, the choice of the modelling parameters and the manner in which the input model is designed, e.g. nodalization, turbulence models, etc. will have great impact on its performance and the accuracy of the results. This master thesis will further validate GOTHIC against available PANDA tests and define a set of modelling guidelines. These modelling guidelines will then be used for post-test analysis of the more complicated HYMERES tests with steam injection, effect of obstacles, etc.

1.2 Goals and Tasks

1.2.1 The goals

Based on the motivation the main goals of this thesis are to:

- Investigate and validate the capability of GOTHIC models in predicting erosion of a stratified helium-rich layer in a containment.
- Develop guidelines for modelling stratification and mixing phenomena for GOTHIC users.

In order to achieve the above mentioned goals a certain number of tasks have been listed to gain more acquaintance with the erosion phenomena and the software itself. The tasks are described below.

1.2.2 Task 1: Investigation of ST1-7 and PANDA Benchmark tests

Both ST1-7 and PANDA Benchmark experiments deal with the erosion of helium-rich layer by vertical low momentum air or air/helium jet. The test conditions and the experiments will be described in more detail in the upcoming sections.

Task 1 includes:

- Continuation of investigation of ST1-7 test and PANDA Benchmark simulations.
- Mapping the conditions present at different locations inside the vessel in order to describe and understand the occurring phenomena.

1.2.3 Task 2: GOTHIC modelling

After understanding the basics of the phenomena for ST1-7 and PANDA Benchmark following procedures will be performed:

- Mesh sensitivity study based on different mesh sizes as well as designs for different models.
Investigation of turbulence models with respect to their accuracy in predicting the erosion of helium and jet behaviour. Special interest is given to understanding the efficiency of the STD k-ε and the ML models combination that has been shown to be successful in the case of ST1-7 test.

Investigation of the submerged jets and modelling of vertical jets.

It is also important to note how the turbulence models and nodalization affect the computational demands. The aim is to find a method for modelling gas stratification and mixing phenomena that will generate accurate results at acceptable computational cost.
2 Theoretical Background

The theoretical background is divided into five subchapters for better acquaintance with the subject of this thesis. The first subchapter deals with some basic knowledge of hydrogen generation, combustion, and mitigation. The following subchapter touches on the subject of turbulence and the use of algebraic models. Short description of turbulence is followed by simplified explanation of the Reynolds-averaged Navier Stokes equations and its applicability on turbulence models. The code GOTHIC is introduced followed by presentation of the HYMERES project and work that has been made within its frame.

2.1 Hydrogen

2.1.1 Hydrogen in NPPs

During severe accidents most of the NPPs will generate hydrogen in large quantities within short period of time. This hydrogen can escape from the primary system and mix within the containment due to natural or forced convection as well as diffusion. The containment forms the ultimate barrier against the release of fission products to the environment. In case of hydrogen combustion, the risk of containment breach increases significantly due following static and dynamic pressure loads. It is also probable that the safety- equipment will suffer damage due to increased pressure and temperature.

We can see that understanding mixing and transport processes are crucial in determining potential risk for combustion and thus improving safety analysis. However, even if the combustion condition is reached, it is not enough to induce a detonation. The flammability criterion needs to be satisfied and an ignition source needs to be present in the system [4]. The flammability criterion can be described by a Shapiro diagram which represents fractions of hydrogen, steam and air that are necessary to reach the detonation limit, see Figure 1.
2.1.2 Hydrogen production

During severe accident there are three sources that can potentially generate large amount of hydrogen for LWRs. The first source is the in-vessel metal (Zr and steel) or neutron absorber (B$_4$C) material oxidation with steam or water [8]. The second source is the ex-vessel metal oxidation during direct containment heating (DCH) or oxidation with water in the cavity pit. In addition ex-vessel oxidation may also occur during molten core concrete interaction (MCCI). Although radiolysis and corrosion also generate hydrogen, their production rates is small enough to assume them negligible in the first phases of the accident.

In the following chapters the basics of hydrogen production reactions are discussed.

In-vessel hydrogen production

For steam-zirconium reaction the rate at which the hydrogen is produced will differ from case to case depending on the accident scenario and thus especially on the clad temperature as well as the amount of available steam. The reaction will take place if the core is partially or totally uncovered, which will result in an increase of the zirconium temperature above 1000°C. The reaction is exothermic (meaning release of energy into the system) and yields:

\[ \text{Zr} + 2\text{H}_2\text{O} \rightarrow \text{ZrO}_2 + 2\text{H}_2 + \text{Energy} \]  

The presence of steam is necessary for the reaction to occur which otherwise is self-propelled.

The amount of produced hydrogen will depend on the reactor type; the size of the core and the number of the fuel assemblies. As an example, a 900 MWe PWR (like the TMI-2) would produce about 1000 kg and a corresponding BWR around 2000 kg assuming total oxidation of the cladding [9].
For the steam-steel reaction the produced hydrogen strongly depends on the surface area of the steel that is exposed to steam and temperature that is favourable for the reaction to occur. The oxidation will start at 1 200°C and will increase exceeding the zirconium oxidation at 1 370°C. In the reaction oxide forms of Fe, Cr and Ni will be present within the reactor vessel.

**Ex-vessel hydrogen production**

In ex-vessel conditions, assuming the existence of the corium in the flooded cavity, uranium dioxide can react with steam to produce UO₂ and hydrogen. If the reactor vessel bottom ruptures and the reactor coolant system is pressurized a DCH is probable to occur. During the event fast oxidation of the metallic part of corium will occur leading to production of H₂. In case of corium drop into the dry cavity hole a MCCI is initiated. It follows oxidation of the metallic part of the corium, Zr and CR, in the steam and CO₂.

Other ex-vessel hydrogen contributors come from radiolysis and corrosion reactions. Radiolysis occurs in the reactor core and in the sump. The water is subjected to radiation which decomposes water molecules into various radicals. Hydrogen is formed during the process, however the production is slow generating only some hundreds of kilogram after approximately three months [8]. The corrosion includes reactions of zinc and aluminium and is affected by changes in the pH values. It has been shown that the amount of hydrogen that is produced reaches some 100 kg within hours.

**2.1.3 Hydrogen transport and mixing**

Due to free or forced convection and mass diffusion, hydrogen will be transferred and mixed around in the containment. Depending on the event sequence fast or slow mixing can occur. In case of large pressure differences within the containment the gases will move fast to the region of low pressure and equalize it. However, in case of density difference, which can occur if hydrogen is released in the upper part of the containment, natural convection will dominate the process of stabilization. Depending on the existing condition free convection can make hydrogen mix within the containment from few minutes to few hours. This process can be accelerated through the actuation of the spray system or the presence of the jets, forming forced convection. Diffusion exists due to concentration differences where the movement of the gases is oriented from high concentrations to low concentration regions. The efficiency of the diffusion depends on the size of the containment and tends to decrease for larger containments. [4]

The pace of the mixing will determine the nature of combustion. Fast mixing has global effect and contributes to a more uniform distribution of hydrogen whereas slow mixing tend to increase the concentration of hydrogen locally and results in local burnings.
2.1.4 Combustion of hydrogen

As previously mentioned combustion of hydrogen requires an ignition source and fulfilment of the flammability criterion. Moreover, depending on the temperature and amount of the available energy in the system auto-ignition or ignition can occur. Chemically the combustion can be described by following reaction:

$$2H_2 + O_2 \rightarrow 2H_2O + Energy$$  \hspace{1cm} (2)

The combustion will appear either as standing diffusion flame, deflagration or detonation [10]. Standing diffusion flames, as the name indicates, are local flames that do not propagate.

Deflagrations are flames transmitted at subsonic speed usually in the range of 1-1000 m/s. The pressure of the reaction is of order of few bar resulting in almost steady state loads. The unburnt gases are heated up through thermal conduction igniting it and propagating forwards. Detonation waves on the other hand travel supersonically at speed of 1500-2000 m/s resulting in strong dynamic loads on containment. The shock wave formed from the compression of the gas raises the temperature and leads to combustion. Moreover, the pressure increases by a factor of over 2 [4] with a typical value of 15 to 20 bar.

2.1.5 Hydrogen mitigation

The hydrogen mitigation measures include use of Passive Autocatalytic Recombiners (PAR), igniters, dilution with CO₂, atmosphere mixing, inertization (for BWRs) and venting of the containment [10]. For PARs, hydrogen comes into contact with the catalyst bed and reacts with the oxygen in air. The heat generated in the reaction establishes the natural circulation, exhausting steam from the recombiner into the containment and supplying air to the recombiner [11]. The efficiency of the PARs is connected to the location at which they are installed. However the reaction rate of PARs is not high, which is why they are insufficient in case of large hydrogen generation.

Igniters are used to combust hydrogen when the flammability criterion is reached. Slow deflagrations are expected which do not jeopardize the containment integrity. Due to early combustions more powerful detonations are avoided through the decrease of the hydrogen concentration.

In case of high local concentrations of hydrogen, CO₂ has been analysed for dilution purposes as well as containment mixing by initiation of the spray system. However, so far these measures have not yet been implemented as they still leave some considerations concerning safety and thus more investigations are awaited.
In most of the BWRs the inertization measures have been adopted in which oxygen is removed by use of nitrogen. Thus the risk of hydrogen combustion due to lack of oxygen is almost non-existing [8].

Lastly the venting of the containment can also be adopted in case of exceeded pressure limits due to steam, air and hydrogen combustion.

### 2.2 Turbulent flow

#### 2.2.1 Turbulence

A turbulent flow is a flow that does not follow any predetermined pattern. It is characterized by its random and chaotic behaviour. Its irregularity is demonstrated in form of eddies, vortices and other instabilities. The kinetic energy is transferred from large to smaller eddies during the turbulence decay until dissipation of eddies into heat occur due to molecular viscosity. Thus turbulent flows are generally dissipative. One of the most important properties is the enhanced diffusivity which contributes to fast mixing of mass, momentum and energy (heat). Furthermore the nature of the turbulence is very complex as it is rotational, time dependent and three dimensional. The most suitable method to address this randomness in turbulence is made through statistical approaches [12] [13].

In order to determine whether a flow is turbulent or laminar Reynolds number is often used. It is a dimensionless unit that describes the ratio of inertial to viscous forces based on characteristic velocity $U$, characteristic length $L$ and the kinematic viscosity $\nu$ of the fluid:

$$ Re = \frac{UL}{\nu} $$

The hydraulic diameter is normally used as the characteristic length in case of pipes and ducts. Reynolds number is always large for turbulent flows. To describe a turbulent flow the time-dependent, three-dimensional Navier-Stokes equation is used.
Figure 2: Laminar and turbulent flow. The parallel, back lines represent the streamlines [14].

2.2.2 The Reynolds-averaged Navier-Stokes equations

The Reynolds-averaged Navier-Stokes equations are time-averaged equations based on the idea of Reynolds decomposition. The solution of the Navier-Stokes equation describes the motion of turbulent flow. For an incompressible Newtonian fluid, the Navier-Stokes equations for mass and momentum conservation are

\[
\frac{\partial u_i}{\partial x_i} = 0
\]  

\[
\frac{\partial u_i}{\partial t} + \rho u_i \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial (\rho u_j u_i)}{\partial x_j} + \frac{\partial (\mu s_{ij})}{\partial x_j}
\]

The position and velocity are defined through the vectors \(x_i\) and \(u_i\), time is denominated as \(t\), pressure as \(p\), density as \(\rho\) and molecular viscosity as \(\mu\). The system has four equations and four unknown variables: pressure and the three velocity components. The strain-rate tensor in equation (5) is defined as

\[
s_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)
\]

Reynolds decomposition implies expression of all quantities in terms of their averages and the fluctuating parts, for visualization see Figure 3. For the velocity field \(u_i\) this yields

\[
u_i(\bar{x}, t) = U_i(\bar{x}, t) + u'_i(\bar{x}, t)
\]
Where the time averaged component is defined as

$$U_i(\bar{x}, t) = \lim_{T \to \infty} \frac{1}{T} \int_0^T u_i(\bar{x}, t) dt$$  \hspace{1cm} (8)$$

Reynolds operator is very useful due to its properties which are applied on the Navier-Stokes equations. Later on the equations are time-averaged and equations (4) and (5) become

$$\frac{\partial U_i}{\partial x_i} = 0$$  \hspace{1cm} (9)$$

$$\rho \frac{\partial U_i}{\partial t} + \rho U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}(2\mu S_{ij} - \rho \overline{u'_j u'_i})$$  \hspace{1cm} (10)$$

The equation above is called Reynolds-averaged Navier-Stokes equation (RANS) [13]. Equation (10) introduces a new term which represents the Reynolds-stress tensor

$$-\rho \overline{u'_j u'_i} = \tau_{ij}$$  \hspace{1cm} (11)$$

Reynolds-stress represents the added stress on the fluid per unit area due to turbulent fluctuations. However due to this term new unknowns are introduced to the system resulting in the closure problem. To close the system Reynolds stress needs to be defined which implies addition of new equations to balance for the unknown quantities. In order to do that the concept of eddy viscosity is introduced. Eddy viscosity is used to model the momentum transfer that is caused by turbulent eddies. In this approximation it is stated that Reynolds-stress tensor is proportional to the gradients of the mean velocity and the coefficient of proportionality is the eddy viscosity. The approximation, also called the Boussinesq eddy-viscosity approximation [13], is used to develop models such as mixing length and the two-equation turbulent models which are described below.
2.2.3 The mixing-length turbulent model

In the mixing-length hypothesis, presented by Prandtl in 1925, the turbulent fluid is simplified to move unidirectionally. Moreover the fluid maintains its momentum in the orthogonal direction to what it’s moving and for a distance called the mixing length, \( l_{mix} \). The Prandtl postulation leads to relation stating proportional relation between the eddy viscosity \( \mu_T \) and shear stress \( \tau_{xy} \)

\[
\tau_{xy} = \mu_T \frac{dU}{dy}
\]  \( (12) \)

where the eddy viscosity is defined as

\[
\mu_T = \rho l_{mix}^2 \left| \frac{dU}{dy} \right|
\]  \( (13) \)

However difficulty emerges from the fact that the mixing length is case specific and thus will differ depending on the flow for shear flows or flows at boundary layers. For jets the mixing length is proportional to the spreading, \( \delta \)

\[
l_{mix} = \alpha \delta(x)
\]  \( (14) \)

where \( \alpha \) is the closure coefficient that can be determined experimentally and for jets it is equal to 0.08, see Figure 4.

![Figure 4: Representation of a free shear flow that is valid for free jets [13].](image)

However as stated before, the mixing length is flow specific, and near the solid boundaries it is almost linear to the distance from the surface by

\[
l_{mix} = \kappa y
\]  \( (15) \)

where \( y \) is distance from the surface and \( \kappa \) is the Kármán constant that has been determined to 0.41. The velocity follows the law of wall which will be discussed further in the following sections.
2.2.4 The two equation k-ε turbulent model

The purpose of the two equation model is to describe the turbulent flow by means of two transport equations. The first one determines the turbulent kinetic energy and the second one its dissipation rate. The k-ε model was presented by Chou in 1945, however it was subjected to many refinements by Davidov in 1961 and Harlow and Nakayama in 1968 [13]. However the true development of the model is credited to Jones and Launder in 1972. Since then it has been referred to as Standard k-ε model. Despite its popularity the model remains complicated introducing many unknown quantities which once again results in the closure problem. Equations for the turbulent kinetic energy and the dissipation rate contain terms for the transport, dissipation and production. These terms in turn contain unknown quantities which why in order to close the system of equations the model must rely on some experimentally determined coefficients also known as the closure coefficients. However firstly the turbulent kinetic energy and its dissipation rate need to be defined. In 1945 Prandtl defined the kinetic energy through the velocity fluctuation terms

\begin{equation}
    k = \frac{1}{2} \overline{u_i' u_i'}
\end{equation}

In order to determine \( k \) the idea of the Reynold's stress tensor is used

\begin{equation}
    \tau_{ii} = -\rho \overline{u_i' u_i'} = -2\rho k
\end{equation}

Likewise the transport equation for \( k \) can be derived

\begin{equation}
    \rho \frac{\partial k}{\partial t} + \rho U_j \frac{\partial k}{\partial x_j} = \tau_{ij} \frac{\partial U_i}{\partial x_j} - \rho \varepsilon + \frac{\partial}{\partial x_j} \left[ \mu \frac{\partial k}{\partial x_j} - \frac{1}{2} \rho \overline{u_i' u_j'} - \overline{p' u_j'} \right]
\end{equation}

In equation above \( \varepsilon \) represents the dissipation energy which is defined as

\begin{equation}
    \varepsilon = \nu \frac{\partial u_i' \partial u_j'}{\partial x_k \partial x_k}
\end{equation}

To close the system the unknown correlations are replaced by introduction of closure approximations until (18) becomes

\begin{equation}
    \rho \frac{\partial k}{\partial t} + \rho U_j \frac{\partial k}{\partial x_j} = \tau_{ij} \frac{\partial U_i}{\partial x_j} - \rho \varepsilon + \frac{\partial}{\partial x_j} \left[ \mu + \mu_T / \sigma_k \right] \frac{\partial k}{\partial x_j}
\end{equation}

The turbulent transport and pressure diffusion have been approximated by

\begin{equation}
    \frac{1}{2} \rho \overline{u_i' u_j'} - \overline{p' u_j'} = -\frac{\mu_T}{\sigma_k} \frac{\partial k}{\partial x_j}
\end{equation}
The eddy viscosity is given by

\[ \mu_T = \frac{\rho C_\mu k^2}{\varepsilon} \]  

(22)

where \( C_\mu \) is the closure coefficient 0.09.

In the two equation k-\( \varepsilon \) model the idea is to have exact solution for the dissipation energy which is defined as

\[ \rho \frac{\partial \varepsilon}{\partial t} + \rho U_j \frac{\partial \varepsilon}{\partial x_j} = C_{e1} \frac{\varepsilon}{k} \tau_{ij} \frac{\partial U_i}{\partial x_j} - C_{e2} \rho \frac{\varepsilon^2}{k} + \frac{\partial}{\partial x_j} \left[ (\mu + \mu_T/\sigma_\varepsilon) \frac{\partial \varepsilon}{\partial x_j} \right] \]  

(23)

where the closure coefficients are \( C_{e1} = 1.44 \), \( C_{e2} = 1.92 \), \( \sigma_k = 1.0 \) and \( \sigma_\varepsilon = 1.3 \). Starting on the left-hand side of the equation, the change and the transport by convection is equal to the production, minus the dissipation plus the transport by diffusion.

### 2.2.5 Jets and plumes

Since this thesis deals with turbulence that is introduced by a jet it is important to understand some physics that will determine the behaviour of the jet. Additionally plumes will also be discussed due to its importance in case of mixing.

By definition, jets are driven by momentum whereas plume are driven by pressure difference or so-called buoyancy force [15]. There are also buoyant jets for which initial flow is controlled by momentum but as the distance from the source grows the behaviour of the jet is governed by buoyancy. In all of the cases the momentum is conserved and the kinetic energy is transferred to turbulence. Investigations of jets have had great importance in understanding the turbulence where the axisymmetric jets constitute a backbone for research of turbulent flow [16]. The work of Wygnaski and Fielders in 1969 is referred to as the standard reference for description of profiles of mean velocity and turbulence stresses among all. These have formed a solid foundation for further research.

Plumes and jet entrainment have been studied already in 1956 by Morton who conducted experiments for vertical convections currents in stratified incompressible fluids with respect to temperature and the height of the jet [17]. Baines and Turner described the behaviour of the plume in a finite closed region as the flow hits the top of containment under different condition [18]. Depending on the value of the inertia of the plume, three different outcomes are possible: for low inertia a linear density gradient is obtained from the top to the bottom, for higher inertia mixing will occur in the upper part of the containment but the density gradients will exist in the lower part. However if the inertial forces are high enough the mixing will occur in the whole containment resulting in a uniform density. Considering jet impingement on a density interface,
the entrainment will depend on the jet properties as it impinges and on the density difference across the interface [19]. The Froude number is often used to describe the impinging conditions

\[
Fr_1 = \sqrt{\frac{U^2}{g \frac{(\rho_{amb} - \rho_0)}{\rho_0} d_0}}
\]  \quad (24)

where \( U \) is the velocity, \( d_0 \) is the diameter of the jet, \( g \) is the gravitational acceleration, \( \rho_0 \) is the density of the injected fluid and \( \rho_{amb} \) is the ambient density. From the Froude number study it is known that for \( Fr < 1 \) the jet will not penetrate the stratified layer and a density gradient from the bottom to the top of the vessel is obtained. However for high values of Froude number, inertia will dominate resulting in the penetration of the stratified layer. Equation (24) is for the initial injection Froude number at the inlet of the jet whereas at the interface with the stratified layer new Froude number is defined due to changes in the velocity and density [20]

\[
Fr_2 = \sqrt{\frac{U_2^2}{g \frac{(\rho_0 - \rho_{i0})}{\rho_{i0}} d_{i0}}}
\]  \quad (25)

\( \rho_{i0} \) is the density at the interface, \( d_{i0} \) is the height of the stratified layer and \( U_2 \) is the fluid velocity at the interface. Thus Froude number is an important indicator of the jet behaviour. However it can be advantageous to have more than one quantity to describe the existing conditions in order to increase the confidence in data. For that Reynolds number should also be calculated for information of the nature of the flow at the interface. For that the velocity and jet diameter need to be determined. Jet diameter \( d \) increases proportionally with the spread rate \( z \) [15].

\[
d \propto z \rightarrow d = 0.107z
\]  \quad (26)

Furthermore for jet velocity along the centreline has been determined:

\[
U_{centerline} = 6.2 \frac{U_0 d_0}{z}
\]  \quad (27)

where \( U_0 \) and \( d_0 \) are the velocity and diameter at the jet nozzle.

Regarding modelling of jets there are still issues that needs to be resolved as the k-ε model seems to be not able to fully predict the behaviour of the jet in all of the modelled cases [21]. Also the process of the entrainment and the interaction of turbulent with non-turbulent flow is not yet fully understood [22].
2.3 The GOTHIC code

GOTHIC is a software package that is used for investigations of the containment integrity, confinement buildings and components in response to accident scenarios. It is meant to provide analytical support for the design and licensing of the NPP [23].

GOTHIC deals with multi-component, multi-phase flow for which the conservation equations for mass, momentum and energy are solved for three primary fields: steam/gas mixture, continuous liquid and liquid droplet fields. Moreover for turbulence calculations GOTHIC apply full treatment of the momentum transport terms in multi-dimensional models with additional models for turbulent shear and turbulent mass and energy diffusion.

A typical model includes at least one control volume that can represent a room, group of rooms within a building or a subsystem in which fluids such as noncondensing gas, steam, drops or liquid water exists. Due to existing noding scheme the control volumes can be treated as lumped system or as subdivided systems divided into one-, two- or three-dimensional computational grid. Each subdivided volume can consist of any number of cells for which fluid properties are calculated. The connection between the cells is made through parameters defined by discretization of the governing equations.

The hydraulic connections are made by the use of flow paths, network models, cell interface connections in subdivided volumes and 3D connectors for subdivided volumes. Flow paths can be used in large diversity as connections between any arbitrary cells within the same volume, lumped and subdivided volume, to model flows through different components such as pipes, vents etc, or to connect boundary conditions to cells where mass, momentum and energy can be subjected to changes.

The initial conditions are specified by stating initial temperatures and fractions of the vapor phase, location and temperature of liquid pools, location and fraction of a liquid component and the temperature of solid structures within the volume.

GOTHIC possesses many features of a typical CFD code such as turbulent models and equations solving for 3-D models [24]. However assuming correct modelling GOTHIC does not require very fine mesh in order to obtain relatively accurate results. This is of great benefit as it lowers computational costs and makes the simulation time relatively short.

GOTHIC includes different types of turbulent models among them the Prandtl mixing length as well as various kinds of the two-equation k-ε model. The turbulent models and their performance with respect to different scenarios are described in the next section.
2.3.1 Turbulence Models

The available turbulence models in GOTHIC include the Mixing-Length (ML) model and various types of the k-ε turbulent models; the standard (STD), renormalized group (RG) and second order approximation of the Reynolds stress term (NL2). Additionally, each two-equation k-ε model includes an approximate transition model from turbulent to laminar conditions. If the volume average Reynolds number is less than 3000, the flow is assumed to be laminar, whereas if the volume average Reynolds number is greater than 5000 the flow is assumed to be turbulent. Between these two values a transition state from turbulent to laminar exists and for which the turbulent kinetic energy is approximated by

\[
k = k \cdot \min \left\{ \begin{array}{c} 1.0 \cdot 10^{-6} \\ \frac{1.0 \cdot 10^{-6}}{\overline{Re} - 3000} \\ \frac{1.0 \cdot 10^{-6}}{2000} \end{array} \right\}
\]

(28)

where \( \overline{Re} \) is the volume average Reynolds number calculated using the volume weighted average phase velocity and the volume hydraulic diameter.

The performance of the mixing-length model will depend on the user defined value which should be carefully evaluated since it is case specific. As it was mentioned in the previous chapter 2.2 the mixing length \( l_{mix} \) is proportional to the width of a round jet by a factor of 0.08. To calculate \( l_{mix} \) the relation between the spreading rate and the radius, \( r_0 \), of a single-phase axisymmetric turbulent jet is used [23]

\[
l_{mix}(x) = 0.08 \cdot (r_0 + x \cdot \tan(10°))
\]

(29)

where \( x \) is a distance from the jet nozzle vertically up. Consequently depending on the distance and the jet diameter, different \( l_{mix} \) are obtained. However since in a CFD simulation only one value of \( l_{mix} \) can be specified per domain, this results in an inability of the code to adjust itself to conditions that are changing during simulations. This was already noticed in previous works where the ML worked well during initial phases of the test but performed poorly in the later stages of the tests [6], [25].

For scenarios of jet impingement (Froude numbers less than one) the law of wall [13] is used, where \( l_{mix} \) is proportional to the distance from the surface, see equation (15). For the turbulent boundary layer three regions are defined

- The sublayer - viscous stresses are dominating.
- The log layer - viscous stresses are negligible due to Reynolds stresses.
- The defect layer - layer close to the edge of the boundary in which the velocity starts to resemble the one in freestream.
The log layer is sometimes referred to as the transition state from the sublayer to the defect layer. Equations used to describe motion in the log layer are very useful due to their relatively easy implementation. Accordingly, the jet impingement on the helium layer can be compared to flows near wall for small Froude number. Under this condition the log layer is assumed to exist close to the helium rich layer. The $l_{\text{mix}}$ yields

$$l_{\text{mix}} = \kappa y = \kappa y^+ v / u_\tau$$

(30)

where $y^+$ is the dimensionless distance from surface, $v$ is kinematic viscosity and $u_\tau$ is shear velocity defined as

$$u_\tau = \sqrt{\frac{\tau}{\rho}} = \frac{1/2 \cdot C_f \cdot \rho \cdot u^2}{\rho}$$

(31)

$\tau$ is wall shear stress, $u$ is the freestream velocity and $C_f$ is the friction coefficient. For turbulent flows the friction coefficient is defined

$$C_f \approx 0.0592 \cdot Re^{-1/5}$$

(32)

For the log layer, the $y^+$ is defined between 30 and 300 for which an interval for $l_{\text{mix}}$ is obtained. Thus in near to wall flows corresponding $l_{\text{mix}}$ is in range between 0.0042 and 0.0420.

The STD k-$\varepsilon$ model is known to be accurate enough for free-shear flows. Its additional advantage is that it is easy to implement and does not require any pre-defined values as in case of the ML. However the simplifications in the RANS models resulted in an error for jet spreading rate overestimating it by up to 40 % [26]. For this reason a correction coefficient has been included in GOTHIC for the calculations of the dissipation rate. However the STD k-$\varepsilon$ model has shown difficulties when applied in case of impinging jets. Instead in that case the RG k-$\varepsilon$ model is preferable. It shows better accuracy as it takes into account the effect of different sized motion scales that contribute to turbulence. This is the reason why it works better for more complex flows like jet impingement. However, in case of shear flows the RNG k-$\varepsilon$ model fails to predict accurately the centreline velocity decay and radial profiles of axial velocities [27]. The NL2 k-$\varepsilon$ model is the most computational demanding model. It takes into account all Reynolds stresses which makes this model very general and applicable for a wide range of flows including wall jets [28]. More information on the performance of the NL2 k-$\varepsilon$ turbulence model in case of stratification and mixing phenomena has not been found as it has not yet been used in in the same extension and as often as the earlier developed turbulence models the ML and the other previously mentioned k-$\varepsilon$ models.
2.4 HYMERES Project

The HYMERES Project was initiated with the main objective of gaining knowledge about hydrogen behaviour in containment in order to improve its modelling and thus improve safety assessments for the already existing and future nuclear power plants [29]. The project for which OECD/NEA are responsible, is planned to take place between 2013 and 2016. Thus the results are hoped to help in enhancing Severe Accident Management and mitigate risks associated with hydrogen generation in NPPs.

In terms computer modelling HYMERES aims to assess realistic flow conditions, interaction of safety components and simulation of specific cases where the system behaviour differs depending on the reactor type [5]. Due to flow conditions necessary information on modelling guidelines such as mesh size or turbulent models can be addressed. Furthermore modelling safety equipment and their performance in case of severe accidents will provide data on their drawbacks and benefits. Moreover different combinations of the systems can be modelled to act in response to hydrogen release.

Two facilities PANDA and MISTRA have been used to provide the project participants with relevant data for the validation of the computational models; the first one being operated by Paul Scherrer Institut in Switzerland and the later one being the property of CEA and located at Saclay nuclear research centre in France [30]. In the frame of the HYMERES project six experimental series are to be conducted at PANDA, where each series aims to analyse specific equipment or system configuration in terms of safety. The first four test series, HP1-HP4, investigate gas stratification break-up and erosion caused by the introduction of jet or by combining multiple of safety components such as cooler, sprays etc. The fifth series, HP5, investigate thermal stratification build-up in a water pool whereas the last sixth, HP6, series deals with multi-compartment convection flows arisen from sudden opening of rupture foil in addition to actuation of the spray system. Due to safety reasons in all experiments hydrogen has been replaced by helium.

Nuclear Safety Division at KTH has actively taken part in the HYMERES project with the purpose of providing analytical support to the experimental program that is carried out at PANDA facility.

This thesis will deal with investigation of the ST1-7 test series and PANDA Benchmark. ST1-7 is a part of the SESAR Thermal-hydraulics (SETH-2) project (a predecessor of the HYMERES project) and deals with low momentum vertical fluid release. The outcome of this thesis can serve as a guideline for the GOTHIC modelling and simulation of the new HYMERES tests, specifically the HP1-HP4 test series.

In the ST1-7 experiment a vertical jet injects hot air in a ~90 m³ large vessel which acts as a containment and where stagnant rich helium layer is present in the upper part of the vessel. The
simulation starts by injecting the air through low momentum vertical jet located close to the wall of the contentment and 4 m above the bottom of the vessel [31]. The air is injected for 12 500 s after which a stabilisation period of 12 500 s follows.

In the PANDA Benchmark hot mixture of air and helium is injected into the vessel through vertical jet. Just like in ST1-7 the aim is to erode the stagnant helium rich layer present in the upper part of the vessel. The location of the pipe is changed and moved towards the centreline of the vessel. The test lasts for 7 200 s under which the air/helium mixture is constantly released.

2.4.1 Description of the PANDA facility

PANDA facility was originally designed for investigations of containment integrity and passive decay heat removal in response to accident scenarios in Light Water Reactors. The design was based on the 670 MWe Simplified Boiling Water Reactor (SBWR) made by General Electric. The operating conditions for PANDA facility include maximum pressure of 10 bar and temperature of 200°C. Initial and boundary conditions for the experiments are set by controlling the auxiliary system and thus addition or removal of water, steam or gas to or from any vessel.

Reactor Pressure Vessel (RPV), Dry-well (DW), Suppression Chamber (SC) or Wet-well (WW) and Gravity Driven Core Cooling System (GDCS) pool are represented by six cylindrical pressure vessels with the total volume of around 460 m$^3$ and a total height of 25 m, see Figure 5.

![Figure 5: PANDA facility. Configuration of the main vessels and pools [30].](image)

The vessels and pools are connected to each other through large number of system lines which facilitates investigation of different containment compartments and allows use of any particular
safety component. As a result separate tests for any part of the reactor can be conducted. The RPV, with the inner diameter of 1.23 m and the height of 19.2 m, includes riser and down-comers as well as 115 electrical heater elements at the lower part of the vessel generating 1.5 MW. The DWs are represented by two cylindrical vessels, each 8 m high and 4 m wide, connected by a 1 m diameter pipe (IP). The WWs, each 10 m high, are connected by two large lines, the first being in the gas space region and the second one in the suppression pool region. Four heat removal condensers, with the total volume of 60 m³, situated inside four pools are situated at the top of the facility, where the Isolation Condenser (IC) is connected to the RPV. The remaining three, the Passive Containment Coolers (PCCs) are connected to the DW.

The PANDA facility is equipped with sensors in all components, systems lines, and auxiliary system in order to measure fluid and wall temperatures, pressure, flow rates, heater power, gas concentration and flow velocities. For temperature measurements, up to 374 thermocouples are available located at different heights, angles and radial distances from the vessel centre axis. For gas concentration and composition measurements, up to 140 sampling lines are installed in the vessel out of which 118 can be connected to two mass spectrometers (MS). The gas sampling ports are located in close vicinity of the thermocouple allowing measuring of both values (temperature and gas concentration) at almost the same spatial location. The measurement sensors are used to monitor facility condition prior to the experiment, at its initiation and afterwards for further post-test evaluation.

2.4.2 Previous work

Since 2001, PANDA facility has been included in large number of projects such as SETH, SETH-2, ERCOSAM-SAMARA and ESFP held by the OECD as well as EURATOM and ROSATOM [30]. The main objective of these projects was to test the predictability of the safety analysis codes for the improvement of the severe accident management. In these cases PANDA acted as a source of the experimental data needed for the validation and comparison of the computational codes and programs. For this reason GOTHIC has been used for simulating gas mixing and stratification in large volumes with interaction of both vertical and horizontal jets. In some cases the modelled scenarios included phenomena such as condensation as well as actuation of some safety components such as spray system. The preferred turbulent models was the k-ε model which in overall has shown good ability in predicting and representing gas transport phenomena and erosion [32], [33]. Concerning the resolution of the models, some sensitivity studies have already been performed [6] to address the importance of appropriate mesh with respect to the modelling subject. It has been shown that too coarse mesh tend to over-predict the mixing time but works good for simulations of stratification build-up [25]. Due to that fine mesh is recommended in the region of the interaction with the density interface. The turbulent models control the interaction of the jet with the stratified layer why they should be chosen carefully. Models for wall plumes, free plumes and horizontal high momentum jets using the k-ε model and 3D approach have been already modelled and tested. This approach delivers satisfying results but
the use of the k-ε models tends to spread the jet without representing the recirculation zones and under-predicts the velocities. The mixing-length on the other hand can be better tuned to adjust for specific scenarios which also permit better agreement with the velocity field at the density interface. However the mixing-length model cannot be recommended for general use. Nevertheless no guidelines have yet been developed for GOTHIC users.

2.5 Summary on the state-of-the-art

The previous sections explained the phenomena and risks of hydrogen release which during severe accidents can accumulate locally or globally inside the reactor containment and combust under certain conditions. This can result in damage of the technical equipment due to high temperature and pressure loads that are associated with the combustion and in worst case disrupt the integrity of the reactor containment causing the release of the radioactive material to the surrounding environment.

Because of it many projects such as HYMERES have been launched in which participants all over the world, including KTH-NPS, deal with simulations and modelling of hydrogen behaviour and erosion phenomena. The codes in use include CFD, which come with high computational costs and long running time, and LP, which are far less time consuming and computer demanding however not as accurate as CFD. The purpose of these projects is to improve severe accident management with better understanding and prediction of hydrogen generation and erosion.

The erosion of hydrogen is a complex phenomenon as it is associated with the rotational, time dependent and three dimensional nature typical for the turbulent flows. Due to that a statistical approach is needed. Through the years, different turbulence models have been developed starting from the simplified mixing-length to more advance two-equation k-ε model which use the Reynolds-Averaged Navier-Stokes equations.

Turbulence models exhibit benefits for different simulation cases such as shear flows, axisymmetric jets, impinging jets etc. Furthermore some turbulence models are more easy to implement than others inclining to their more frequent use and thus continuous attempts of improvements. The k-ε turbulence model constitutes such an example with its multiple variants. Nevertheless there is still much to be improved in terms of time efficiency and accuracy. For this reason large part of the engineering work focuses on the validation of the existing models to ensure that the issue of turbulence can be properly modelled. Thus simulations are conducted and validated against experimental data to ensure the credibility of the codes. Moreover high demands are set for the codes to be affordable, have high reliability through low computational codes and at the same time easy to implement.
3 Approach and Methodology

This chapter aims to describe ST1-7 test and PANDA Benchmark. A pre-test analysis of the conditions inside Vessel 1 is determined by the author of this thesis and completed with the data provided from PSI. In total, four general GOTHIC models have been created: two for ST1-7 and two for PANDA Benchmark. All of them are described and presented here. A simulation matrix is provided for each of the tests explaining the difference between each simulation.

3.1 ST1-7 Test

In ST1-7 test, GOTHIC was used to simulate the interaction of a low-momentum air jet with a stagnant helium rich layer in a large volume. In the experiment, both drywells, Vessel 1 and Vessel 2, in PANDA facility were used. The data and the results provided by PSI were used to set up the computational model and to validate GTH.

3.1.1 Test Conditions

Vessel 1 and 2 consist of two cylinders with an inner height of approximately 8 m and a diameter of 4 m. The vessels are connected to each other through 1 m long pipe situated around 3 m above the bottom of the vessels. At distance of around 0.5 m from the wall an injection pipe can be observed, see Figure 6. The nozzle of the pipe is 0.075 m and the outlet from the injection line is located 4 m from the bottom of the vessel.

![Figure 6: Configuration of the ST1-7 experiment in which both Vessel 1 and 2, Interconnecting Pipe (IP) and the injection pipe are shown [20].](image)
The vessels are made of stainless steel (DIN 1.4571) with the top covered with rock wool. Vessel 2 contains a venting pipe which is used to keep stable pressure in the system. In Vessel 1 a nominal 40% stagnant helium rich layer is present at 6 m from the bottom of the vessel [34]. Below that level as well as in the IP and Vessel 2 the atmosphere consists of air. The nominal temperature and pressure in Vessel 2 are 20°C and 97.4 kPa respectively. For Vessel 1 the initial temperature is 15°C. The test starts by injecting 15 g/s of air at ~30°C through the injection pipe in Vessel 1 for 12500 s. After that another 12500 s runs during which the system stabilizes and gases inside Vessel 1 are mixing.

To describe the conditions present in Vessel 1, the Reynolds number and Froude number, recall equations (3), (24) and (25), are used. For illustration of the conditions and the regions of interest see Figure 7.

![Figure 7: Illustration of the initial conditions inside Vessel 1.](image)

Froude number, Reynolds number together with conditions concerning the jet and Vessel 1 for both regions are presented in Table 1.

**Table 1: Initial conditions determined at the air jet nozzle 4 m from the bottom of the vessel and at the density interface 6 m above the bottom of the vessel.**

<table>
<thead>
<tr>
<th>Region</th>
<th>Velocity [m/s]</th>
<th>Density [kg/m³]</th>
<th>Jet diameter [m]</th>
<th>Reynolds number</th>
<th>Froude number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Region I</td>
<td>2.93</td>
<td>1.16</td>
<td>0.075</td>
<td>13800</td>
<td>18.39</td>
</tr>
<tr>
<td>Region II</td>
<td>0.68</td>
<td>0.78</td>
<td>0.214</td>
<td>9100</td>
<td>0.67</td>
</tr>
</tbody>
</table>
It has been previously concluded [20] and can be confirmed by analysing data in Table 1 that the air jet will not penetrate the helium layer, rather impinge on it in the early phase of the test. However its length will increase in time as the helium layer is subjected to continuous erosion.

3.1.2 GOTHIC Models

For ST1-7 experiment various types of GTH models were tested and the two final versions are described below. The main difference between the two models consists in subdivision of Vessel 1 for the first model whereas in the second model Vessel 1 is modelled as one unit. Although the amount of computational grids differs from the first and the second model by a factor of 2, the mesh in the vicinity of the jet is similar. The turbulence models applied on the models include the STD, RG, NL2 k-ε, the ML as well as the combination of the STD k-ε and the ML. For the ML model different \( l_{mix} \) will be tested to find good accuracy for the jet region and the density interface. The strategy includes use of equation ( ) and an adjustment made through trial and error attempts as well as tests of previous successful results with \( l_{mix} = D/4 \) [6].

Model 1

Figure 8 presents the general idea and schematics of Model 1. The 3D model of Model 1 with the visible computational grid can be seen in Figure 9. Vessel 1 is divided into four control volumes, ‘1s’, ‘2s’, ‘3s’, ‘4s’, with an additional volume ‘5s’ assigned to the jet region in which the injection pipe was modelled. The size of the jet volume (1m x 1m x 2m) was chosen in order to fully capture the jet for investigation of its profile. The height of the volume captures also the density interface making it possible to observe the reaction of the impinging jet.
Figure 8: Model 1. The subdivided Vessel 1 is connected to Vessel 2 through the interconnecting pipe (IP). Small squares represent the 3D connectors and two additional rectangles outside the vessels are boundary conditions.

Due to subdivision, the volumes with higher velocity and temperature gradients, like the jet volume and the upper part of Vessel 1 where the helium layer is present, can be refined whereas other parts of the model can still be relatively coarse. In this manner the total amount of cells can

Figure 9: The schematics of Model 1 where the grid can be seen. Vessel 1 has significantly finer mesh. Also jet volume has been brought outside the model for better visualisation and is represented as the dark square above Vessel 1.
be kept low, improving the computational time. In latter modifications of Model 1 the mesh was increased to match it with the total number of cells for Model 2, described later on in this section, in order to compare the two models with respect to their mesh sensitivity. Vessel 2, ‘7s’, was modelled as a unit with a coarse mesh. Same is valid for the interconnecting pipe, ‘6s’. The manhole which is located at the top of the vessels and insulated with wool rock is fully represented in the model. The control volumes are connected to each other through 10 3D connectors. As the venting occurs in Vessel 2, this control volume was provided with a boundary condition for pressure, ‘1P’ connected to the vessel through a flow path. The boundary conditions for the air injection, ‘2F’, are connected to the jet volume. Following the instructions and recommendations found in [6], [25] the size of the cells in the vicinity of the injection was kept small and has the same size as the injection nozzle for all directions, see Figure 10. For the whole model the ratio between the adjacent cells sizes was kept to maximum of 2.

The turbulence models tested on Model 1 include the ML and the STD k-ε. The STD k-ε is chosen to be applied in the jet volume and the ML model in the remaining control volumes. This is made based on previous research and work that have shown that by combining these two models accurate results can be obtained [6]. The idea is based on the assumption that the STD k-ε will be optimal in the jet volume due to its good performance in shear flows whereas in the rest of the model where conditions are not turbulent the ML should do. However some research points out difficulties for the STD k-ε in case of round jets; this is why other turbulence models and their performance on round jets will be tested as well.

The nodalization of the jet volume for Model 1.

**Model 2**

Figure 11 illustrates Model 2. It consists of three control volumes (‘1s’, ‘2s’, ‘3s’) that represent Vessel 1, 2 and the interconnecting pipe. Unlike Model 1, Vessel 1 is not subdivided however it has very fine mesh which can be observed in Figure 12. The total number of cells is 46403. This is mainly due to refined regions of the jet and the density interface. Due to lack of the subdivision
the fine mesh is stretched out throughout the whole model resulting in large number of cells in total. This is unfortunately a disadvantage of the integrated models versus subdivided models. The injection pipe is modelled in the same manner as in the previous model and the two manholes are represented in both vessels. Two boundary conditions are defined; first one for the jet injection which is connected to Vessel 1 and the second one for the ventilation that occurs in Vessel 2. The amount of control volumes that needs to be connected determines number of 3D connectors. For this model, it has been reduced to two due to its lack of the subdivided volumes.

One of the purposes of this model is to compare it to the previous one from the modelling perspective. One conclusion can be drawn directly concerning the mesh of the model; model without any subdivisions will contain more cells if the parts of interest (in this case the jet volume and density interface) have the same resolution as in the model with subdivisions. Thus leads to longer simulation time as the computational costs increase with larger models.

Turbulence models that will be tested on Model 2 include the STD, RG, NL2 k-ε and the ML models. Due to the construction of the model the combination of any of the above mentioned models is thus impossible.

Figure 11: Model 2. The vessels are connected to each other through the interconnecting pipe (IP) for which 2 3D connectors are used. Just like in Model 1, two boundary conditions are present within the system to define the air jet conditions and to stabilise the pressure. Figure to right shows the mesh of Vessel 1 which is refined in the location of the air jet and helium rich layer.
3.1.3 The simulation matrix

Table 2 and Table 3 present the sub-models that have been used for the simulation of ST1-7 experiment. Table 2 includes different variants of Model 1 which was modified with respect to mesh, turbulence models, and design as some models in contrast to others, the injection pipe was modelled. The same applies for Table 3 which refers to Model 2 and its variations.

Table 2: Simulation matrix for Model 1, where different design and simulation parameters have been varied.

<table>
<thead>
<tr>
<th>Model no.</th>
<th>Total no. of cells</th>
<th>Turbulence model</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>15100</td>
<td>STD k-(\epsilon)</td>
<td>No injection pipe modelled</td>
</tr>
<tr>
<td>1b</td>
<td>15100</td>
<td>STD k-(\epsilon)</td>
<td>Injection pipe modelled</td>
</tr>
<tr>
<td>1c</td>
<td>20897</td>
<td>STD k-(\epsilon)</td>
<td>Injection pipe modelled</td>
</tr>
<tr>
<td>1d</td>
<td>21407</td>
<td>STD k-(\epsilon) &amp; ML</td>
<td>STD k-(\epsilon) in the jet volume, ML in the rest of the model with (l_{mix} = D/4)</td>
</tr>
<tr>
<td>1e</td>
<td>21407</td>
<td>STD k-(\epsilon) &amp; ML</td>
<td>STD k-(\epsilon) in the jet volume, ML in the rest of the model with (l_{mix} = D/8)</td>
</tr>
<tr>
<td>1f</td>
<td>21479</td>
<td>ML &amp; STD k-(\epsilon)</td>
<td>ML in the jet volume with (l_{mix} = D/4), STD k-(\epsilon) in the rest of the model</td>
</tr>
<tr>
<td>1g</td>
<td>21479</td>
<td>ML &amp; STD k-(\epsilon)</td>
<td>ML in the jet volume with (l_{mix} = 0.0312) m, STD k-(\epsilon) in the rest of the model</td>
</tr>
<tr>
<td>1h</td>
<td>21479</td>
<td>STD k-(\epsilon) &amp; ML</td>
<td>STD k-(\epsilon) in the jet volume, ML in the rest of the model (l_{mix} = D/6)</td>
</tr>
<tr>
<td>1i</td>
<td>21479</td>
<td>ML</td>
<td>ML with (l_{mix} = 0.0312) m in the jet volume, (l_{mix} = D/6) into the rest of the model</td>
</tr>
</tbody>
</table>
Table 3: Simulation matrix for Model 2, where different design and simulation parameters have been varied.

<table>
<thead>
<tr>
<th>Model no.</th>
<th>Total no. of cells</th>
<th>Turbulence model</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>2a</td>
<td>14711</td>
<td>STD k-ε</td>
<td>No injection pipe modelled</td>
</tr>
<tr>
<td>2b</td>
<td>40078</td>
<td>STD k-ε</td>
<td>No injection pipe modelled</td>
</tr>
<tr>
<td>2c</td>
<td>40078</td>
<td>STD k-ε</td>
<td>Injection pipe modelled</td>
</tr>
<tr>
<td>2d</td>
<td>46703</td>
<td>STD k-ε</td>
<td>Injection pipe modelled</td>
</tr>
<tr>
<td>2e</td>
<td>46703</td>
<td>RG k-ε</td>
<td>Injection pipe modelled</td>
</tr>
<tr>
<td>2f</td>
<td>46703</td>
<td>ML</td>
<td>$l_{mix} = 0.0312 \text{ m}$</td>
</tr>
<tr>
<td>2g</td>
<td>46703</td>
<td>NL2 k-ε</td>
<td>Injection pipe modelled</td>
</tr>
<tr>
<td>2h</td>
<td>24240</td>
<td>STD k-ε</td>
<td>Coarser mesh at the injection line</td>
</tr>
</tbody>
</table>

3.2 PANDA Benchmark

To validate the models presented in section 3.1 for the ST1-7 test, additional validation was done against the PANDA Benchmark test. This chapter summarizes the experiment and the modifications of Model 1 and Model 2 that were needed in order to fit new conditions concerning PANDA Benchmark. All conditions and specifications for the experiment are provided by PSI [35].

3.2.1 Test conditions

For PANDA Benchmark only Vessel 1 is used. At the distance of 0.65 m from the centre axis of the vessel a vertical injection pipe is located. Its nozzle diameter is 0.075 m, that is, identical as the injection pipe in ST1-7 experiment. The outlet of the pipe is located 3 m above the bottom of the vessel. The venting of the vessel is made in the lower part of the vessel through a funnel found at the height of around 0.16 m. The interconnecting pipe has been blocked off, however a small hole is made and connected to the funnel via a pipe, see Figure 13. At the elevation of 6 m a stagnant helium rich layer of nominal 40% is present. Below the 6 m the vessel is filled with air. The pressure and temperature for the experiment are 99.4 kPa and 20°C respectively.

The test starts by injecting a mixture of air and helium through the injection pipe. The gas consisting of 13.5% helium and 86.5% air has a total mass flow of 21.95 g/s. The temperature of the gas raises starting from 23°C and reaching 29.3°C during the course of the experiment. The experiment lasts for 7200 seconds under which the gas is constantly injected. A comparison of ST1-7 experiment and PANDA Benchmark is presented in Table 4.
Table 4: Comparison of ST1-7 test and PANDA Benchmark.

<table>
<thead>
<tr>
<th></th>
<th>ST1-7 test</th>
<th>PANDA Benchmark</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal pressure</td>
<td>97.4 kPa</td>
<td>99.4 kPa</td>
</tr>
<tr>
<td>Nominal temperature</td>
<td>15°C (in Vessel 1)</td>
<td>20°C</td>
</tr>
<tr>
<td>Venting</td>
<td>Vessel 2</td>
<td>Lower part of Vessel 1</td>
</tr>
<tr>
<td>Gas composition at 6 m in Vessel 1</td>
<td>40 % Helium, 60 % Air</td>
<td>40 % Helium, 60 % Air</td>
</tr>
<tr>
<td>Pipe nozzle diameter</td>
<td>0.075 m</td>
<td>0.075 m</td>
</tr>
<tr>
<td>Injecting gas</td>
<td>100 % Air</td>
<td>86.5 % Air and 13.5 % Helium</td>
</tr>
<tr>
<td>Location of the pipe outlet</td>
<td>4 m above bottom of Vessel 1</td>
<td>3 m above bottom of Vessel 1</td>
</tr>
<tr>
<td>Transient</td>
<td>12500 sec of gas injection and 12500 sec of stabilisation</td>
<td>7200 sec of gas injection</td>
</tr>
<tr>
<td>Total time of experiment</td>
<td>25000 sec</td>
<td>7200 sec</td>
</tr>
</tbody>
</table>

The procedure is identical as for ST1-7 case; two regions are determined, the outlet of the jet and the density interface at 3 m and 6 m respectively. For both regions the initial conditions are determined and presented in Table 5.

Table 5: Initial conditions determined at the jet nozzle 3 m from the bottom of the vessel and at the density interface 6 m above the bottom of the vessel.

<table>
<thead>
<tr>
<th></th>
<th>Velocity [m/s]</th>
<th>Density [kg/m³]</th>
<th>Jet diameter [m]</th>
<th>Reynolds number</th>
<th>Froude number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Region I</td>
<td>4.73</td>
<td>1.05</td>
<td>0.075</td>
<td>22200</td>
<td>14.56</td>
</tr>
<tr>
<td>Region II</td>
<td>0.73</td>
<td>0.79</td>
<td>0.321</td>
<td>14700</td>
<td>0.71</td>
</tr>
</tbody>
</table>

As seen in Table 5, higher velocity for PANDA Benchmark is expected to cause larger turbulence in comparison with ST1-7. However, at the region of density interface, as the pipe is located 1 m lower than for ST1-7 the Froude number remains similar for both tests. Thus, it is expected that the jet will not penetrate the density interface. Nevertheless, the high turbulence that has been determined from Reynolds number will enhance the diffusion process of the gases. Also, the warmer gas injected into the vessel causes a temperature difference that will aim to equalize throughout the vessel contributing to the mixing process.
3.2.2 GOTHIC Models

Model 3

For PANDA Benchmark Vessel 2 and the interconnecting pipe have been removed. The jet volume is higher as it is aimed to capture the jet profile and the density interface. Due to the new size of it, the middle part of the model has to be merged, see Figure 14. However the remaining control volumes remain the same. The cell size in the jet volume is homogenous in all directions and the pipe is modelled at the bottom of the control volume. The venting through funnel has been solved by adding a boundary condition at the bottom of the vessel. The boundary condition for the jet volume has been changed to inject air and helium for 7200 seconds and new initial conditions concerning helium volume fraction, temperature, and pressure inside the vessel are applied to match the PANDA Benchmark test.
Figure 14: Schematics of Model 3. In figure to right the square outside the volume represents the jet control volume. Also the mesh of Model 3 with refined grid lines for the jet and helium rich layer can be observed.

The turbulence models that are applied include the STD $k$-$\varepsilon$, the ML and the combination of these two.

**Model 4**

The modifications for Model 4 include removal of Vessel 2 and the interconnecting pipe. The injection pipe has been relocated to 3 m above the bottom of the vessel as well as the mesh was adjusted to its new position. The venting through the funnel was made by adding a boundary condition to the lower part of the vessel. Boundary condition for the jet has been changed to inject a mixture of helium and air. The initial conditions concerning helium volume fraction and the temperature along the vessel have been changed to match PANDA Benchmark.
Figure 15: Schematics of Model 4. In figure to the right fine mesh of the model can be observed. The available turbulence model included use of the STD k-ε model.

### 3.2.3 The simulation matrix

Table 6: The simulation matrix for PANDA Benchmark test with the description of the models and the most important parameters.

<table>
<thead>
<tr>
<th>Model no.</th>
<th>Total no. of cells</th>
<th>Turbulence model</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>3a</td>
<td>19002</td>
<td>STD k-ε</td>
<td>Injection pipe modelled, model based on Model 1 from ST1-7</td>
</tr>
<tr>
<td>3b</td>
<td>19002</td>
<td>ML &amp; STD k-ε</td>
<td>STD k-ε in the jet volume, ML in the rest of the model $l_{mix} = D/6$</td>
</tr>
<tr>
<td>3c</td>
<td>19002</td>
<td>ML</td>
<td>$l_{mix} = D/2$ for the jet volume and $l_{mix} = D/6$</td>
</tr>
<tr>
<td>3d</td>
<td>19002</td>
<td>ML</td>
<td>$l_{mix} = D$ for the jet volume and $l_{mix} = D/6$</td>
</tr>
<tr>
<td>3e</td>
<td>40296</td>
<td>STD k-ε</td>
<td>The jet volume is refined in the x and y direction with a minimum cell size of $D/2$</td>
</tr>
<tr>
<td>4a</td>
<td>46575</td>
<td>STD k-ε</td>
<td>Injection pipe modelled, model based on Model 2 from ST1-7</td>
</tr>
</tbody>
</table>
4 Results and Discussions

The results will be validated against experimental data obtained from PSI and presented in form of graphs. Also to quantify the validation the root mean square error \[ \text{RMS} = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{n}} \] will be provided for the experiment compared with the simulation where \( \hat{y}_i, y_i \) are values for the experiment and simulation and \( n \) is the total number of the data points. Data points subjected for comparison include helium volume fractions and temperature at different locations inside Vessel 1 for ST1-7 test, see Figure 16. For PANDA Benchmark the measurement locations differ due to the new position of the jet, see Figure 17. The validation will be conducted against the experimental data concerning helium volume fractions at different heights and velocity fields at different heights and time.

First chapter of this section considers ST1-7 whereas in the second one the results from PANDA Benchmark are discussed.

![Figure 16: Data points for helium volume fractions are presented in the left figure where red stars indicate points for the centreline and green stars are points for the injection line. The figure on the right presents locations for the temperature data points with brown stars indicating the centreline and grey stars indicating the injection line [30].](image)
Figure 17: Data points for helium volume fractions can be observed in the figure to the left where the locations have been marked with red stars. In the figure to the left locations for the measurements of the velocity fields are presented [35].

4.1 ST1-7 Test

The RMSE for Model 1 are presented in Table 7 and for Model 2 in Table 8. The results are further discussed in the following chapters.

Table 7: Root Mean Square Error (RMSE) for different variants of Model 1, validated for the ST1-7 experiment.

<table>
<thead>
<tr>
<th>Model no.</th>
<th>Helium Volume Fraction along the centreline</th>
<th>Helium Volume Fraction along the injection line</th>
<th>Temperature along the centreline [°C]</th>
<th>Temperature along the injection line [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>0.031</td>
<td>0.045</td>
<td>6.17</td>
<td>5.71</td>
</tr>
<tr>
<td>1b</td>
<td>0.020</td>
<td>0.027</td>
<td>1.86</td>
<td>2.34</td>
</tr>
<tr>
<td>1c</td>
<td>0.021</td>
<td>0.027</td>
<td>1.82</td>
<td>2.46</td>
</tr>
<tr>
<td>1d</td>
<td>0.023</td>
<td>0.027</td>
<td>1.84</td>
<td>3.47</td>
</tr>
<tr>
<td>1e</td>
<td>0.018</td>
<td>0.027</td>
<td>1.56</td>
<td>3.52</td>
</tr>
<tr>
<td>1f</td>
<td>0.030</td>
<td>0.030</td>
<td>1.85</td>
<td>2.85</td>
</tr>
<tr>
<td>1g</td>
<td>0.014</td>
<td>0.016</td>
<td>1.88</td>
<td>3.13</td>
</tr>
<tr>
<td>1h</td>
<td>0.014</td>
<td>0.016</td>
<td>1.81</td>
<td>3.44</td>
</tr>
<tr>
<td>1i</td>
<td>0.017</td>
<td>0.027</td>
<td>1.83</td>
<td>2.26</td>
</tr>
</tbody>
</table>
Table 8: Root Mean Square Error (RMSE) for different variants of Model 2, validated for the ST1-7 experiment.

<table>
<thead>
<tr>
<th>Model no.</th>
<th>Helium Volume Fraction along the centreline</th>
<th>Helium Volume Fraction along the injection line</th>
<th>Temperature along the centreline [°C]</th>
<th>Temperature along the injection line [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2a</td>
<td>0.051</td>
<td>0.068</td>
<td>7.60</td>
<td>8.52</td>
</tr>
<tr>
<td>2b</td>
<td>0.027</td>
<td>0.045</td>
<td>1.64</td>
<td>2.39</td>
</tr>
<tr>
<td>2c</td>
<td>0.019</td>
<td>0.026</td>
<td>1.69</td>
<td>1.84</td>
</tr>
<tr>
<td>2d</td>
<td>0.015</td>
<td>0.026</td>
<td>1.77</td>
<td>1.90</td>
</tr>
<tr>
<td>2e</td>
<td>0.016</td>
<td>0.033</td>
<td>1.65</td>
<td>1.80</td>
</tr>
<tr>
<td>2f</td>
<td>0.038</td>
<td>0.045</td>
<td>1.86</td>
<td>1.96</td>
</tr>
<tr>
<td>2g</td>
<td>0.016</td>
<td>0.026</td>
<td>1.82</td>
<td>2.20</td>
</tr>
<tr>
<td>2h</td>
<td>0.015</td>
<td>0.029</td>
<td>1.74</td>
<td>2.20</td>
</tr>
</tbody>
</table>

4.1.1 Jet instabilities

This section focuses on the evaluation of Model 1 and Model 2 based on their design; the subdivision and the modelling of the injection pipe.

Initial models of Model 1 have shown large instabilities, especially in the jet volume region. The instabilities were observed in the form of large oscillations in helium volume fractions and temperatures obtained for the injection line for the first 2350 seconds. This in turn affected negatively the results in the centreline. The origin of the oscillations is believed to come from the instabilities of the turbulent kinetic energy, which oscillated strongly at the same time, see Figure 18. The turbulent kinetic energy is zero during first ~1000 seconds of the simulation after which it oscillated for another ~1000 seconds before it finally stabilises. At the same time instabilities appear at the centreline and are most visible for the levels closest to the jet, which are 3.676 m, 4.326 m, 4.976 m and 6. It can be speculated that the reason for these oscillations can be found in the fine mesh used at the jet region near the wall.
Figure 18: Turbulent kinetic energy at the jet outlet is shown in the figure to the left whereas the right figure shows the decreasing helium volume fraction at the centreline for the corresponding time.

However, different models designed to investigate the stability of the turbulent kinetic energy showed that these oscillations could be avoided if the injection pipe was modelled (Model 1b). This modelling allowed the flow to maintain its turbulent kinetic energy before being injected into the vessel, enhancing the stability of the turbulent kinetic energy at the outlet. The results can be observed in Figure 19: Model 1a (which did not include the pipe) is represented by the dashed lines, Model 1b by straight line, and the experimental data by dots. It can be seen that up to 2300-2500 seconds the results are unstable for Model 1a as it was also shown in Figure 18. After modelling the injection pipe, the oscillations along the injection line were lowered and an improvement for the results along the centreline was observed, as it can be seen in Figure 19 by observing the straight line representing Model 1b. Slight increase of helium is noted at the time of the jet inactivation and the erosion from this point onwards is governed by the mixing phenomena due to density difference in the vessel.
Figure 19: The effect of pipe modelling on helium volume fraction along the centreline as function of height and time: no pipe modelled in Model 1a (15100 cells), pipe modelled in Model 1b (15100 cells).

In case of Model 2, the comparison is made between Model 2b and Model 2c. Both models consist of exactly the same amount of cells (40078 cells) however the injection pipe has been modelled only for Model 2c. The results can be observed in Figure 20. Also in these models oscillations appeared along the injection line and do not disappear when the injection pipe is modelled. The performance of Model 2c is slightly more accurate as the erosion of helium is more precisely predicted for levels 6.926 m and 6.496 m. However the mixing in the containment after the inactivation of the jet is over-predicted. The reason for the small impact of the injection pipe may be due to very fine mesh of the models which accurately captures the erosion of helium.
Figure 20: The effect of pipe modelling on helium volume fraction along the centreline for Model 2b which lacks the injection pipe and Model 2c in which the pipe is modelled.

4.1.2 Mesh sensitivity

Since the results obtained from models 1a and 1b were unsatisfying, a decision to refine the mesh was made. Thus, additional grid lines were added in the part of helium rich layer. In Figure 21 Model 1b consisting of 15100 cells and Model 1c consisting of 20897 cells are shown. As it can be observed both models behave in a similar manner, suggesting that the 20897 cells mesh can give converged results and that any further refinements might result in much higher computational costs but only gain minimal accuracy. The calculation time for Model 1b and Model 1c using 4 cores of an i7 3.40 GHz is 85 hours and 125 hours respectively which is already a relatively long time compared to previous experiments in which simulations conducted on the same computer but with 1 core instead of 4, lasted for 19.2 hours, 63.1 hours and 106.3 hours for models consisting of 3011 cells, 7415 cells and 10859 cells [6]

The mesh sensitivity is made for Model 2a (14711 cells) and Model 2b (40078 cells). In Figure 22 the decrease of helium volume fraction with respect to time along the centreline is presented and compared to experimental data. Model 2a fails to capture the behaviour of the system and the helium erosion is strongly over-predicted especially for heights above 6 m. The decrease of helium volume fraction along the centreline was due to the numerical oscillations of the jet. These are caused by large oscillations in turbulent kinetic energy, causing errors in the energy for the whole system and additionally affecting other parameters such as temperature, density, velocity, etc. The mesh is increased significantly for Model 2b by addition of approximately 35000 cells. The improvement is noticeable as the model remains stable for longer period of time
compared to Model 2a. However, the oscillations reappears even for this model and the system starts to behave in a similar way as Model 2a developing instabilities some hundred seconds after the initiation of the simulation. This model consists of twice as many cells as Model 1b and yet does not deliver satisfactory results. Moreover, among all performed simulations this lasted the longest time which is an additional reason why this method is unaffordable.

Figure 21: The effect of mesh on helium volume fraction along the centreline: Model 1b consists of 15 100 cells whereas Model 1c consists of 20 897 cells.

In neither Model 2a nor Model 2b the injection pipe was modelled. For comparison the mesh sensitivity was conducted for the models containing it, see Figure 23. Model 2d is a modified Model 2c in which additional grid lines have been added in the region of density interface resulting in additional 6000 cells. This was made as the helium volume fraction at height 8.030 m for Model 2c was very inaccurate. However the results were not improved significantly and the helium erosion remains over-predicted at the highest level. For most of the models the mesh size in the jet volume and in the vicinity of the injection pipe was set to the size of the pipe nozzle (0.075 m) which delivered acceptable results. However in Model 2h the mesh in the vicinity of the jet was reduced to its double size to test its effect on the jet profile. Some of the grid lines in the x- and y- direction were removed whereas the grid lines in the z-direction were kept unchanged. As the jet spreading becomes less accurate, it results in underestimation of the helium erosion. However as the erosion of helium at 8.030 m has been overestimated for most of the models due to previous mentioned reason it becomes accurate for Model 2h. It is possible that the difficulty in prediction of the helium erosion for the height of 8.030 m comes from the change in the geometry of the vessel. The man-hole is located there and it is possible that even finer mesh is needed just for that region. Due to insufficient refinement it is believed that the simulation fails to recreate the correct event and the helium layer is eroded too fast.
Figure 22: Mesh sensitivity for Model 2a and Model 2b consisting of 14,711 cells and 40,078 cells. Also for both models the injection pipe is not modelled.

Figure 23: Mesh sensitivity for Model 2c, Model 2d and Model 2h consisting of 40,078 cells, 46,403 cells and 24,240 cells. In all models the injection pipe is modelled.

4.1.3 Turbulence models

The main issue of the STD k-ε turbulence model is the appearance of large oscillations along the injection line. The magnitude of the oscillations increases with the size of the model: the larger
number of cells the larger the oscillations. An explanation of this behaviour may be found in the performance of the turbulence model for this specific case of integrated models. As it was mentioned before the STD k-ε model is optimal for shear flows and fully developed turbulence. However in Vessel 1, such conditions exist only in the jet volume. At more distant regions of the model the flow will be laminar. The GOTHIC Technical Manual [23] warns for this kind of situation and points out that it can result in non-physical turbulence in the solution. Also there is a possibility that due to large and fast changes in local Reynolds number near to the transition state from the turbulent to laminar flow the approximate transition model is activated leading to sudden drops of the turbulent kinetic energy. As the jet increases in length in time and the transition to laminar moves upwards this issue appears firstly at lower levels and moves upwards in the vessel.

The best results are achieved for the combination of the turbulence models, however changes in the parameters have large consequences on its performance. In Model 1d the STD k-ε model is applied in the jet volume and the ML model with $l_{mix} = D/4$ in the remaining control volumes resulting in strong under-prediction of the helium erosion. When the mixing length is reduced to $D/8$ the erosion is on the other hand over-predicted. The best results are thus found for $l_{mix} = D/6$ which correctly predicts the helium erosion up to ~7 m but slightly over-predicts it at higher levels. When the location of the turbulence models is reversed, applying the ML in the jet volume with $l_{mix} = D/4$ and the STD k-ε in the rest of the model (Model 1f) tends to over-predict the helium erosion, see Figure 25. The best results are found with $l_{mix} = 0.0312$ m although slight over-prediction still occurs. Also by analysing the figure it can be seen that the agreement with the experimental data does not occur until ~6000 s for the height of 6.496 m and ~9000 s for 6.926 m after the start of the transient. This emphasises the need of careful choice of $l_{mix}$ as it is very case specific and will not perform accurately unless the mixing length is chosen correctly depending on the condition in the vessel. It also implies that although the ML model with $l_{mix} = 0.0312$ m produces acceptable results, the fixed values of mixing length over long periods of time are not optimal and would probably work better under steady state conditions. As the conditions differ from each other in the control volumes so should $l_{mix}$. Due to models 1h and 1g two values for the mixing length were found; one which works satisfactory in the upper part of the vessel ($l_{mix} = D/6$) and one that can be applied in the jet volume ($l_{mix} = 0.0312$ m). Model 1i uses these values and the results can be observed in Figure 26.
Figure 24: The effect of the combined turbulence models on helium volume fraction along the centreline: The models use the STD k-ε model in the jet volume and the Mixing Length in the remaining control volumes. The mixing lengths are $D/4$ for Model 1d, $D/8$ for Model 1e and $D/6$ for Model 1h.

Figure 25: The effect of the combined turbulence models on helium volume fraction along the centreline: Both models use STD k-ε in Vessel 1, except for the jet volume where Mixing Length is applied with $l_{mix} = D/4$ for Model 1f and $l_{mix} = D/2$ for Model 1g.
Figure 26: The effect of the Mixing Length turbulence model on helium volume fraction along the centreline. In Model 1i the ML is applied with $l_{mix} = D/2$ for the jet volume and $l_{mix} = D/6$ for the remaining control volumes.

Figure 27 presents the performance of different turbulence models on Model 2 which consists of 46703 cells. It should be noticed how the choice of fixed $l_{mix}$ for the ML model influences the outcome. With $l_{mix} = 0.0312$ m the helium erosion is strongly under-predicted and the error increases with the increased distance from the air jet. The RMSE is almost twice as large as for cases with the two-equation turbulence models, see Table 8. Thus fixed mixing length is a faulty method for dealing with the turbulence considering the size of the model and different conditions existing at different levels.

The different k-ε turbulence models perform relatively well which is believed to be attributed to the adequate mesh of the model. However helium erosion at the top of the vessel is over-predicted by all of the turbulence models. The results for the centreline are relatively accurate and no significant difference in the performance for the two-equation turbulence models is noticed. The only difference was noted in form of the simulation time which, when using the NL2 k-ε model was couple of hours longer than when other turbulence models were applied.
4.1.4 Erosion of the helium layer

The general behaviour of the helium layer is presented in Figure 28 and Figure 29 which show temperature and helium volume fraction distribution at 1000 s, 4000 s and 10000 s. Furthermore Model 1h and Model 2d have been chosen to the analysis due to their high agreement with the experimental data. The helium volume fraction along the injection line is shown for both models in Figure 30 and Figure 33.
Figure 28: Snapshots of temperature profiles at times 1000 s, 4000 s and 10000 s after the start of the simulation.

The initial temperature in Vessel 1 is relatively uniform across the whole vessel and is approximately 15°C. Figure 28 shows the distribution of the temperature during the simulation. Air at around 30°C is vertically injected to the containment however due to its low momentum the jet does not penetrate the helium layer. At 1000 s it has nearly reached the density interface, see Figure 29. The blue region in the figure presents regions where the helium concentration is low whereas the highest concentration is represented by the red region at the top of the vessel. The hot temperature from the jet spreads radially towards the centreline of the vessel. The warmed air that now exists in the middle part of the vessel is lighter than the gases in the upper part of the vessel. This density and temperature difference will thus try to spread uniformly in the vessel, propagating the warmer gas upwards and contributing to the mixing inside the containment. The cold air will be “pushed” downwards creating recirculation patterns inside the vessel. As the hot air propagates upwards the jet continues to erode the stratified layer creating turbulence that contributes to the mixing through diffusion of the gases. The highest concentrations of helium will be found in the manhole where the gas allocates.

As it can be observed in Figure 30, the experiment is generally well captured. Some discrepancies occur for the levels at 5.3-5.6 m. Also the erosion of the helium layer is under-predicted for the 5.6 m level and does not follow the steep decrease that is observed for the experiment. Although good agreement with the experimental data exists for the levels above 6 m, the same trend the smooth helium decrease is observed at 6.276 m starting at ~4000 s. When the injection of air is stopped after 12500 s an increase of helium is observed as a result of the buoyancy forces due to previous mentioned density difference inside the vessel. However the mixing is over-predicted at all levels.
Figure 29: Snapshots of helium volume fractions profiles at times 1000 s, 4000 s and 10000 s after the start of the simulation.

Continuing with the temperature profiles, Figure 31 and Figure 32 show the temperature distribution along the centreline and the injection line for Model 1h. Although the general idea of temperature increase as the hot air enters the vessel is captured, large discrepancies exist between the simulation and the experiment. It is believed that this is due to initial assumption concerning the temperature of the walls which was set to 15°C. This is the reason why the temperatures converge towards that value as the simulation goes on and can be observed in both figures. Also, due to the vicinity to the wall and because the hot air from the jet does not reach the top of the vessel the data at 8.030 m level differs significantly from the experiment (red line) and the temperature behaviour at that level is poorly captured. Consequently, the highest temperatures are observed at 5 m and 6 m due to the near location of the measurement points to the jet. The temperature profile along the injection line is under-predicted, possibly due to its proximity to the wall. However, like in the experiment, the temperature increases first for the level nearest to the injection pipe. The wall proximity may not be the only reason for the temperature underestimation. Due to that the jet profile should also be analysed. It is possible that the combination of the two turbulence models which are the STD k-ε and the ML models has some effect on the prediction of the jet spreading by under-predicting it. Unfortunately no velocity profile data is available for the comparison and this assumption cannot be confirmed.
Figure 30: Helium volume fraction along the injection line for Model 1h in which the STD k-ε is applied in the jet volume and the ML in the remaining control volumes.

To analyse results obtained from Model 2 and its different variants Figure 33, Figure 34, and Figure 35 are used. In the previous chapters, oscillations along the injection line were mentioned which can also be observed in Figure 33. Despite the oscillations the behaviour of helium is however nicely captured. It is believed that the oscillations originate from the turbulent to laminar flow transition model that was previously mentioned. Due to large amount of cells in Model 2d, velocity gradients are expected to affect local Reynolds number which in some cases can become very small leading to the activation of the transition model. When the air jet is shut down at 12500 s and the turbulence is cancelled the values become also stable and the oscillatory behaviour disappears.

The temperature profiles are presented for the centreline and the injection line in Figure 34 and Figure 35. The temperature at level 8.030 m (red line) in Figure 34 behaves in the similar way to Model 1h probably due to the same reason. However data for levels 4.326 m, 4.976 m and 6 m indicate larger spreading of the jet and more vigorous transport of the gases especially for the middle part of the vessel. As the simulation goes on the temperature decreases at lower levels as the hot air drifts upwards which can be observed by the increase of temperature at level 6.926 m (green line) and decrease at other levels.
Figure 31: Temperature profile along the centre line for Model 1h in which the STD k-ε is applied in the jet volume and the ML in the remaining control volumes.

Figure 32: Temperature along the injection line for Model 1h where the STD k-ε is applied in the jet volume and the ML in the remaining control volumes.
Figure 33: Helium volume fraction along the injection line for Model 2d in which the STD k-ε model is applied.

For the injection line the general trend is captured with the high temperature increase in the vicinity of the injection line, however large discrepancies are observed at 6.276 m and later on at 6.926 m. The oscillations in temperature profiles appear at the same time as the oscillation along the injection line for helium volume fraction, Figure 33.

Figure 34: Temperature profile along the centre line for Model 2d where the STD k-ε model was applied.
4.1.5 Velocity profiles

In this section the investigation and comparison of the vertical jets for Model 1h, Model 2d and Model 1i is conducted. In Model 1h a combination of the STD $k$-$\varepsilon$ and the ML was applied, in Model 2d the STD $k$-$\varepsilon$ model was applied whereas in Model 1i the ML was applied. All models have homogenous cell size in $x$-, $y$- and $z$-direction for uniform spread of the jet.

During the simulation it was noticed that changes or fluctuations in the turbulent kinetic energy affected the jet profile. Since the oscillations appeared most frequently in Model 2d, it contributed to the disturbance of the jet profile for most of the tests.

Although the combination of the STD $k$-$\varepsilon$ and the ML turbulence model gave accurate results for the helium volume fractions, an unphysical behaviour was noticed when observing the velocity profile (Figure 36). The velocity field obtained through GOTHIC might be misleading as it indicates strong movements in the upper part of the vessel. This is only due to the scaling factor used for the velocity arrows. When plotting the contours of the velocity magnitudes, we can see that the velocity in the lower region is very small. We can see in Figure 36 that the air jet is deflected to one side instead of showing a vertical profile, which was also observed in other GOTHIC models in which the combination of the STD $k$-$\varepsilon$ and the ML was used. The right side of Vessel 1 (opposite the injection pipe) contains no source for disturbance, yet strong and unphysical movements can be noticed in that region. Figure 37 presents a slice of the velocity profile for Model 1h taken from another side. In this figure, we can see that the jet turns towards
one of the walls of the vessel. This profile would explain the low temperature rise for the injection line and the centreline, Figure 31 and Figure 32. It is important to note that even if the helium volume fractions were well predicted with this model, the velocity profile is unreasonable. There is nothing on the way of the jet that can cause its sudden right angle turn. As the air leaves the injection pipe nozzle, it enters free and large space and should without any obstacle move upwards until it hits the helium-rich layer. Although, the model provides good fit with the experimental data for helium volume fraction, the velocity profile remains questionable challenging the credibility of the model.

Figure 36: Velocity vector profile taken 1000 s after the initiation of the simulation for Model 1h in which the STD k-ε is applied in the jet volume and the ML in the remaining control volumes. Figure to left is made in GTH whereas figure to right was made using ParaView [37].

For comparison, Model 2d is used. The velocity field obtained from the STD k-ε turbulence model is presented in Figure 38. As it can be seen the air jet has a fountain-like shape with two light blue shades on each side indicate the downward oriented flow. The temperature profile for Model 2d was previously shown in Figure 28, indicating the movement of the jet and its propagation upward along the vessel. In overall, large recirculation patterns are observed for the model.

Due to strange behaviour of the jet in Model 1h, questions arise concerning the combination of the STD k-ε and the ML turbulence model. It has been shown that the STD k-ε model alone works satisfactorily; thus, the next step is to investigate the accuracy of the ML model alone. For this reason Model 1i is chosen; this model uses the ML turbulence model predicts accurately the erosion of the helium along the centreline and the injection line. Figure 39 shows the velocity field taken at the same time as for Model 1h and Model 2d; that is, 1000 s after the start of the
The jet profile is slightly crooked; however, it remains vertical unlike Model 1h. Very small movements are observed in the upper part of the model like in the previous models. The jet does not have the same fountain-like shape like in Model 2d and the STD k-ε model. There is also a strong downward circulation which is represented by the colourful “flame” to the left of the air jet. In Figure 40 the temperature distribution throughout the vessel is shown for Model 1i at three different times. Similar to Model 2d, the jet impinges on the helium layer but as it cannot penetrate it, the temperature spreads radially and later on propagates upwards as it erodes the helium layer. Also in this figure it can be seen that the jet is not symmetrical and more activity is visible on the side closest to the wall.

![Temperature Distribution](image)

Figure 37: Snapshot of velocity magnitude taken at 1000 s for Model 1h.

Why this anti-symmetry appears and the reason why the same trend of downward flow is not visible on the other side of the air is uncertain. It is probable that it is related to the vicinity to the wall.

Although no experimental data was available for velocities for ST1-7, velocities for all three models are taken in order to make a simple evaluation and comparison between the models. Figure 41 shows the velocity at 1000 s, 4000 s and 10000 s after the start of the simulation. The measurement location was at 1.8 m above the pipe exit. Model 2d and Model 1i are comparable except for the first value taken at time 1000 s which for Model 2d is close to 0 m/s. It is suggested that this is due to the oscillating behaviour of Model 2d along the injection line (Figure 33) as the velocities at times 4000 s and 10000 s for both models are very similar. Also, the profile is shifted towards the wall at time 4000 s for Model 1i. However in the remaining cases the highest velocities are correctly found to be located along the injection line. Although the width of the jet is similar for models 1i and 2d as the jet evolves at time 10000 s it can be seen
that for Model 1i it gets wider. Due to lack of the experimental data it is though impossible to conclude if the correct width is modelled through the ML or the STD k-\(\varepsilon\) model. In contrast to the good agreement between models 1i and 2d, Model 1h did not show any resemblance between the models indicating no similarity in the jet behaviour. This is an important discovery which shows that the combination of different turbulence models may be erroneous despite the accurate results for the helium volume fractions and the temperatures profiles. The reason for the good agreement between the simulation and the experimental data for Model 1h is not yet understood. Other models that use the combination of the turbulence models that is models 1d, 1e as well as models 1f and 1g where the ML was applied in the jet volume and the STD k-\(\varepsilon\) model in the remaining volumes were also analysed. The results are not shown here due to restriction of the size of this report. Nevertheless in all of the models the skewness of the jet profile was visible and resembles the one presented for Model 1h, in Figure 37.

Figure 38: Velocity vector profile taken 1000 s after the initiation of the simulation for Model 2d in which the STD k-\(\varepsilon\) turbulence model is applied. Figure to left is made in GTH whereas figure to right was made using ParaView.
Figure 39: Snapshot of velocity field for Model 1i taken at 1 000 s after the start of the simulation.

Figure 40: Snapshot of temperature profile for Model 1i in which the Mixing-Length turbulence model is applied.
Figure 41: Velocity profile for Model 1h (the STD k-ε + the ML), Model 2d (the STD k-ε) and Model 1i (the ML) taken 1.8 m above the injection pipe at times 1000 s (black line), 4000 s (blue line) and 10000 s (red line).

### 4.2 PANDA Benchmark

The results are compared with the experimental data and discussed further in the following sections. To quantify the accuracy between the experiment and the simulation the root mean square error is calculated for parameters helium volume fraction and velocity field. It is presented in the table below.

Table 9: Root Mean Square Error (RMSE) for different variants of Model 3 and Model 4, validated against PANDA Benchmark.

<table>
<thead>
<tr>
<th>Model no.</th>
<th>Helium Volume Fraction [-]</th>
<th>Velocity Field [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>3a</td>
<td>0.012</td>
<td>0.083</td>
</tr>
<tr>
<td>3b</td>
<td>0.015</td>
<td>0.280</td>
</tr>
<tr>
<td>3c</td>
<td>0.031</td>
<td>0.230</td>
</tr>
<tr>
<td>3d</td>
<td>0.019</td>
<td>0.140</td>
</tr>
<tr>
<td>3e</td>
<td>0.025</td>
<td>0.197</td>
</tr>
<tr>
<td>4a</td>
<td>0.017</td>
<td>0.130</td>
</tr>
</tbody>
</table>
4.2.1 Design and mesh sensitivity

Mesh sensitivity was performed on Model 3a, 3e and 4a. Helium volume fractions for the models can be observed in Figure 42, Figure 43, and Figure 44. Models 3a and 4a show similarity by under-predicting the erosion of helium at lower levels and over predicting it at the top level. Based on the results it is believed that the over prediction is due to location of the injection pipe and manhole which lies along the same axis. Instead of accumulating helium in the manhole and thus concentrating it there the helium is dispersed too quickly. The turbulence is relatively large due to high Reynolds number which also contributes to fast diffusion of the gases. Nevertheless, the over-prediction of helium indicates high velocities at the top levels. It is believed that this is related to mesh rather than to the turbulence model. To confirm this assumption, the mesh in the jet volume was refined in the x- and y-direction for Model 3e. The results can be observed in Figure 43. The erosion of helium is still strongly under predicted at all levels. However as the cells become wider for Model 3e (the cell size is 0.0375 m x 0.0375 m x 0.075 m), it affects spreading of the jet which becomes radial. This makes the penetration of the density interface less efficient causing under-prediction of the helium erosion. The velocity profiles for the models will be discussed further in the next section.

Figure 42: Helium volume fraction decrease at different levels with respect to time for Model 3a which consists of 19002 cells and uses the STD k-ε turbulence model.
Figure 43: Helium volume fraction at different levels along the injection line for Model 3e which consists of 40296 cells in total. In the jet volume contains the homogenous cells in the x- and y-direction have size of 0.0375 m (half of the pipe diameter).

Figure 44: Helium volume fraction decrease at different levels with respect to time for Model 4a which consists of 46575 cells and uses the STD k-ε turbulence model.

Due to the very fine mesh of Model 4a, large oscillations are observed along the injection line. The same behaviour was visible for Model 2 for ST1-7 when using the k-Epsilon STD model as presented in Figure 33. Further, it is believed that the reason for the oscillations is the same as in
the previous ST1-7 case: velocity gradients in the control volume which contribute to large variation of the local Reynolds numbers and results in the activation of the approximate transition model.

4.2.2 Turbulence models

The turbulence models used for PANDA Benchmark include the STD $k$-$\varepsilon$, the ML and their combination.

The STD $k$-$\varepsilon$ model delivers relatively accurate results which were shown for Model 3a in Figure 42. However, increased mesh results in oscillatory behaviour which was presented for Model 4a. This emphasises the strong relation between the nodalisation and the performance of the STD $k$-$\varepsilon$ turbulence model. As it was presented in Model 3e, inaccurate mesh in the region of the jet under-predicts the helium erosion.

The combination of the STD $k$-$\varepsilon$ and the ML models resulted in code crash at $\sim$4000 s. Additional four other sub-models to Model 3b were made in which the porosity and time step were changed in hope to improve the results. Unfortunately this method was unsuccessful and the simulations continued to crash. Instead it was decided to emphasize on other turbulence models due to restricted time of the thesis. It is difficult to state any reason for the crashes as GOTHIC does not provide its users with detailed crash reports. The only difference between models 3a, 3b and 3c was the turbulence model. All the other parameters were kept unchanged suggesting the choice of the turbulence model as the primary reason of the code crashing. Still, helium volume fraction for the first 4000 s for Model 3e can be observed in Figure 45.

Once again, the individual turbulence models are investigated. The STD $k$-$\varepsilon$ model worked satisfactorily as it was observed for Model 3a and Model 4a. For this reason the focus was transferred for the ML turbulence model. Due to similar test conditions for PANDA Benchmark and ST1-7 test, concerning the Froude number and the velocity at the region of density interface, the $l_{\text{mix}}$ was set to same values as in Model 1i for ST1-7. This resulted in accurate helium erosion for heights up to 5 m. For heights above this level the helium erosion is over-predicted. Comparing the results with ST1-7 it should be pointed out that the jet volume in PANDA Benchmark is 1 m higher than for ST1-7 which was 2 m high. Thus, the chosen $l_{\text{mix}}$ works satisfactorily only for some levels while at other levels, a large disagreement with the experiment is observed. The mixing length in the jet volume will determine the behaviour of the jet, so it should be chosen very carefully. Analysing equation (13) shows that since the velocity at the top of the vessel is very small, small values of mixing length will only result in small eddy viscosity. Thus, large values must be set to compensate for the low velocity; however, this will have impact on other locations inside the vessel where the velocity is larger. To solve this issue more divisions of the vessel are needed or if the present design should be kept the mixing length in the jet volume should be readjusted if better agreement with the experiment is wished to be achieved at
the top of the vessel. It seems that in neither way the full agreement with the experiment will not be achieved with this model. Still the ML is capable of producing satisfactory results.

Figure 45: Performance of the combined turbulence model where the STD k-ε was applied in the jet volume and the ML in the remaining control volumes. The simulation crashed after 4 000 s.

Figure 46: Comparison of Model 3c and Model 3d in which the ML is applied. For Model 3c $l_{mix} = D/2$ for the jet volume and $l_{mix} = D/6$ for the remaining control volumes whereas for Model 3d $l_{mix} = D$ for the jet volume and $l_{mix} = D/6$ for the remaining control volumes.
4.2.3 Velocity profiles

Figure 47 shows the snapshot of the velocity field for Model 3a, 3000 s after the start of the simulation. The jet has a fully developed profile with the fountain-like shape at the top and streamlines coming back down on both sides of the jet. Very similar behaviour was observed also for Model 4a although the jet spread was wider, see Figure 49. For Model 3b (with the combined turbulence model) the skewed profile was once again discovered. The jet of models 3c and 3d are very wide due to user defined mixing lengths.

Best agreement with the experimental data was achieved with Model 3a, see Figure 48. The velocities are slightly underestimated for most of the levels; however, the overall result is satisfactory. The first velocity measurement taken at 111 s (red line) coincides with the oscillatory behaviour noted during first 250-300 s which could explain the disagreement with the experimental data. All models oscillated for the first hundred seconds and the agreement for the first data point is not achieved for any of them. The sudden drop of velocity at 6.110 m (yellow line) is for now inexplicable as this trend appeared also in other models despite relatively good agreement for the velocity at 5.900 m (dark blue line) which was taken at the same time at 715 s. The worst results were obtained for Model 3b with the combined turbulence model. Very low velocities were observed at all times and all levels. The profile was skewed in the same way as in case of ST1-7 out of the jet volume. Thus relatively large movements are noted for the middle part of the vessel whereas the upper part remains still. It is remarkable that velocity profiles measured in PANDA Benchmark were not captured by the combination of the STD k-ε and the ML models (see Figure 51) while overall prediction of the transient concentration was quite reasonable (Figure 45).
Figure 47: Velocity field for Model 3a, in which the STD k-ε turbulence model is applied, taken at time 3000 s. Figure to left is made using GOTHIC built-in function whereas figure to right is made using software ParaView.

Figure 48: Velocity profiles for Model 3a taken different levels and at different times.
Figure 49: Velocity profiles for Model 4a taken different levels and at different times.

Figure 50: Velocity profiles for Model 3e taken for different levels and at different times. The model consists of 40296 cells and uses the STD k-ε turbulence model.
4.3 Discussion

This section aims to integrate the knowledge that has been obtained from the results from ST1-7 and PANDA Benchmark and form the basis for the conclusion chapter.

4.3.1 The design and mesh sensitivity

For ST1-7 and PANDA Benchmark, two types of models were investigated. The first one consisted of subdivided control volumes whereas the second one was an integrated model. Based on the results it is recommended to always use the subdivision feature when modelling large objects such as reactor containment. Both models need adequate mesh resolution to capture the stratification phenomena which is why the mesh was refined in the jet volume and the density interface. However in the integrated model these regions could not be separated as it was made in the subdivided model, and because of that the mesh was refined even in the regions that did not require it. Due to that the integrated model consisted of 3 times more cells when compared to the subdivided model resulting in the total amount of around 46000 cells. The large size of the integrated model increases the simulation time and computational costs making the model unaffordable.
Concerning mesh, it is important to have sufficient resolution for regions with higher gradients. In the case of ST1-7 and PANDA Benchmark, these regions are the jet and the density interface. It is important to resolve the jet in order to obtain correct spreading. The smaller the mesh, the better accuracy is achieved; however, the choice of the resolution should be a balance between good agreement and affordability. In this work, it was observed that a mesh size equal to the pipe diameter provided acceptable results. It was also observed that a homogenous cell size in the jet region for x-, y- and z-directions is preferred over gradually increasing size mesh. For the density interface, the grid lines in the x- and y-direction were sparser than in the jet volume; however, the cell size in the z-direction was kept unchanged with values of 0.075 m. The results are satisfactory leading to the conclusion that in the upper stratified part of the vessel the resolution in the vertical z-direction needs to be refined; whereas the grid lines in the other directions can be kept coarser.

4.3.2 Turbulence models

The turbulence models that were analysed include the STD k-ε, the ML, the RG k-ε, the NL2 k-ε and combination of the STD k-ε and the ML. The ML model is an algebraic model which requires a user-defined value for the mixing length, which will be treated as a constant value during the transient. For ST1-7 test, too small mixing length resulted in an over-prediction of the helium erosion, whereas too large mixing length under-predicted it. Also, the mixing length needs to be adjusted to different conditions that exist inside the vessel. Consequently if the ML model is to be used, subdivided model is necessary to capture these specific conditions. For ST1-7 the subdivision was relatively successful and produced good results. For PANDA Benchmark, the mixing lengths that could fully capture the existing condition in that range were not found, leading to the conclusion that the middle part and the upper part of the vessel should be divided into smaller parts. With the current model, the helium erosion is either under- or over-predicted at different levels. To set mixing length in the jet volume equation () was used. For the rest of the control volumes an engineering judgement was used. The values for $l_{mix}$ for the two models which gave most accurate results for ST1-7 and PANDA Benchmark tests are summarized in Table 10.

Table 10: Values for the mixing-length which gave most accurate results for ST1-7 and PANDA Benchmark test.

<table>
<thead>
<tr>
<th>Model</th>
<th>$l_{mix}$ in the jet volume</th>
<th>$l_{mix}$ in the vessel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model 1i (ST1-7)</td>
<td>0.0312 m</td>
<td>D/6 m</td>
</tr>
<tr>
<td>Model 3d (PANDA Benchmark)</td>
<td>D=0.075 m</td>
<td>D/6 m</td>
</tr>
</tbody>
</table>

For Model 1i, the distance x in equation () was set to 2 m which gave $l_{mix}$ equal to 0.0312 and provided accurate results. However, when similar value for $l_{mix}$ in the jet volume was used for PANDA Benchmark (Model 3c) the helium erosion became strongly over-predicted suggesting a need for a higher value. This was then modified and the new $l_{mix}$ was set to the same size as the jet nozzle. When examining the conditions for the jet exit for ST1-7 and PANDA Benchmark, which are presented in Table 1 and Table 5, it is noticed that this coincidences with the velocity
magnitude and Reynolds number which are also approximately twice the size of PANDA Benchmark compared to ST1-7. This observation suggests that the choice of $l_{mix}$ should not only depend on the jet spreading, which equation (1) is based on, but also take into account the Reynolds number at the jet exit, which depends on the jet exit velocity. It is assumed that $l_{mix}$ depends on the magnitude of the turbulence and can be determined based on the Reynolds number. In this case $l_{mix}$ is the product of Reynolds number and a constant, $\beta$, which depends on the type of flow:

$$l_{mix} = Re \cdot \beta$$  \hspace{1cm} (34)

Based on the results of ST1-7 and PANDA Benchmark the constant $\beta$ is roughly $2.8 \cdot 10^{-6}$ m. Certainly, more tests and simulations are needed to confirm this approximation. In the remaining domains $l_{mix}$ is estimated based on the law of wall and equation (15) which was also suggested in previous experiments [6].

All the two-equation turbulence models delivered similar results; thus, since the RG k-\(\varepsilon\) and the NL2 k-\(\varepsilon\) models required higher computational costs and longer simulation time, they are not recommended. The STD k-\(\varepsilon\) model has shown to work satisfactory; however, its performance is very dependent on the mesh. The larger the mesh, the larger oscillations can be observed in the results. This trend occurred for Model 2 and Model 4 which were used in ST1-7 test and PANDA Benchmark respectively. It should be pointed out that both models consisted of more than 40000 cells. For the subdivided models which consisted of ~20000 cells this trend did not occur. A probable reason for the appearance of the oscillations is the effect of the model used for the transition from turbulent to laminar conditions; something which has been observed to be a problem in most of the high-Reynolds turbulence models. In GOTHIC, this transition is determined by the local (cell) Reynolds number; thus, finer cell size can induce more sudden variations at a certain cell which will trigger the laminar/turbulent transition model and lead to a instability of the solution. Despite this oscillations, the STD k-\(\varepsilon\) model was observed to provide good results in the Helium volume fractions and velocity fields; thus, it is recommended to be used as it relatively general model and can be applied for different types of engineering flows without any user-defined parameters.

Even though the STD k-\(\varepsilon\) and the ML can individually deliver reasonable results, more research is necessary in order to understand better the combination of these two. It was observed that when the STD k-\(\varepsilon\) and the ML is applied on the same model the jet profile is not vertical and tends to skew towards one of the walls of the vessel, leading to extremely low vertical velocities. Still, the helium data shows that the erosion occurs and the results are surprisingly accurate. Further understanding of how GOTHIC deals with the combination of the turbulence models is necessary before the model can be recommend.
4.3.3 Low momentum vertical jet

In the early models the jet pipe was not modelled as it was assumed that it was not needed. However the addition of the vertical pipe improved the results by stabilising the system and suppressing some of the oscillations. In the “free and open spaces” the kinetic turbulent energy oscillates; however, inside more restricted volumes such as pipes, it has a more stable value. This behaviour was observed especially for the subdivided model where the pipe had bigger effect than for the integrated model. It is possible though that this is related to the resolution of the model as the integrated model was twice the size of the subdivided model. Furthermore it can be speculated that the changes in the local Reynold number were dominating for the large models why modelling a pipe had such small effects.

Analysing the jet profile most of the turbulence models could predict it correctly. For the STD k-ε turbulence model the jet velocity depended on the chosen resolution why relatively large variation was observed for different models. This fact emphasises the importance of the correct nodalization for the models. As the ML model is user dependent, the velocities and the jet profile will also depend on the values of the mixing length chosen by the user: for example, the larger mixing length, the wider jet profile is obtained. The combination of the STD k-ε and the ML results in flat velocity profile which was shown for PANDA Benchmark.

5 Conclusions

GOTHIC was found to be reliable when dealing with stratification and mixing phenomena in a containment. However, it is crucial to follow some modelling standards and guidelines in order to obtain reliable results. In ST1-7 and PANDA Benchmark simulations the helium rich layer is eroded by a vertical low momentum jet and the injection of air or air/helium. The conducted simulations show good agreement with the experimental data. In this chapter, conclusions considering the adequate mesh, the preferable turbulence model, the jet, and the overall design will be presented in form of modelling guidelines.

5.1 The guidelines

For simulations involving erosion of a helium rich layer by a low-momentum vertical jet following steps are recommended based on the performed analysis in this work:

- Calculate Reynolds number at the jet nozzle exit to determine the magnitude of turbulence.
• Identify domains in which large velocity, temperature and density gradients are expected such as jet volume and density interface regions.
• Determine the spreading of the jet in order to choose the size of the control volume and fully capture the jet profile.
• The cell size in the jet volume should be homogenous in the x-, y- and z-direction. Also the cells size should not exceed the size of the jet nozzle.
• Keep fine mesh in the z-direction at the density interface with a minimum size equal the jet diameter. The remaining grid lines in the x- and y-direction can be sparser.
• Keep the mesh in the remaining domains relatively sparse to minimize computational costs.
• For stability improvement model the injection pipe inside the jet volume.
• For the choice of turbulence model following is recommended:
  • The STD k-ε turbulence model is preferable as it predicts accurately the erosion of helium and jet velocities.
  • If the ML turbulence model should be used, use equation (34) to calculate \( l_{mix} \) in the jet volume.
  • Lastly use the combination of the STD k-ε model in the jet volume and the ML model in the remaining parts of the vessel. However, further investigation of this method with respect to the prediction of the velocity field of the jet is necessary.

5.2 Outlook

For future studies it is recommended to focus on the jet conditions and turbulence models. The location of the jet inside the vessel as well as the pipe exit diameter have interesting effects on the nodalization and subdivision of the model which in turn affects the results and performance of turbulence model. For this thesis the Froude number at the density interface was similar for both cases, however it would be interesting to see how higher Froude numbers affect the helium erosion, jet velocity field and the performance of the turbulence models. It is believed that through this manner more understanding could be obtained concerning the choice of the mixing lengths if the ML model was of interest. It would be preferable to find a relation between the mixing length in the jet region and the corresponding Froude number to simplify the determination of the mixing lengths parameters. Moreover the relation found between Reynolds number and \( l_{mix} \) needs further validation and more tests are needed to determine whether this is a proper method for the choice of \( l_{mix} \). Since the ML turbulence model is an approximative model it would also be interesting to test its performance in other types of flows and situations when other complex phenomena appears such as condensation. Also more consideration should be given to the nodalization. Tests with smaller or bigger injection pipes should be conducted to see if the adequate mesh depends on the jet diameter.
Bibliography


Pisa, 2013.


