CFD Study of Gas Dispersion and Jet Fires in Complex Geometries

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Abstract

An implementation and validation of a gas dispersion model and a radiation model in the Computational Fluid Dynamics (CFD) code EXSIM (Sæter 1998, Hjertager et al. 1992) have been performed. The extended code is named FLEXSIM (Fire Leak Explosion Simulator). The computational simulations have been performed with different wind speeds, geometries, gas types, release directions, leak rates, and discharge orifices. Results have been validated against experimental findings.

A computational study of air changes and jet leaks, using a buoyant neutral gas, in highly confined and congested geometries has been performed. The results have been compared to large scale experimental findings (Savvides et al. 1999, BG Technology & Shell Global Solutions April 1999). The pre-release ventilation rates are in good quantitative agreement with experiments and well within the criteria for acceptable performance.

The predicted flammable gas volumes show an acceptable quantitative agreement with the majority of the measurements within a factor of two. The flammable gas volumes inside the module are in general over predicted but show an acceptable overall quantitative statistical performance. Two simulations with decaying release rate have been simulated and show good agreement with experimental findings.

A series of buoyant gas releases have been simulated and compared to experimental findings (Roberts et al. 2006, Shell Global Solutions 2003). The releases were performed with methane and hydrogen. The methane releases were over predicted and the hydrogen releases were under predicted. The predicted results are in the high end of acceptable performance.

A numerical study of open field dense gas dispersion has been per-
formed. The predicted transient development compares quantitatively well with experimental results (Hall 1997, McQuaid & Roebuck 1985) and (Sklavouuos & Rigas 2004).

The Composite Radiosity Gap radiation model has been implemented in EXSIM. The predicted heat fluxes obtained from horizontally released natural gas jet fires have been compared to experimental findings reported by Johnson et al. (1994). The radiation levels are slightly under predicted but compares qualitatively well with measurements.
Synopsis

Denne afhandling omhandler implementering og validering af en gas spredningsmodel og en termisk strålingsmodel i EXSIM. EXSIM er en Computational Fluid Dynamics (CFD) kode, der nu omtales som FLEXSIM (Fire Leak Explosion Simulator). Computersimuleringer er blevet udført med forskellige vindhastigheder, geometrier, gassammensætninger, udslingsretninger, masserater, og lækagehuller. Resultaterne er blevet valideret mod eksperimentelle værdier.

Et numerisk studie af luftudskiftninger og gasvolumener som følge af jetlækager med neutral opdrift i et fuldskala offshore procesmodul, er udført. Resultaterne er blevet valideret mod eksperimentelle værdier (Savvides et al. 1999, BG Technology & Shell Global Solutions April 1999). Der er god kvantitativ oversættelse mellem de målte og de prædikerede værdier for luftudskiftning. Størstedelen er indenfor accept kriterierne for acceptabel ydelse.

Der er kvantitativ acceptabel oversættelse mellem de beregnede og eksperimentelle gasvolumener hvoraf majoriteten af beregningerne er indenfor en faktor 2. De brændbare gasvolumener i modulet er generelt overprædikerede, men de er statistisk kvantitativt acceptabel. Der er udført to simuleringer med aftagende masserater. Der er for disse beregninger god oversættelse mellem eksperimentelle resultater.

Der er udført simuleringer af gasudslip med metan og brint. Resultaterne er blevet valideret mod eksperimentelle værdier for volumetrisk gaskoncentration (Roberts et al. 2006, Shell Global Solutions 2003). Metanudslippet er overestimeret mens brintudslippene er overestimeret. Simuleringerne er i den høje ende af accept kriterierne.

Gaspredning på åben mark er udført. Der blev benyttet gas med højere molvægt end luft. Der er god kvalitativ oversættelse mellem simulerede
og målte værdier, (Hall 1997, McQuaid & Roebuck 1985) og (Sklavonuos & Rigas 2004), af den transiente udvikling af volumenkoncentrationer.

Strålingsmodellen 'The Composite Radiosity Gap' er blevet implementeret i EXSIM. Beregnede strålingsfluxer fra horisontale jetbrande med naturgas er blevet valideret med eksperimentelle værdier Johnson et al. (1994). Strålingsniveauet er noget underestimeret, men der er kvalitativ god overensstemmelse mellem de beregnede og eksperimentelle resultater.
Acknowledgements

This work has been carried out at the Chemical Engineering Laboratory, Aalborg University Esbjerg, Denmark.

Foremost, I would like to thank my supervisors Professor Tron Solberg and Bjørn Helge Hjertager for their patience and encouragement during my studies.

I would like to thank my colleagues during my stay in Esbjerg; Kim Granly Hansen, Stefano Bove, Rolf Hansen, Jesper Madsen, Claus H. Ibsen, Niels Deen, and Peter Naamansen. I would also like to thank Dr. Simon Chynoweth at Shell Global Solutions for providing experimental data. It has been a great help in the validation of my work. EXSIM Consultants AS is thanked for making the EXSIM code available for the Ph.d. project.

I want to acknowledge Otto Mønsted Fond for their financial support to my conference expenses.

Finally, a gigantic hug to my wife Lene for her love, patience and understanding during my long hours, and to Synne and Endre for their everyday laughter.
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<th>Definition</th>
<th>Unit</th>
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<tr>
<td>a</td>
<td>Absorption coefficient</td>
<td>[m²]</td>
</tr>
<tr>
<td>A</td>
<td>Area</td>
<td>[m²]</td>
</tr>
<tr>
<td>A_x</td>
<td>Area of control volume</td>
<td>[m²]</td>
</tr>
<tr>
<td>A_s</td>
<td>Area of a control volume occupied by an obstacle</td>
<td>[m²]</td>
</tr>
<tr>
<td>c</td>
<td>Sound of speed</td>
<td>[m/s]</td>
</tr>
<tr>
<td>d</td>
<td>Diameter</td>
<td>[m]</td>
</tr>
<tr>
<td>D</td>
<td>Gap</td>
<td>[m]</td>
</tr>
<tr>
<td>e_b</td>
<td>Black body emissivity</td>
<td>[-]</td>
</tr>
<tr>
<td>f</td>
<td>Mixture fraction</td>
<td>[-]</td>
</tr>
<tr>
<td>g_i</td>
<td>Gravitational acceleration in the i-th direction</td>
<td>[ms⁻²]</td>
</tr>
<tr>
<td>G</td>
<td>Turbulent production term</td>
<td>[kg(ms³)]</td>
</tr>
<tr>
<td>G_i</td>
<td>Incident radiation</td>
<td>[W/m²]</td>
</tr>
<tr>
<td>h</td>
<td>Enthalpy</td>
<td>[J/kg]</td>
</tr>
<tr>
<td>h</td>
<td>Heat transfer coefficient</td>
<td>[W/m²K]</td>
</tr>
<tr>
<td>i</td>
<td>Radiative intensity</td>
<td>[W/m²]</td>
</tr>
<tr>
<td>J_h,j</td>
<td>Enthalpy flux</td>
<td>[kg/s³]</td>
</tr>
<tr>
<td>J_i,j</td>
<td>Mass diffusive flux of species Y_j</td>
<td>[kg species/m²s]</td>
</tr>
<tr>
<td>k</td>
<td>Turbulent kinetic energy</td>
<td>[m²/s²]</td>
</tr>
<tr>
<td>k'</td>
<td>Extinction coefficient</td>
<td>[1/m]</td>
</tr>
<tr>
<td>L</td>
<td>Length</td>
<td>[m³]</td>
</tr>
<tr>
<td>M</td>
<td>Mach number</td>
<td>[-]</td>
</tr>
<tr>
<td>Y_fu</td>
<td>Mass fraction of fuel</td>
<td>[kg fuel/kg]</td>
</tr>
<tr>
<td>Y_O2</td>
<td>Mass fraction of oxygen</td>
<td>[kg oxygen/kg]</td>
</tr>
<tr>
<td>Y_pr</td>
<td>Mass fraction of product</td>
<td>[kg product/kg]</td>
</tr>
<tr>
<td>p</td>
<td>Pressure</td>
<td>[Pa]</td>
</tr>
<tr>
<td>q</td>
<td>Radiative heat flux</td>
<td>[W/m²]</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>--------</td>
<td>------------------------------------------------------------</td>
<td>----------------</td>
</tr>
<tr>
<td>R</td>
<td>Radiosity</td>
<td>W/m²</td>
</tr>
<tr>
<td>R_i</td>
<td>Additional flow resistance</td>
<td>kg/(m²s²)</td>
</tr>
<tr>
<td>R_j</td>
<td>Rate of production or consumption of species</td>
<td>kg species/(m³s)</td>
</tr>
<tr>
<td>R_fu</td>
<td>Combustion rate</td>
<td>kg fuel/(m³s)</td>
</tr>
<tr>
<td>s</td>
<td>Stoichiometric oxidant/fuel ratio</td>
<td>[-]</td>
</tr>
<tr>
<td>S_φ</td>
<td>Source term for conserved variable</td>
<td>kg/(m³s)</td>
</tr>
<tr>
<td>S</td>
<td>Distance (radiation)</td>
<td>m</td>
</tr>
<tr>
<td>t</td>
<td>Time</td>
<td>s</td>
</tr>
<tr>
<td>T</td>
<td>Temperature</td>
<td>K</td>
</tr>
<tr>
<td>U_i</td>
<td>Velocity in the i-th direction</td>
<td>m/s</td>
</tr>
<tr>
<td>U_w</td>
<td>Averaged velocity, wind profile</td>
<td>m/s</td>
</tr>
<tr>
<td>V</td>
<td>Volume</td>
<td>m³</td>
</tr>
<tr>
<td>V_f</td>
<td>Volume available for fluid flow</td>
<td>m³</td>
</tr>
<tr>
<td>V_s</td>
<td>Volume occupied by an obstacle</td>
<td>m³</td>
</tr>
<tr>
<td>Y_j</td>
<td>Mass fraction of a species i</td>
<td>kg species/kg</td>
</tr>
<tr>
<td>x_i</td>
<td>Spatial coordinate in the i-th direction</td>
<td>m</td>
</tr>
<tr>
<td>z_0</td>
<td>Roughness length</td>
<td>m</td>
</tr>
</tbody>
</table>

**Greek symbols**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>β_i</td>
<td>Area porosity</td>
<td>[-]</td>
</tr>
<tr>
<td>β_v</td>
<td>Area porosity</td>
<td>[-]</td>
</tr>
<tr>
<td>Γ_φ</td>
<td>Diffusion coefficient for conserved variable</td>
<td>kg/(m s)</td>
</tr>
<tr>
<td>τ_ij</td>
<td>Turbulent flux momentum</td>
<td>kg/(m s²)</td>
</tr>
<tr>
<td>τ_mix</td>
<td>Local mixing time</td>
<td>s</td>
</tr>
<tr>
<td>τ_crit</td>
<td>Critical extinction time</td>
<td>s</td>
</tr>
<tr>
<td>δ_ij</td>
<td>Kronecker delta</td>
<td>[-]</td>
</tr>
<tr>
<td>ε</td>
<td>Turbulent dissipation rate</td>
<td>m²/s³</td>
</tr>
<tr>
<td>ε_w</td>
<td>Wall emmisivity</td>
<td>[-]</td>
</tr>
<tr>
<td>λ</td>
<td>Volumetric expansion coefficient</td>
<td>K⁻¹</td>
</tr>
<tr>
<td>ν</td>
<td>Kinematic viscosity</td>
<td>m²/s</td>
</tr>
<tr>
<td>μ</td>
<td>Viscosity</td>
<td>kg/ms</td>
</tr>
<tr>
<td>ρ</td>
<td>Density</td>
<td>kg/m³</td>
</tr>
<tr>
<td>φ</td>
<td>Conserved variable</td>
<td>[-]</td>
</tr>
<tr>
<td>σ_s</td>
<td>Scattering coefficient</td>
<td>1/m</td>
</tr>
</tbody>
</table>
Greek symbols continued

$\sigma_b$  Stefan-Boltzmann constant  [Wm$^{-2}$K$^{-4}$]

$\omega$  Angle

Subscripts

$\lambda$  Wave length

eff  effective

lam  laminar

turb  turbulent

Abbreviations

CFD  Computational Fluid Dynamics

CRG  Composite Radiosity Model

HVAC  Heating, Ventilation and Air Conditioning

PDA  Porosity Distributed Resistance

RTE  Radiative Transport Equation

SIMPLE  Semi-Implicit Method for Pressure-Linked Equations

TDMA  Tri-Diagonal Matrix Algorithm (Thomas Algorithm)
Chapter 1

Introduction

With activity involving petroleum components there is always a risk for a gas or oil leakage, which creates a risk for these to be ignited causing fire, smoke, and in worst case an explosion. These elements can have severe consequences as demonstrated by the Piper Alpha accident (UKOOA 2004).

A gas leak can be ignited immediately or build up to an explosive gas cloud. An immediate ignition of a gas leak, causing a fire, can result in structural damages due to heat effects and reduced visibility due to smoke generation. Other consequences are BLEVE’s (Boiling Liquid Expanding Vapor Explosion) and ignition of gas clouds from other leaks. An ignited gas cloud is likely to explode causing fatal damage to structures and to personnel. Prediction of gas dispersion, fires, heat loads and smoke concentrations is therefore of great importance in order to optimize the design of detection and protection systems providing a safer working environment.

In the following sections it will be given an introduction to the most essential features characterizing gas dispersion, liftoff, combustion process, soot, as well as radiation. For all of these phenomenas their respective properties can be described using one of the following generic models:

- Empirical
- Phenomenological
- Field (Computational Fluid Dynamics, CFD)
- Physical
Empirical models are often very simple and derived from experimental data or simplifications of physics found in more complex models such as phenomenological and CFD types. Empirical models are easy to use and provides a quick first estimate, but their validity are often limited to the range of data they have been derived from. Phenomenological models offers a higher degree of details compared to empirical ones and often consists of sub-models. Phenomenological models are often limited to a specific type of problems and have, as empirical models, a limited range of validity. Field models solve fundamental fluid flow equations and are a general purpose technique. Additional properties such as turbulence, combustion, and detailed kinetics can be implemented. However, field models are computational demanding and are to be used for detailed analysis and calculations in confined geometry. Finally, a physical model represents a scaled or full-scale representations of the object of interest e.g. a scaled offshore platform in a wind tunnel. It provides a detailed understanding of flow fields and fluctuations, but can be expensive and time consuming to build and run, as well as difficult to scale-up to full scale.

1.1 Gas dispersion

In case of a gas release the worst-case explosion scenario, that the entire offshore module is filled with a stoichiometric or a slightly rich mixture of air and flammable gas, is often too conservative. A realistic scenario, however, requires a gas dispersion analysis that accurately can describe the interactions between the gas release, the wind field and the complex, highly congested and partially confined geometry defined by e.g. on- and offshore installations.

The physics of a gas leak and a gas cloud build-up depends on a number of parameters such as wind speed and direction, release orientation, flow rate, reservoir pressure, molecular weight, hole size, and location. In congested areas the flow is significantly affected by the presence of turbulence generating obstructions.

There are several methods with different complexity available to calculated gas dispersion both in 2- and 3-dimensions. These varies from less complex models, such as empirical and phenomenological models, to more advanced models using CFD (Hanna et al. 2004, Chynoweth 2001, Health & Safety Executive 1996). The less complex models have the
benefit of providing a rather easy implementation but less detail. They are computationally more time efficient compared to CFD models that are more computational demanding. However, in congested and partially confined geometry, the less complex models are not as accurate as CFD models so there is a trade off between accuracy and computational time citeChynoweth:2001.

In the 1970's several experimental programs regarding heavy gas dispersion were initiated. They ranged from full scale open field experiments with and without obstacles, to experiments performed in wind tunnels and laboratories. The objective was to create a database in order to validate mathematical models for predicting gas dispersion in open terrain and in industrial areas and process plants. An extensive review of research programs are given in McQuaid & Roebuck (1985). Also, a comprehensive dataset of laboratory and field experiments are listed and available trough the Comprehensive Atmospheric Modeling Program, CAMP, at George Mason University (CAMP Research Group 2005).

The dispersion experiments cited by McQuaid & Roebuck (1985) and CAMP Research Group (2005), are related to dispersions of dense gas into open terrain with a limited amount of obstacles.

In 1998, the Joint Industry Project, JIP, performed a series of neutrally buoyant gas releases in a full scale offshore module, at Spadeadam in Cumbria, England. Discharge pressures, orifices, and directions were varied together with the confinement of the module (Savvides et al. 1999). The ambient weather conditions were logged as well as the ventilation rate and gas concentration within the module. These experiments resulted in an extensive database related to sonic jet releases of neutral gas inside installations related to petrochemical industry.

### 1.2 Flame liftoff

If a high pressure sonic jet release is ignited the flame base will be established at a distance downstream the discharge point known as the liftoff distance. Increasing the flow rate will move the flame base further downstream the release exit, eventually extinguish the flame when the blowout criteria is exceeded. The flame is referred to as turbulent non-premixed, or diffusion, flame.
Over the years a significant amount of research has been performed trying to understand the mechanisms controlling liftoff and blowout. No conclusive results have been presented although three main theories exist. The first is based on the work of Vanquickenborne & Van Tiggelen (1966), and is regarded as one of the earliest contributions in the understanding of the liftoff phenomena. They argued that at the base of a lifted flame the fuel and oxidizer are fully premixed. The stabilization of the flame base would occur at a distance downstream of the discharge point where the average flow velocity is equal to the turbulent burning velocity of a premixed flame. Kalghatgi (1984) utilized the theory of Vanquickenborne & Van Tiggelen (1966) to analyze the experiments of jet diffusion flames using hydrogen, propane, methane, and ethylene. Kalghatgi (1984) proposed that the liftoff distance was independent of the burner diameter and linearly increasing with increasing exit velocity. He found that the base of the flame was established where the ratio of the turbulent burning velocity and laminar burning velocity was equal to the square root of the local turbulent Reynolds number. Byggstøyl & Magnussen (1978) described liftoff and blowout criterias based on the Eddy Dissipation Concept (Magnussen 1981) and on the premixed combustion theory. They concluded that the lifted flame base would be established where the fine structure mixing time scale is close to the chemical time scale.

The second model was proposed by Peters & Williams (1983). They questioned the theory presented by Vanquickenborne & Van Tiggelen (1966) arguing that there would not be sufficient time for molecular mixing between fuel and air to occur in the period between the release exit and the flame base. Peters & Williams (1983) suggested an approach using the concept of laminar diffusion flamelets where the liftoff distance is determined by the quenching of the flamelets due to the strain rate exceeding a critical quenching value as reported by Liñán (1979). Peters (1984) presented the possibility of a partially premixed flamelets model utilizing mechanisms from both premixed flame theory and the flamelet approach.

In the third approach, Broadwell et al. (1984) proposed that the criteria for flame extinction is related to large-scale turbulent structures. Hot combustion products are believed to re-entrain the jet and ignite the unburned fuel-air mixture. When the products are mixed faster than
a critical time required for ignition the flames are extinguished and a liftoff distance is established.

In the paper of Pitts (1989) all of the theories above have been reviewed. Pitts (1989) concludes that although the theories show good agreement with experiments, none of them can be regarded as universal and valid for predicting liftoff in all situations. Pitts (1989) proposed a new model for predicting the liftoff supporting the stabilizations mechanism proposed by Broadwell et al. (1984) and suggesting that the small-scale turbulent structures are of less importance.

More recently triple flames have been introduced as the stabilization mechanism (Muñiz & Mungal 1997, Peters 2000). The triple flame is described as a diffusion flame surrounded by two premixed flames, one fuel-rich and one fuel-lean. In the thesis of Watson (2002) a thorough review have been given regarding triple flame and leading-edge structures together with experimental results obtained using laser based techniques such as particle image velocimetry, planar laser-induced fluorescence, and Rayleigh scattering, supporting the theory of triple flames.

1.3 Combustion and radiation

Within fire safety engineering, computer analysis of combustion processes, reaction kinetics, soot formation, thermal radiation from e.g. flares and large scale accidental high-pressure jet fires are of great importance. Output from fire simulations helps understanding smoke generation and visibility, and heat loads on process equipment and structure. Results obtained from such analysis will be dimensional within the design phase of HVAC and exhaust systems, escape routes, and the extend and need of active and passive fire protection as well as isolation.

The eddy dissipation model (EDM) (Magnussen & Hjertager 1976) and eddy dissipation concept (EDC) (Magnussen 1981) are widely used and accepted for both premixed and diffusion flames. The methods only solves a transport equation for the mass fraction of fuel and mixture fraction, from which the mass fractions of oxygen and product can be calculated. The reaction rate of fuel is taken as the smallest of the turbulent dissipation rates of fuel, oxygen and products. The EDM and EDC can be extended to include chemical kinetics using the Ar-
1.3. COMBUSTION AND RADIATION

Rhenius expression for the turbulent reaction rate of fuel (Versteeg & Malalasekera 1996).

Recent combustion modeling uses a laminar flamelet model. Here, the turbulent flame is assumed to consist of an ensemble of laminar flames, called flamelets. The most common approach is to assume an one-dimensional laminar strained flame, solving for the mixture fraction and scalar dissipation using Probability Density Functions (PDF). The advantage is that the chemistry can be calculated separately from the flow field and and stored in look-up tables (Yan 1999, Peters 1984, Peters 2000). The chemical kinetics involved in the combustion process can be calculated using databases such as CHEMKIN (Reaction Design 2005) and NIST (NIST 2005).

In the presence of flaring, jet fires and/or hot smoke, thermal radiation will be the dominating heat transfer mechanism. Solving the Radiative Transfer Equation (RTE) is mathematically complex since the RTE is an integro-differential equation. To make it applicable to practical engineering approaches, a number of assumptions have to be introduced before the RTE can be solved. Furthermore, the absorption, emission, and scattering coefficients have to be derived. The simplest solution is to assume these to be constant. A more accurate, but more time demanding, approach is to related them to pressure, temperature, type of gas participating, wavelengths, soot and particles. Finally, a suitable method to solve the RTE algorithm must be found (Carlsson & Karlsson 2001).

Over the last few decades numerous methods to solve the RTE have been developed and is summarized in Karlsson & Quintiere (2000), Siegel & Howell (2002) and Carcalho & Farias (1998). It is beyond the scope of this work to describe in detail all available radiation models, but a brief overview is given. Hottel’s zone model (Hottel 1954, Hottel & Cohen 1958) is mostly used within simpler geometries such as combustion chambers and is based on known data for heat transfer. Monte Carlo simulations (Howell 1968) treats the radiation statistically. It can be used for complex geometries but the results will be affected by statistical errors. The zone model and Monte Carlo method do not easily combine with flow field calculations. Flux methods such as the six-flux model proposed by De Marco & Lockwood (1975), spherical harmonics models (PN-method), (Siegel & Howell 2002), and the Dis-
crete Ordinates (DO) method (Raithby & Chui 1990) are finite volume models where the flux is solved by partial differential equations for the three coordinate directions. The Discrete Transfer Radiation Model (DTRM), (Shah 1979, Lockwood & Shah 1981), is also solved by ray tracing. All models have their advantages and disadvantages depending on participating medium and optical properties. The radiative properties such as absorption, scattering, and emission coefficients have to be accounted for. This is related to the spectral properties of the gas by using narrow band models, wide band models, and weighted sum of gray gases models, but also to the shape and distribution of particles by applying models for e.g. soot, fuel droplets, char, and ash (Carcalho & Farias 1998). The key to realistic modeling of thermal radiation is that the designer should know the advantages and disadvantages of the combustion and radiative model used in a computer analysis.

1.4 Objective

Over the years EXSIM (Sæter 1998, Hjertager et al. 1992) have been used solely for gas explosion simulations. The objective of this thesis will be to extend the capabilities of EXSIM to include the possibility to simulate wind fields, gas dispersion and jet fires. As a result a model for jet gas dispersion, flame liftoff, and radiation will be implemented in EXSIM and validated against experimental data.

Programs to visualize geometry and simulation results in general will be developed using Matlab (The MathWorks Inc. 2005).

The extended EXSIM code will be referred to as FLEXSIM; Fire, Leak, and EXplosion simulator.

1.5 Thesis overview

The thesis has been divided in five main chapters. In Chapter 2 the transport equations solved in FLEXSIM are presented. An introduction to the wind- and dispersion model is given together with theory regarding liftoff and radiation.

Theory regarding statistical analysis of model performance is given in Chapter 3. Implementation, simulations, and results regarding gas dispersion of neutral, dense, and buoyant gases are also described here.
1.5. THESIS OVERVIEW

Chapter 4 describes the implementation and validation of the radiation model, whereas conclusions and recommendations for future work are given in Chapter 5.
Chapter 2

Theoretical Formulation

2.1 Introductory remarks

FLEXSIM solves the density averaged Navier-Stokes equation for the mean turbulent flow. The governing equations are written in Cartesian coordinates using tensor notation.

2.2 Geometrical representation

On- and offshore modules consist of a large number of process equipment making the overall geometry complex and congested. Representing the geometry using CFD can be done by resolving the obstacles exactly with a high resolution, performing a detailed computation. This is very computer time and memory demanding and is with the existing computer power not feasible. Instead, using a coarser resolution, the obstacles can be solved by using a Porosity Distributed Resistance, PDR, formulation of the governing transport equations (Sæter 1998). The PDR method was first proposed by Patankar & Spalding (1974) and have been extended to include turbulence modeling (Sha & Launder 1979, Sha et al. 1982). Hjertager et al. (1992) have formulated and used the PDR methodology for simulation of gas explosions in complex three-dimensional geometries.

2.3 Volume and area porosities

The PDR formulation modifies the governing equations in two ways. Only non-blocked areas are available for fluid flow and obstacles occupying a control volume give an additional flow resistance and turbulence
2.3. VOLUME AND AREA POROSITIES

production (Sæter 1998). The volume porosity, $\beta_v$, is defined as:

$$\beta_v = 1 - \frac{V_s}{V_f + V_s} \quad (2.1)$$

where $V_f$ is the volume available for fluid flow and $V_s$ is the volume occupied by the obstacle, see Figure 2.1.

Figure 2.1: A control volume with a cylindrical obstacle inside. The gray area shows the volume occupied by the obstacle, $V_s$.

Similar, the area porosity, $\beta_x$, is illustrated in Figure 2.2 where the surface in the x-direction, $A_x$ is partially occupied by an obstacle, $A_s$. The area porosity is defined as:

$$\beta_x = 1 - \frac{A_s}{A_x + A_s} \quad (2.2)$$

where $A_x$ is the control volume area in the x-direction and $A_s$ is the area occupied by the obstacle. The definition of area porosities in the y- and z-direction is similar.
The volume and area porosities have values between zero and one, indicating completely blocked and fully open, respectively.

2.4 General transport equation and solution procedure

The conservation equations in the following sections can be considered as convection-diffusion processes where the conservation of any property $\phi$, can be expressed in a general transport equation:

$$\frac{\partial}{\partial t} (\beta_\phi \rho \phi) + \frac{\partial}{\partial x_j} (\beta_j \rho U_j \phi) = -\frac{\partial}{\partial x_i} \left( \beta_j \Gamma_\phi \frac{\partial \phi}{\partial x_i} \right) + S_\phi \quad (2.3)$$

The transient term and the convective term are on the left hand side and the diffusive term and the source term on the right hand side, respectively.

The solution of the conservation equations is obtained using the finite volume method with a structured mesh. The computational domain is
subdivided into contiguous Control Volumes, CVs, with a nodal point at the center of each control volume. All scalar properties are stored at the nodal points whereas the velocity components are stored at the control volume surfaces. The conservation equations are integrated over the control volumes both in space and time. The numerical differencing schemes are the hybrid scheme in space and the Euler implicit scheme in time. The time step is limited by the courant number.

The procedure above results in a set of algebraic equations which are solved using the tri-diagonal matrix algorithm, also known as the Thomas algorithm. To solve the coupling between the pressure, velocity, and density in the mass- and momentum conservation equations, the SIMPLE method by Patankar & Spalding (1972), modified by Hjertager (1982) to handle compressible flows, is used.

### 2.5 Mass and momentum conservation

Applying the mass conservation principle to a general control volume gives the following equation:

\[
\frac{\partial}{\partial t} (\beta_v \rho) + \frac{\partial}{\partial x_i} (\beta_i \rho U_i) = 0
\]  

(2.4)

where \( \rho \) is the density, and \( U_i \) is the velocity component in the \( x_i \) coordinate direction. The conservation of momentum can be expressed as

\[
\frac{\partial}{\partial t} (\beta_v \rho U_i) + \frac{\partial}{\partial x_j} (\beta_j \rho U_j U_i) = -\beta_v \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} (\beta_j \tau_{ij}) + \beta_v \rho g_i + R_i
\]

(2.5)

Here, \( p \) is the pressure; \( \tau_{ij} \) is the momentum flux, and \( g_i \) is the gravitational acceleration force. \( R_i \) is a subgrid model for additional resistance caused by obstacles present in the control volume. \( R_i \) is referred to as CRX in Chapter 3.
2.6 Energy and chemical species conservation equations

The first law of thermodynamics can be expressed by an overall energy balance equation:
\[
\frac{\partial}{\partial t} (\beta_v \rho h) + \frac{\partial}{\partial x_j} (\beta_j \rho U_i h) = -\frac{\partial}{\partial x_j} (\beta_j J_{h,j}) + \beta_v \frac{Dp}{Dt} + \beta_v S_h \quad (2.6)
\]
Here, \( h \) is the enthalpy and \( J_{h,j} \) is the enthalpy diffusive flux. Frictional losses inside the control volume and radiative properties are included in the source term \( S_h \).

The conservation equation for a chemical specie \( j \) is expressed by the mass fraction \( Y_j \):
\[
\frac{\partial}{\partial t} (\beta_v \rho Y_j) + \frac{\partial}{\partial x_j} (\beta_j \rho U_i Y_j) = -\frac{\partial}{\partial x_j} (\beta_j J_{j,i}) + R_j \quad (2.7)
\]
where \( J_{j,i} \) is the mass diffusive flux of species \( Y_j \) and \( R_j \) is the rate of production or consumption due to chemical reactions.

2.7 Turbulence model

The turbulence model used is the standard \( k - \epsilon \) model by Launder & Spalding (1972), where the distribution of turbulent kinetic energy \( k \), and its rate of dissipation, \( \epsilon \), is determined. The model has been modified to include the effect of buoyancy (Versteeg & Malalasekera 1996). The Reynolds stresses are modeled using an extended Boussinesq relationship:
\[
\tau_{ij} = \mu_{\text{eff}} \left[ \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right] - \frac{2}{3} \delta_{ij} \left( \rho k + \sigma_{\phi} \frac{\partial U_k}{\partial x_k} \right) \quad (2.8)
\]
where the Kroenecker delta \( \delta_{ij} = 1 \) if \( i = j \) and \( \delta_{ij} = 0 \) if \( i \neq j \). The turbulent diffusive fluxes are modeled by the gradient hypothesis:
\[
J_{\phi, j} = -\Gamma_{\phi} \frac{\partial \phi}{\partial x_i} = -\frac{\mu_{\text{eff}}}{\sigma_{\phi}} \frac{\partial \phi}{\partial x_i} \quad (2.9)
\]
Here, \( \Gamma_{\phi} \) is the effective turbulent exchange coefficient, \( \sigma_{\phi} \) is the effective Prandtl/Schmidt number, and \( \mu_{\text{eff}} \) is the effective viscosity given as the sum of the laminar and turbulent viscosity:
\[
\mu_{\text{eff}} = \mu_{\text{lam}} + \mu_{\text{turb}} \quad (2.10)
\]
The turbulent viscosity is related to $k$ and $\epsilon$ by:

$$\mu_{turb} = C_\mu \rho \frac{k^2}{\epsilon} \quad (2.11)$$

The conservation equations for $k$ and $\epsilon$ read:

$$\frac{\partial}{\partial t}(\beta_\nu \rho k) + \frac{\partial}{\partial x_j}(\beta_j \rho U_j k) = -\frac{\partial}{\partial x_j}\left(\beta_j \frac{\mu_{eff} \partial k}{\sigma_k \partial x_j}\right) + G + G_b - \beta_\nu \rho \epsilon \quad (2.12)$$

and

$$\frac{\partial}{\partial t}(\beta_\nu \rho \epsilon) + \frac{\partial}{\partial x_j}(\beta_j \rho U_j \epsilon) = -\frac{\partial}{\partial x_j}\left(\beta_j \frac{\mu_{eff} \partial \epsilon}{\sigma_\epsilon \partial x_j}\right) + C_1 \frac{\epsilon}{k} (G + C_3 \epsilon G_b)$$

$$- C_2 \beta_\nu \rho \frac{\epsilon^2}{k} \quad (2.13)$$

respectively. The constants used in the turbulence model are listed in Table 2.1.

Table 2.1: Modeling constants used in the $k - \epsilon$ model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$C_\mu$</th>
<th>$C_{1_\epsilon}$</th>
<th>$C_{2_\epsilon}$</th>
<th>$\sigma_k$</th>
<th>$\sigma_\epsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>0.09</td>
<td>1.44</td>
<td>1.79</td>
<td>1.0</td>
<td>1.30</td>
</tr>
</tbody>
</table>

The turbulent production term, $G$, is the sum of the generation rate of turbulence due to shear, $G_S$, and the internal frictional resistance, $G_R$, related to obstacles inside the control volume (Sæter 1998), expressed as:

$$G = G_S + G_R = \beta_\nu \tau_{ij} \frac{U_j}{x_i} + C_B |U_i| R_i \quad (2.14)$$

Here, $R_i$ is the flow resistance due to objects present in the control volume, whereas $C_B$ is a modeling constant calibrated against explosion experiments (Sæter 1998). In Chapter 3, $G_R$ will be referred to as CTX.

The production of turbulence due to buoyancy in Eq. 2.12 is expressed by $G_b$ as:

$$G_b = \lambda g_i \frac{\mu_t}{\sigma_T} \frac{\partial T}{\partial x_i} \quad (2.15)$$
where $g_i$ is the gravitational acceleration vector in the $i$th direction. $\lambda$ is the volumetric expansion coefficient defined by:

$$\lambda = -\frac{1}{\rho} \frac{\partial \rho}{\partial T}$$  \hspace{1cm} (2.16)

For ideal gases Eq. 2.15 can be reduced to:

$$G_b = -\frac{1}{\rho} g_i \frac{\mu_t}{\sigma_T} \frac{\partial \rho}{\partial x_i}$$  \hspace{1cm} (2.17)

In Eq. 2.13 for dissipation, $C_{3_\epsilon}$ is calculated according to:

$$C_{3_\epsilon} = \tanh \left| \frac{u}{u} \right|$$  \hspace{1cm} (2.18)

where $u$ is the flow velocity parallel to the gravitational vector and $v$ is the velocity perpendicular to the gravitational vector (Fluent Inc. 2004).

### 2.8 Combustion model

The combustion process in a jet fire is assumed to be an infinitely fast, single-step, irreversible chemical reaction expressed as:

$$1 \text{ kg fuel} + s \text{ kg oxygen} \rightarrow (1 + s) \text{ products}$$  \hspace{1cm} (2.19)

where $s$ is the stoichiometric oxygen/fuel ratio by mass. Using this simple reaction scheme results in a system where the conservation equation for only two variables have to be solved, namely the mass fraction of fuel, $Y_{fu}$:

$$\frac{\partial}{\partial t} (\beta_v \rho Y_{fu}) + \frac{\partial}{\partial x_j} (\beta_j \rho U_j Y_{fu}) = \frac{\partial}{\partial x_j} \left( \beta_j \Gamma_{fu} \frac{\partial Y_{fu}}{\partial x_j} \right) + R_{fu}$$  \hspace{1cm} (2.20)

and the mixture fraction, $f$:

$$\frac{\partial}{\partial t} (\beta_v \rho f) + \frac{\partial}{\partial x_j} (\beta_j \rho U_j f) = \frac{\partial}{\partial x_j} \left( \beta_j \Gamma_f \frac{\partial f}{\partial x_j} \right)$$  \hspace{1cm} (2.21)

For this to be valid it is assumed that the exchange coefficients are the same for all species, implying the Schmidt numbers are equal for all species (Versteeg & Malalasekera 1996). This is reasonable for turbulent flows.
2.8. COMBUSTION MODEL

The mixture fraction \( f \) is defined by a passive scalar \( \zeta \) as:

\[
f = \frac{\zeta - \zeta_{\infty}}{\zeta_0 - \zeta_{\infty}} \tag{2.22}
\]

where \( \zeta \) is a conserved combined variable of, for example, mass fraction of fuel \( Y_{fu} \) and mass fraction of oxygen \( Y_{O_2} \), expressed as

\[
\zeta = Y_{fu} - \frac{Y_{O_2}}{s} \tag{2.23}
\]

The suffix '0' in Eq. 2.22 denotes an oxygen rich reference point whereas '\( \infty \)' denotes a fuel rich reference point.

The mean reaction rate of combustion, \( R_{fu} \), is modeled according to the eddy break-up model (Versteeg & Malalasekera 1996):

\[
R_{fu} = -\rho C_R C_A \frac{\zeta}{k} Y_{\text{lim}} \tag{2.24}
\]

where \( C_R \) is the reaction rate constant and \( C_A \) is a quenching factor. The limiting mass fraction for a jet fire is defined as the minimum of the mass fraction of fuel, oxygen, and products (Magnussen & Hjertager 1976):

\[
Y_{\text{lim}} = \min \left[ Y_{fu}, \frac{Y_{O_2}}{s}, \frac{Y_{pr}}{1 + s} \right] \tag{2.25}
\]

The ignition/extinction model implemented is based on the theory that the local mixing time is less than a critical time required for ignition. The extinction is assumed to take place in the fine structures similar as proposed by Byggstøyl & Magnussen (1978):

\[
\tau_{\text{mix}} < \tau_{\text{crit,ext}} \tag{2.26}
\]

The local mixing time is defined as:

\[
\tau_{\text{mix}} = \frac{\gamma^s}{\hat{m}} = 0.41 \frac{k}{\epsilon} \left( \frac{\nu \epsilon}{k^2} \right)^{0.0833} \tag{2.27}
\]

where \( \nu \) is the kinematic viscosity:

\[
\nu = \frac{\mu}{\rho} \tag{2.28}
\]

The critical extinction time is kept constant, \( \tau_{\text{crit,ext}} = 0.009 \).
2.9 Wind field and dispersion modeling

2.9.1 Wind field

The background flow field is calculated separately for a given wind speed and direction and all relevant variables are stored e.g. velocities and turbulence. This is to obtain a stationary wind field in the calculation domain before the leak is introduced.

The inflow wind profile is assumed to have a logarithmic shape typical of atmospheric boundary layers. The averaged velocity, $\bar{U}_w$, at given a height $z$, is defined as:

$$\bar{U}_w(z) = \frac{u_r}{k} \ln \left( \frac{z}{z_0} \right)$$

Here, $u_r$ is the shear velocity and $k$ is the von Karman’s constant, with a value of 0.41 (AICHE 1999). The surface roughness length, $z_0$, depends on the surrounding terrain. Typical values for the roughness lengths are taken from AICHE (1999) and are listed in Table 2.2.

Table 2.2: Surface roughness lengths for different types of terrain.

<table>
<thead>
<tr>
<th>Terrain classification</th>
<th>Terrain description</th>
<th>Roughness length - $z_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Highly urban</td>
<td>Centers of cities with tall buildings, very hilly or mountainous area</td>
<td>3 - 10</td>
</tr>
<tr>
<td>Urban area</td>
<td>Centers of towns, villages, fairly level wooded country</td>
<td>1 - 3</td>
</tr>
<tr>
<td>Residential area</td>
<td>Areas with dense but low buildings, wooded area, industrial site without large obstacles</td>
<td>1</td>
</tr>
<tr>
<td>Large refineries</td>
<td>Distillation columns and other tall equipment pieces</td>
<td>1</td>
</tr>
<tr>
<td>Small refineries</td>
<td>Smaller equipment, over a smaller area</td>
<td>0.5</td>
</tr>
<tr>
<td>Cultivated land</td>
<td>Open area with great overgrowth, scattered houses</td>
<td>0.3</td>
</tr>
<tr>
<td>Flat land</td>
<td>Few trees, long grass, fairly level grass plains</td>
<td>0.1</td>
</tr>
</tbody>
</table>
Table 2.2: continued from previous page

<table>
<thead>
<tr>
<th>Terrain classification</th>
<th>Terrain description</th>
<th>Roughness length - $z_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Open water</td>
<td>Large expanses of water, desert flats</td>
<td>0.001</td>
</tr>
<tr>
<td>Sea</td>
<td>Calm open sea, snow covered flat, rolling land</td>
<td>0.0001</td>
</tr>
</tbody>
</table>

The wind profiles for different roughness lengths are illustrated in Figure 2.3. It is assumed that a wind speed of 3 m/s is measured 5 meters above the ground. It is seen that a small roughness length results in a more vertical/flatter wind profile than for higher values of the roughness length. The calculated wind profile is then applied to the appropriate boundaries.

![Figure 2.3: The relation between the roughness length and the shape of the wind profile applied at boundaries.](image-url)
2.9.2 Dispersion

In gas dispersion simulations using FLEXSIM, the leak source is represented as one or several control volumes. The direction of the leak is controlled by altering the area porosity of the control volume.

The gas jet leak is treated as high pressure flow through a nozzle. The gas is discharged from a high pressure reservoir into ambient atmospheric pressure and temperature conditions. In cases of a supersonic flow the dispersion model assumes two regions just outside the orifice, as illustrated in Figure 2.4. In the first region the jet is adjusting from the choked exit conditions to the ambient pressure, $P_{o,1}$. In this region the flow is supersonic and entrainment of surrounding fluid is neglected.

The second region is downstream of the normal shock. Here, the jet is adjusting to the back pressure, $P_{o,2}$, and is growing in width while being decelerated due to entrainment of surrounding fluid. Over the distance $x_2$ there is an undisturbed core of fuel where no mixing occurs (Lamkin et al. 1980).

The discharged fuel temperature and the shock area can be calculated using isentropic expansion relations from the reservoir to the upstream region, and normal shock relations over the shock. Numerical details can be found in Appendix A.

The porosity of the leak is calculated from the area of the control volume and the area of the normal shock wave. In case of subsonic flow there is no shock area and the porosity is calculated from the area of the discharge control volume and the area of the leak orifice.
2.9. WIND FIELD AND DISPERSION MODELING

Figure 2.4: Description of a supersonic jet leak and terminology.
2.10 Radiation modeling

2.10.1 Radiative Transport Equation

Thermal radiation will be the dominant heat transfer mechanism in fires and is described by the Radiative Transfer Equation, RTE. The change in radiation intensity is due to gains and losses of radiative energy by absorption, emission, and scattering. This is illustrated in Figure 2.5 where a single ray is passing a volume (Fluent Inc. 2004).

![Figure 2.5: Gains and losses to the radiative heat transfer process.](image)

The RTE is valid for all angles $\omega'$, wavelengths $\lambda$, and distances $ds$, about the $\omega$-direction, and can be written as (Siegel & Howell 2002):

\[
\frac{dI_\lambda}{ds} = -\frac{a_\lambda I_\lambda}{II} + \frac{a_\lambda I_\lambda b}{II} - \frac{\sigma_s I_\lambda}{IV} + \frac{\sigma_\lambda}{4\pi} \int_{\omega'=0}^{4\pi} I_\lambda(\omega')\Phi_\lambda(\omega, \omega')d\omega' \tag{2.30}
\]
2.10. RADIATION MODELING

The terms marked by roman letters are:

I: Change in radiative intensity

II: Loss by absorption (includes induced emission)

III: Gain by spontaneous emission

IV: Loss by scattering

V: Gain by scattering into the $\omega$ direction

By integrating Eq. 2.30 over all wavelengths and angles, and assuming that the radiative transfer occurs through an absorbing, emitting, and nonscattering medium, the RTE can be re-written as:

$$\frac{dI}{ds} = -K_R I + K_R I_b$$

(2.31)

where, $K_R$ is the extinction coefficient:

$$K_R = a + \sigma_s$$

(2.32)

If the contribution from the scattering coefficient, $\sigma_s$ is neglected, the extinction coefficient can be determined as a function of the mass fraction of fuel and products (Khalil et al. 1975):

$$a = 0.2 \cdot Y_{fu} + 0.1 \cdot Y_{pr}$$

(2.33)

In Eq. 2.31, $I_b$ is the total black body intensity defined as:

$$I_b(T) \equiv n^2 \frac{\sigma_b T^4}{\pi}$$

(2.34)

where $n$ is the refractive index which for gases is close to unity, $n \approx 1$ (Özişik 1973). $\sigma_b$ is the Stefan-Boltzmann constant ($= 5.6710^{-8}[W m^{-2}K^{-4}]$).

The RTE can then be expressed as:

$$\frac{dI}{ds} = -K_R I + K_R \frac{\sigma_b T^4}{\pi}$$

(2.35)

The influence of thermal radiation is calculated as a radiative heat flux and included as a source term in the energy conservation equation, Eq. 2.6. An expression for the heat flux is obtained by integrating the radiative intensity over all angles, $\omega'$ (Siegel & Howell 2002):

$$\frac{\partial}{\partial x_i}(q_r) = \int_{\omega'=0}^{4\pi} \frac{dI}{ds} d\omega' = -4\pi K_R (I - \frac{\sigma_b T^4}{\pi})$$

(2.36)
2.10.2 P1 approximation

In the general PN method the radiation intensity, $I$, is expressed as an expansion into an orthogonal series of spherical harmonics denoted $P$, and truncated after a selected number of terms, $N$ (Siegel & Howell 2002). By applying the P1 radiation model, the radiative intensity becomes a set of differential equations of the zeroth, $I^{(0)}$, and the first order moment, $I^{(1)}$:

\[
\frac{d(I^{(1)})}{d\kappa} + (1 - \Omega)I^{(0)} = 4\pi(1 - \Omega)I_b \\
\frac{d(I^{(0)})}{d\kappa} + 3I^{(1)} = 0
\] (2.37) (2.38)

Here, $\Omega$:

\[
\Omega \equiv \frac{\sigma_s}{K_R} = \frac{\sigma_s}{a + \sigma_s}
\] (2.39)

and

\[
1 - \Omega = \frac{a}{K_R} = \frac{a}{a + \sigma_s}
\] (2.40)

and $d\kappa = K_R ds$.

The zeroth and first order moment have the physical interpretation:

\[
I^{(0)} = G(\kappa) = \text{incident radiation}
\] (2.41)

\[
I^{(1)} = q_r(\kappa) = \text{net radiative heat flux}
\] (2.42)

Inserting the physical interpretation for the zeroth and first order moment into the differential Eqs. 2.37 and 2.38 gives:

\[
\frac{dq_r}{dx} + (1 - \Omega)G = 4\pi(1 - \Omega)I_b
\] (2.43)

\[
\frac{dG}{d\kappa} + 3q_r = 0
\] (2.44)

By differentiating Eq. 2.44 and inserting it into Eq. 2.43 the transport equation for the incident radiation, $G$, becomes:

\[
\frac{d^2G}{d\kappa^2} = 3(1 - \Omega)(G - 4\pi I_b)
\] (2.45)
Rearranging Eq. 2.45 and inserting the properties of \( I_b, d\kappa, \) and \( \Omega \) give:

\[
\frac{\partial}{\partial x_i} \left( \frac{1}{3(a + \sigma_s)} \frac{\partial G}{\partial x_i} \right) = a\left[ G - 4\sigma_b T^4 \right]
\]

\[ (2.46) \]

when the refractive index is assumed equal to unity. The radiative heat flux is found from Eq. 2.44 to be:

\[
\frac{\partial q_{ri}}{\partial x_i} = -\frac{\partial}{\partial x_i} \left( \frac{1}{3(a + \sigma_s)} \frac{\partial G}{\partial x_i} \right)
\]

\[ (2.47) \]

and can be substituted into the energy equation, Eq. 2.6, as heat source due to radiation. The radiative heat flux is obtained by solving Eq. 2.46 for the incident radiation.

**Boundary condition**

In low order PN approximations Marshak’s wall boundary conditions are widely used. The radiative heat flux on the wall is (Özişik 1973):

\[
q_{r,w} = -\frac{4\epsilon_w\sigma_b T_w^4 - (1 - \rho_w)G_w}{2(1 + \rho_w)}
\]

\[ (2.48) \]

where \( \rho_w \) is the wall reflectivity. If the wall is assumed to be a grey diffusive surface, then \( \rho_w = 1 - \epsilon_w \) and Eq. 2.48 becomes:

\[
q_{r,w} = -\frac{\epsilon_w}{2(2 - \epsilon_w)}(4\sigma_b T_w^4 - G_w)
\]

\[ (2.49) \]

2.10.3 Composite Radiosity Gap model


**The Radiosity model**

The radiosity model proposed by Spalding (2001) is very similar to the P1-method for the RTE. The radiosity \( R \), represents the average of the incoming and outgoing radiation for all directions and angles and can be expressed as:

\[
\frac{\partial}{\partial x_i} \left( \frac{4}{3(a + \sigma_s)} \frac{\partial R}{\partial x_i} \right) = 4a(R - \sigma_b T^4)
\]

\[ (2.50) \]
CHAPTER 2. THEORETICAL FORMULATION

The radiative heat flux is then related to the radiosity by:

$$\frac{\partial q_{r,i}}{\partial x_i} = - \frac{\partial}{\partial x_i} \left( \frac{4}{3(a + \sigma_s)} \frac{\partial R}{\partial x_i} \right)$$ (2.51)

The Radiosity model is accurate for optical thick media but is less valid for thin to medium cases. The CRG model (Rasmussen 2002) proposes a method, the Gap model, to overcome this problem.

The Gap model

Consider two parallel, infinite plates with different temperature $T_1$ and $T_2$. The plates are treated as black bodies and there is no absorption, emission or scattering in the medium between the plates, hence an optical thin case. The radiative heat flux normal to the plates is given as:

$$q_{r,x} = -\Delta e_b = \sigma_b(T_2^4 - T_1^4)$$ (2.52)

Rasmussen (2002) assumes that a solution for the radiosity between the plates with a distance of $dx$ can be related to the radiative heat flux as:

$$\frac{dR}{dx} = \frac{\Delta e_b}{D}$$ (2.53)

where $D$ is the gap (distance) between the two plates.

Combining Eqs. 2.52 and 2.53 gives the following expression for the radiative heat flux:

$$q_{r,x} = -D \frac{dR}{dx}$$ (2.54)

The heat flux based on radiosity for optical thick cases is:

$$q_r = -\frac{4}{3(a + \sigma_s)} \frac{dR}{dx}$$ (2.55)

Rasmussen (2002) proposes a relation between the radiative stopping distance for the optical thick cases, $1/(a + \sigma_s)$ and the geometrical stopping distance for optical thin cases, $D$. Based on the two expressions for stopping distance Rasmussen (2002) proposed a new extinction coefficient:

$$k' = (a + \sigma_s) + \frac{4}{3D}$$ (2.56)
The transport equation for the composite radiosity, Eq. 2.50, then becomes:
\[
\frac{\partial}{\partial x_i} \left( \frac{4}{3k'} \frac{\partial R}{\partial x_i} \right) = 4a(R - \sigma_b T^4) \tag{2.57}
\]
and the radiative heat flux becomes the negative of the radiosity:
\[
\frac{\partial q_{r,i}}{\partial x_i} = -\frac{\partial}{\partial x_i} \left( \frac{4}{3k'} \frac{\partial R}{\partial x_i} \right) \tag{2.58}
\]
In order to solve the transport equation for radiosity the gap, D, in the extinction coefficient has to be solved. From the IMMERSOL model of Spalding (2001) the gap, D, is calculated as:
\[
D = 2 \left[ \left( \frac{dL}{dx_i} \right)^2 + 2L \right]^{0.5} \tag{2.59}
\]
where L is defined as:
\[
\frac{\partial}{\partial x_i} \left( \frac{\partial L}{\partial x_i} \right) + 1 = 0 \tag{2.60}
\]
and can be solved as a transport equation with no transient or convective terms.

A property often referred to is the temperature related to radiosity given as:
\[
T_R = \left( \frac{R}{\sigma_b} \right)^{0.25} \tag{2.61}
\]

**Boundary Conditions**

Intuitively the wall boundary conditions for the CRG model would be the same as for the P1-approximation with the relation of \( R = G/4 \). Modifying Eq. 2.49 gives a wall heat flux:
\[
q_{r,w} = -\frac{\epsilon_w}{2(2 - \epsilon_w)} (4\sigma_b T_w^4 - 4R) = -\frac{2\epsilon_w}{(2 - \epsilon_w)} (\sigma_b T_w^4 - R) \tag{2.62}
\]
A problem is that Eq. [2.62] is only valid for optical thick cases. To make the CRG model suitable for all optical thicknesses, Rasmussen (2002) proposed two empirical equations for the radiosity at the boundary:

\[
R_w = \frac{\sigma_b T_w^4 + C_{ad} \sigma_b T_c^4}{1 + C_{ad}}
\]  

(2.63)

where:

\[
C_{ad} = \frac{\ln(aD + 1)}{\ln(2)}
\]

(2.64)

T_c is the temperature of the fluid in the computational cell adjacent to the wall boundary cell.

The heat flux on the boundary then becomes:

\[
q_{r,w} = -h_R (R_w - R)
\]

(2.65)

where the heat transfer coefficient is:

\[
h_R = -\frac{2\epsilon_w}{(2 - \epsilon_w)}
\]

(2.66)

Rasmussen (2002) suggested that if the emissivity of the walls, \(\epsilon_w\), are less than one, an additional resistance is added to the radiosity through a heat transfer coefficient:

\[
h_R = \frac{1}{\left(\frac{3k' \Delta y}{4} + \frac{1-\epsilon_w}{\epsilon_w}\right)}
\]

(2.67)
Chapter 3
Dispersion - Simulations and Validation

3.1 Statistical analysis

The performance of the dispersion model in FLEXSIM may be quantified using the statistical measures suggested by Hanna et al. (2004). For a value $\Phi$, the fractional bias (FB), the normalized mean square error (NMSE), the geometric mean bias (MG), the geometric variance (VG) and the fraction of predictions within a factor of two of observations (FAC2) are expressed as:

$$FB = \frac{(\bar{\Phi}_p - \bar{\Phi}_o)}{0.5(\bar{\Phi}_p + \bar{\Phi}_o)}$$  \hspace{1cm} (3.1)

$$NMSE = \frac{(\Phi_p - \Phi_o)^2}{\Phi_p \Phi_o}$$  \hspace{1cm} (3.2)

$$MG = exp(\ln(\Phi_p) - \ln(\Phi_o))$$  \hspace{1cm} (3.3)

$$VG = exp[(\ln(\Phi_p) - \ln(\Phi_o))^2]$$  \hspace{1cm} (3.4)

$$FAC2 = \text{fraction of data that satisfy } 0.5 \leq \frac{\Phi_p}{\Phi_o} \leq 2.0$$  \hspace{1cm} (3.5)

Here, the subscripts $o$ and $p$ denote observations and predictions, re-
3.2 Neutral gas dispersion

3.2.1 The Spadeadam experiments

In 1998 a Joint Industry Project, JIP, was carried out to study the dispersion of high-pressure gas releases in congested, partially confined geometry. The experiments were performed at British Gas’ test site at Spadeadam in Cumbria, England. The geometry represented a full-scale offshore process module with a high number of obstacles. The module was constructed to be 28 meters long, 12 meters wide and 8 meters high in x-, y-, and z-direction (east, north, and up) (Savvides et al. 1999). The module is illustrated in Figure 3.1 with the roof, walls and floor removed.

Three test series, denoted A, B and C, were performed, each with different confinements denoted C1, C2 and C3, respectively. The three confinements have been illustrated in Figure 3.2 looking down at the module. Confinement C1 had open east and west faces, whereas the north and south walls were closed. In confinement C2 the north and south walls were closed and the east and the west ends were blocked approximately 80%. In confinement C3 the west and south walls were closed whereas the north and east faces were open.
CHAPTER 3. DISPERSION - SIMULATIONS AND VALIDATION

Figure 3.1: The Spadeadam module geometry as drawn in FLEXSIM. The roof, floor and walls have been made transparent to better see the level of congestion.

Figure 3.2: Top view of the three confinements, C1, C2, and C3 used in the Spadeadam experiments.

Inside the module the ventilation rate was measured as Air Changes Per Hour, from now referred to as ACPH, (Savvides et al. 1999). The ACPH
for configuration C1 was determined from averaged values deduced from measurements registered by ten anemometers. Five were placed in a vertical cross section at the opening of the west side and five in a vertical cross section at the east opening of the module, both in the yz-plane. In configuration C2, the ACPH was deduced from ten anemometers located in a vertical cross section in the yz-plane, eight meters inside the module from the west side. Configuration C3 had five anemometers in the vertical yz-plane eight meters inside the module and another five, twenty meters inside the module from the west side (BG Technology & Shell Global Solutions April 1999).

There were 192 monitoring points, evenly distributed, measuring the gas concentration inside the module. The gas mixture released was weakly buoyant with a molecular weight of 25.6 [kg/kmol], and lower- and upper flammability limits of 5% and 15% by volume, respectively (Savvides et al. 1999). The ambient wind speeds and directions were measured approximately 20 meters upstream of the module 5 meters above the ground. Also the ambient temperature and pressure were logged prior to a gas release.

### 3.2.2 Implementation of the Spadeadam experiments

The mesh used were generated with the coordinates of the leak point as origin. The leak point control volume was assumed to be cubic with sides of 0.3 meters. The mesh was expanded with a factor of 5% from the leak point to the edges of the module, and a factor of 10% from the edges to the domain boundaries.

Test series A experiments with confinement C1 was modeled using a computational domain of 88 by 52 by 20 meters in x-, y-, and z-direction, respectively. The module was inserted in the calculation domain with the lower south-west corner of the module located at the coordinates [30,20,0] meters. The total number of control volumes in the domain was typically in the order of 216,000 [80×60×45], with the module occupying in average 36,288 [48×28×27] cells. The cases with confinement C1 simulated in FLEXSIM are summarized in Table 3.1.
Table 3.1: Details for Spadeadam experiments simulated in FLEXSIM. Test series A with confinement C1.

<table>
<thead>
<tr>
<th>Test case</th>
<th>Wind dir.*</th>
<th>Wind angle**</th>
<th>Wind speed [m/s]</th>
<th>Leak dir.***</th>
<th>Leak diam [mm]</th>
<th>Leak rate [kg/s]</th>
<th>Ambient Temp. [°C]</th>
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</table>
3.2. NEUTRAL GAS DISPERSION

* - Wind direction where the wind is flowing towards (n=north, s=south, e=east, w=west)
** - Degrees from north, counting clockwise
*** - Flow direction where the leak is discharged towards the given direction (n=north, s=south, e=east, w=west, u=upwards)

Trans. - Transient release with decaying mass flow rate

The calculation domain used for test series B with confinement C2 was 88 by 72 by 20 meters in x-, y-, and z-direction, respectively. The lower south-west corner of the module was located at the coordinates [30,30,0] meters. Steel plates were mounted on east and north ends of the module covering approximately 80% of the opening. The total number of control volumes in the domain was approximately in the order of 234,000 [80×65×45]. The module occupied in average approximately 38,400 control volumes. The cases with confinement C2 simulated in FLEXSIM are summarized in Table 3.2

Table 3.2: Details for Spadeadam experiments simulated in FLEXSIM. Test series B with confinement C2.

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<th>Test case</th>
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<th>Wind angle**</th>
<th>Wind speed [m/s]</th>
<th>Leak dir.***</th>
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<th>Leak rate [kg/s]</th>
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* - Wind direction where the wind is flowing towards (n=north, s=south, e=east, w=west)
** - Degrees from north, counting clockwise
*** - Flow direction where the leak is discharged towards the given direction (n=north, s=south, e=east, w=west, u=upwards)
Test series C experiments with confinement C3 were modeled using the same mesh properties as for test series A, but with the west and south face blocked and the north and south ends open. The cases with confinement C3 simulated in FLEXSIM are summarized in Table 3.3.

Table 3.3: Details for Spadeadam experiments simulated in FLEXSIM. Test series C with confinement C3.

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<th>Wind angle**</th>
<th>Wind speed [m/s]</th>
<th>Leak dir.***</th>
<th>Leak diam [mm]</th>
<th>Leak rate [kg/s]</th>
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<td>32</td>
<td>5.11</td>
<td>14.9</td>
</tr>
<tr>
<td>C 07</td>
<td>e</td>
<td>97.6</td>
<td>4.5</td>
<td>e</td>
<td>13</td>
<td>0.97</td>
<td>15.6</td>
</tr>
<tr>
<td>C 08</td>
<td>e</td>
<td>90.2</td>
<td>2.9</td>
<td>s</td>
<td>32</td>
<td>5.13</td>
<td>14.7</td>
</tr>
<tr>
<td>C 09</td>
<td>e</td>
<td>84.4</td>
<td>3.1</td>
<td>s</td>
<td>13</td>
<td>0.83</td>
<td>14.9</td>
</tr>
<tr>
<td>C 10</td>
<td>e</td>
<td>91.1</td>
<td>5.4</td>
<td>u</td>
<td>32</td>
<td>5.11</td>
<td>13.4</td>
</tr>
<tr>
<td>C 11</td>
<td>e</td>
<td>78.0</td>
<td>5.1</td>
<td>u</td>
<td>13</td>
<td>0.83</td>
<td>14.9</td>
</tr>
<tr>
<td>C 12</td>
<td>e</td>
<td>80.6</td>
<td>3.4</td>
<td>s</td>
<td>32</td>
<td>5.0</td>
<td>14.1</td>
</tr>
<tr>
<td>C 13</td>
<td>e</td>
<td>84.1</td>
<td>5.2</td>
<td>s</td>
<td>13</td>
<td>0.83</td>
<td>14.9</td>
</tr>
<tr>
<td>C 14</td>
<td>e</td>
<td>80.7</td>
<td>6.3</td>
<td>s</td>
<td>43</td>
<td>9.58</td>
<td>12.7</td>
</tr>
<tr>
<td>C 15</td>
<td>e</td>
<td>73.5</td>
<td>5.4</td>
<td>u</td>
<td>43</td>
<td>9.53</td>
<td>12.2</td>
</tr>
</tbody>
</table>

* - Wind direction where the wind is flowing towards (n=north, s=south, e=east, w=west)
** - Degrees from north, counting clockwise
*** - Flow direction where the leak is discharged towards the given direction (n=north, s=south, e=east, w=west, u=upwards)

For all simulations the wind fields were calculated for 300 to 500 seconds prior to the gas releases with a constant roughness parameter of $z_o = 0.0001$, producing an almost flat inlet wind profile. The ACPH was monitored in the same cross sections as the gas concentrations. The pre-
dicted ACPH was used as an indication of the stability of the velocity profile inside the module. A developed flow pattern inside the module was assumed achieved when the ACPH approached a steady state. The predicted ACPH was compared to experimental findings reported by BG Technology & Shell Global Solutions (April 1999) and Savvides et al. (1999).

All gas releases ran for 200 to 500 seconds until a steady state gas volume was achieved. The volumetric gas concentration between 5-15% and above 5% were predicted for the entire module volume and compared to the measured flammable volumes presented in the technical report of BP Amoco et al. (May 2000).

For all figures comparing ventilation rates and flammable volumes, filled markers represent results obtained with the subgrid model for drag, CRX, and turbulence production, CTX, included. Markers with no fill (white) indicate results obtained without the subgrid models included. For the figures in this section compass north is parallel with the positive y-axis. All slices have been plotted at a height of five meters above the ground unless stated otherwise.

3.2.3 General observations - confinement C1

Test cases A22 and A28 have been chosen to illustrate general trends related to wind direction, release orientation, and gas build-up. For case A22 the wind was coming from east toward west with a speed of 1.7 m/s and the leak rate was 5.68 kg/s and oriented toward west. For case A28 the wind was from west toward east with a speed of 1.6 m/s and the release rate was 5.08 kg/s directed toward west.

A general pre-release flow observation for all cases with confinement C1, was that the module configuration produced a canalized flow causing high ventilation rates. Wind directions almost perpendicular to the open faces produced a calm through flow with no recirculation areas outside the construction as can be seen in Figure 3.4 illustrating the speed- and streamlines for case A28. For wind directed with an angle toward the module, wake areas were predicted on the leeward side of the rig as illustrated in Figure 3.3 for test case A22.
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Figure 3.3: Wind speed and streamlines for case A22 five meters above the ground. The wind was directed toward west with a velocity of 1.7 m/s.

Figure 3.4: Wind speed and streamlines for case A28 five meters above the ground. The wind was in the east direction with a velocity of 1.6 m/s.
In general, releases directed cocurrent with the wind increased the ventilation rate in the module due to the high momentum of the jet leakage. For small flow rates around 1 kg/s released cocurrent with the wind, upwards or downwards, the discharged gas was well mixed and swept out of the module due to the momentum of the wind and jet. As a result, the flammable volumes inside the module were close to zero as summarized in Table 3.7. For higher release rates, the degree of filling inside the module increased. There was also a considerable amount of gas exiting the structure forming large flammable volumes outside of the module as illustrated for case A22 in Figure 3.5. Here, the predicted 5 vol.% isosurface of gas after reaching steady state have been plotted with streamlines.

Releases with a small flow rate oriented against the wind, the amount of gas exiting the module was dominated by the momentum of the wind forcing the released gas back into the module. For higher release rates, gas was exiting the module due to the high momentum of the jet leakage. Outside the rig the flow pattern of the exited gas was dominated by the orientation and momentum of the wind, as can be seen for case A28 in

Figure 3.5: Isosurface of gas cloud at 5 vol.% with stream lines five meters above the ground for case A22. The leak rate was 5.68 kg/s and the leak orientation was toward west.
Figure 3.6: Figure 3.6 also illustrates how the leak caused a recirculating flow pattern at the east face resulting in an additional airflow into the module.

The flow pattern and ventilation rate inside the module changed significantly for releases oriented against the wind. The flow pattern have been illustrated with streamlines in Figure 3.7 for case A28. The wind flowed calmly through the module and no recirculation areas were predicted. Introducing the leak changed the flow pattern significantly both on the inside and on the outside of the module, as seen in Figure 3.8 and 3.9. The momentum of the jet caused entrainment of air from the module opening downstream of the leak point. Large recirculation areas were formed both inside the module but also on the east and west side of the construction. It can also be seen how the wind forced the exited gas over the module. This would imply that on an on- or offshore installation, sections surrounding the discharge area would be subject to filling of flammable gas.

1 All slices are through the center of the leak point 5.2 meters inside the module in the xz-plane. For Figure 3.8 and 3.9 the isosurface of 5 vol.% is shown with contours. Red indicates a high gas concentration.
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Figure 3.7: Pre-release streamlines for case A28, 5.2 meters inside the module in the xz-plane.

Figure 3.8: Streamlines, isosurface at 5 vol.%, and concentration contours for case A28, 5.2 meters inside the module in the xz-plane.

Figure 3.9: Streamlines, isosurface at 5 vol.%, and concentration contours for case A28, 5.2 meters inside the module in the xz-plane.
3.2.4 Results and discussion - confinement C1

The predicted and measured ACPH’s for test series A with confinement C1, have been compared in Figure 3.10. The results have been categorized to analyze what influence the subgrid drag and turbulence models have on the prediction of the ventilation rate. The model performance, according to Chapter 3.1, has been summarized in Table 3.4. The variable $\Phi$ analysed is the ventilation rate.

Simulations performed including the subgrid models for drag and turbulence under predicted the ventilation rates. This was due to the over prediction of the resistance in the momentum equation (Eq. 2.5), and k-$\epsilon$ model (Eq. 2.14). Neglecting the submodels improved the ACPH significantly with all the predictions within a factor two of measured. As a result, the gas dispersion simulations were performed without the subgrid drag and turbulence models.
Table 3.4: Dispersion model performance comparing observed and predicted ventilation rates obtained from Spadeadam module confinement C1; test series A.

<table>
<thead>
<tr>
<th>CRX and CTX included</th>
<th>CRX and CTX not included</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max observed</td>
<td>361</td>
</tr>
<tr>
<td>Max predicted</td>
<td>182.57</td>
</tr>
<tr>
<td>Min observed</td>
<td>58</td>
</tr>
<tr>
<td>Min predicted</td>
<td>39.17</td>
</tr>
<tr>
<td>Max observed/Max predicted</td>
<td>1.98</td>
</tr>
<tr>
<td>Mean observed</td>
<td>210.97</td>
</tr>
<tr>
<td>Mean predicted</td>
<td>100.37</td>
</tr>
<tr>
<td>FB [-0.3 , 0.3]</td>
<td>-0.71</td>
</tr>
<tr>
<td>NMSE [ &lt;4 ]</td>
<td>0.67</td>
</tr>
<tr>
<td>MG [0.7 , 1.3]</td>
<td>0.48</td>
</tr>
<tr>
<td>VG [ &lt;1.6]</td>
<td>1.8</td>
</tr>
<tr>
<td>FAC2 [ &gt;0.5]</td>
<td>0.4</td>
</tr>
</tbody>
</table>

The predicted and measured volumetric gas concentrations between 5 and 15 vol.% have been compared in Figure 3.11. The results have been arranged according to the orientation of the leak relative to the wind direction. The label With indicates that the wind and leak were oriented in the same direction, whereas Against indicates that the wind and leak were directed towards each other. Leaks directed upwards or downwards were labeled Vertical, and leaks released horizontally towards north or south perpendicular to the nominal wind direction and have been labeled Across. The volumetric gas concentrations have been statistically analyzed according to Chapter 3.1 with \( \Phi \) beeing the flammable volume \([m^3]\). The results have been summarized in Table 3.5.

The analysis shows that the majority of the predicted concentrations between 5 and 15 vol.% are within a factor of two. The fractional bias, geometric mean variance, and normalized mean square error are in the high end of acceptable performance whereas the geometric mean bias is outside acceptable performance criteria.

The predicted volumetric gas concentrations above 5 vol.% have been compared to measured concentrations in Figure 3.12 with the same
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Figure 3.11: The predicted versus measured concentrations between 5 and 15 vol.% for the Spadeadam module confinement C1; test series A.

Table 3.5: Statistical performance of the observed and predicted concentrations between 5 and 15 vol.% for Spadeadam module confinement C1; test series A.

<table>
<thead>
<tr>
<th>CRX and CTX not included</th>
<th>Max observed</th>
<th>Max predicted</th>
<th>Min observed</th>
<th>Min predicted</th>
<th>Max observed / Max predicted</th>
<th>Mean observed</th>
<th>Mean predicted</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max observed</td>
<td>1631.71</td>
<td>1633</td>
<td>43.2</td>
<td>107</td>
<td>0.999</td>
<td>600.36</td>
<td>815.61</td>
</tr>
<tr>
<td>Max predicted</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Min observed</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Min predicted</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Max observed / Max predicted</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mean observed</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mean predicted</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>FB [-0.3 , 0.3]</td>
<td>0.3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NMSE [ &lt;4]</td>
<td>0.36</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MG [0.7 , 1.3]</td>
<td>1.51</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>VG [ &lt;1.6]</td>
<td>1.53</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>FAC2 [ &gt;0.5]</td>
<td>0.67</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
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categorization as for the results presented in Figure 3.11. The statistical performance have been summarized in Table 3.6.

The analysis shows that the majority of the predicted concentrations above 5 vol.% are within a factor of two but are over predicted. The statistical performance parameters exceeds acceptable performance criterias.

Volumetric gas concentrations that have been measured equal to zero have been excluded from the statistical performance measures due to the logarithmic functions in geometric mean bias and geometric variance. The measured and predicted concentrations have been listed in Table 3.7 and it can be seen that there is good agreement between the predicted and measured volumes.

Figure 3.12: The predicted versus measured concentrations above 5 vol.% for the Spadeadam module confinement C1; test series A.
Table 3.6: Statistical performance of the measured and predicted concentrations above 5 vol.% for the Spadeadam module confinement C1; test series A.

<table>
<thead>
<tr>
<th>CRX and CTX</th>
<th>CRX and CTX</th>
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<tbody>
<tr>
<td>Max observed</td>
<td>1631.71</td>
</tr>
<tr>
<td>Max predicted</td>
<td>2214</td>
</tr>
<tr>
<td>Min observed</td>
<td>43.2</td>
</tr>
<tr>
<td>Min predicted</td>
<td>108</td>
</tr>
<tr>
<td>Max observed / Max predicted</td>
<td>0.74</td>
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<tr>
<td>Mean observed</td>
<td>621.38</td>
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<tr>
<td>Mean predicted</td>
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<td>FB ([-0.3 , 0.3]]</td>
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<tr>
<td>NMSE (&lt;4]</td>
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</tr>
<tr>
<td>MG ([0.7 , 1.3]]</td>
<td>1.65</td>
</tr>
<tr>
<td>VG (&lt;1.6]</td>
<td>1.6</td>
</tr>
<tr>
<td>FAC2 (&gt;0.5]</td>
<td>0.67</td>
</tr>
</tbody>
</table>

Table 3.7: Measured and predicted volumetric concentrations, using Spadeadam module confinement C1; test series A. These results are not included in the statistical performance calculations.

<table>
<thead>
<tr>
<th>Test concentration</th>
<th>Measured concentration</th>
<th>Predicted concentration</th>
<th>Measured concentration</th>
<th>Predicted concentration</th>
</tr>
</thead>
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<tr>
<td>Test series</td>
<td>5-15 vol.%</td>
<td>5-15 vol.%</td>
<td>5-100 vol.%</td>
<td>5-100 vol.%</td>
</tr>
<tr>
<td>A 09</td>
<td>0</td>
<td>0.4</td>
<td>0</td>
<td>0.4</td>
</tr>
<tr>
<td>A 13</td>
<td>0</td>
<td>1.7</td>
<td>0</td>
<td>1.8</td>
</tr>
<tr>
<td>A 14</td>
<td>0</td>
<td>0.9</td>
<td>0</td>
<td>0.9</td>
</tr>
<tr>
<td>A 18</td>
<td>0</td>
<td>0.5</td>
<td>0</td>
<td>0.6</td>
</tr>
<tr>
<td>A 25</td>
<td>0</td>
<td>0.4</td>
<td>0</td>
<td>0.4</td>
</tr>
<tr>
<td>A 27</td>
<td>0</td>
<td>3.5</td>
<td>0</td>
<td>3.6</td>
</tr>
<tr>
<td>A 31</td>
<td>0</td>
<td>0.5</td>
<td>0</td>
<td>0.5</td>
</tr>
<tr>
<td>A 33</td>
<td>0</td>
<td>0.42</td>
<td>0</td>
<td>0.56</td>
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</table>
3.2.5 General observations - confinement C2

To illustrate flow patterns related to confinement C2; test series B, the pre-release wind speed and streamlines as well as gas build-up have been illustrated for case B07 and case B11. For case B07 the wind was coming from east toward west with a speed of 3.9 m/s and the leak rate was 5.09 kg/s and oriented upward. For case B11 the wind was from east toward west with a speed of 0.86 m/s and the release flow rate was 5.14 kg/s and directed toward west. For the figures in this section compass north is parallel with the positive y-axis and all slices have been plotted at a height of five meters above the ground.

Reducing the free flow area on the east and west faces had a significant effect on the flow pattern reducing the ventilation rate considerably compared to findings using confinement C1. On the leeward side of the module large recirculation areas were predicted, but also close to the module face on the windward side. The length of the wake zones increased for wind directions not facing the east or west face directly. The pre-release wind speed and streamlines for case B07 and B11 have been plotted in Figure 3.13 and Figure 3.14, respectively, clearly illustrating the wake zones.

All release rates equal to 0.5 kg/s for test series B, independent of leak orientation, were predicted to produce no flammable volumes. This is consistent with experimental findings and has been summarized in Table 3.11.

For flow rates of 1 kg/s, there were no flammable volumes predicted for releases oriented cocurrent with the wind directed close to perpendicular toward the east or west face. The gas volumes increased when introducing vertical leaks and with the wind directed with an angle toward the module opening.

Flow rates of 5 kg/s were filling up the rig with a flammable gas concentration, independent of leak orientation and wind- speed and direction. Figure 3.15 and Figure 3.16 show the predicted 5 vol.% isosurface of gas and streamlines after reaching steady state for case B07 and B11, respectively. It can be seen how the module was filled up with only small flammable volumes exiting the panel openings.
Figure 3.13: Wind speed and streamlines for case B07 five meters above the ground. The wind was in the east direction with a velocity of 3.9 m/s.

Figure 3.14: Wind speed and streamlines for case B11 five meters above the ground. The wind was in the west direction with a velocity of 0.86 m/s.
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Figure 3.15: Isosurface of gas cloud at 5 vol.% with stream lines at z=5 meters for case B07. The leak rate is 5.09 kg/s and the leak orientation is upwards.

Figure 3.16: Isosurface of gas cloud at 5 vol.% with stream lines at z=5 meters for case B11. The leak rate is 5.14 kg/s and the leak orientation is towards west.
To illustrate a typical pre-release flow pattern, streamlines of the wind have been plotted in Figure 3.17. It can be seen how the wind enters and exits the panel openings. There were areas of recirculation inside the module as well as on the outside. The introduction of the jet leak changed the flow pattern inside the construction as seen in Figure 3.18. The momentum of the jet dominated the internal module flow, but the momentum of the wind on the east side of the module caused gas to exit through the openings on the eastern top side. It can also be seen how this caused a higher gas concentration in the east end of the module compared to the west side. The extent of the exited gas volume was small due to the low velocity and high degree of mixing on the outside of the module.

In general the time to reach steady state, both for the ventilation rates and gas volumes, was longer than for simulations of configuration C1 due to the increased domain size and enclosed confinement used in C2.

Figure 3.17: Pre-release streamlines for case B07, 4.3 meters inside the module in the xz-plane.

\footnote{All slices are through the center of the leak point 4.3 meters inside the module in the xz-plane. In Figure 3.18 the isosurface of 5 vol.% is shown with contours. Red indicates a high gas concentration.}
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The predicted and measured ACPH’s for test series B with confinement C2 have been compared in Figure 3.19. The results have been categorized to analyze what influence the subgrid drag and turbulence models have on the prediction of the ventilation rate. The model performance, according to Chapter 3.1, has been summarized in Table 3.8. The variable Φ analyzed is the ventilation rate.

The predicted ventilation rates for confinement C2 were lower than for confinement C1 due to the increased flow resistance. The effect of the subgrid models for drag and turbulence was not so dominating as for configuration C1. The calculated ventilation rates were under predicted but neglecting the subgrid models gave some improvements. As a result, the gas dispersion simulations were performed without the subgrid drag and turbulence models.

The predicted and measured volumetric gas concentrations between 5 and 15% have been compared in Figure 3.20. The results have been arranged according to the orientation of the leak relative to the wind direction. The label With indicates that the wind and leak are oriented in the same direction. Leaks directed upwards or downwards are labeled Vertical and leaks released horizontally towards north or south perpendicular to the nominal wind direction have been labeled Across. The volumetric gas concentrations have been statistically analyzed according to Chapter 3.1 with the Φ being the flammable volume [m$^3$] and the results have been summarized in Table 3.9.
Figure 3.19: Predicted versus measured ACPH of the Spadeadam module with configuration C2; test series B, with and without subgrid drag and turbulence models.

Table 3.8: Performance measures of the predicted and measured ACPH obtained by FLEXSIM for the Spadeadam test series B.

<table>
<thead>
<tr>
<th></th>
<th>CRX and CTX included</th>
<th>CRX and CTX not included</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max observed</td>
<td>63</td>
<td>63</td>
</tr>
<tr>
<td>Max predicted</td>
<td>28.3</td>
<td>34.29</td>
</tr>
<tr>
<td>Min observed</td>
<td>12</td>
<td>12</td>
</tr>
<tr>
<td>Min predicted</td>
<td>2.66</td>
<td>3.26</td>
</tr>
<tr>
<td>Max observed / Max predicted</td>
<td>2.22</td>
<td>1.84</td>
</tr>
<tr>
<td>Mean observed</td>
<td>37.91</td>
<td>37.91</td>
</tr>
<tr>
<td>Mean predicted</td>
<td>16.47</td>
<td>19.06</td>
</tr>
<tr>
<td>FB [-0.3, 0.3]</td>
<td>-0.79</td>
<td>-0.66</td>
</tr>
<tr>
<td>NMSE [&lt;4]</td>
<td>0.96</td>
<td>0.66</td>
</tr>
<tr>
<td>MG [0.7, 1.3]</td>
<td>0.4</td>
<td>0.46</td>
</tr>
<tr>
<td>VG [&lt;1.6]</td>
<td>2.72</td>
<td>2.1</td>
</tr>
<tr>
<td>FAC2 [&gt;0.5]</td>
<td>0.37</td>
<td>0.45</td>
</tr>
</tbody>
</table>
Figure 3.20: The predicted versus measured concentrations between 5 and 15 vol.% for the Spadeadam module confinement C2; test series B.

Although the ventilation rate was under predicted the flammable volumes between 5 and 15 vol.% are qualitively in good agreement with measured concentrations. The statistical performance are well within the acceptance criterias.

The predicted volumetric gas concentrations above 5 vol.% have been compared to experimental findings reported in BP Amoco et al. (May 2000), and are illustrated in Figure 3.21 with the same categorization as for the results above. The statistical performance have been summarized in Table 3.10 and it can be seen the predicted flammable volumes are well within the criterias for acceptable performance with all volumes within a factor two of the measured.
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Table 3.9: Statistical performance of the measured and predicted concentrations between 5 and 15 vol.% for Spadeadam module confinement C2.

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>Max observed</td>
</tr>
<tr>
<td>Max predicted</td>
</tr>
<tr>
<td>Min observed</td>
</tr>
<tr>
<td>Min predicted</td>
</tr>
<tr>
<td>Max observed / Max predicted</td>
</tr>
<tr>
<td>Mean observed</td>
</tr>
<tr>
<td>Mean predicted</td>
</tr>
<tr>
<td>FB [-0.3, 0.3]</td>
</tr>
<tr>
<td>NMSE [&lt;4]</td>
</tr>
<tr>
<td>MG [0.7, 1.3]</td>
</tr>
<tr>
<td>VG [&lt;1.6]</td>
</tr>
<tr>
<td>FAC2 [&gt;0.5]</td>
</tr>
</tbody>
</table>

Figure 3.21: The predicted versus measured concentrations above 5 vol.% for the Spadeadam for Spadeadam module confinement C2; test series B.
The volumetric concentrations that have been measured equal to zero have been excluded from the statistical performance measures due to the logarithmic functions in geometric mean bias and geometric variance. Those concentrations have been listed in Table 3.11. There is good agreement between the predicted and observed flammable volumes measured equal to zero, except for case B05 where the flammable volume was significantly over predicted.

Table 3.10: Statistical performance of the measured and predicted concentrations above 5vol.% for Spadeadam module confinement C2.

<table>
<thead>
<tr>
<th>CRX and CTX</th>
<th>Max observed</th>
<th>Max predicted</th>
<th>Min observed</th>
<th>Min predicted</th>
<th>Max observed / Max predicted</th>
<th>Mean observed</th>
<th>Mean predicted</th>
<th>FB [-0.3, 0.3]</th>
<th>NMSE [&lt;4]</th>
<th>MG [0.7, 1.3]</th>
<th>VG [&lt;1.6]</th>
<th>FAC2 [&gt;0.5]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max observed</td>
<td>2389.4</td>
<td>2460</td>
<td>42.34</td>
<td>23</td>
<td>0.97</td>
<td>1582</td>
<td>1800</td>
<td>0.13</td>
<td>0.043</td>
<td>1</td>
<td>1.11</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 3.11: Measured and predicted volumetric concentrations, using Spadeadam module confinement C2; test series B. Not included in the statistical performance calculations.

<table>
<thead>
<tr>
<th>Test number</th>
<th>Measured 5-15 vol.%</th>
<th>Predicted 5-15 vol.%</th>
<th>Measured 5-100 vol.%</th>
<th>Predicted 5-100 vol.%</th>
</tr>
</thead>
<tbody>
<tr>
<td>B 04</td>
<td>0</td>
<td>0.3</td>
<td>0</td>
<td>0.3</td>
</tr>
<tr>
<td>B 05</td>
<td>0</td>
<td>145</td>
<td>0</td>
<td>147</td>
</tr>
<tr>
<td>B 14</td>
<td>0</td>
<td>0.14</td>
<td>0</td>
<td>0.17</td>
</tr>
<tr>
<td>B 16</td>
<td>0</td>
<td>1.01</td>
<td>0</td>
<td>1.07</td>
</tr>
<tr>
<td>B 19</td>
<td>0</td>
<td>1.6</td>
<td>0</td>
<td>1.6</td>
</tr>
</tbody>
</table>
3.2.7 General observations - confinement C3

Test cases C02 and C05 have been chosen to illustrate the interaction between wind speed and direction, leak direction and momentum, and how the flow pattern depends on these parameters. For both cases the wind was from west toward east with a wind speed of 4.4 m/s and 3.3 m/s for case C02 and C05, respectively. Regarding releases case C02 had a flow rate of 5.17 kg/s oriented toward the west wall. As for case C05, the mass flow rate was 9.14 kg/s directed toward east.

The nominal wind direction was toward east for all experiments with confinement C3; test series C. The flow pattern, illustrated with speed slice and streamlines, in Figure 3.22 and 3.23 are therefore general for all cases in this section. The flow field inside the module was more complex compared to findings from confinement C1 and C2. Due to the open wall configuration, wake zones were predicted on the north and east faces causing in- and outflow on the boundaries of the module. As seen from Figure 3.26 the flow direction inside the module was shifted against the nominal wind direction because of recirculation areas. This was also observed during the experiments and have been reported by BG Technology & Shell Global Solutions (April 1999) and BP Amoco et al. (May 2000).

For gas releases with confinement C3 flow rates of 1, 5, and 10 kg/s were used. Leaks of 1 kg/s directed towards west were measured and predicted to accumulate only minor gas volumes. Release orientations different from west resulted in flammable gas concentrations equal to zero, see comparison of measured and predicted flammable volumes in Table 3.15.
3.2. NEUTRAL GAS DISPERSION

Figure 3.22: Wind speed and streamlines for case C02 at z=5 meters. The wind is in the east direction with a velocity of 4.4 m/s.

Figure 3.23: Wind speed and streamlines for case C05 at z=5 meters. The wind is in the east direction with a velocity of 3.3 m/s.
Flow rates of 5 and 10 kg/s caused build-ups of flammable gas volumes, independent of release orientation. It was however observed and predicted that releases towards west were caught by the recirculation area on the north face leaving the the east side of the module empty of gas within the flammable range, see Figure 3.24. Leaks directed against east impinged on an tank installed in the middle of the module at ground floor (see Figure 3.28). This reduced the momentum of the released gas, limiting the amount of gas outside the rig as shown in 3.24.

A typical pre-release flow pattern have been illustrated in Figure 3.26. Introducing a leak changed the internal flow pattern of the module. In Figure 3.27, taken from case C02, the release increased the entrainment of air into the module from the east face and areas of recirculation were formed. It was also seen how the area upstream the leak point contained no gas. Figure 3.28 shows the release from case C05 where the discharged gas impinged on a tank located close to the release point.

Figure 3.24: Isosurface of gas cloud at 5 vol.% with stream lines at z=5 meters for case C02. The leak rate is 5.17 kg/s and the leak orientation is towards west.

---

\[\text{All slices are through the center of the leak point, 4.3 meters inside the module in the xz-plane. In Figure 3.27 and 3.28 the isosurface of 5 vol.% is shown with contours. Red indicates a high gas concentration.}\]
3.2. NEUTRAL GAS DISPERSION

Figure 3.25: Isosurface of gas cloud at 5 vol.% with stream lines at z=5 meters for case C05. The leak rate is 9.11 kg/s and the leak orientation is towards east.

Figure 3.26: Pre-release streamlines for case C02 4.3 meters inside the module in the xz-plane.
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Figure 3.27: Streamlines, isosurface at 5 vol.%, and concentration contours for case C02, 4.3 meters inside the module in the xz-plane.

Figure 3.28: Streamlines, isosurface at 5 vol.%, and concentration contours for case C05, 4.3 meters inside the module in the xz-plane.
3.2.8 Results - confinement C3

The predicted and measured ACPH’s for test series C with confinement C3 have been compared in Figure 3.29. The results have been categorized to analyze what influence the subgrid drag and turbulence models have on the prediction of the ventilation rate. The model performance, according to Chapter 3.1, has been summarized in Table 3.12. The variable Φ analyzed is the ventilation rate.

For configuration C3 the ventilation rates were under predicted when the submodels for drag and turbulence were included, whereas excluding the submodels over predicted the ACPH. In both cases the calculated ventilation rates were within a factor of two. The ACPH shows a symmetric behavior regarding over- and under prediction with respect to having the submodels for drag and turbulence included or not. The normalized mean square error and geometric mean variance are close to equal, independent of the status of the submodels. Although the analysis of the ventilation rates gave no conclusive results regarding whether to use the subgrid models for drag and turbulence or not, the gas dispersion simulations were performed without in order to be consistent with previous calculations.

The predicted and measured volumetric gas concentrations between 5 and 15% have been compared in Figure 3.30. The results have been segregated according to the orientation of the leak relative to the wind direction.
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Figure 3.29: Predicted versus measured ACPH of the Spadeadam module with confinement C3, with and without subgrid drag and turbulence models.

Table 3.12: Performance of the predicted and measured ACPH for the Spadeadam module confinement C3.

<table>
<thead>
<tr>
<th></th>
<th>CRX and CTX included</th>
<th>CRX and CTX not included</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max observed</td>
<td>36</td>
<td>36</td>
</tr>
<tr>
<td>Max predicted</td>
<td>33.1</td>
<td>44.6</td>
</tr>
<tr>
<td>Min observed</td>
<td>11</td>
<td>11</td>
</tr>
<tr>
<td>Min predicted</td>
<td>12.24</td>
<td>9.94</td>
</tr>
<tr>
<td>Max observed / Max predicted</td>
<td>1.09</td>
<td>0.81</td>
</tr>
<tr>
<td>Mean observed</td>
<td>24.93</td>
<td>24.93</td>
</tr>
<tr>
<td>Mean predicted</td>
<td>21.78</td>
<td>27.94</td>
</tr>
<tr>
<td>FB [-0.3, 0.3]</td>
<td>-0.13</td>
<td>0.11</td>
</tr>
<tr>
<td>NMSE [ &lt;4]</td>
<td>0.047</td>
<td>0.05</td>
</tr>
<tr>
<td>MG [0.7, 1.3]</td>
<td>0.88</td>
<td>1.09</td>
</tr>
<tr>
<td>VG [ &lt;1.6]</td>
<td>1.06</td>
<td>1.06</td>
</tr>
<tr>
<td>FAC2 [ &gt;0.5]</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>
The label *With* indicates that the wind and leak are oriented in the same direction, whereas *Against* indicates that the wind and leak are directed towards each other. Leaks directed upwards or downwards are labeled *Vertical*, and leaks released horizontally towards north or south perpendicular to the nominal wind direction have been labeled *Across*. The volumetric gas concentrations have been statistically analyzed according to Chapter 3.1 with the variable $\Phi$ being the flammable volume in $[\text{m}^3]$. The results have been summarized in Table 3.13.

The predicted flammable volumes between 5 and 15 vol.% are in good agreement with measurements. The statistical analysis is affected by the single outlier but the results are well within the criteria for acceptable performance.

![Figure 3.30: The predicted versus measured concentrations between 5 and 15 vol.% for the Spadeadam module confinement C3; test series C.](image)

The predicted volumetric gas concentrations above 5% have been compared to experimental findings reported in BP Amoco et al. (May 2000), and have been illustrated in Figure 3.31 with the same categorization as for the results above. The statistical performance have been summarized in Table 3.14.
Table 3.13: Statistical performance of the measured and predicted concentrations between 5 and 15 vol.% for the Spadeadam module confinement C3; test series C.

<table>
<thead>
<tr>
<th>CRX and CTX not included</th>
<th>CRX and CTX not included</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max observed</td>
<td>1646</td>
</tr>
<tr>
<td>Max predicted</td>
<td>2113</td>
</tr>
<tr>
<td>Min observed</td>
<td>32.32</td>
</tr>
<tr>
<td>Min predicted</td>
<td>8.3</td>
</tr>
<tr>
<td>Max observed / Max predicted</td>
<td>0.78</td>
</tr>
<tr>
<td>Mean observed</td>
<td>1146.99</td>
</tr>
<tr>
<td>Mean predicted</td>
<td>1351.23</td>
</tr>
<tr>
<td>FB [-0.3, 0.3]</td>
<td>0.16</td>
</tr>
<tr>
<td>NMSE [&lt;4]</td>
<td>0.18</td>
</tr>
<tr>
<td>MG [0.7, 1.3]</td>
<td>1.04</td>
</tr>
<tr>
<td>VG [&lt;1.6]</td>
<td>1.51</td>
</tr>
<tr>
<td>FAC2 [&gt;0.5]</td>
<td>0.8</td>
</tr>
</tbody>
</table>

Figure 3.31: The predicted versus measured concentrations above 5 vol.% for the Spadeadam module confinement C3; test series C.
Table 3.14: Statistical performance measures of the measured and predicted concentrations above 5 vol.% for the Spadeadam module confinement C3; test series C.

<table>
<thead>
<tr>
<th>CRX and CTX not included</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max observed</td>
</tr>
<tr>
<td>Max predicted</td>
</tr>
<tr>
<td>Min observed</td>
</tr>
<tr>
<td>Min predicted</td>
</tr>
<tr>
<td>Max observed / Max predicted</td>
</tr>
<tr>
<td>Mean observed</td>
</tr>
<tr>
<td>Mean predicted</td>
</tr>
<tr>
<td>FB [-0.3, 0.3]</td>
</tr>
<tr>
<td>NMSE [&lt;4]</td>
</tr>
<tr>
<td>MG [0.7, 1.3]</td>
</tr>
<tr>
<td>VG [&lt;1.6]</td>
</tr>
<tr>
<td>FAC2 [&gt;0.5]</td>
</tr>
</tbody>
</table>

The majority of the calculated volumes above 5 vol.% are within a factor of two. The flammable volumes are over predicted and the results exceeds the criteria for acceptable performance. This is mainly due to the single outlier.

The volumetric concentrations measured equal to zero have been excluded from the statistical performance measures due to the logarithmic functions in geometric mean bias and geometric variance. The concentrations are listed in Table 3.15. There are good agreement between the predicted and measured flammable volumes close to zero.

Table 3.15: Measured and predicted volumetric concentrations not included in the statistical performance in the Spadeadam module confinement C3; test series C.

<table>
<thead>
<tr>
<th>Test number</th>
<th>Measured 5-15 vol.%</th>
<th>Predicted 5-15 vol.%</th>
<th>Measured 5-100 vol.%</th>
<th>Predicted 5-100 vol.%</th>
</tr>
</thead>
<tbody>
<tr>
<td>C 09</td>
<td>0</td>
<td>2.68</td>
<td>0</td>
<td>2.78</td>
</tr>
<tr>
<td>C 13</td>
<td>0</td>
<td>1.4</td>
<td>0</td>
<td>1.5</td>
</tr>
<tr>
<td>C 11</td>
<td>0</td>
<td>1.4</td>
<td>0</td>
<td>1.5</td>
</tr>
</tbody>
</table>
3.2.9 Transient releases - confinement C1

The Spadeadam experiments performed two releases with a decaying discharge pressure, namely case A10 and A23. The transient mass flow rates were measured during the two test series. The geometry, mesh properties, and pre-release wind calculations have previously been described in section 3.2.2.

Test case A10 had a rapid pressure decay using a 75 mm orifice with an initial release pressure of approximately 15 bar. Test case A23 was a slow decaying release with a leak orifice of 25 mm and an initial release pressure of 60 bar (BG Technology & Shell Global Solutions April 1999). Input to the simulations were the measured mass flow rate versus time.

Due to the decaying pressure the area porosity of the leak control volume should be re-calculated every time the pressure changes. In order to see what effect the porosity, hence the effective diameter, has on the transient gas build-up, two approaches have been investigated. In the first approach the porosity was based on the initial release pressure and kept constant for the release period. The same transient case was then performed with a constant porosity based on the mean pressure taken as the arithmetic mean between the peak pressure and the ambient pressure.

Calculating the area porosity from the peak pressure the initial conservation of mass and momentum will be correct. Over time the mass flow rate will be correct but the velocity will be too small, hence the calculated momentum will be too low. Using the mean pressure to calculate the area porosity the leak velocity and momentum will be over predicted for the first half of the release. Halfway through the transient release the leak velocity and momentum will be correct, but for the remaining period they will be under predicted.

The predicted volumetric gas concentrations between 5 and 15% and above 5% for case A10 have been illustrated in Figure 3.32. Similar predictions for test case A23 have been shown in Figure 3.33.
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(a) Time history of total gas volume for concentrations between 5 and 15 vol.% inside the module

(b) Time history of total gas volume for concentrations above 5 vol.% inside the module

Figure 3.32: Time history of total gas volume for concentrations between 5 and 15 vol.% and above 5 vol.% inside the module for Spadeadam test series A10.
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(a) Time history of total gas volume for concentrations between 5 and 15 vol.% inside the module

(b) Time history of total gas volume for concentrations above 5 vol.% inside the module

Figure 3.33: Time history of total gas volume for concentrations between 5 and 15 vol.% and above 5 vol.% inside the module for Spadeadam test series A23.
In case A10 the leak impinged on the south wall reducing the momentum of the discharged gas. This can also be seen in Figure 3.32 where the difference between the two approaches is small. In case A23 the leak is directed toward the open west face and the approach using the mean pressure shows good agreement with experimental findings. It is seen in Figure 3.33 how the mean pressure approach under predicts the flammable volumes in the beginning of the transient development where the momentum is over predicted. This can be explained by the high momentum resulting in a better mixing between air and released gas. The amount of gas exiting the module will increase with a high momentum. When the momentum decreases the flammable volumes are over predicted. For the approach using the peak pressure the momentum is under predicted for the whole transient period and the volumes are therefore over predicted.

The dispersion model captures the transient development of the flammable volumes of both the slow and rapid decaying releases. Using the arithmetic mean pressure as initial condition for calculating the porosity of the leak area gives a better result than using the peak pressure. To few simulations have been performed to give a conclusive explanation to why, but there seems to be a relation between the calculated momentum, degree of mixing, and the transient gas build-up.

3.2.10 Overall Performance

In this section the overall statistical performance of the dispersion model with respect to neutral buoyant gas releases will be presented. All of the results from the Spadeadam experiments for module configurations C1, C2, and C3 with respect to ventilation rates (ACPH) and gas volumes have been analyzed. All predictions presented in this section are calculated without the subgrid model for drag and turbulence, CRX and CTX, respectively.

The predicted versus the measured ventilation rates have been plotted in Figure 3.34. The results have been organized according to their respective module confinement. The statistical performance for the ventilation rates have been summarized in Table 3.16.
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Figure 3.34: Predicted versus measured ACPH for Spadeadam experiments module C1, C2, and C3.

Table 3.16: Statistical performance of the observed versus predicted ACPH for Spadeadam experiments module C1, C2, and C3.

<table>
<thead>
<tr>
<th>CRX and CTX not included</th>
<th>Max observed</th>
<th>361</th>
</tr>
</thead>
<tbody>
<tr>
<td>CRX and CTX not included</td>
<td>Max predicted</td>
<td>364</td>
</tr>
<tr>
<td>CRX and CTX not included</td>
<td>Min observed</td>
<td>11</td>
</tr>
<tr>
<td>CRX and CTX not included</td>
<td>Min predicted</td>
<td>3.26</td>
</tr>
<tr>
<td>CRX and CTX not included</td>
<td>Max observed / Max predicted</td>
<td>0.991</td>
</tr>
<tr>
<td>CRX and CTX not included</td>
<td>Mean observed</td>
<td>129</td>
</tr>
<tr>
<td>CRX and CTX not included</td>
<td>Mean predicted</td>
<td>122.29</td>
</tr>
<tr>
<td>CRX and CTX not included</td>
<td>FB [-0.3 , 0.3]</td>
<td>-0.053</td>
</tr>
<tr>
<td>CRX and CTX not included</td>
<td>NMSE [&lt;4]</td>
<td>0.0445</td>
</tr>
<tr>
<td>CRX and CTX not included</td>
<td>MG [0.7 , 1.3]</td>
<td>0.86</td>
</tr>
<tr>
<td>CRX and CTX not included</td>
<td>VG [&lt;1.6]</td>
<td>1.2</td>
</tr>
<tr>
<td>CRX and CTX not included</td>
<td>FAC2 [&gt;0.5]</td>
<td>0.89</td>
</tr>
</tbody>
</table>
The predicted ventilation rates are in good qualitative and quantitative agreement with measurements. The statistical analysis indicates that the calculated ventilation rates are under predicted, but they are well within the criteria of acceptable performance. As seen from Figure 3.34 the main contribution to the under prediction comes from results calculated for confinement C2.

A comparison of the measured and predicted gas volumes for concentrations between 5-15 vol.% and above 5 vol.% have been shown in Figure 3.35. The results have been segregated according to their respective module confinement. The statistical performance have been summarized in Table 3.17.

Figure 3.35: The predicted versus measured gas volumes for concentrations between 5-15 vol% and above 5 vol.% for Spadeadam module confinements C1, C2, and C3.
Table 3.17: Statistical performance for predicted versus measured gas volumes between 5-15 vol% and above 5 vol.% for Spadeadam module confinements C1, C2, and C3.

<table>
<thead>
<tr>
<th></th>
<th>NO CRXCTX</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max observed</td>
<td>2389.4</td>
</tr>
<tr>
<td>Max predicted</td>
<td>2460</td>
</tr>
<tr>
<td>Min observed</td>
<td>32.32</td>
</tr>
<tr>
<td>Min predicted</td>
<td>8.3</td>
</tr>
<tr>
<td>Max observed / Max predicted</td>
<td>0.97</td>
</tr>
<tr>
<td>Mean observed</td>
<td>863</td>
</tr>
<tr>
<td>Mean predicted</td>
<td>1144</td>
</tr>
<tr>
<td>FB [-0.3 , 0.3]</td>
<td>0.28</td>
</tr>
<tr>
<td>NMSE [&lt;4]</td>
<td>0.26</td>
</tr>
<tr>
<td>MG [0.7 , 1.3]</td>
<td>1.31</td>
</tr>
<tr>
<td>VG [&lt;1.6]</td>
<td>1.50</td>
</tr>
<tr>
<td>FAC2 [&gt;0.5]</td>
<td>0.76</td>
</tr>
</tbody>
</table>

The calculated concentrations are over predicted but they show an acceptable quantitative performance. The majority of the predictions are within a factor of two but the fractional mean bias (FB) and geometrical mean bias (MG) are in the high end of acceptable performance.

There is also good agreement between the predicted and measured concentrations equal to zero as can be seen in Table 3.7, 3.11 and 3.15 for module configuration C1, C2, and C3, respectively.

The transient simulations show good agreement with the experimental findings. Using the arithmetic mean transient pressure as input to calculate the porosity of the leak point gave the best fitting with measured data.
3.3 Buoyant gas dispersion

3.3.1 The Buxton experiments

In 2002 Shell performed a series of buoyant gas dispersion and jet fire experiments using hydrogen and methane (Roberts et al. 2006, Shell Global Solutions 2003). The experiments were performed at the Blast Range at the Health and Safety Laboratory at Buxton, England. The module had a cubic shape with a volume of 1m$^3$, a solid floor, roof, and backplate, as illustrated in Figure 3.36. Vertical rods were inserted to vary the degree of congestion inside the structure.

Figure 3.36: The experimental setup used in the Buxton experiments.

The ambient weather conditions such as temperature, wind speed and direction were monitored and logged prior to the gas releases. The predominant wind direction was towards north-west. Hydrogen and methane were released into the module, and the concentration was measured using 13 oxygen depletion sensors inside the module. All jets were released 1.5 meter above the ground and the point of discharge was located one meter from the south face of the module. All releases were directed towards north, i.e. positive x-direction, see Figure 3.37. The leak orifice diameter varied from 3 mm to 12 mm in diameter, and the stagnation pressure varied from 5 bar to 40 bar.
3.3.2 Implementation of the Buxton experiments

Identical geometries and numerical meshes were used for the methane and hydrogen dispersion simulations. The calculation domain was 20 by 20 by 15 meters in the x-, y-, and z-direction, respectively, with a total of 465,120 [120 by 68 by 57] control volumes. The high number of control volumes was necessary in order to capture the physics of the release, the confinement of the module, and each measurement sensor. The leak point control volume was modeled with a cubic shape, with sides of 0.1 meters. The coordinates of the leak source was at [10, 11.5, 1.5] meters and the mesh was expanded from the leak point coordinates to capture the shape of the module. The geometry and the numerical mesh are shown in Figure 3.38 a) and b) for the xz- and xy-planes, respectively.

Figure 3.37: The Buxton module used in FLEXSIM.
3.3. BUOYANT GAS DISPERSION

(a) XZ-plane illustration of the geometry and meshgrid used in the simulation of the Buxton experiments.

(b) XY-plane illustration of the geometry and meshgrid used in the simulation of the Buxton experiments.

Figure 3.38: The geometry and numerical mesh used in the simulation of the Buxton experiments for methane and hydrogen releases.
The wind-speed and direction used in the simulations were calculated from time averaged weather observations provided by Shell Global Solutions (2003). All calculations have been performed without the subgrid models for turbulence and drag. Figure 3.39 and 3.40 illustrate the measured wind direction counted in degrees clockwise from north axis and the measured wind speed for hydrogen test series 01, respectively. The averaged wind field data was used as boundary conditions, and a steady state wind field was calculated prior to the introduction of the leak.

The dispersion calculations ran until the concentration in the thirteen monitoring points had reached steady state. The predicted concentrations were compared to the time averaged experimental concentration measurements. The oscillatory behavior of the measured gas concentrations, obtained from the first six of total thirteen monitoring points in hydrogen dispersion test series 01, have been illustrated in Figure 3.41.

Figure 3.39: Measured wind direction in Buxton hydrogen test series 01.
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Figure 3.40: Measured wind speed in Buxton hydrogen test series 01.

Figure 3.41: Examples of concentration measurements from six of the thirteen monitoring points in Buxton hydrogen test series 01.
A general observation for the methane and hydrogen releases was the effect of buoyancy due to the differences in density between air and the discharged gases. This have been illustrated in Figure 3.42 for hydrogen series 01, with the isosurface of gas at 4 vol.%. The released gas was dominated by the momentum of the wind soon after the discharge. The leak would fill the module but pockets with no gas were predicted as illustrated in Figure 3.44. Also, a significant amount of gas was predicted outside of the module. As seen from the measurements the local gas concentration depends on the fluctuating weather conditions. Averaging the weather conditions will not reproduce this oscillatory behaviour and clearly introduces a source of error.

![Figure 3.42: The predicted isosurface of 4 vol.% of hydrogen release 01.](image)

### 3.3.3 Simulations and results - Methane releases

Eight of the methane jet releases have been simulated and analyzed. Figure 3.43 (a-h) show scatter plots of predicted versus measured volumetric gas concentrations of varying leak orifice diameter, and discharge pressure. The triangles indicate the measured concentration, and the dotted lines are factor of two limits.
In Test series no. 9, 17, and 18 there were large discrepancies between the measured and predicted concentrations in some of the monitoring points. Predictions indicated areas with a concentration equal to zero whereas the experiments had registered concentrations above zero.

(a) Test 03 - Orifice 6 mm - 20 bar.

(b) Test 05 - Orifice 6 mm - 10 bar.

Figure 3.43: Scatter plots of predicted versus measured volumetric concentrations for the Buxton methane releases for different orifice diameters and stagnation pressures.
CHAPTER 3. DISPERSION - SIMULATIONS AND VALIDATION

(c) Test 07 - Orifice 4 mm - 30 bar.

(d) Test 09 - Orifice 4 mm - 20 bar.

(e) Test 11 - Orifice 4 mm - 10 bar.

Figure 3.43: continued from previous page.
3.3. BUOYANT GAS DISPERSION

(f) Test 13 - Orifice 3 mm - 40 bar.

(g) Test 17 - Orifice 3 mm - 30 bar.

(h) Test 18 - Orifice 3 mm - 20 bar.

Figure 3.43: continued from previous page.
In Figure 3.44 the streamlines and concentration distribution for test series 18 have been visualized, with red being high concentration areas. It can be seen how the interaction between the momentum of the released gas and wind resulted in areas with no gas concentration. Areas with recirculation have been predicted on the north side of the module. The highest concentrations have been predicted between the release point and south face of the module. Considerable gas volumes have been predicted outside the module as well.

Figure 3.44: Predicted volumetric gas concentration for Buxton methane Test series 18. The colorbar is only valid for volumetric concentrations between zero and five.

The median performance measures, according to Chapter 3.1, omitting the concentrations equal to zero, have been summarized in Table 3.18. The variable Φ analyzed is the mean concentration $[c]$. 

66% of the predicted concentrations are within a factor two of the measured. The calculated concentrations are under predicted and the statistical measures exceed the criterias of acceptable performance.
Table 3.18: Median performance measures for the Buxton methane releases

<table>
<thead>
<tr>
<th></th>
<th>Median for methane releases</th>
</tr>
</thead>
<tbody>
<tr>
<td>FB</td>
<td>[-0.3 , 0.3] -0.32</td>
</tr>
<tr>
<td>NMSE</td>
<td>[&lt;4] 0.33</td>
</tr>
<tr>
<td>MG</td>
<td>[0.7 , 1.3] 0.68</td>
</tr>
<tr>
<td>VG</td>
<td>[&lt;1.6] 1.88</td>
</tr>
<tr>
<td>FAC2</td>
<td>[&gt;0.5] 0.66</td>
</tr>
</tbody>
</table>

3.3.4 Simulations and results - Hydrogen releases

Eleven hydrogen jet releases have been simulated. Figure 3.45 (a-k) show scatter plots of predicted versus measured volumetric gas concentrations, for varying leak orifice diameter, and discharge pressure. The triangles indicate the measured points, and the dotted lines are factor of two limits.

![Scatter plots of predicted versus measured volumetric gas concentrations for the Buxton hydrogen releases for different orifice diameters and stagnation pressures.](image)

(a) Test 01 - Orifice 12 mm - 5 bar.

Figure 3.45: Scatter plots of predicted versus measured volumetric concentrations for the Buxton hydrogen releases for different orifice diameters and stagnation pressures.
(b) Test 03 - Orifice 12 mm - 10 bar.

(c) Test 06 - Orifice 6 mm - 30 bar.

(d) Test 07 - Orifice 6 mm - 30 bar.

Figure 3.45: continued from previous page.
3.3. BUOYANT GAS DISPERSION

(e) Test 08 - Orifice 6 mm - 20 bar.

(f) Test 09 - Orifice 6 mm - 20 bar.

(g) Test 10 - Orifice 6 mm - 10 bar.

Figure 3.45: continued from previous page.
(h) Test 13 - Orifice 4 mm - 30 bar.

(i) Test 17 - Orifice 4 mm - 10 bar.

(j) Test 18 - Orifice 4 mm - 40 bar.

Figure 3.45: continued from previous page.

85
The statistical median performance measures according to the procedure described in chapter 3.1, with $\Phi$ being the mean concentration $[c]$, are summarized in Table 3.19. The analysis indicates that the hydrogen releases are over predicted with 77% of the predicted concentrations within a factor two of the measured. The fractional bias and geometric variance are higher than performance criterias. Releases with an orifice of 12 mm and high pressure releases with 6 mm orifice have the largest scatter and overpredictions.

Table 3.19: Median performance measures for the Buxton hydrogen releases

<table>
<thead>
<tr>
<th>Performance Measure</th>
<th>Median [FB, NMSE, MG, VG, FAC2]</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>FB</td>
<td>[-0.3, 0.3]</td>
<td>0.5</td>
</tr>
<tr>
<td>NMSE</td>
<td>[&lt;4]</td>
<td>0.32</td>
</tr>
<tr>
<td>MG</td>
<td>[0.7, 1.3]</td>
<td>1.78</td>
</tr>
<tr>
<td>VG</td>
<td>[&lt;1.6]</td>
<td>1.49</td>
</tr>
<tr>
<td>FAC2</td>
<td>[&gt;0.5]</td>
<td>0.77</td>
</tr>
</tbody>
</table>
3.3.5 Overall performance

In this section the overall statistical performance of the dispersion model with respect to buoyant gas releases performed in the Buxton experiments will be presented. In Figure 3.46 the predicted versus the measured concentrations have been illustrated. The statistical analysis of the Buxton releases have summarized in Table 3.20.

Based on the statistical data in Table 3.18 and 3.19 the dispersion model under predicts the methane releases whereas the hydrogen releases are over predicted. The main contribution to the over predictions comes from high pressure releases with 6 and 12 mm orifices. For a buoyant release in general Table 3.20 indicates that 77% of the predicted concentrations are within a factor two of the measured. The statistical performance is in the high end of the criterias of acceptable model performance.

Figure 3.46: Predicted and measured concentrations for the methane and hydrogen releases performed in the Buxton experiments.
Table 3.20: Median statistical performance of the observed versus predicted gas concentrations for the Buxton methane and hydrogen releases.

<table>
<thead>
<tr>
<th></th>
<th>Median for methane and hydrogen releases</th>
</tr>
</thead>
<tbody>
<tr>
<td>FB</td>
<td>[-0.3 , 0.3] 0.18</td>
</tr>
<tr>
<td>NMSE</td>
<td>[&lt;4] 0.32</td>
</tr>
<tr>
<td>MG</td>
<td>[0.7 , 1.3] 1.21</td>
</tr>
<tr>
<td>VG</td>
<td>[&lt;1.6] 1.6</td>
</tr>
<tr>
<td>FAC2</td>
<td>[&gt;0.5] 0.77</td>
</tr>
</tbody>
</table>

3.4 Dense gas dispersion

3.4.1 The Thorney Island experiments

In 1983 the Health and Safety Executive performed a series of dense gas experiments. The experiments were performed on an open field with a fixed volume gas cloud of approximately 2000 m$^3$. The gas source was a cylindrical container approximately 14 meters in diameter and 14 meters high. The container was covered with plastic material and filled with gas. At the start of the experiment the plastic walls collapsed to the ground leaving a cylindrical gas cloud. The gas released was a mixture of Refrigerant-12, Freon, diluted with nitrogen, with an initial relative density ratio of two (McQuaid & Roebuck 1985). The wind speed and direction, ambient temperature, and pressure were monitored. The gas concentration was measured at various locations and at different heights upstream of the release point (McQuaid & Roebuck 1985).

To investigate how dense gas disperses over built environment three types of obstructions were examined:

1. Solid barrier - a five meter high, impermeable fence was built on a 180$^o$ arc around the gas container. The diameter was 100 meter with the gas cloud as centre.

2. Porous barrier - ten meter high porous fences built on a 180$^o$ arc around the gas container. The first row was located with a diameter of 100 meters from the leak point and subsequent rows were places at 3.3 meter intervals. The number of rows was from 2 to 4.
3. Solid Building - a 9 meter mobile cubical building was placed at various locations shortly before the release of gas.

Trial no. 21 and no. 26 have been selected to validate the dispersion of dense gases. Trial no. 21 was performed with obstruction type one; i.e. solid barrier, whereas trial no. 26 was performed with obstruction type three; i.e. solid building. For both trials the measured time history of concentration at given positions and heights have been compared with predicted concentrations.

3.4.2 Simulations and Results - Trial 21

Thorney Island trial no. 21 was simulated using a computational domain of 450 by 200 by 70 meters in x-, y-, and z-direction, respectively. The structure enclosing the gas cloud, as well as the gas cloud itself, was modeled as a rectangular box with the lower left corner at [50, 93.5, 0] meters. The total number of control volumes used was 183,825 [75×57×43]. A semi-circle impermeable fence with a diameter of 100 meters surrounded the cloud. The mesh was designed to capture the size of the gas cloud and the shape of the fence.

The wind speed was measured to be 3.9 m/s 10 meters above ground level with the mean wind direction being 61°, measured counter clockwise, relative to the positive x-axis (McQuaid & Roebuck 1985). The wind field was simulated for 200 seconds prior to the release to obtain a steady flow pattern. Similar to the simulations done by Hall (1997) the roughness parameter \( z_0 \) was chosen to be 0.068. In Figure 3.47 the steady state wind speed and streamlines have been illustrated at a height of 1.25 meters after two hundred seconds. The structure containing the gas is shown as the red box.

Wake areas have been predicted on the leeward side of the spill point and the fence. In both areas the wind speed was reduced, which will affect the mixing and flow pattern of the released gas.

The gas cloud was approximately 2050 m\(^3\) with the gas having a relative density ratio of two. The cloud was surrounded by an impermeable fence modeled as a semi-circle with a diameter of hundred meters. The time history of the gas concentration was monitored at coordinates [71.7, 30.51, (0.4, 2.4, 4.4, 6.4, 10.4)] meters, relative to the center of the gas cloud. The isosurface of the gas at 1 vol.%, is illustrated in Figure 3.48.
and Figure 3.49 after two and sixty seconds, respectively.

Figure 3.47: Wind speed and streamlines for Thorney Island trial no. 21 at z=1.25 meters after 200 seconds.

Figure 3.48: Isosurface of gas 1 vol.%, 2 seconds after release for the Thorney Island trial no. 21.
The flow pattern of the released gas volume is determined by the wind speed and direction. The dense gas is blocked and accumulated by the fence. Over time the gas will be diluted and carried over the fence by the wind. From Figure 3.47 it is seen that the wind speed is higher on the sides of the fence than in the center. This is also reflected in Figure 3.49 where gas clearly follows the areas with a higher speed, hence faster mixing.

Hall (1997) performed a simulation of trial no. 21 with the CFD-code STAR-CD. An un-structured grid with a total of 171,540 control volumes was used and the domain was 650 by 30 by 80 meters in x-, y-, and z-direction, respectively. Figure 3.50(a-e) compares the time history of the gas concentrations predicted in FLEXSIM to the results obtained by Hall (1997) and the experimental data also reported in Hall (1997).

The predicted concentration follows the measured transient behavior very good but over predicts the peak concentrations. The predictions by Hall (1997) appears to capture the peak concentrations somewhat better.
3.4. DENSE GAS DISPERSION

(a) Height = 0.4 meters

(b) Height = 2.4 meters
(c) Height = 4.4 meters

(d) Height = 6.4 meters
3.4.3 Simulations and Results - Trial 26

The Thorney Island trial no. 26 was modeled using a computational domain of 150 by 100 by 35 meters in x-, y-, and z-direction, respectively. The gas cloud was modeled as a rectangular box with the lower left corner at [50, 44, 0] meters. A total number of 425,088, \([123 \times 72 \times 48]\), control volumes was used. A impermeable mobile building was placed 50 meters downwind of the gas volume. The mesh was designed to capture the size of the gas cloud and the shape of the building.

The wind speed was measured to be 1.9 m/s measured 10 meters above ground level with the mean wind direction being 5.0° relative to the positive x-axis counting clockwise, (McQuaid & Roebuck 1985). The roughness parameter \(z_0\) used was 0.005, the same as used by Sklavonuos & Rigas (2004). Figure 3.51 illustrate the steady state wind speed and streamlines after two hundred seconds. The slice is at a height of 1.25 meters and the red box represents the structure containing the gas.

Figure 3.50: Time history of the predicted and measured gas concentration at different heights for Thorney Island Trial no. 21.
The gas cloud size was roughly 1944 m$^3$ with the gas having a relative density ratio of two. The time history of the gas concentration was monitored in front of the building at a height of 6.4 meters, and behind the building at a height of 0.4 meters. The isosurface of the gas at 1 vol.%, is illustrated in Figures 3.52 and 3.53 after two and eighteen seconds, respectively.

The released gas volume is dispersed in symmetrical flow pattern. Because of the low wind speed the momentum of the wind is not so dominating compared to trial no. 21.

The time history comparison is presented in Figure 3.54 together with simulations performed with CFX reported by Sklavonuos & Rigas (2004) and experimental measurements. Sklavonuos & Rigas (2004) used a unstructured mesh with 33,791 volume elements and the $k-\varepsilon$ turbulence model.
3.4. DENSE GAS DISPERSION

Figure 3.52: Isosurface of gas 1 vol.%, 2 seconds after release for the Thorney Island trial no. 26.

Figure 3.53: Isosurface of gas 1 vol.%, 18 seconds after release for the Thorney Island trial no. 26.

The dispersion model in FLEXSIM over predicts the time it takes for the gas to reach the building, whereas the predicted concentrations themselves are under predicted. The peak concentration is higher on the front side of the building then on the rear, but the duration of detected gas is longer on the rear side of the structure. There is good agreement with the measured transient development of the concentration both in front
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and at the rear of the building.

Figure 3.54: Time history of the predicted and measured gas concentration at different heights for Thorney Island Trial no.26.

(a) Time history of gas concentration in front of the building at $z = 6.4$ meters.

(b) Time history of gas concentration at the rear of the building at $z = 0.4$ meters.
Chapter 4

Fire and Radiation

In this chapter a validation of the implemented CRG model (Rasmussen 2002) will be presented. Radiation in a furnace (Mills 1995) has been simulated with only heat transfer between surfaces and no participating mediums in the enclosed volume. Furthermore, an experiment with horizontally released jet fires has been simulated (Bennett et al. 1991) including a model for the reaction rate and extinction coefficient.

4.1 Radiant transfer in a furnace

The Composite Radiosity and Gap, CRG, model by Rasmussen (2002) has been implemented in FLEXSIM. The mesh used was 50 by 50 and the simulations ran until steady state was obtained. The results from FLEXSIM has been compared against example 6.5, page 516, in the textbook of Mills (1995):

A furnace is 3m × 3m in cross section. The side wall and roof are at 1700 K and 1400 K, respectively. The floor is at 600 K. All the surfaces are gray and diffusive and have an emittance $\epsilon = 0.5$. The furnace is illustrated in Figure 4.1.

The gas enclosed by the furnace walls is neither absorbing or emitting so that the radiation will occur between the wall surfaces.

Mills uses his own computer program, RAD2, to solve the problem. The method is a radiosity-shape factor method where algebraic equations are solved.
4.1. RADIANT TRANSFER IN A FURNACE

Figure 4.1: Illustration of furnace used in the example of Mills (1995).

4.1.1 Results and discussions

The heat flux in the vertical direction and the radiosity temperature distribution is reported from Mills (1995) and compared to similar results obtained from FLEXSIM and Zhubrin (2000). The simulation results by Mills and FLEXSIM are summarized in Table 4.1 and 4.2, respectively. Zhubrin (2000) reports a heat flux of $-1.597 \times 10^5$ W/m² on surface one. Results obtained with FLEXSIM are in good agreement with data reported by Mills (1995) and Zhubrin (2000). Comparing the profile of the heat flux in vertical direction and the radiosity temperature from FLEXSIM and Zhubrin (2000) show very good agreement. The profiles are illustrated in Figure 4.2 and Figure 4.3.
CHAPTER 4. FIRE AND RADIATION

Figure 4.2: The radiative heat flux in the vertical direction and the radiosity temperature profiles, calculated by FLEXSIM.
Figure 4.3: The radiative heat flux in the vertical direction and the radiosity temperature profiles (Zhubrin 2000).
4.2 Horizontally released jet fires

4.2.1 Experiments

As a part of a CEC project a series of gas jet experiments were performed at Spadeadam in Cumbria, UK. The experimental setup has been reported by Bennett et al. (1991). A selection of these experiments have been presented in the paper of Johnson et al. (1994), namely test 1083, 1033, and 1089, which from now on are denoted case C, D, and E, respectively. These cases have been used to validate the CRG radiation and fire models implemented in FLEXSIM. The experimental details have been summarized in Table 4.3.

The molar composition of the gas used in the experiments was by volume 94% methane, 5.31% ethane, 0.425% nitrogen, and 0.265% propane and other hydrocarbons, similar to natural gas (Johnson et al. 1994).
4.2. HORIZONTALLY RELEASED JET FIRES

Table 4.3: Experimental gas jet fire releases

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Test 1083</th>
<th>Test 1033</th>
<th>Test 1089</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow rate</td>
<td>kg/s</td>
<td>8.4</td>
<td>7.9</td>
<td>3.8</td>
</tr>
<tr>
<td>Stagnation pres.</td>
<td>barg</td>
<td>2.1</td>
<td>11.1</td>
<td>66</td>
</tr>
<tr>
<td>Stagnation temp.</td>
<td>K</td>
<td>267</td>
<td>279</td>
<td>281</td>
</tr>
<tr>
<td>Ambient temp.</td>
<td>K</td>
<td>281</td>
<td>282</td>
<td>286</td>
</tr>
<tr>
<td>Release diameter</td>
<td>mm</td>
<td>152</td>
<td>75</td>
<td>20</td>
</tr>
<tr>
<td>Release height above ground</td>
<td>m</td>
<td>3.0</td>
<td>3.0</td>
<td>3.0</td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td>0.3</td>
<td>3.9</td>
<td>6.9</td>
</tr>
<tr>
<td>Wind direction degrees</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>clockwise from north</td>
<td></td>
<td>146</td>
<td>91</td>
<td>89</td>
</tr>
</tbody>
</table>

4.2.2 Simulation and results for test case C

For case C the thermal radiation flux was measured at the positions illustrated in Figure 4.4a. In the experimental setup the release point was located at origo and directed along the positive x-direction with north being in the positive y-direction. Figure 4.4b illustrates the predicted heat flux with and without liftoff compared to experimental findings reported in Johnson et al. (1994).

The experimental data have been marked with an error band of +/- 50%. The predicted heat fluxes are well within the error band, except for the three points along the release axis 50-60 meters from the release point, where the calculated heat fluxes are underpredicted. There are no significant differences in the level of radiation when introducing the liftoff model.

In Figure 4.5, the absorption coefficient, extinction coefficient, fuel concentration, combustion product, radiosity, reaction rate, length according to Eq. 2.60, and temperature are illustrated as contour plots through the release point in the xz-plane. Note that in the simulations the point of discharge was at x equal to 10 meters. The left column shows plots without a liftoff criteria and the right column shows plots with a liftoff criteria.
CHAPTER 4. FIRE AND RADIATION

(a) Monitoring points for heat flux. Release point in origo and directed along the positive x-axis.

(b) Measured and predicted heat fluxes, with and without liftoff criteria. 50% limits are indicated at measured data bar.

Figure 4.4: Monitoring points and predicted versus measured heat fluxes for test case C.
4.2. HORIZONTALLY RELEASED JET FIRES

Figure 4.5: Contour plots in the xz-plane through the release point of relevant physical variables for test case C. With and without liftoff criteria.
Figure 4.5: Continued.
Figure 4.5: Continued.
4.2.3 Simulation and results for test case D

Figure 4.6a illustrates the monitoring points for thermal radiation in case D. The release point is still at origo directed along the positive x-axis. The predicted heat flux with and without a liftoff criteria compared to experimental findings, as reported in Johnson et al. (1994), is shown in Figure 4.6b. The experimental data have been marked with an error band of +/- 50%. The predicted heat fluxes are within a factor of two of experiments. However, the measured heat fluxes are in general underpredicted. Introducing the liftoff model appears to deteriorate the predictions.

In Figure 4.7 the absorption coefficient, extinction coefficient, fuel concentration, combustion product, radiosity, reaction rate, length according to Eq. 2.60 and temperature are illustrated as contour plots through the release point in the xz-plane. Note that in the simulations the discharge point was at x equal to 5 meters. The left column shows plots without a liftoff criteria and the right column shows plots with a liftoff criteria.

(a) Monitoring points for heat flux. Release point in origo and directed along the positive x-axis.
4.2. HORIZONTALLY RELEASED JET FIRES

(b) Measured and predicted heat fluxes, with and without liftoff criteria. 50% limits are indicated at measured data bar.

Figure 4.6: Monitoring points and predicted versus measured heat fluxes for test case D.

(a) Absorption coefficient-without (b) Absorption coefficient-with

Figure 4.7: The absorption coefficient, extinction coefficient, fuel concentration, combustion product, radiosity, reaction rate, length, and temperature are illustrated as contour slices through the release point in the xz-plane for case D.
Figure 4.7: Continued.
4.2. HORIZONTALLY RELEASED JET FIRES

Figure 4.7: Continued.
CHAPTER 4. FIRE AND RADIATION

4.2.4 Simulation and results for test case E

Figure 4.7 illustrates the monitoring points for thermal radiation in case E. The release point is at origo directed along the positive x-axis. The predicted heat flux with and without a liftoff criteria compared to experimental findings, as reported in Johnson et al. (1994), is shown in Figure 4.8. The experimental data have been marked with an error band of +/- 50%. The predicted heat fluxes are within a factor of two of experiments, and are in general underpredicted. Again the introduction of the liftoff model appears to deteriorate the predictions.

In Figure 4.9 the absorption coefficient, extinction coefficient, fuel concentration, combustion product, radiosity, reaction rate, length according to Eq. 2.60, and temperature are illustrated as contour plots through the release point in the xz-plane. Note that in the simulations the discharge point was at x equal to 5 meters. The left column shows plots without a liftoff criteria and the right column shows plots with a liftoff criteria.
4.2. HORIZONTALLY RELEASED JET FIRES

(a) Monitoring points for heat flux. Release point in origo and directed along the positive x-axis.

(b) Measured and predicted heat fluxes, with and without liftoff criteria. 50% limits are indicated at measured data bar.

Figure 4.8: Monitoring points and predicted versus measured heat fluxes for test case E.
CHAPTER 4. FIRE AND RADIATION

Figure 4.9: Contour plots in the xz-plane through the release point of relevant physical variables for test case E. With and without liftoff criteria.
4.2. HORIZONTALLY RELEASED JET FIRES

Figure 4.9: Continued.
4.2.5 Overall performance

The predicted and measured heat flux for test cases C, D, and E, have been compared in Figure 4.10. The model performance, according to Chapter 3 has been summarized in Table 4.4. The variable Φ analyzed is the heat flux.

The calculated heat fluxes compare qualitatively very well with experiments. The statistical parameters in Table 4.4 shows that the predicted levels of radiative heat flux are well within acceptable performance criteria. There are insignificant differences between the results obtained with and without the lift-off model. Case C is the only test series with measurement points far from the discharge exit. These levels are under predicted just outside the experimental error bar of +/- 50%.
4.2. HORIZONTALLY RELEASED JET FIRES

Figure 4.10: Predicted versus measured heat flux for case C, D, and E.

Table 4.4: Statistical performance of the observed and predicted heat fluxes for case C, D, and E.

<table>
<thead>
<tr>
<th></th>
<th>Without liftoff</th>
<th>With liftoff</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max observed</td>
<td>20.2</td>
<td>20.2</td>
</tr>
<tr>
<td>Max predicted</td>
<td>15.8</td>
<td>14.97</td>
</tr>
<tr>
<td>Min observed</td>
<td>0.7</td>
<td>0.7</td>
</tr>
<tr>
<td>Min predicted</td>
<td>1.09</td>
<td>0.92</td>
</tr>
<tr>
<td>Max observed / Max predicted</td>
<td>1.34</td>
<td>1.35</td>
</tr>
<tr>
<td>Mean observed</td>
<td>7.05</td>
<td>7.05</td>
</tr>
<tr>
<td>Mean predicted</td>
<td>6.0</td>
<td>5.76</td>
</tr>
<tr>
<td>FB [-0.3 , 0.3]</td>
<td>-0.16</td>
<td>-0.20</td>
</tr>
<tr>
<td>NMSE [ &lt;4]</td>
<td>0.07</td>
<td>0.11</td>
</tr>
<tr>
<td>MG [0.7 , 1.3]</td>
<td>0.84</td>
<td>0.80</td>
</tr>
<tr>
<td>VG [ &lt;1.6]</td>
<td>1.14</td>
<td>1.2</td>
</tr>
<tr>
<td>FAC2 [ &gt;0.5]</td>
<td>0.87</td>
<td>0.87</td>
</tr>
</tbody>
</table>
Chapter 5

Conclusions and Recommendations

This thesis presents the implementation and validation of a gas dispersion and radiation model in EXSIM (Sæter 1998, Hjertager et al. 1992). Simulations have been performed with different wind speeds, geometries, gas types, release directions, leak rates, and discharge orifices. Results have been validated against experimental findings. This chapter will present conclusions and also recommendations for future work.

5.1 Conclusions

A computational study of air changes and jet leaks, using a buoyant neutral gas, in highly confined and congested geometries has been performed. The results have been compared to large scale experimental findings as reported by Savvides et al. (1999) and BG Technology & Shell Global Solutions (April 1999). The pre-release ventilation rates are in good quantitative agreement with experiments. The ventilation rates are under predicted but well within the criterias for acceptable performance. Air changes predicted for module configuration C2, where the flow in- and outlet areas are blocked by 80%, are the main contributors to the under prediction.

The predicted flammable gas volumes show an acceptable quantitative performance with the majority of the predictions within a factor of two. The flammable gas volumes inside the module are in general over predicted but show an acceptable over all quantitative statistical performance. Two simulations with decaying release rate have been simulated
5.2 Recommendations

The analytical approach to calculate the boundary conditions of the leak point should be studied. The convergent-divergent nozzle approach used in this thesis results in subsonic outlet conditions for the discharge area. The supersonic core existing downstream of the release point will not be captured using the nozzle approach, resulting in an under prediction of the momentum. An alternative is the pseudo-diameter method by Birch et al. (1987) which conserves both momentum and energy.

To account for the non-isotropic effects on the turbulence due to buoyancy a hybrid of the $k - \epsilon$ model and the Algebraic Reynolds Stress
Model (ASM) as proposed by Davidson (1990) and Yan & Holmstedt (1998) should be implemented and validated. The advantages of the hybrid model are that:

i) it accounts for non-isotropic effects on the turbulence due to buoyancy in the same way as Reynolds stress models (which the $k-\epsilon$ cannot handle)

ii) it is expected to be numerically much more stable than the Reynolds stress models and, thus, to decrease the computational effort for a convergent solution

This model is mainly derived for buoyant driven diffusion flames but should be tested against both gas dispersion and turbulent jet fires.

Since soot particles contribute to radiative heat transfer in combustion processes, as they absorbs and emits heat, a model for soot formation has to be implemented. Khan & Greeves (1974) have presented a single step soot formation model solving only a single transport equation for the soot mass fraction. The soot generation is then given by empirical expressions for the soot formation and soot combustion. Another approach is the soot formation model of Magnussen & Hjertager (1976) solving two transport equations; first soot nuclei and from the nuclei the soot particles are formed. The combustion rates of soot nuclei and particles are related to the combustion rate of the gaseous fuel.

A further investigation of the liftoff model should be done, and the validity of the radiation model in enclosed jet fires should be investigated. Furthermore, pool fires should also be investigated.
5.2. RECOMMENDATIONS
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Appendix A

Convergent-divergent Nozzle

In FLEXSIM the following assumptions are used:

- $P_{o,1}$ = Upstream stagnation pressure
- $P_{o,2}$ = Downstream stagnation pressure
- $T_{o,2}$ = Downstream stagnation temperature
- $T_{o,1} = T_{o,2}$ : Upstream stagnation temperature is equal to downstream stagnation temperature
- $d_p$ = The pipe outlet diameter is known
- $\gamma$, Kappa for the specific gas

1. An expression for the Mach number upstream of the shock, $M_1$, can be found using isentropic expansion and normal shock relations:

\[
\frac{P_{o,1}}{P_{o,2}} = \frac{P_{o,1}}{P_1} \times \frac{P_1}{P_2} = \frac{P_{o,1}}{P_1} \times \frac{P_1}{P_{o,2}}
\]  
(A.1)

This can be written as (Lamkin et al. 1980):

\[
\frac{P_{o,1}}{P_{o,2}} = \frac{(1 + (\frac{\gamma-1}{2})M_1^2)^{\frac{2}{\gamma-1}}}{(\frac{2\gamma}{\gamma+1})M_1^2 - \frac{\gamma-1}{\gamma+1}}
\]  
(A.2)

Eq. [A.2] has to be solved iterally in order to obtain a solution for $M_1$. 

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2. From normal shock relations the Mach number downstream of the shock can be expressed as (Lamkin et al. 1980):

\[ M_2 = \left[ \frac{(1 + \left(\frac{\gamma - 1}{2}\right)M_1^2)}{\gamma M_1^2 - \left(\frac{\gamma - 1}{2}\right)} \right]^{1/2} \]  \hspace{1cm} (A.3)

3. From isentropic expansion and normal shock relations the temperature relation can be described as (Moran & Shapiro 1999):

\[ \frac{T_2}{T_{o,1}} = \frac{T_1}{T_{o,1}} \cdot \left(\frac{T_2}{T_1}\right) = \frac{T_1}{T_{o,1}} \cdot \left(\frac{P_2}{P_1} \cdot \frac{v_2}{v_1}\right) \]  \hspace{1cm} (A.4)

where (Moran & Shapiro 1999)

\[ \frac{P_2}{P_1} \cdot \frac{v_2}{v_1} = (1 + \frac{2\gamma}{\gamma + 1} (M_1^2 - 1)) \cdot (1 - \frac{2}{\gamma + 1} (1 - \frac{1}{M_1^2})) \]  \hspace{1cm} (A.5)

4. Using the assumption that the reservoir temperature is equal to the temperature of the surroundings and using isentropic expansion relations the temperature downstream of the shock \(T_1\) can be expressed as: (Thompson 1972):

\[ \frac{T_{o,1}}{T_1} = 1 + \frac{\gamma - 1}{2} M_1^2 \Rightarrow \]

\[ T_1 = \frac{T_{o,1}}{1 + \frac{\gamma - 1}{2} M_1^2} \]  \hspace{1cm} (A.6)

5. The temperature after the shock \(T_2\) can be found by inserting Eq. \[A.5\] and Eq. \[A.6\] into Eq. \[A.4\]

\[ T_2 = T_{o,1} \frac{T_1}{T_{o,1}} \left(\frac{P_2}{P_1} \cdot \frac{v_2}{v_1}\right) \]

\[ = T_1 \left(\frac{P_2}{P_1} \cdot \frac{v_2}{v_1}\right) \]

\[ = \frac{T_{o,1} \cdot \frac{P_2}{P_1} \cdot \frac{v_2}{v_1}}{1 + \frac{\gamma - 1}{2} M_1^2} \left(1 + \frac{2\gamma}{\gamma + 1} (M_1^2 - 1)\right) \cdot (1 - \frac{2}{\gamma + 1} (1 - \frac{1}{M_1^2})) \]  \hspace{1cm} (A.7)
6. The speed of sound downstream of the shock, $c_2$, can be found from:

$$c_2 = \sqrt{\gamma RT_2}$$

$$= \sqrt{\frac{\gamma R}{Mw} T_2} \quad (A.8)$$

7. The velocity downstream of the shock can then be found from (Thompson 1972):

$$u_2 = M_2 \cdot c_2 \quad (A.9)$$

8. The relation between the pipe outlet area, $A^*$, and the area at the shock, $A_2$, can be expressed as (Moran & Shapiro 1999):

$$\frac{A_2}{A^*} = \frac{1}{M_2 \left[\left(\frac{2}{\gamma + 1}\right) \cdot (1 + \frac{\gamma - 1}{2}) M_2^2 \right]^{\frac{\gamma + 1}{\gamma - 1}}} \quad (A.10)$$

From Eq. (A.10) the shock area, $A_2$, and diameter can be found.

9. From the Eq. (A.9) and Eq. (A.10) the mass flow rate can be found as:

$$\dot{m} = \rho_2 A_2 u_2$$

$$= \frac{P_2}{\frac{R}{Mw} T_2} A_2 u_2 \quad (A.11)$$

10. The area porosity for the leak can be found from:

$$\beta = \frac{A_2}{A_{cv}} \quad (A.12)$$