CFD Simulation of Aerosol Flow and Hydrocarbon Fouling on a Circular Disk

by

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Abstract

Coking is one of the key technologies used in upgrading of oil sands bitumen. In coking units, the bitumen is thermally cracked in the presence of steam to produce valuable lighter species and by-product solid coke. Hot vapours which contain these valuable species from the fluid coker pass through cyclones before entering the scrubber section of the coker, so that coke and heavy droplets are removed. However, some micron-sized heavy hydrocarbon droplets are not removed in the cyclones and enter the scrubber grid packing. These droplets can deposit on the scrubber grid and react over time to form coke as a result of high temperatures. A model is developed for calculation of deposition from a droplet-gas mixture at similar conditions. A simple geometry of a circular disk was used to be able to evaluate the validity of model at different conditions. The model combined Computational Fluid Dynamics (CFD) for calculating the flow hydrodynamics and droplet transport to the surface, and HYSYS simulation for prediction of mixture phase equilibrium at different temperatures.

Effects of parameters such as droplet size and gas velocity were studied. Based on modeling results, Stokes number seemed to be a very important parameter on deposition of droplets. At low Stokes number, the main mechanism for deposition was molecular and eddy diffusion, and deposition did not change very much with change in droplet size and velocity. At higher Stokes number impaction was the main mechanism, and the deposition rates increased with increases in droplet size and gas velocity.

The effect of surface properties on deposition was also studied. For the applied conditions and surfaces the perfect sticking assumption was considered satisfactory. Calculations suggested that application of hydrophobic material might help to decrease deposition by increasing the possibility of rebounding for droplets.

Model was tested against room-temperature data for air-droplet systems and hot-unit experiments with heavy hydrocarbons carried out in parallel with the modeling work. For the latter, increases in the temperature decreased the deposition rates both by decreasing the droplet concentration and by the evaporation of volatiles formed in coking reaction.
Finally, the model showed good ability in the prediction of deposition rates at different conditions.
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Nomenclature

$A_d$  
Total disk surface area, m$^2$

$A_p$  
Particle (droplet) surface area, m$^2$

$a$  
Attraction parameter for Peng-Robinson equation, N.m$^4$

$B$  
Dimensionless repulsion Parameter for Peng-Robinson equation, $B = bP/RT$

$b$  
Repulsion parameter for Peng Robinson equation, N/m$^2$

$C_b$  
Bulk concentration, kg/m$^3$

$C_{1e}, C_{2e}, C_{3e}, C_1, C_2$  
Constants for turbulence dissipation rate

$C_{\mu}$  
Eddy viscosity constant, dimensionless

$C_e$  
Cunningham correction, dimensionless

$C_D$  
Drag coefficient, dimensionless

$c_p$  
Heat capacity of the particle (droplet), J/(kg.K)

$D$  
Diffusion coefficient of vapour in the bulk, m$^2$/s

$D_{r,p}$  
Thermophoretic coefficient, kg/m$^2$s$^2$

$d_{ij}$  
Deformation tensor

$d$  
Diameter, m

$d_m$  
Droplet maximum spread diameter, m

$d_c$  
Disk diameter, m
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d_p$</td>
<td>Particle (droplet) diameter, m</td>
</tr>
<tr>
<td>$E$</td>
<td>Total energy of droplet at a certain stage, J</td>
</tr>
<tr>
<td>$E_a$</td>
<td>Activation energy, J/mol</td>
</tr>
<tr>
<td>$E_{ERE}$</td>
<td>Dimensionless excess rebound energy</td>
</tr>
<tr>
<td>$F$</td>
<td>Force, N</td>
</tr>
<tr>
<td>$F_b$</td>
<td>Amplitude of Brownian force, N</td>
</tr>
<tr>
<td>$f$</td>
<td>Fugacity, N/m$^2$</td>
</tr>
<tr>
<td>$G_b$</td>
<td>Turbulence kinetic energy generation due to the buoyancy, kg/m.s$^3$</td>
</tr>
<tr>
<td>$G_k$</td>
<td>Turbulence kinetic energy generation due to the mean velocity, kg/m.s$^3$</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravity acceleration, 9.81 m/s$^2$</td>
</tr>
<tr>
<td>$h$</td>
<td>Heat transfer coefficient, W/(m$^2$K)</td>
</tr>
<tr>
<td>$h_{fb}$</td>
<td>Latent heat, J/kg</td>
</tr>
<tr>
<td>$K$</td>
<td>Constant in the Saffman lift force equation, $K = 2.594$</td>
</tr>
<tr>
<td>$k$</td>
<td>Turbulence kinetic energy, m$^2$/s$^2$</td>
</tr>
<tr>
<td>$k_B$</td>
<td>Boltzmann constant = $1.38 \times 10^{-23}$ J/K</td>
</tr>
<tr>
<td>$k_d$</td>
<td>Deposition coefficient (velocity), m/s</td>
</tr>
<tr>
<td>$k_r$</td>
<td>Reaction rate constant, min$^{-1}$</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------</td>
<td>-------------------------------------------------------</td>
</tr>
<tr>
<td>$k_{\infty}$</td>
<td>Thermal conductivity of the continuous phase, W/(m.K)</td>
</tr>
<tr>
<td>$KE$</td>
<td>Droplet kinetic energy, J</td>
</tr>
<tr>
<td>$L$</td>
<td>Liquid phase fraction</td>
</tr>
<tr>
<td>$m$</td>
<td>Accumulated mass, kg</td>
</tr>
<tr>
<td>$m_p$</td>
<td>Particle mass, kg</td>
</tr>
<tr>
<td>$\dot{m}_d$</td>
<td>Deposition rate, kg/s</td>
</tr>
<tr>
<td>$\dot{m}_{volatile}$</td>
<td>Rate of formation of volatiles from reaction, kg/s</td>
</tr>
<tr>
<td>$MCR$</td>
<td>Micro carbon residue, measure of potential coke in an oil fraction determined by a specific testing procedure</td>
</tr>
<tr>
<td>$M_w$</td>
<td>Molecular weight, kg/mol</td>
</tr>
<tr>
<td>$Oh$</td>
<td>Ohnesorge number, $Oh = u_p / \sqrt{\rho_p \nu_p d_p}$</td>
</tr>
<tr>
<td>$P$</td>
<td>Pressure, N/m$^2$</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number, $Pr = c_p \mu / k_p$</td>
</tr>
<tr>
<td>$R$</td>
<td>Gas constant = 8.314 J/(mol.K)</td>
</tr>
<tr>
<td>$r$</td>
<td>Radial direction</td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>$Re_p$</td>
<td>Particle Reynolds number</td>
</tr>
<tr>
<td>$S_k$</td>
<td>Source term for turbulent kinetic energy</td>
</tr>
<tr>
<td>$S_{n,ff}$</td>
<td>Spectral density of the Brownian motion</td>
</tr>
</tbody>
</table>
$S_e$  
Source term for the turbulence dissipation rate

$Sc$  
Schmidt number, $Sc = \mu/(\rho_d d_p)$

$SE$  
Droplet surface energy, J

$Stk$  
Stokes number, $Stk = \tau u_g/d_c$

$T$  
Temperature, K

$T_L$  
Lagrangian fluid time scale, s

$T_\infty$  
Temperature of the continuous phase, K

$t$  
Time, s

$\bar{u}$  
Velocity vector, m/s

$u$  
Velocity, m/s

$u_g$  
Gas velocity, m/s

$u_p$  
Droplet (particle) velocity, m/s

$V$  
Vapour fraction

$V_m$  
Molar volume, m$^3$/mol

$W$  
Work, J

$We$  
Weber number, $We = \rho_d d_p u_p^2/\gamma$

$x$  
First axis direction, m

$x_i$  
Fraction of component $i$ in the liquid phase

$Y$  
Yield of volatiles in coking reaction
Maximum yield of volatiles in coking reaction

Second axis direction, m

Fraction of the component $i$ in the gas phase

Compressibility factor, dimensionless

Third axis direction

Fraction of the component $i$ in the mixture

Greek symbols

Surface tension, N/m

Turbulence dissipation rate, m$^2$/s$^3$

Kronecker delta function

Fugacity coefficient, dimensionless

Viscosity, Pa.s

Droplet viscosity, Pa.s

Kinematic viscosity, m$^2$/s

Contact angle, degree

Density, kg/m$^3$

Turbulence Prandtl number

Particle relaxation time, $\tau = \rho_p d_p^2 / 18 \mu_g$
Normal Gaussian distribution function
Acknowledgement

I would like to take this opportunity to express my profound gratitude to my supervisors, Dr. A.P. Watkinson, Dr. F. Taghipour and Dr. D. Posarac for their great help, support and guidance throughout my program.

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I would like to dedicate this thesis to my mother, my father and my friend Sarah for their great help, patience and encouragement throughout my difficulties.
Chapter 1. Introduction

With over 174 billion barrels of oil reserves, the oil sands of Alberta are a secure source of petroleum that rivals the resources of the Middle East (Reynolds, 2005). However, there is a great challenge to turn these reserves into productive capacity. Oil sands are naturally occurring mixtures of bitumen, water, sand and clay. After removing the water, sand and clay, the aim of upgrading the bitumen is to produce synthetic crude oil that can be used in refineries for the production of gasoline, diesel and other useful products. The process used by Syncrude Canada Ltd. one of the world's largest producers of synthetic crude oil from oil sands, involves mining, extraction and upgrading steps. A detailed description of the above steps is given in Appendix I.

A major challenge is to find better ways of upgrading the oil to meet consumer and environmental needs. One of the important problems in the upgrading of oil-sands bitumen that can have significant effects on the system operability is unwanted coke formation in different parts of the upgrading process.

1.1. Fouling in the scrubber section of the coker

In a synthetic crude oil production unit, the main function of the fluid coker is to break down heavy hydrocarbons in bitumen to produce volatiles and solid coke. The coker consists of three main parts: stripper section, fluidized bed coking reactor and scrubber section. The coking reaction occurs on the surface of particles in the fluidized bed reactor. The stripper is located at the bottom of the coking reactor and strips off the remaining liquid on the coke. The volatiles move through a cyclone to the scrubber section of the fluid coker. The main function of the scrubber is to cool and scrub heavy components from the hot vapour rising from the fluid coker. The scrubber overhead goes to a fractionator where Naphtha, Light Gas Oil (LGO) and Heavy Gas Oil (HGO) are separated. A part of HGO is used to cool the vapours in the scrubber. The schematic diagram of the scrubber can be seen in Figure 1.1. Although the cyclones are supposed to
remove coke particles and liquid droplets, some liquid droplets enter the scrubber. The scrubber has sets of sheds in the middle and a Koch-grid at the top. Heavy components are first cooled and scrubbed at the sheds by 325°C Atmospheric Topped Bitumen (ATB) and then enter the scrubber Koch-grid that is a structured packing with ten layers. The vapours are cooled in the grid by 325°C HGO. Fouling can occur in the structured grid packing of the scrubber section in the fluid coker.

**Figure 1.1** Schematic diagram of the scrubber section

The fouling process in the grid packed bed is assumed to occur as follows (Subudhi, 2006):

There are droplets of heavy hydrocarbons in the vapour some of which contact the packing surface and deposit on it. The deposit reacts to produce coke and volatiles at temperatures of 380–400°C. The volatiles evaporate whereas coke and non-volatile
fractions remain on the packing. This can increase the pressure drop in the grid section of the scrubber and eventually result in costly shutdowns of the fluid coker.

1.2. Application of Computational Fluid Dynamics (CFD)

Fouling is caused by attachment of fine droplets, deposition of which will be affected by their flow in the vicinity of packing surface. As a result, using CFD (Computational Fluid Dynamics) software such as FLUENT (ANSYS, Inc. Canonsburg, PA, USA) can give more information on the system by providing details of the flow and droplet transport to the surface. CFD can be applied in situations where the complete experimental study of the process is not economical. In such cases, CFD results are first validated for a simpler case by means of a simple experimental model and then simulations can be extended for the real process conditions and complex geometrical configurations to predict the behaviour of the system. In general, CFD is the science of predicting the flow hydrodynamics, heat transfer, mass transfer and other related phenomena by means of numerical calculations.

Subudhi (2006) developed a mathematical model for vapour/liquid counter-current pressure drop across the scrubber grid surface based on empirical equations for pressure drop, mass-transfer and coking kinetics. Finally, he suggested that the vapour, liquid flow and droplet size distribution need to be studied to give some accuracy to the calculation.

In the development of fouling or deposition, the essential steps are transport and adhesion of the fouling agents on the surface. CFD can be a valuable tool to improve our knowledge of the effect of different parameters on the deposition of droplets on the surface. It has been widely used previously for studying aerosol flow in different applications (Brandon and Aggarwal, 2001). Particle dispersion and deposition of aerosols have attracted attention of many researchers in the past few decades due to its wide applications (Tian and Ahmadi, 2007). As mentioned before, deposition of micro particles in the scrubber section of the synthetic crude oil production unit is considered the main factor in build-up of coke. Coke formation which increases pressure drop, can affect production costs; and can ultimately force shut down of the coker. As a result, any improvement in understanding the mechanism of deposition would result in direct
economic benefits in crude oil production. In this work, a CFD model is developed to study aerosol flow and deposition on a circular disk. One reason for using a simple geometry is to check the CFD model experimentally and to assess predictive power of CFD for predicting the trends in deposition behaviour as conditions such as droplet size distribution and flow parameters are changed. The developed model is extended to more closely simulate the industrial practice by including the phase equilibrium and reaction at high temperature.

1.3. Objectives

The overall objective of this project is to use CFD simulation to study the hydrodynamics of aerosol flow close to the surface of a circular disk in order to calculate the deposition rates of fine heavy oil droplets under a range of conditions applicable to fouling in the scrubber gird section of a fluid coker. The fouling process in the structured packing of a scrubber is assumed to occur as follows. The vapours that enter the scrubber contain some heavy hydrocarbon droplets, which were not removed in the cyclone. These droplets contact the packing surface and deposit on it. The heavy oil deposit reacts to produce coke and volatiles. The volatiles evaporate whereas coke and non-volatile fractions remain on the packing as the final deposit. The investigation of the fouling phenomena therefore is performed in two steps. First, the model will investigate the droplet deposition at room temperature and then it will be extended to high temperature hydrocarbon fouling conditions.

So, the specific objectives of this work are:

1-To study the hydrodynamics of gas-liquid flow close to a circular disk and the droplet deposition at room temperature, and to determine the capability of the model to predict effect of different parameters such as superficial gas velocity and droplet size. The model is to be verified with experimental data from the literature, and from experimental study.

2-To extend the model to high temperature conditions where phase equilibrium and reaction also play a role, to map out the effect of temperature and hydrocarbon mixture
composition on deposition and reaction, and to investigate the validity of results for high temperature conditions by comparison with an on-going experimental study.

3- To study the effect of different parameters in minimizing hydrocarbon fouling, with application to the grid fouling of the coker scrubber unit.
Chapter 2. Literature review

The transport of particles and fine droplets, and their deposition on surfaces is of great importance in numerous engineering and science applications. It is applicable to areas such as: air pollution and health physics including dust inhalation and deposition on human respiratory systems, micro-contamination in electronic industry, spray coatings, fire suppression, design of sampling and cleaning devices and fouling on heat transfer surfaces. For design improvements, developing reliable models that can predict the behaviour in these systems is important.

Much of the past work on particle deposition focuses on deposition in laminar flow. Levich (1972) has extensively reviewed particle deposition in laminar flow. Ramarao and Tien (1989) investigated aerosol deposition in two-dimensional laminar stagnation point flow including inertial impaction, interception and gravity, using analytical solution. Tsai and Liang (2002) used a similar approach for deposition on an axisymmetric plate also including the effects of Brownian diffusion.

For turbulent gas streams, the work in the area of aerosol deposition has been mostly devoted to deposition in ducts and pipes. An early model to study the deposition from turbulent gas streams was developed by Friedlander and Johnstone (1957). They defined the concept of stopping distance from which particles carried by eddies from turbulent core, move in free-flight towards the wall. One of the problems of their method was that they assumed a constant free-flight velocity whereas the velocity of particles will decrease as they approach the wall; another issue was that they did not account for the effects of molecular diffusion in their work. Cleaver and Yates (1975) tried to solve the problems associated by the concept of stopping distance by basing their work on a detailed study of the turbulent boundary layer. Their deposition model was based on the idea that particles are convected to the wall by turbulent “downsweeps”. Fluid is continually being swept towards the wall (i.e., in “downsweeps”) and ejected away from it in turbulent bursts. They assume that particles move to a certain distance from the surface by turbulent diffusion and then are carried to the surface by turbulent downsweeps. A viscous two-dimensional stagnation point method was used to model the
near-wall turbulence in their work. They calculated the particle trajectories by solving the equation of motion (Lagrangian approach) only accounting for Stokes drag force and neglecting gravity, buoyancy and lift forces. Papavergos and Hedley (1984) reviewed the existing work on particle deposition in turbulent flows. The theories were divided into main areas of classical turbulence concepts and more recent particle eddy interaction methods based on stochastic approaches. However, based on their review, existing models lacked the effect of external forces such as gravity and lift on deposition.

Fan and Ahmadi (1993) included the effect of external forces in their work. They extended the turbulent sub-layer model of Cleaver and Yates (1975) by including gravity and lift force in their calculation. They also accounted for the effect of Brownian diffusion and surface roughness. In their next paper, Fan and Ahmadi (1995) claimed that the plane stagnation method used previously provided discontinuous near wall vortices. So, they developed a model based on the results of stability analyses in channel flows to provide a continuous variation of velocity field for near-wall vortices. They also included particle rebounding in their model.

As precise modeling of turbulence can have major effects on prediction of particle deposition, exact simulation of turbulence has been also used in prediction of turbulent deposition in pipes. McLaughlin (1989) applied the Direct Numerical Simulation (DNS) method to simulate the three-dimensional, time-dependent flow. He used pseudo-spectral methods to examine the validity of inertial deposition by Friedlander and Johnstone (1957) and Cleaver and Yates (1975) by modeling the turbulence at the smallest scales. Later, Uijittewaal and Oliemans (1996) used both DNS and LES (Large Eddy Simulation) to model particle deposition in a cylinder at different Reynolds numbers. They showed that the capability of LES method was more limited at higher Reynolds numbers in comparison with DNS prediction.

As the Direct Numerical Simulation (DNS) is computationally so expensive despite its strong predictive power, Matida et al. (2000) used the near wall turbulence parameters estimated from the Direct Numerical Simulation (DNS) for the channel flow and fitted them to the k-epsilon method for the wall region. They showed that accurate prediction of particle deposition highly depends on the sufficient resolution of near wall turbulence,
which cannot be totally provided using conventional Reynolds Averaged Navier-Stokes (RANS) approaches. They claimed that their present approach may not be extended to more complex geometries with high Reynolds numbers for which DNS data is not available; however application of recent experimental techniques together with this method would be a possibility for providing accurate results. They use a one-way coupling Lagrangian model to simulate the particle trajectories.

Commercial software has also been used for prediction of deposition in duct flow. Tian and Ahmadi (2007) used FLUENT 6.1.22 and a series of different turbulence models and compared their results with available experimental data to evaluate the accuracy of various approaches. They showed that the use of an appropriate turbulence model was important in predictions of micro-particle flow in transport in turbulent flow fields. They showed that their “two zonal model” boundary condition together with Reynolds Stress Model (RSM) could reproduce the results of DNS simulation with a better agreement in comparison with k-epsilon methods. That is because RSM accounts for the anisotropy of turbulence whereas models such as k-epsilon do not account for it. They suggested that these guidelines could be applied for deposition at more complex conditions.

Whereas most of the work on modeling particle deposition has been devoted to deposition in ducts, there has been limited work on deposition on more complex geometries. The deposition of particles on bluff bodies can occur by different mechanisms of molecular diffusion, turbulent diffusion, and impaction. Sub-micron particles usually follow the flow path but might be carried to the wall by the Brownian motion of the fluid (molecular diffusion). For turbulent diffusion, particles might follow the flow path but have enough size that gain some velocity from the turbulent eddies, and are carried to the wall. Larger particles that have larger inertia follow their original path and are not affected by the flow until they hit the surface by inertial impaction. Li et al. (1994) studied the deposition on bluff bodies in an obstructed duct. They used a thermodynamically consistent algebraic stress model to simulate the mean fluid flow, and solved the equation of motion for particles accounting for Brownian motion, Stokes drag and Saffman lift force. They calculated the capture efficiencies for trapezoidal and rectangular blocks at different Stokes numbers. They showed that higher Stokes numbers
lead to higher capture efficiencies on the front side of the block. In addition, the slope on the front side of the trapezoidal block reduces the effectiveness of the inertial impaction mechanism. Brandon and Aggarwal (2001) studied the particle deposition on a cylinder placed in a two-phase unsteady laminar flow field. They included the drag and lift force in the equation of motion of particles and their work was extended by Salmanzadeh et al. (2007), by including the effects of gravity and studying the effects of blockage and obstruction aspect ratios.

Although theoretically, fluid mechanics can predict and explain how the particles transport to the wall as suggested above, it cannot predict if the particles would adhere to the wall. For prediction of particle deposition, the phenomena associated with contact of particles to the surface should also be included in the model. In the case of liquid droplets, there has been much effort devoted to investigating the behaviour of single droplets contacting a surface.

As suggested by Bai and Gossman (1995), seven different regimes can be defined as droplets impact the wall: (1) stick, in which droplets with little energy impact on a relatively cool surface and remain there in a spherical state (2) spread, in which the drop forms film on a dry wall or merges with a pre-existing film on a wetted surface, (3) rebound, in which the drop bounces in from the surface, (4) rebound with break up, in which the drop breaks up into two or three drops after impacting with a hot surface, (5) boiling-induced break-up caused by rapid boiling on a hot surface, (6) break up in which a film is first formed and subsequently disintegrates in a random manner, and (7) splash, in which the drop impacts at high velocity, forming a liquid crown from which disintegrating jets form. Clearly, regimes (1) and (2) lead to deposition, hence it is of value to determine the conditions which favour these regimes.

Mundo et al. (1995) reviewed droplet impingement on heated surfaces, cold surfaces and existing liquid films. Based on their review, droplet rebound was only possible for heated surfaces or existing liquid film under low droplet impingement energy (low Weber number normal to the wall). Weber number is a measure of droplet’s inertia compared to its surface tension and is defined as:
\[ We = \frac{\rho_p d_p u_p^2}{\gamma} \]  

(2.1)

On the cold surfaces, Mundo et al. (1995) restricted the associated phenomena to deposition and splashing. They used phase Doppler anemometry to determine the boundary of splashing and deposition regimes and characterize the size and velocity of the secondary droplets formed in the case of splashing. They defined the parameter \( K \) as:

\[ K = Oh \cdot Re^{1.25} \]  

(2.2)

Where \( Re \) is the droplet Reynolds number, and \( Oh \) is the droplet Ohnesorge number that relates the viscous and surface tension force. These dimensionless groups are defined by the following equations:

\[ Re = \frac{\rho_p d u_p}{\mu_p} \]  

(2.3)

\[ Oh = \frac{\mu_p}{\sqrt{\rho_p \gamma d}} \]  

(2.4)

Mundo et al. (1995) suggested that threshold for sticking and splashing regimes occurs at \( K = 57.7 \) i.e., with \( K < 57.7 \) for the cold surface deposition is favoured. Gavaises et al. (1996) suggested that rebounding or spreading of the liquid droplet depends on different factors such as droplet size, surface temperature, droplet velocity and surface material and roughness. They claim that an impinging droplet can rebound (with or without break up) or stick to the wall depending on the Weber number. Their model assumes that droplet is reflected from the surface if the Weber number just before impaction is smaller than a critical value. However, they believe that a general critical Weber number does not exist for all the cases. Their model does not differentiate between the rebounding and splashing regimes, and the critical Weber numbers applied by them are more likely to distinguish the splashing and sticking droplets.

Although droplet rebounding from a surface was reported in many studies, little theoretical work or experimental investigation exists to define conditions under which
rebounding can occur. Sikalo et al. (2005) investigated droplet rebound for dry and wetted surfaces of different material with liquids including water, isopropanol and glycerin and found a wide range of critical Weber numbers at different conditions.

Chandra and Avedisian (1991) in their investigation of droplet/surface impact showed that droplets can rebound under surface temperatures higher than the Leidenfrost temperature of the liquid and low impact energy. Leidenfrost temperature is the surface temperature beyond which a vapour layer forms between the droplet and surface before the droplet impacts the surface. Chandra and Avedisian (1991) used energy conservation of droplet before and after impact, and showed that maximum spread of the droplet depends on the droplet/surface contact angle. Contact angle is defined as the angle between the liquid/vapour interface and the solid surface. They claimed that at temperatures higher than the Leidenfrost temperature of the droplet, quick formation of a vapour film between droplet and surface largely increases the droplet/surface contact angle and facilitates rebounding of the droplet.

Mao et al. (1997) extended the use of the energy conservation of a liquid droplet to propose a model for rebounding of droplets from smooth surfaces. Their model showed that rebounding probability was a function of the droplet maximum spread and static contact angle. Their model suggested that the possibility of rebounding would increase as the static contact angle is increased, which qualitatively agreed with their experimental observations. Hsiao et al. (2009) extended the method of Mao et al. (1997) and developed an analytical model to also consider the effects of wetting and wall roughness. They defined a dimensionless droplet bouncing potential and performed high-speed image tests that correlated well with their model prediction.

Considering that surface properties can be changed in order to minimize or maximize sticking to the surface, in order to decrease or increase deposition, droplet/surface contact can be an important part of the deposition process. These phenomena must be incorporated in the Eulerian/Lagrangian simulation of gas/droplet flow to include droplet-wall interactions. There has been a limited amount of work which considers the droplet/surface contact in modeling droplet transport and deposition on the surfaces. Langrish and Kota (2007) studied the deposition rates for a water spray on a plate in a rectangular
box configuration using a simple RANS approach. They assumed a critical Weber number to distinguish rebounding and sticking droplets. Although as suggested before, the critical Weber number could depend on the surface and liquid properties, they did not consider any experimental measurement of the critical Weber in their case and. Their assumed value of the critical Weber number was very small (0.05) compared to values suggested by Sikalo et al. (2005) which was in the range of 1.03-15.6. Finally their simulation under predicted their own experimental data by about 75%.

Yoon et al. (2006) examined the transport of water droplets around a circular cylinder. They used the energy conservation method developed by Passandideh-Fard et al. (1996). The principles of their model were the same as given by Mao et al. (1997). However, claiming no relation was available on rebounding work from the surface, they based their model on experimental studies of molten metal droplets by Aziz and Chandra (2000) whereas their assumptions clearly could not be concluded from that work.

In the present case of deposition of heavy hydrocarbons at high temperatures, a deposition model also must deal with the phase equilibrium of the heavy hydrocarbon droplet-vapour system to estimate droplet concentration and size distribution at different temperatures. Jankovic (2005) simulated the scrubber section of the fluid coker using HYSYS and estimated the average droplet size, which could pass through the coker cyclone. Subudhi (2006) used HYSYS to calculate the gas/droplet properties in the scrubber section and used a mass transfer model on dry and irrigated surfaces to calculate deposition and pressure drop in the scrubber grid. His deposition model was based on the work of Papavergos and Hedley (1984), although these authors investigated deposition in duct flow (parallel flow) and did not consider deposition on obstructing surfaces.

To summarize, although different models has been developed for deposition of particles on surfaces, first of all to our knowledge there was no published work using commercial software for deposition on bluff bodies in turbulent flow. Moreover, the available models usually did not consider the effects of droplet/surface contact, or lacked logical assumptions in doing so. In addition, we are aware of no work on simultaneous usage of CFD and HYSYS to include the effects of temperature on the multi-component mixture phase equilibrium in this area.
This work tries to develop a precise droplet deposition model on a circular disk accounting for droplet transport and interaction with the wall for both turbulent and laminar flow, and finally extends the prediction of droplet deposition by a CFD model, to conditions where the hydrocarbon phase equilibrium and reaction play a role in fouling and coke formation.
Chapter 3. Experimental setup for model verification

The aim of this work is to use mathematical modeling to study the effect of different parameters on deposition in the scrubber section. However, the model will be developed for simpler conditions where the capability of model in prediction of deposition can be evaluated experimentally. So, the model is based on the experimental setups used in our group to study the same problem experimentally. In experimental work the problem is divided into two main parts: room temperature (cold) and high temperature (hot) unit tests. The room temperature unit tests are mostly used for the general study of deposition phenomena at room temperature and studying the effect of flow conditions and droplet size. The high temperature unit tests are applied to study deposition of heavy hydrocarbon material, mostly focusing on the effects of temperature and mixture composition. The detailed description of both setups can be found below.

3.1. Cold unit setup

The model will be first used to simulate experiments at room temperature and atmospheric pressure performed by B. Petkovic in the cold unit, schematically shown on Figure 3.1. The unit consists of a 7.5 cm diameter and 150 cm height glass column, in which a 5 cm diameter circular disk is placed normal to the upward flow. The disk is positioned 30 cm below the top of the column and is connected to the load cell above the unit through a 1.6 mm diameter rod.

Droplets are generated in the atomizer where air is used to atomize tri-ethylene glycol, or sugar solution. Generated aerosol flows through two elbows where large droplets are removed from it and collected as wash down. A gas distributor placed around the nozzle is used to add secondary air in order to obtain higher velocities in the column, up to 1.4 m/s. Flow of the liquid in the aerosol is measured using the balance (0.1g precision) placed below the column, as the difference between liquid flow to the nozzle and wash down liquid flow rates. Droplet size distribution in the flow is measured with
shadowgraphy, 45cm below the disk. The droplet size distribution is measured after stopping the flow. The droplet size distribution on the disk is also studied by means of a microscope. The deposition rates are read through load cell during the run times and also by initial and final weighing of the disk. By changing the air to nozzle flow rate and secondary air flow rate, gas superficial velocities between 0.4 to 1.4 m/s are covered. By changing the ratio of liquid/air to nozzle, the droplet size distribution changes can be measured by means of the shadowgraphy system.

![Figure 3.1 Schematic diagram of the cold unit](image-url)
3.2. Hot unit setup

The diagram of the flow sheet of the hot unit is shown in Figure 3.2.

**Figure 3.2** Schematic diagram of the hot unit
The hot unit consists of a stainless steel spray chamber with atomization system and a circular disk similar to the one in the cold unit. The chamber has 7.5 cm diameter and 1 m length. Because of the high temperature conditions and safety concerns high temperature unit is equipped with additional features to control the temperature and also reduce the amount of H₂S in the outlet gases. Downstream of the chamber are condenser and liquid accumulator tank, demister, scrubber and the afterburner system. The liquid feed is a mixture of bitumen (MEBR) and Voltesso. The bitumen contains heavy oil fraction with normal boiling points above 425°C, the maximum temperature used; whereas the Voltesso is a lighter hydrocarbon mixture and is primarily in the vapour phase in the spray chamber. The mixture is stored in a storage tank and is fed through a pump to the nozzle. Nitrogen is used for atomization of the liquid. Additional nitrogen is injected through the gas distributor to achieve higher velocities. High temperatures are provided by two different heaters known as lower and upper heaters and temperature is controlled with two controllers. The wash down liquid is collected at an oil receiver at the bottom of the spray chamber. The experiments were performed at disk temperatures of 295, 340, 370, 390 and 425°C for 5% and 10% MEBR mixtures by J. Song. The range of superficial velocities covered was between 0.2–0.9 m/s.

In both cases the modeling focused on the flow around the disk and deposition. As a result, the upper 0.7 m of the column was modeled assuming uniform inlet velocity profile at the inlet of the column to diminish complexities associated with flow through nozzle, gas distributor and atomization process. The uniform inlet velocity assumption was evaluated by comparing simulation of unit with nozzle and a fine mesh resolution in nozzle vicinity.
Chapter 4. Mathematical model

The mathematical modeling of hydrocarbon fouling on a circular disk is complex. So, the problem is broken into several steps. At the first step, a model is developed to study the transport and deposition of droplets to the circular disk. In order to do this, first gas flow hydrodynamics is simulated and particle (droplet) transport and deposition is modeled independently (Eulerian-Lagrangian approach). Next, droplet surface interaction is added to the model, and finally the effects of high temperature and reactions that lead to formation of coke are considered.

4.1. Droplet Transport model

The Eulerian-Lagrangian approach is applied to model the droplet transport to the surface. First, the mass and momentum conservation equations are solved for the primary phase (gas flow). Then the droplet trajectories are tracked in a Lagrangian frame of reference by solving the force balance (Newton's second law) for droplets. This method is applicable where the volume fraction of the secondary phase, in our case droplets, is small.

4.1.1 Governing equations for the primary phase flow

To model the gas flow, equations of motion are solved together with the equation of continuity. These equations result from the conservation of momentum and mass in the system. Under the laminar flow condition for a Newtonian fluid, these equations will be as following in the general form (Bird et al., 2001):

\[
\frac{\partial p}{\partial t} + \nabla \cdot \rho \vec{u} = 0
\]  \hspace{1cm} (4.1)

\[
\rho \left( \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right) = -\nabla P + \mu \nabla^2 \vec{u} + \vec{F}
\]  \hspace{1cm} (4.2)
FLUENT 6.1.22 solver is used to solve these equations numerically. Since the geometry is cylindrical, the 2D axisymmetric method is used, which will solve the equations below under the laminar flow conditions neglecting the $\theta$-direction:

$$\frac{1}{r} \frac{\partial}{\partial r} (ru_r) + \frac{\partial u_r}{\partial x} = 0$$  \hspace{1cm} (4.3)

$$r: \rho \left( \frac{\partial u_r}{\partial t} + u_r \frac{\partial u_r}{\partial r} + u_x \frac{\partial u_r}{\partial x} \right) = \frac{\partial p}{\partial r} + \mu \left[ \frac{1}{r} \frac{\partial}{\partial r} (ru_r) + \frac{\partial^2 u_r}{\partial x^2} \right] + \rho g_r$$  \hspace{1cm} (4.4)

$$x: \rho \left( \frac{\partial u_x}{\partial t} + u_r \frac{\partial u_x}{\partial r} + u_x \frac{\partial u_x}{\partial x} \right) = \frac{\partial p}{\partial x} + \mu \left[ \frac{1}{r} \frac{\partial}{\partial r} (ru_r) + \frac{\partial^2 u_x}{\partial x^2} \right] + \rho g_x$$  \hspace{1cm} (4.5)

Solving these equations consists of several steps:

1. Dividing the flow domain into discrete control volumes using computational grids
2. Integration of the governing equations in the control volumes to convert differential equations to algebraic equations
3. Linearization of the discretized equations and solution of the linear equations to get the values of dependant variables such as velocity and pressure

Pre-processing step (first step above) is performed in GAMBIT to create the geometry and generate the grids. Then FLUENT segregated solver is used to solve the governing differential equations.

4.1.2 Turbulent flow

Turbulent flow has fluctuating velocity fields that are computationally too demanding to be exactly solved. So, instead of the exact governing equations, usually averaged equations are developed to be solved less expensively. Each of these averaged models will have their own restrictions and choosing a suitable turbulence model will strongly depend on the nature of the problem and available resources. The Reynolds-averaged Navier-Stokes (RANS) equations govern the transport of the averaged flow quantities, with the whole range of the scales of turbulence being modeled. k-epsilon and its variants
and Reynolds Stress Model (RSM) are two forms of RANS models. (Fluent User’s Guide, 2005). In this method, solution variables are decomposed into mean and fluctuating components. For example, for the velocity component:

\[ u_i = \bar{u}_i + u'_i \] (4.6)

Substituting above equation in continuity and momentum conservation equations, and taking a time average leads to the following equations in the Cartesian tensor form:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0
\] (4.7)

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} [\mu (\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_i}{\partial x_i})] + \frac{\partial}{\partial x_j} (-\overline{\rho u'_i u'_j})
\] (4.8)

Additional term, the Reynolds stress \( \overline{\rho u'_i u'_j} \), must be modeled in order to account for effects of turbulence.

4.1.2.1. The k-epsilon model

k-epsilon model applies the Boussinesq hypothesis to relate the Reynolds stress term to the mean velocity gradients.

\[
-\overline{\rho u'_i u'_j} = \mu_t (\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}) - \frac{2}{3} (\rho k + \mu_t \frac{\partial u_i}{\partial x_i}) \delta_{ij}
\] (4.9)

\( \mu_t \) is the turbulent viscosity. In the case of k-epsilon model, two additional equations must be solved for turbulence kinetic energy \( k \), and turbulence dissipation rate \( \epsilon \), and \( \mu_t \) is calculated from them. For the standard k-epsilon method the equations for turbulence kinetic energy \( k \) and turbulence dissipation rate \( \epsilon \) are as follows:
\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) = \frac{\partial}{\partial x_j} [\left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j}] + G_k + G_b - \rho \varepsilon - Y_M + S_k
\]  
(4.10)

\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho \varepsilon u_i) = \frac{\partial}{\partial x_j} [\left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j}] + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \frac{\varepsilon^2}{k} + S_\varepsilon
\]  
(4.11)

And \( \mu_t \) is calculated by combining \( k , \varepsilon \):

\[
\mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon}
\]  
(4.12)

FLUENT uses the following default values for model constants:

\[ C_{1\varepsilon} = 1.44 , \ C_{2\varepsilon} = 1.92 , \ C_{\mu} = 0.09 , \ \sigma_k = 1.0 \ \text{and} \ \sigma_\varepsilon = 1.3 \]

These calculations are based on the work of Launder and Spalding (1972).

A different version of the k-epsilon method is the realizable k-epsilon model. The realizable k-epsilon model is a relatively recent development (Fluent User’s Guide, 2005) and differs from the standard k-epsilon model in two important ways:

1-The realizable k-epsilon model contains a new formulation for the turbulent viscosity.

2-A new transport equation for the dissipation rate \( \varepsilon \) has been derived from an exact equation for the transport of the mean-square vorticity fluctuation.

The term realizable means that the model satisfies certain mathematical constraints on the Reynolds stresses, consistent with the physics of turbulent flows.

For this model the epsilon equation will be:
\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_j} (\rho \varepsilon u_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_e} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \rho C_1 S \varepsilon \\
- \rho C_2 \varepsilon^2 \frac{\varepsilon}{k+\sqrt{\varepsilon}} + C_{1e} \frac{\varepsilon}{k} C_{3e} G_b + S \varepsilon
\]  

(4.13)

\( C_\mu \) will no longer be a constant number and will be defined as a function of mean strain and rotation rates, the angular velocity of the system rotation, and the turbulence fields.

4.1.2.2. Reynolds Stress Model (RSM)

The Boussinesq approach considers the same Reynolds stresses at all directions, so it does not account for anisotropy of the turbulence. A better representation of the turbulence in the system will need to calculate the Reynolds stresses in different directions individually. The Reynolds stress model involves calculation of the individual Reynolds stresses, using differential transport equations. The individual Reynolds stresses are then used to obtain the Reynolds-averaged momentum equation.

4.1.3 Discrete Phase model (Droplet transport)

As described before, the Eulerian/Lagrangian approach is used to model the droplet transport. After solving the flow equations for the primary phase flow (gas flow) as a continuum, the force balance will be applied on the secondary phase (droplets). The effects of droplets on gas phase and on each other are not included as the droplets are dispersed. The force balance will equate the droplet inertia with the forces acting on it. Writing the force balance in Cartesian coordinates in the x-direction will lead to:

\[
\frac{du_p}{dt} = \frac{18 \mu}{\rho_p d_p^2} C_p \text{Re}_p \frac{g_x}{24} (u - u_p) + \frac{g_x (\rho_p - \rho)}{\rho_p} + F_x
\]  

(4.14)

\[
\frac{du_p}{dt} = \frac{dx}{dt}
\]  

(4.15)

Where first term in the right hand side is the drag force per unit mass, the second term is gravity term and the last term is the external force. The external force in our case is a
combination of lift and Brownian forces for the cold unit, in addition to thermophoretic force for the hot unit.

4.1.3.1. Drag force

Drag is generally the resistant force that acts opposite to the flow direction of a particle moving in a fluid. The particle Reynolds number in the drag force is defined as:

\[
\text{Re}_p = \frac{\rho d_p |u - u_p|}{\mu}
\]  

(4.16)

The drag coefficient is calculated based on Hinds (1984), and at \(\text{Re}_p < 1\) it will be calculated by:

\[
C_D = \frac{24}{\text{Re}_p}
\]  

(4.17)

For \(1 < \text{Re}_p < 400\), it will be calculated by the following equation:

\[
C_D = \frac{24}{\text{Re}_p} (1 + 0.15 \text{Re}_p^{0.687})
\]  

(4.18)

4.1.3.2. Lift force

The Saffman (1965) lift force or lift due to shear is one of the forces that must be calculated as the forces acting on the droplets. The generalization by Li and Ahmadi (1995) is applied here as follows:

\[
F_i = \frac{2K\sqrt{\mu}}{\rho d_p (d_h d_k)^\frac{1}{4}} (u_j - u_{ij})
\]  

(4.19)

Where \(K = 2.594\) and \(d_{ij}\) is the deformation tensor.

4.1.3.3. Thermophoretic force
As a result of the temperature gradient in the gas phase a force known as thermophoretic force acts in the opposite direction on the suspended particles. This force is only included in the hot unit simulation. It can be calculated as (Fluent User’s Guide, 2005):

$$F_x = -D_{r,p} \frac{1}{m_p T} \frac{\partial T}{\partial x}$$  \hspace{1cm} (4.20)

$D_{r,p}$ is the thermophoretic coefficient (Talbot, 1980) and is a function of particle size, gas viscosity and mean free path of the fluid and $m_p$ is the particle mass.

4.1.3.4. Brownian motion

For submicron particles, the effect of Brownian motion can be considerable. Brownian forces are calculated as Gaussian white noise with spectral density:

$$S_{n,ij} = S_0 \delta_{ij}$$  \hspace{1cm} (4.21)

Where $\delta_{ij}$ is the Kronecker delta function and

$$S_0 = \frac{216 \kappa B T}{\pi^2 \rho d_p^5 \left( \frac{\rho_p}{\rho} \right)^2 C_c}$$  \hspace{1cm} (4.22)

Amplitudes of the Brownian forces are of the form:

$$F_{b_i} = \zeta_i \sqrt{\frac{\pi S_0}{\Delta t}}$$  \hspace{1cm} (4.23)

where $\zeta_i$ are zero-mean Gaussian random numbers. The amplitudes are calculated at each time step.
4.1.3.5. *Stochastic tracking*

When the flow is turbulent, the mean velocity will be applied to calculate the trajectories of droplets. To include the effects of fluctuating velocities due to turbulence, a stochastic approach can be applied. The Discrete Random Walk Model (DRW) is used to consider the interaction of particles with the turbulent eddies. Each eddy is characterized by a Gaussian distributed random velocity fluctuation, $u'$, $v'$, $w'$ and a time scale, $\tau_e$.

The values of fluctuating velocities during the lifetime of the turbulent eddy are sampled by assuming a Gaussian probability distribution as in the following equation:

$$ u' = \zeta \sqrt{u'^2} \quad (4.24) $$

where $\zeta$ is a normally distributed random number generated from a Gaussian probability density function of zero mean and $\sqrt{u'^2}$ is the root mean square of the fluctuating velocity. For the k-epsilon model assuming isotropic turbulence:

$$ \sqrt{u'^2} = \sqrt{v'^2} = \sqrt{w'^2} = \sqrt{2k/3} \quad (4.25) $$

When the Reynolds Stress Model (RSM) is used, the anisotropy of the turbulence included in the velocity fluctuations is considered.

$$ u' = \zeta \sqrt{u'^2} \quad (4.26) $$

$$ v' = \zeta \sqrt{v'^2} \quad (4.27) $$

$$ w' = \zeta \sqrt{w'^2} \quad (4.28) $$

The characteristic eddy time scale $\tau_e$ is either defined as a constant,

$$ \tau_e = 2T_L \quad (4.29) $$

or by the following equation:
\[ \tau_s = -T_L \log(r) \]  
(4.30)

where \( r \) is a uniform random between 0 and 1, and \( T_L \) is the Lagrangian fluid integral time that describes the time spent in turbulent motion along the particle path, and can be approximated as:

\[ T_L \approx 0.15 \frac{k}{\varepsilon} \]  
(4.31)

for the k-epsilon model. For RSM method \( T_L \) can be approximated as:

\[ T_L \approx 0.30 \frac{k}{\varepsilon} \]  
(4.32)

The particle is assumed to interact with the eddy during the eddy lifetime; after each eddy life time, the instantaneous velocity is updated by applying a new amount of \( \zeta \) (a random number generated from a Gaussian density function) in equation 4.24.

### 4.2. Droplet/Surface interaction model

The impact of the droplet to the surface is divided to several steps and energy conservation is applied to model the maximum spread and rebounding of the droplets. The rebounding criterion is mostly based on the work of Mao et al. (1997). For the low impact energy case that splashing does not occur, \( K < 57.7 \) (Mundo et al., 1995), the impact stages are shown in Figure 4.1.
Before the impact, the droplet energy will be a combination of the kinetic and surface energies.

\[ E_1 = KE_1 + SE_1 = \frac{\pi}{12} \rho d^3 + \pi d^2 \gamma_{LV} \]  

(4.33)

At stage 2, the droplet reaches its maximum spread diameter and is assumed to be a thin circular disk. The droplet energy at stage 2 is estimated as:

\[ E_2 = SE_2 = SE_{2,LV} + SE_{2,SL} - SE_{2,SV} \]  

(4.34)

\[ E_2 = A_p LV \gamma_{LV} + A_p SL \gamma_{SL} - A_p SV \gamma_{SV} \]  

(4.35)

Where \( LV \), \( SL \) and \( SV \) refer to liquid-vapour, solid-liquid and solid-vapour surfaces.

Using the Young equation \( \gamma_{SL} - \gamma_{SV} = \gamma_{LV} \cos \theta \) will give:
The energy conservation between stages (1) and (2) can be written as:

\[ KE_1 + SE_1 = SE_2 + W_{\text{Diss,2}} \quad (4.37) \]

\( W_{\text{Diss,2}} \) can be estimated from the work of Pasandideh-Fard et al. (1996) for stagnation point flow as following:

\[ W_{\text{Diss,2}} = \frac{\pi}{3} \rho u^2 d_n^2 d \frac{1}{\sqrt{\text{Re}}} \quad (4.38) \]

The maximum spread of droplets is calculated based on equations 4.37 and 4.38. Stage (3) is the maximum extent that droplet recoils or bounces and stage (4) is a virtual stage that droplet has rebounded.

\[ E_3 = E_2 - W_{\text{rebound}} \quad (4.39) \]

If the droplet bounces or recoils from the surface the droplet energy will be:

\[ E_3 = E_4 = SE_4 + KE_4 \quad (4.40) \]

So based on this equation if \( E_3 > SE_4 \) the droplet will have a kinetic energy to rebound, as a result the normalized excess energy can be used to describe tendency of a droplet to rebound:

\[ E_{\text{ERE}} = \frac{E_3 - SE_4}{SE_4} = \frac{E_2 - W_{\text{rebound}} - SE_4}{SE_4} > 0 \quad (4.41) \]

Using the empirical equation of Mao et al. (1995) for the rebounding work:
The excess rebound energy will have the following form:

\[
E_{\text{ERR}} = \frac{1}{4} \left( \frac{d_m}{d} \right)^2 (1 - \cos \theta) - 0.12 \left( \frac{d_m}{d} \right)^{2.3} (1 - \cos \theta)^{0.63} + \frac{2}{3} \left( \frac{d}{d_m} \right) - 1
\] (4.43)

In the modeling of droplet/surface interaction, first the critical value for splashing is checked for the droplets and then the droplets rebounding/sticking criteria are evaluated by calculating the rebounding excess energy. A User Defined Function (UDF) is developed for calculation of the droplet rebounding energy as it contacts the disk surface based on equations 4.37, 4.38 and 4.43.

4.3. Mixture phase equilibrium and flash calculations

To calculate the temperature-dependant concentrations of the liquid droplets in hydrocarbon mixture, and properties at high temperatures HYSYS is used. The objective here was to use the flash calculations at the desired temperature to get the essential information required for the CFD model and calculate the droplet concentration. Flash calculations use the mass balance for each component in the mixture.

\[
L + V = 1 \quad (4.44)
\]

\[
z_i = x_i L + y_i V \quad (4.45)
\]

\[
\sum x_i = 1 \quad (4.46)
\]

\[
\sum y_i = 1 \quad (4.47)
\]

Where \( L \) and \( V \) are the fraction of liquid and vapour. \( x_i \) and \( y_i \) present the fraction of the \( i \)-component in liquid and vapour phase. Another equation that will be used is the equilibrium constraint that fugacity of a component must be equal in both phases:
\[ f_i^l = f_i^* \] (4.48)

That can be written as:

\[ x_i \phi_i^l = y_i \phi_i^v \] (4.49)

where \( \phi_i^l \) and \( \phi_i^v \) are fugacity coefficients of \( i \)-component in vapour and liquid, and can be calculated from the following equation:

\[ RT \ln \phi_i = \int_0^P \left( \frac{\dot{V}_i}{P} - \frac{RT}{P} \right) dP \] (4.50)

\[ \dot{V}_i = \frac{\partial V}{\partial n_i} \] (4.51)

The above equations need to be solved iteratively to find the composition and molar fraction of each phase. However, for calculation of fugacity an equation of state must be defined. In the case of petroleum material, the Peng-Robinson equation is an appropriate equation of state. The Peng-Robinson equation of state can be presented in the following form:

\[ P = \frac{RT}{V-b} - \frac{a}{V(V+b)+b(V-b)} \] (4.52)

\[ Z = \frac{PV}{RT} \] (4.53)

where \( a \) and \( b \) represent deviation from ideal behaviour. The fugacity coefficient is defined for Peng-Robinson equation by:

\[ \ln \phi_i = \frac{b_i}{b} (Z - 1) - \ln(Z - B) \]

\[ -\frac{A}{2\sqrt{2B}} \left( \frac{2 \sum x_j a_{ij}}{a} - \frac{b_i}{b} \right) \ln \left( \frac{Z + (1 + \sqrt{2})B}{Z + (1 - \sqrt{2})B} \right) \] (4.54)
HYSYS solves the flash equations for the multi-component mixture, defined by means of the available boiling curves. The Peng-Robinson equation is used for calculation of the fugacity as stated above. Finally, the mass fraction of liquid and vapour is used for calculation of the droplet concentration. In addition, properties of the droplets are used for CFD modeling.

Concentrations calculated from HYSYS can be used together with the deposition velocity calculated from CFD to find out the deposition rate. The deposition rate is calculated by the following equation:

$$\dot{m}_d = k_d C_b A_d$$  \hspace{1cm} (4.55)  
where \( k_d \) is the deposition velocity coefficient, \( C_b \) is the bulk concentration of the droplets, and \( A_d \) is the disk surface area.

### 4.4. Heat and mass transfer model for droplets

The effect of temperature is not limited to the change in concentration; in the hot unit the droplet size distribution can change as a result of evaporation of the droplets. So, a heat transfer model is needed to calculate the evaporation of droplets and essential time for reaching equilibrium with their surroundings. Neglecting the effect of radiation, the energy conservation equation for the droplets is expressed as follow:

$$m_p c_p \frac{dT}{dt} = h A_p (T_\infty - T_p) + h_{lb} \frac{dm_p}{dt}$$  \hspace{1cm} (4.56)  

Here \( T_\infty \) refers to the surrounding gas temperature, and \( h_{lb} \) is the droplet latent heat. Feed is considered as a combination of fraction that can evaporate and fraction that stays in the liquid phase at each temperature. Physical properties and the percentage of the evaporating fraction at the desired conditions are calculated from HYSYS.

\( h \) can be calculated from the below correlation (Ranz and Marshall, 1952):

$$h = \frac{k_{in}}{d_p} (2.0 + 0.6 \text{Re}_p \text{Pr})$$  \hspace{1cm} (4.57)
And the rate of evaporation can be estimated by (Ranz and Marshall, 1952):
\[
\frac{dm_p}{dt} = D_p \left( 2.0 + 0.6 \text{Re}_p \text{Sc} \right) (C_0 - C) A_p M_w, \tag{4.58}
\]

where $C_0$ and $C$ refer to concentration of the component on the surface and in the bulk.

### 4.5. Reaction modeling

In the hot unit, the deposited droplets can go through reactions to form coke and volatiles. So, at high temperatures, evaporation of the volatiles resulting from the reaction can lead to the changes in the amount of the deposit on the disk.

\[
\text{Heavy oil deposit} \xrightarrow{\Delta} \text{Coke + Volatiles} \tag{4.59}
\]

Based on the work of Yue et al. (2004), the volatile yield for Athabasca pitch (+524°C) correlates well with a simple first order empirical model. The yield of volatiles follows the equation:
\[
\frac{dY}{dt} = k_r (Y^* - Y) \tag{4.60}
\]

where
\[
Y^* = 1 - \text{MCR} \tag{4.61}
\]
\[
k_r = k_{r0} \exp \left( \frac{-E_a}{RT} \right) \tag{4.62}
\]

and $Y^*$ is the maximum potential volatile forming in the oil. MCR (Micro Carbon Residue) is a measure of potential coke in an oil fraction, determined by a specific testing procedure. The MCR for Athabasca pitch is 27.1 wt%.

In integrated form this is written as:
\[
Y = Y^* (1 - \exp(-k_r t)) \tag{4.63}
\]
Writing the equation for transport and reaction together:

\[
\frac{dm}{dt} = \dot{m}_d - \dot{m}_{volatile} \tag{4.64}
\]

\[
\dot{m}_{volatile} = k_r [Y^* - Y(0)] m(0) + \ldots + k_r [Y^* - Y(t)] m(t) \tag{4.65}
\]

\[
= \int k_r Y^* \exp(-k_r t) m(t) dt
\]

Approximating \( m(t) \) that is the amount of mass added at time \( t \) with the deposition rate \( \dot{m}_d \), the final accumulation rate is calculated from:

\[
\frac{dm}{dt} = \dot{m}_d \left[ 1 - Y^* + Y^* \exp(-k_r t) \right] \tag{4.66}
\]
Chapter 5. CFD and HYSYS simulation

Simulation of the high temperature unit consists of two main parts using FLUENT and HYSYS, first part for modeling the flow hydrodynamics and transport and second part for modeling the mixture phase equilibrium. The simulation of the room temperature unit is limited to the first part. The following chapter will first discuss the steps in CFD simulation of gas-liquid flow including convergence criteria, mesh independence, effect of different turbulence models and will follow with the results of gas flow simulation and droplet tracking for specific cases. Finally, a description of the HYSYS setting used for approximation of droplet properties and concentration is provided.

5.1. CFD simulation

First the system was simulated together with nozzle with a very fine mesh in nozzle vicinity (total number of 389000 meshes). However, as the focus of the work was the flow around the disk, to avoid complexities associated with flow through the nozzle and gas distributor, and demanding computational effort, 0.7 m length column with uniform inlet velocity (same mass flow rate) was assumed and validity of this assumption was evaluated by comparing the flow upstream the disk for both cases with nozzle and uniform velocity at 1 m/s gas velocity.

<table>
<thead>
<tr>
<th>Table 5.1 Geometrical parameters of the base case</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column length used in simulation (m)</td>
</tr>
<tr>
<td>Column diameter (m)</td>
</tr>
<tr>
<td>Disk diameter (m)</td>
</tr>
<tr>
<td>Disk distance from the top (m)</td>
</tr>
</tbody>
</table>
The geometrical parameters of the base case are given in Table 5.1. Figure 5.1 compares the axial velocities upstream the disk for these cases.

![Graph showing axial velocity vs. radial position for uniform and non-uniform inlet velocities](image)

**Figure 5.1** Axial velocity vs. radial position for uniform inlet velocity and nozzle and secondary air simulation 0.3 m upstream the disk (Average inlet velocity 1m/s, standard k-epsilon model)

A two-dimensional axisymmetric model is applied, neglecting the terms in the angular direction. The computational domain for the base case simulation is shown in Figure 5.2.
Figure 5.2 The schematic diagram of the computational domain

The walls are considered as no slip and the outlet boundary condition is defined as being at atmospheric pressure. Primary simulation is performed with 24035 quadrilateral structured grids for inlet gas superficial velocity of 1 m/s, and to reach mesh independent results, simulations are repeated with total grid number of 95990 and 290000. The inlet gas material is air for the room temperature unit and nitrogen for the high temperature unit (with additional vapours from the evaporation of the hydrocarbon mixture). The properties of air and Tri-ethylene-glycol at room temperature are given in Table 5.2.
Table 5.2 Properties of gas (air) and liquid (tri-ethylene-glycol) at (15°C)

<table>
<thead>
<tr>
<th></th>
<th>Density (kg/m³)</th>
<th>Viscosity (cp)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>1.225</td>
<td>0.00179</td>
</tr>
<tr>
<td>Tri-ethylene-glycol</td>
<td>1146.022</td>
<td>48.5</td>
</tr>
</tbody>
</table>

The second order up-winding scheme is used for discretization of momentum, energy, turbulent kinetic energy and turbulent dissipation rate. To check convergence three different criteria were investigated:

1-Reduction of the scaled residuals to less than 10E-4 for momentum, velocities, turbulent kinetic energy and turbulent dissipation rate and less than 10E-7 for energy

2-Achievement of a stable mass flow rate at the outlet and total mass balance in the system

3-Checking the value of $y^+$ at the walls (for standard wall function $y^+$ at the center of the adjacent cell was checked to be between 30 and 300, $y^+$ close to 30 was the most desired. For enhanced wall treatment $y^+$ is checked to be lower than 5, where $y^+$ close to 1 was the most desired.)

A sample of the residuals can be observed in Figure 5.3 for the 1 m/s with the standard k-epsilon turbulence model and for 95990 meshes. Outlet mass flow rate is shown in Figure 5.4.
Figure 5.3 A sample residual curve during convergence ($u_g = 1$ m/s, standard k-epsilon model, 95990 meshes)

Figure 5.4 Outlet mass flow rate monitored as a convergence criteria ($u_g = 1$ m/s, standard k-epsilon model, 95990 meshes)
5.1.1 Mesh independence

To determine that results are independent of number of meshes, the axial and radial velocities are plotted close to the disk where the changes in the flow are steep for different mesh resolutions. The radial velocity is plotted for both mesh resolutions 1 cm upstream of the disk at different radial positions in Figure 5.5. In Figure 5.6 the axial velocity is plotted on the column centerline from one disk diameter upstream the disk to the disk.

A good agreement between the velocity profiles for both resolutions is observed; also increasing the number of mesh to 290000 did not cause considerable change in the velocity prediction. As a result, the resolution of 95990 was considered satisfactory for our purpose.

![Radial velocity profile](image)

**Figure 5.5** Radial velocity 1 cm upstream the disk for different mesh resolutions ($u_g = 1$ m/s, standard k-epsilon model)
Figure 5.6 Axial velocity on the centerline vs. distance from the disk for two different mesh resolutions ($u_g = 1$ m/s, standard k-epsilon model)

5.1.2 Effect of turbulence model

The simulation is first performed using the standard k-epsilon model and standard wall function. Then it is repeated with realizable k-epsilon and RSM (Reynolds Stress Model) using enhanced wall treatment and results are compared in Figure 5.7, Figure 5.8, and Figure 5.9 for axial and radial velocities close to the disk. It can be observed that using a different turbulence model does not change the main structure of the flow. However, the up to 15% variation can be observed in prediction of velocity magnitude between RSM and standard k-epsilon models. The average difference between predicted velocities from RSM and realizable k-epsilon model is less than 7%. Turbulent kinetic energy is shown in Figure 5.10, 1 mm upstream the disk at different radial positions. It seems standard k-epsilon model predicts much higher values for turbulence kinetic energy in comparison with RSM and realizable k-epsilon models. Although, this difference did not affect the general flow field that much, its effects on droplet deposition and dispersion can be very important.
Figure 5.7 Radial velocity 1 cm upstream the disk for different turbulence models ($u_g = 1$ m/s)

Figure 5.8 Radial velocity 1 mm upstream the disk for different turbulence models ($u_g = 1$ m/s)
Figure 5.9 Axial velocity on the centerline vs. distance from the disk for different mesh turbulence models ($u_g = 1 \text{ m/s}$)

Figure 5.10 Turbulence kinetic energy 1 mm upstream the disk versus radial position for different turbulence models ($u_g = 1 \text{ m/s}$)
RSM model is chosen for its greater strength in prediction of anisotropic turbulence (as discussed in Chapter 4) and droplet deposition (Tian and Ahmadi, 2007). Where achieving convergence for the RSM method was not possible, realizable k-epsilon model was used instead.

5.1.3 Gas flow velocity

![Figure 5.11](image)

**Figure 5.11** (a) Axial and (b) radial velocity contours for 1m/s gas inlet velocity, \( \text{Re}_g = 3440 \)
Axial and radial steady-state velocities are shown for air with gas inlet velocity of 1m/s \((Re_g = 3440)\) in Figure 5.11.

**Figure 5.12** Velocity vectors colored by velocity magnitude for 1m/s and 2m/s inlet gas velocity, \((Re_g = 3440, 6880)\)
Figure 5.12 shows the velocity vectors (the length of vectors can be representative of velocity magnitudes) around the disk at two different inlet velocities of 1m/s and 2m/s ($\text{Re}_g = 3440, 6880$). Some general features of the flow are:

1- Highest velocity magnitudes occur between the disk and the wall

2- The radial velocity increases from the centerline to the disk edge and as axial distance from the disk decreases

3- Backward flow and formation of vortices occurs downstream of the disk

5.1.4 Tracking droplets

As the gas velocity profile is calculated, the equation of motion of droplets can be solved to track them. Droplets are injected uniformly from the gas inlet. Different droplet diameters from 1–100 microns are tested. FLUENT uses droplet parcels as representative of greater numbers of real droplets. When stochastic tracking is applied, the number of parcels should be large enough to result in statistically dependable information. The number of injected droplets is increased until we can get results independent of the number of injections. Perfect sticking is assumed at column walls.

The particle traces are shown for 1m/s inlet gas velocity and different droplet sizes in the following figures accounting only for drag and lift forces, and neglecting stochastic behaviour and diffusion. Gravity force is neglected in Figure 5.13, but included in Figure 5.14. The droplets of size 1, 20 and 100 micron are plotted as samples. The larger droplets seem to have greater tendencies to follow their original paths, whereas smaller droplets are more likely to follow the general flow path. The effect of gravity seems to be more pronounced for the larger droplets. In the case without stochastic tracking, injection of 80 droplets leads to reproducible results. However, with stochastic tracking injection of a minimum number of 4000 parcels seemed necessary to get reproducible results. In Figure 5.14 for 100 micron droplets as a result of gravity some of them fall down close to the disk upstream surface and do not reach the disk while the effect of turbulent eddies is not considered.
Figure 5.13 Droplet tracking for (a) 1, (b) 20 and (c) 100 micron diameter droplets including drag and lift force on the droplets ($u_g = 1 \text{ m/s}$)

Figure 5.14 Droplet tracking for (a) 1, (b) 20 and (c) 100 micron droplets including drag, lift force and gravity on the droplets ($u_g = 1 \text{ m/s}$)
Figure 5.15 shows the droplet tracking for the same case, including the effects of stochastic tracking. As only 100 droplets are shown from the 4000 injected droplets, the shown droplet paths might not be a complete representation of the droplets behaviour. However, as the droplet size increases, greater number of droplets seem to reach the disk upstream surface and fewer droplets seem to be captured in the vortices downstream of the disk.

![Droplet tracking](image)

**Figure 5.15** Droplet tracking for (a) 1, (b) 20 and (c) 100 micron droplets including drag, lift force, gravity, and stochastic tracking on the droplets ($u_g = 1$ m/s)

### 5.2. HYSYS simulation

As described in chapter 3, a mixture of Voltesso and MEBR is fed as the liquid, atomized and carried up the column by nitrogen gas. The aim of the HYSYS simulation is to calculate the concentration of the liquid at different temperatures, and the properties of both vapour and liquid to be used for hot unit calculations. Voltesso and MEBR are
characterized in HYSYS based on the laboratory data available from their boiling curves. The boiling curves for MEBr and Voltesso are given in Appendix II. The mixed oil feed and nitrogen enter the column at different temperatures. As the lower heater and upper heater are at various temperatures, two different equilibrium stages are considered in the column. Flash calculations are performed to calculate the properties and liquid fraction. The PFD of the HYSYS setting used for calculations is shown in Figure 5.16. The properties of liquid and vapour from second stage are used for CFD simulation.

![Figure 5.16 PFD for the HYSYS setting for simulating the hot unit](image)

Properties of vapour and liquid for 5% and 10% MEBr mixture at hot unit conditions are calculated by HYSYS. Table 5.3 and Table 5.4 show the liquid properties at different temperatures for 5 and 10% MEBr mixture.
Table 5.3 Properties of liquid at different temperatures for 5% MEBR mixture

<table>
<thead>
<tr>
<th>Hot unit run number</th>
<th>Disk estimated temperature (˚C)</th>
<th>Density (kg/m³)</th>
<th>Viscosity (cp)</th>
<th>Surface tension (dyne/cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>296</td>
<td>873.1</td>
<td>8.76</td>
<td>18.2</td>
</tr>
<tr>
<td>17</td>
<td>340</td>
<td>867.6</td>
<td>8.65</td>
<td>16.7</td>
</tr>
<tr>
<td>18</td>
<td>370</td>
<td>855.6</td>
<td>8.45</td>
<td>15.4</td>
</tr>
<tr>
<td>11</td>
<td>425</td>
<td>839.1</td>
<td>6.23</td>
<td>13.6</td>
</tr>
</tbody>
</table>

Table 5.4 Properties of liquid at different temperatures for 10% MEBR mixture

<table>
<thead>
<tr>
<th>Hot unit run number</th>
<th>Disk estimated temperature (˚C)</th>
<th>Density (kg/m³)</th>
<th>Viscosity (cp)</th>
<th>Surface tension (dyne/cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>296</td>
<td>873.1</td>
<td>7.75</td>
<td>18.8</td>
</tr>
<tr>
<td>15</td>
<td>340</td>
<td>861.6</td>
<td>7.69</td>
<td>17.3</td>
</tr>
<tr>
<td>16</td>
<td>370</td>
<td>855.3</td>
<td>7.59</td>
<td>16.1</td>
</tr>
<tr>
<td>12</td>
<td>425</td>
<td>846.1</td>
<td>5.80</td>
<td>13.9</td>
</tr>
</tbody>
</table>

The calculated viscosities for the liquid phase for 5% MEBR mixture were higher than the calculated viscosities for the liquid phase for 10% MEBR mixture. This seemed counter-intuitive, and it might be because of the error in calculation of the mixture viscosity.
Chapter 6. Results and discussions

As mentioned previously, first the effect of flow parameters at low temperature unit is studied and then the effects of governing parameters in the high temperature unit are investigated. The following chapter will discuss the effect of different parameters on deposition, for both cold and hot unit, by comparing the prediction of developed model with literature data and experimental results in our group.

6.1. Room temperature unit conditions

The parameters that can play a role in the droplet deposition are those that govern the flow of the gas, transport of droplets to the disk and sticking of droplets to the surface. The effect of gas and liquid flow rates on atomization and as a result on the generated size distribution is not studied in this work, as in the industrial case droplets are not generated with the same procedure. As a result, droplet size distribution is not considered a function of gas flow rate in our simulations and effects of these two parameters are studied independently.

Although deposition velocity (deposition flux over bulk concentration) is usually the key parameter for deposition on surfaces, impaction capture efficiency is the parameter usually referred for deposition on bluff bodies. Impaction capture efficiency is defined as the number of deposited particles to the number of particles swept by the bluff body (disk in our case). To be able to check the CFD results with data from literature, for the room temperature unit the capture efficiency will be used to present deposition results.

6.1.1 Effect of droplet size and gas velocity

Larger droplets have larger inertia, so generally they are more likely to follow their original path and do not change their path as the flow diverges around the disk. Their relaxation time is large and so before they react to the change in gas flow they will reach the upstream surface of the disk. This can be also observed from droplet path lines in Figure 5.13 and Figure 5.15. Figure 6.1 shows capture efficiency of the upstream surface of the disk at different droplet sizes for three different superficial gas velocities of
1, 2 and 5 m/s. It can be seen that for different gas velocities the capture efficiency increases as the droplet size increases. However, the trends are different at different velocities showing that the capture efficiency is also a function of gas velocity.

![Graph showing capture efficiency vs droplet diameter for different gas velocities.]

Figure 6.1 The capture efficiency of the disk upstream surface at different droplet sizes ($\rho_p = 1146$ kg/m$^3$, $\mu = 0.00178$ cp)

As a result, a proper way of showing deposition on the bluff bodies would be to plot capture efficiency versus Stokes number. Stokes number is defined as the ratio of the stopping distance of a particle to a characteristic dimension of the obstacle.

$$Stk = \frac{\tau u_g}{d_c} = \frac{\rho_p d_p^2 u_g}{18\mu d_c}$$

(6.1)

Where, $\tau$ is the particle relaxation time defined as $\tau = \frac{\rho_p d_p^2}{18\mu}$, and $d_c$ is the disk diameter.

For higher Stokes numbers, particles will continue in a straight line as the fluid turns around the obstacle therefore impacting on the obstacle. For low Stokes numbers, particles will follow the fluid streamlines closely.
For smaller droplet sizes (lower $Stk$), the dependence of capture efficiencies on droplet size and gas velocity is weaker, as the main mechanism for deposition is not inertial impaction, and deposition is mainly controlled by molecular and eddy diffusion (Chapter 2).

The results were first checked in comparison with analytical solution of Ranz and Wong (1952) for the horizontal flow normal to a disk. The capture efficiencies are plotted for these two cases in Figure 6.2 versus Stokes number. The CFD simulation shows a very good agreement with results of the analytical solution of Ranz & Wong (1952). The fact that results of the analytical solution only based on drag force shows consistency with our numerical model, shows that eddy and molecular diffusion are not significant as the inertial impaction prevails ($Stk$ higher than 0.1).

![Figure 6.2 Capture efficiency vs. Stokes number for horizontal flow, from CFD simulation and analytical solution of Ranz and Wong (1952)](image)
Note that at a gas velocity of 1 m/s, $Stk = 0.1$ for the present system corresponds to a droplet diameter of 30 microns. For upward flow including the effects of gravity, the capture efficiencies are shown in Figure 6.3 together with experimental results of May & Clifford (1967) for air and di-butyl-phthalate. Their experiments were done for uniform droplet sizes from 20–40 microns and gas velocities of 2–6 m/s, where the diameters of the disk were between 0.1–2.9 cm. The predicted simulation results for upward flow seem to be lower in comparison with horizontal flow (Figure 6.2) due to the effects of gravity which also is observed in the experimental results of May and Clifford (1967). CFD simulation predicts the trend in the capture efficiency shown in experimental results of May and Clifford, but over predicts their results by 15%. This might be because of neglecting re-entrainment of the droplets in the model.

Figure 6.3 Capture efficiency vs. Stokes number for upward flow, from CFD simulation and experimental results of May & Clifford (1967)
Figure 6.4 shows the modeling results in comparison with the capture efficiency from the experimental work of Petkovic (2009). His capture efficiencies for different droplet sizes were calculated by means of measuring the droplet size distribution in the aerosol flow by shadowgraphy system, the size distribution of droplets on the disk upstream surface with a microscope, and the upstream deposition rate by analytical balance. Based on the measured parameters the capture efficiency was calculated by the following equation:

\[
E = \frac{m_{d,\text{upstream}} \cdot v_{i,\text{upstream}}}{u \cdot A_{\text{upstream}} \cdot c_b \cdot v_{i,\text{aerosol}}}
\]  

(6.2)

where \( v_{i,\text{upstream}} \) and \( v_{i,\text{aerosol}} \) are mass fractions of each droplet size obtained from measured size distribution in the aerosol and on the disk upstream surface.

Figure 6.4 The Capture efficiency vs. Stokes number for the disk upstream surface from CFD and experimental work
At Stokes higher than 0.2 the capture efficiencies of Petkovic are higher than 1, which is not logically possible. This might be because of problem in measuring the mass fraction of larger droplets by the shadowgraphy system. As described before, shadowgraphy measurements were performed after stopping the flow, whereas under this condition large droplets might fall down before being captured by the shadowgraphy. This can lead to considerable under prediction of the mass fraction of large droplets that causes unreasonable capture efficiencies for higher Stokes numbers. There is on-going work to improve these measurements. However, the model prediction and experimental measurements of Petkovic show a similar trend with the increase in the droplet size.

The calculated droplet capture efficiency versus Stokes number at different duct Reynolds numbers can be seen in Figure 6.5.

Figure 6.5 The calculated upstream capture efficiency vs. Stokes number at different gas Reynolds numbers
Although higher gas velocities (higher Stokes numbers) lead to larger amounts of deposition as shown in Figure 6.1, when the capture efficiency is plotted versus Stokes number, deposition shows a weak dependence on Reynolds number.

6.1.2 Deposition mechanisms on upstream/downstream surface
At higher Stokes number, the inertia of the droplets is larger and the possibility to follow their original path will be greater (Chapter 2). For higher droplet size and higher velocity (larger inertia) inertial impaction is the main mechanism for the upstream surface and the inertial capture efficiency on the upstream surface increases with Stokes number. At lower droplet sizes and lower velocities (lower Stokes) the governing mechanisms are eddy and molecular diffusion which are small in comparison with inertial impaction at high Stokes number.

Deposition on the downstream (back) surface of the disk is going to be small at high Stokes numbers, as in high Stokes numbers the droplets will follow their primary path and will not be captured in the vortices downstream of the disk.

![Figure 6.6 Capture efficiency of upstream and downstream surfaces of the disk at low Stokes number (u_g = 1 m/s)](image-url)
The capture efficiency is shown in Figure 6.6 for upstream/downstream surfaces at low Stokes numbers. It can be seen that the CFD model predicts the same trend as expected qualitatively, and that back surface capture efficiency is negligible for Stokes numbers larger than 0.1 where impaction is the main regime for deposition. These calculations are in basic agreement with experimental results of Vincent and Humphries (1978) who suggest that downstream capture efficiency is always very small and only comparable with front deposition at Stokes lower than 0.1.

6.1.3 Deposition for non-uniform size distribution

For a sample of non-uniform inlet droplet size distribution as shown in Figure 6.7, the simulation is performed for superficial gas velocity of 1 m/s ($Re_g = 3440$) for conditions of room temperature unit. The mass fractions of different droplet sizes are calculated on the disk upstream and downstream surfaces.

![Histogram of droplet size distribution](image)

**Figure 6.7** The distribution of different droplet sizes in the flow, disk upstream and downstream surfaces ($u_g = 1$ m/s, $\rho_p = 1146$ kg/m³ and $\mu = 0.00178$ cp)
The simulations suggest that no large droplets are deposited where the largest mass fraction of droplets have the size 5 micron. For the upstream surface the opposite is observed and the mass fraction of larger droplets in the deposit is greater than their fraction in the flow.

6.1.4 Effects of surface properties and contact angle

The surface material and properties can change the amount of deposition on the surface by two different means: roughness and contact angle. Roughness can change the droplet transport to the surface by changing the flow close to the surface. Roughness generally increases the amount of deposition. Lai et al. (1999) measured the aerosol deposition velocity in a duct and found that for a surface with two-dimensional ribs, the deposition velocity increased by a factor of 2–3 relative to the smooth surface.

Contact angle (the angle between vapour/droplet interface and solid surface) is a critical parameter for the surface-liquid interaction. Contact angle is a measure of wetting the surface by the droplet. At contact angles higher than 90 degrees, surface is not wetted by the droplet, which can have direct effect on rebounding of droplets. For 1 m/s droplet velocity ($\mu_p = 48.5 \text{ cp}$ and $\gamma = 0.00455 \text{ N/m}$), and different droplet sizes, the average dimensionless excess rebound energy (equation 4.43) is plotted versus the contact angle in Figure 6.8. It can be observed that for the above mentioned conditions only at contact angles higher than 150 degrees, is rebounding possible for 1 micron droplets. For larger droplet sizes, the excess rebound energy is negative at contact angles less than 170 degrees. As in the case of usual material like stainless steel and glass with contact angles of 50 and 20 degrees, based on these calculations respectively, perfect sticking is a reliable assumption. It can be observed that rebounding is very sensitive to the surface contact angle, and as the contact angle increases the possibility of rebounding is increasing. For low contact angles that the surface is wetted with the droplets, an increase in droplet size increases the maximum spread diameter. This decreases the chance for rebounding because the dissipation work is large, although the initial droplet energy is higher.
Figure 6.8 Dimensionless excess rebound energy vs. surface contact angle for 1 m/s droplet velocity and different droplet sizes ($\mu_p = 48.5$ cp and $\gamma = 0.00455$ N/m)

Figure 6.9 Dimensionless excess rebound energy vs. surface contact angle for 5 micron droplets at different droplet velocities ($\mu_p = 48.5$ cp and $\gamma = 0.00455$ N/m)
However, for high contact angles that the surface is not wetted with the surface, an increase in the droplet size increases the possibility of rebounding because the increase in the total energy is more important than the increase in dissipation work which is very small for high contact angles.

The effect of different contact angles on rebounding of a 5 micron droplet at different velocities is shown in Figure 6.9. It can be seen that at a given contact angle, for very low and high droplet velocities the excess rebound energy is higher.

![Graph showing the effect of droplet velocity on rebounding excess energy for different fixed contact angles](image)

**Figure 6.10** The effect of droplet velocity on the rebounding excess energy for different fixed contact angles ($\mu_p = 48.5$ cp and $\gamma = 0.00455$ N/m).

The same information on the effect of droplet velocity on excess rebound energy for a 5 micron droplet is shown, plotted for different contact angles in Figure 6.10. The potential for rebounding first decreases with the increase in the droplet velocity and at some velocity this pattern changes and the rebounding potential increases with increase in the velocity. By increasing the velocity, first rebounding work increases more than the droplet initial energy, as a result the excess rebound energy decreases, but increasing the
velocity more, makes the effect of droplet energy dominant and increases the potential for rebounding.

6.2. **High temperature unit conditions**

At high temperature conditions, the composition and concentration of the hydrocarbon liquid droplets, as well as the droplet size distribution change based on the operating conditions. Droplet deposition rates are calculated for conditions in the high temperature unit and compared with experimental measurements from load-cell and analytical balance. First the droplet concentrations are calculated based on liquid and vapour flow rates by HYSYS, and then deposition velocities are calculated from CFD modeling. The results of the two parts are merged for calculation of the deposition rates.

6.2.1 **Effect of droplet concentration**

The concentration of droplets which approach the disk, will depend on the upper and lower heater zone temperatures, liquid flow rate, liquid composition, wash down rate and gas superficial velocity. These parameters are read from the experimental measurements given in Appendix III for different experimental conditions at hot unit. Amount of the liquid and vapour phases (droplet concentration) calculated via HYSYS are tabulated in Appendix IV.

The calculated droplet concentrations are plotted versus the disk temperature in Figure 6.11. The mean droplet size in the hot unit was estimated by Petkovic (2009) to be in the range of 5 to 10 microns. In addition, from the calculation for the scrubber section of the fluid coker (Jankovic, 2005) the same range of droplet size was calculated in the scrubber section. Figure 6.12 shows the total deposition rates calculated from CFD for 5 and 10 micron droplets, together with experimental deposition rates (Song, 2009) versus the concentrations calculated from HYSYS. The effect of different temperatures on droplet size and reaction were not considered, and this calculation was only based on the change in the deposition rate by change in droplet concentration. For the experimental work however different temperatures could also affect the droplet size, properties and reaction of the deposited material.
Figure 6.11 Droplet concentration calculated by HYSYS vs. temperature for 10% and 5% MEBR mixture in Voltesso at superficial gas velocity of 0.3 m/s.

Figure 6.12 Total deposition rate on the disk vs. calculated droplet concentration for 10% and 5% MEBR at disk temperatures of 340–425°C, for 5 and 10 micron droplets.
The reproducibility of experimental data is discussed by Song (2009). The model prediction for 5 and 10 micron droplets differs with experimental measurements within the range of 17% and 6%. Run numbers and conditions of experiments for Figure 6.12 are given in Appendix III. Based on Figure 6.12 deposition rate is changing linearly with droplet concentration both from experimental and modeling results.

6.2.2 Effect of droplet size and velocity for high temperature unit
At the range of operation of the high temperature unit (velocities between 0.2–0.9 m/s) the deposition rate is not a strong function of velocity and average droplet size (Stokes number) and the downstream to upstream deposition ratio is high. At Stokes numbers less than 0.1, the deposition is mostly by molecular and eddy diffusion mechanisms and does not increase with Stokes number (as shown in Figure 6.6 for Stk < 0.02). Experimental data shown from the hot unit in Figure 6.13 for velocities lower than 0.9 m/s supports this trend. The conditions of the experimental runs used here are given in Table III.2.

![Graph](image)

**Figure 6.13** The total deposition rate for the high temperature unit vs. the superficial gas velocity at different droplet sizes (constant concentration)
By extending simulation to higher velocities, and larger diameters, the deposition rate seems to increase as the dominant deposition mechanism shifts from diffusion towards impaction and ratio of upstream to downstream deposition increases. For the 10 micron droplets, as Stokes number is higher the switch from diffusion to impaction regime happens at lower velocity. So, for larger droplets the effect of gas velocity on deposition will be more important. The downstream to upstream deposition ratio is plotted in Figure 6.14. This ratio decreases with the increase in velocity and as the inertial impaction becomes the dominating mechanism.

![Figure 6.14 Downstream to upstream deposition ratio vs. superficial velocities for different droplet size](image)

In addition, experimental results showed high ratios of downstream to upstream surface deposition, which supports the argument that these runs were in the diffusion regime which was also observed in CFD prediction for low Stokes numbers as shown in Figure 6.6.
6.2.3 The effect of temperature on deposition rates

Temperature can affect the deposition by several ways. First, by changing the droplet properties, concentration and size distribution in the system, temperature can change the droplet transport in the system. It can also change the droplet surface contact by changing the contact angle and surface properties. Finally high temperature will promote chemical reactions. Figure 6.11 showed the effect of temperature on droplet concentration for 5% and 10% mixture at different disk temperatures. The droplet size can also change as a result of evaporation of droplets in the column. To determine the droplet size at each temperature, first HYSYS is used to calculate what fraction of droplets can be volatilized at the desired temperature. The HYSYS assumes that the droplet is in equilibrium with the environment. Assuming that droplets enter the column at 150°C, and inlet average droplet size is 10 microns, the outlet average diameter and the volatile fraction of the 10% mixture at each temperature are shown in Table 6.1.

Table 6.1 The average outlet diameter for 10 micron inlet diameter droplets at different temperatures

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Volume fraction of volatiles (%)</th>
<th>Average outlet diameter (micron)</th>
</tr>
</thead>
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<tr>
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<tr>
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<tr>
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<td>0.897</td>
<td>4.486</td>
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</table>

As shown in Figure 6.13 the deposition rate in this size range does not highly depend on the change in droplet size. As a result for operating conditions similar to ours, the effect of changes of droplet size with temperature would not strongly influence the deposition
rates. However, if the operation is at high velocity conditions with larger droplet sizes the decrease in droplet size with temperature will influence the deposition rates more importantly.

The deposition rate for 10% MEBR mixture is shown in Figure 6.15 assuming 10 micron uniform droplets at the inlet (the effect of temperature on droplet size is included).

![Deposition rate vs. disk temperature](image)

**Figure 6.15** Total deposition rate vs. the disk temperature for 10% MEBR, gas velocity of 0.3 m/s and uniform inlet droplet size of 10 micron

The deposition rate decreases with temperature mainly as a result of change in the droplet concentration. Model prediction for deposition rate shows a good agreement with the trend of accumulation rate on the disk. At higher temperature the model prediction over-predicts the experimental measurements by 22%. This can be due to droplet re-entrainment and reaction.

For the 5% mixture shown in Figure 6.16, a larger discrepancy is observed between the model prediction and experimental measurements. The conditions of the experimental results used in Figure 6.15 and Figure 6.16 are given in Appendix III.

For the 5% low temperature run at 295°C, since the lower furnace temperature is much lower in comparison with other runs (205°C), and as shown in Figure 6.11, at this
temperature the concentration of droplets is much higher, assuming that droplets reach the disk temperature, might be the source of error in prediction of real droplet concentration.

Figure 6.16 Total deposition rate vs. the disk temperature for 5% MEBR, gas velocity of 0.3 m/s and uniform inlet droplet size of 10 micron

For both model prediction and experimental measurements, deposition rates are higher for the 10% mixture because of the higher concentration of liquid droplets

6.2.4 Effects of reaction

At high temperatures as the deposit is formed on the disk it can react to form volatiles and coke. The volatiles are then released and the non-volatiles remain on the disk as deposit. The yield of the volatiles is a function of temperature and run length for high temperature unit.

Figure 6.16 shows the effect of temperature on formation of volatiles for the same run length as in high temperature unit experiments based on equation 4.61 and 4.62. The MCR for Athabasca pitch is 27.1 wt%, $E_a = 197.5$ kJ/mol and $k_{r0} = 1.233E13$ min$^{-1}$. The
yield of volatiles increases by increase in temperature and as a result the amount of deposit on the disk will decrease because of evaporation of volatiles formed.

Increasing the length of runs can also have the same effect at conditions similar to high temperature unit experiments by reducing the deposit amount because of evaporation of the formed volatiles. Figure 6.18 shows the effect of run length on the yield of volatiles at different operating temperatures, according to equation 4.62. The increase in the run length generally increases the yield of volatile, but this effect is more important in lower run length. Including the effect of reaction on calculation of accumulated mass on the disk will lead to reductions in the predicted deposition rates on the disk especially at higher temperatures.

![Graph showing the effect of temperature on formation of volatiles in coking reaction for 260 min run](image)

**Figure 6.17** The effect of temperature on formation of volatiles in coking reaction for 260 min run
Figure 6.18 Effects of run length on the yield of volatiles at different temperatures

Figure 6.18 shows the deposition rates after including the effect of reaction at different temperatures (equation 4.65). Better agreement is observed at higher temperatures between modeling and experimental results after including the reaction effects.

It can be seen that the effect of reaction is more significant at higher temperatures. Also it can be predicted that increasing the length of runs will lead to lower accumulation on the disk as the deposit will lose weight by reacting and realising volatiles (aging). Figure 6.20 shows the same predictions for 5% MEBR mixture, the discrepancy between model and experimental measurements also decreases for this case, as the reaction is included in the model.
Figure 6.19 Deposition rates vs. temperature including the effects of reaction for 10% MEBR mixture and 0.3 m/s gas velocity.

Figure 6.20 Deposition rates vs. temperature including the effects of reaction for 5% MEBR mixture and 0.3 m/s gas velocity.
7.1. Concluding remarks

A model was developed to study deposition of heavy hydrocarbon droplets on a circular disk at different conditions, combining CFD and HYSYS simulation. First, the model was developed for deposition of droplets on the disk surface at room temperature. Then, the model was extended to conditions of the hot unit experiments where temperature also affected the deposition, and phase equilibrium and reaction were also of importance.

The predicted results for deposition in the cold unit were in agreement with results existing in the literature for both horizontal and vertical flow over a disk. They were also tested for tri-ethylene glycol experiments done as part of the present project. The capture efficiency of the disk increases as droplet size and gas velocity increase and can be characterized by means of the droplet Stokes number $\frac{\rho_p d_p^2 u_g}{18 \mu d_e}$. The cold unit simulation showed that deposition strongly depends on the droplet size and gas velocity at Stokes numbers higher than 0.1. Deposition in this range is controlled by the inertial impaction of droplets on the upstream surface of the disk. At Stokes numbers smaller than 0.1 where eddy and molecular diffusion are the main deposition mechanisms, the downstream to upstream deposition ratio is larger than 1 and capture efficiency shows much less dependence to Stokes number. The capture efficiency for the upstream surface slightly decreases with increase in Stokes number at very low stoke numbers, but starts to increase as inertial impaction starts to prevail. The capture efficiency for the downstream surface is important at very low Stokes and becomes negligible in Stokes higher than 0.1. As a result, for a non-uniform size distribution of droplets at inlet gas velocity of 1 m/s, the upstream surface showed greater capability in capturing the larger droplets (droplets larger than 20 micron) and small droplets (less than 10 micron) showed more tendency for deposition on the downstream surface. Although the effects of geometrical
configuration of the disk were not directly investigated, it can be stated that by increasing
the disk diameter in the impaction regime, the decrease in Stokes number will lead to
decrease in the capture efficiency.

The perfect sticking of droplets to the surface seemed to be a logical assumption
considering the range of contact angles that were tested for both cold and hot unit.
Rebounding of droplets was limited to contact angles larger than 120 degrees in our range
of operation. The possibility of rebounding increased with increase in the contact angle.
Moreover, for sufficiently high contact angles that the surface was not wetted, increase in
the droplet size increased the possibility for rebounding as the droplet initial contact
energy increased. For low contact angles such that the surface was wetted, increase in the
droplet size increased the dissipation work more than the initial droplet energy, and as a
result decreased the possibility of rebounding.

The deposition showed almost a linear relation with droplet concentration which was also
demonstrated by experimental measurements.

For hydrocarbon mixture atomized in nitrogen, temperature seemed to have major effects
on deposition rate mainly by changing the droplet concentration. Generally, higher
temperatures led to lower concentration of droplets in the system and as a result, a
smaller deposition rate. Changes in droplet properties with temperature did not
significantly affect the deposition rate. However, temperature has a direct effect on the
average droplet size; if impaction is the main mechanism for the hot unit deposition, this
would also decrease the deposition rate by decreasing the droplet size (Stokes number).
However, in the range of operation of the hot unit, droplet transport mostly occurs by
eddy and molecular diffusion (low Stokes numbers), and changes of droplet size with
temperature did not have major effects on the deposition rates.

For hot unit, high ratio of downstream to upstream deposition from experiments, also
approved that inertial impaction was not important at the range of operation of hot unit.
This was also in agreement with CFD prediction that at low Stokes numbers a high ratio
of downstream to upstream deposition is expected.
The combination of CFD and HYSYS simulations could provide good agreement with the deposition rates measured from experiments at different temperatures. However, the model prediction seemed to over predict the deposition rates at high temperatures by 22%. The reaction of the deposited material would reduce the final amount of deposit because of the release of the formed volatiles. Effects of temperature and run duration were studied on formation of volatiles. Higher temperatures and longer runs increased the yield of volatiles, leading to lower accumulation of deposits. By including this effect of reaction on the depositing mass, a better prediction of the deposition rates was provided at higher temperatures.

To summarize, the model showed good agreement with the available data from the literature for deposition on the disk and effects of droplet size and gas velocity. In addition, when combined with HYSYS predictions for system phase behaviour, it showed a good capability in predicting the effects of temperature and concentration on heavy oil deposition rates. Moreover, the model could provide information on droplet rebounding and surface properties that would associate with minimization of droplet sticking to the surface.

7.2. Recommendations

The developed model showed good capability for prediction of deposition and fouling under non-irrigated conditions on a simple geometry of a circular disk at different temperatures. Gas velocity and droplet size controlled the deposition at these conditions. Although controlling these parameters in the industrial coker might not be possible, the minimization of both will generally decrease the rate of deposition and fouling. If possible, process conditions leading to impaction regime for the droplets (Stokes higher than 0.1) should be avoided. Moreover, choosing a suitable configuration for the surface to minimize the capture efficiency, for example by using a sloped or curved surface might help. The effect of different geometries can be further studied by applying the developed model for such conditions.

To give more accuracy to the study, the measurement of droplet size distribution for the cold unit should be improved and a method should be developed for direct measurement.
of the droplet size distribution in the hot unit. In addition, the droplet concentrations calculated from HYSYS should be verified independently especially at low temperatures by an experimental method. A study of droplet re-entrainment at different conditions and including its effects in our model would improve the model predictions. Direct Numerical Simulation (DNS) can be used for a more precise presentation of the near wall turbulence and as a result an improved prediction of the deposition. Effect of surface roughness and surface change over time can be included in the model to more closely simulate the real conditions.

Although increasing contact angles directly increases the possibility of rebounding, rebounding seemed to be limited to the conditions that droplet did not wet the surface. As a result, in order to minimize the deposition by means of change in surface properties in addition to minimizing the surface roughness, using super-hydrophobic material such as some Teflon products might be useful. Further investigations with super hydro-phobic material that can be used at high temperatures or conditions leading to high surface contact angles like where Leidenfrost phenomenon takes place can be another direction to extend the work. Experimental Study of the contact of a single heavy oil droplet at high temperatures with different surfaces would provide a better understanding of such phenomena. Moreover, modeling of the system under conditions that rebounding is applicable and its experimental verification can be helpful.

On the effect of temperature, from this work, increase in temperature decreased the deposition rates both by decreasing the droplet concentration and evaporation of volatiles formed in coking reaction on a non-irrigated surface. For improving the model at high temperature conditions effect of non-equilibrium conditions can be studied by by-passing some of the feed for better prediction of droplet concentration. Also, HYSYS and FLUENT can be integrated to calculate the heat transfer and evaporation simultaneously. For the industrial case, as the droplets are heavier at higher temperature and the surface is washed down frequently, any general statement on the effect of temperature would require further investigation.
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Appendix I. Production of Synthetic Crude oil from Oil Sands

A detailed description of different steps for turning oil sands to crude oil is provided in this section based on the process used at Syncrude (http://www.syncrude.ca/).

Figure I.1 The block diagram for the synthetic crude oil production.
The schematic diagram of the whole process can be seen in Figure I.1.

I.I. Mining

The process of turning oil sand into crude oil begins with mining the resource. Because the oil sand in Syncrude’s leases is not deeply buried, surface mining is the most viable method of recovery.

- Layers of muskeg and earth are removed first. Suitable soil materials are used in ongoing reclamation.
- Beneath the muskeg is a layer of overburden, which is removed to expose the thick deposit of oil sand.
- Trucks and shovels remove the overburden and mine the oil sand.
- The oil sand is trucked to crushers, where large chunks are broken down for transport via hydrotransport or conveyor to bitumen extraction facilities.

I.II. Bitumen Extraction

Separating the bitumen from the sand is the primary objective of Extraction. Bitumen is extracted from the oil sand using the hot water process.

- Oil sand is fed into tumblers where steam, hot water and caustic soda are added to form slurry and condition it for bitumen separation.
- Froth mixes with this slurry in the tumblers, and then the combined slurry is discharged onto vibrating screens where large material is rejected.
- This feed is blended with the oil sand slurry from the North mine hydrotransport system.
- The blended slurry is fed into four Primary Separation Vessels (PSVs) and two Auxiliary Settling Areas (ASAs). The bitumen primary froth floats to the top, the sand settles to the bottom, and middlings are pumped to Tailings Oil Recovery (TOR) vessels.
- Froth from the TOR vessels is recycled through the PSVs to improve its quality.
• Bitumen recovered from TOR vessel middlings is processed by a secondary flotation plant, and then combined with the PSV’s primary froth.

• The feed is then deaerated, heated and fed into the Froth Treatment Plant.

• Oil sand slurry is hydrotransported to PSVs, during which time it has already been conditioned for bitumen separation, eliminating the need for tumblers. The froth then travels via pipeline to the operation for froth cleaning, treatment and bitumen upgrading.

I.III. Bitumen Upgrading

Through upgrading, Syncrude converts bitumen into hydrocarbon streams – Naphtha, Light Gas Oil (LGO) and Heavy Gas Oil (HGO) – that are blended to create high quality, light, low sulphur crude oil known as Syncrude Crude Oil. There are two basic steps to this upgrading process: Primary Upgrading and Secondary Upgrading.

Primary Upgrading

In Primary Upgrading, the process begins with diluted bitumen fed into the Diluent Recovery Units (DRU) where water is removed and naphtha is recovered to be recycled through Extraction. The resulting dry bitumen is fed to the cokers, the LC-Finer and the Vacuum Distillation Unit (VDU) for further processing.

• LGO and HGO are distilled off in the VDU and sent to hydrotreaters. The remaining bitumen is sent to the LC-Finer and cokers.

• LGO and HGO are formed in the LC-Finer, through the use of hydrogen addition via a catalyst, and sent to hydrotreaters. The remaining bitumen is sent to the cokers.

• Naphtha, LGO, HGO are produced in the cokers, through chemical reaction using hot coke, and sent to hydrotreaters.

Secondary Upgrading
Secondary Upgrading is where the impurities such as sulphur and nitrogen are removed from the naphtha, LGO and HGO by hydrotreating. The treated gas oils and naphtha are then blended together forming Syncrude Crude Oil and shipped to downstream refineries.
Appendix II. Distillation curves for Voltesso and MEBR

Table II.1 ASTM D2877 distillation curve for Voltesso

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<th>wt%</th>
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### Appendix III. Run numbers and conditions of experiments

#### Table III.1 The conditions of runs for Figure 6.12

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<th>Top furnace temperature</th>
<th>Wash-down rate (g/min)</th>
<th>Gas velocity (m/s)</th>
<th>Deposition rate (mg/hr)</th>
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<th>Oil flow (g/min)</th>
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<th>Top furnace temperature</th>
<th>Wash-down rate (g/min)</th>
<th>Gas velocity (m/s)</th>
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#### Table III.3 The conditions of runs for Figure 6.15

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<th>Oil flow (g/min)</th>
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<th>Wash-down rate (g/min)</th>
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Appendix IV. HYSYS Simulation results

Table IV.1 Vapour and liquid flow rates calculated by HYSYS

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