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Modeling Fluid Coker Cyclone Fouling

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Abstract

Fluid Coking^{TM} is a continuous process that thermally converts heavy hydrocarbons, such as oil-sands bitumen, to lighter and higher-value products by horizontal injection onto a fluidized bed of hot coke particles. The deposition of carbonaceous materials in the cyclone sections of commercial Fluid Cokers has been observed throughout each run. The main objective of this work is to improve unit reliability by proposing cyclone fouling mitigation strategies based on a localized phenomenological model using Aspen Plus®. The heavy ends condensation fouling mechanism was studied by incorporating vapour-liquid thermodynamics, thermal cracking reactions, and overall fluid dynamics in the Fluid Coker. Four case studies were performed to determine the impacts of transfer line temperature, hot coke flow rate, hot coke entrainment and scouring coke flow rate on the predicted temperatures and liquid flow rates. Scouring coke flow rate was identified as the most promising process lever to mitigate Fluid Coker cyclone fouling.

Keywords

Cyclone fouling, Aspen Plus modeling, thermal cracking, vapour condensation, Ranque-Hilsch

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Nomenclature

A	Arrhenius pre-exponential factor, s^{-1}
β	Ratio of two squared pipe diameters in a pipe contraction
d_1	Diameter of smaller pipe in a pipe contraction, m
d_2	Diameter of the larger pipe in a pipe contraction, m
D_b	Cyclone barrel diameter, m
d_{hi}	Hydraulic diameter of cyclone inlet, m^2
E_a	Activation energy, kJ/mol
f	Fanning friction factor
f_{tc}	Thermal cracking fraction, mass. frac.
ΔH_r	Heat of reaction, kJ/kg
θ	Angle of contraction in a pipe contraction
K	Resistance coefficient due to contraction
K_{fi}	Contraction coefficient for flow from freeboard to cyclone inlet
K_o	Contraction coefficient for flow from cyclone barrel to cyclone outlet
k_{VR}	Rate constant, s^{-1}
L	Solids loading, kg of solids/m^3 of gas
μ	Gas viscosity, kg/(m·s)
N_s	Number of solid spirals in a cyclone
ΔP_{bf}	Cyclone barrel friction pressure drop, kPa
$\Delta P_{(f-i)g}$	Gas contraction pressure drop from freeboard to cyclone inlet, kPa
$\Delta P_{(f-i)p}$	Acceleration of solids pressure drop, kPa
ΔP_o	Cyclone exit pressure drop, kPa
ΔP_r	Gas reversal pressure drop, kPa
ρ_g	Gas density, kg/m^3
ρ_p	Particle density, kg/m^3

Q_{VR}	Heat loss in a Fluid Coker zone due to thermal cracking, kJ/s
R	Gas constant, kJ/mol·K
Re_{hi}	Reynold's number at the cyclone inlet based on d_{hi} (average velocity)
r_{VR}	Rate of conversion of vacuum residue, s^{-1}
T	Temperature of a Fluid Coker zone, ˚C
U_b	Gas velocity in the cyclone barrel, m/s
U_f,	Gas velocity in freeboard of fluidized bed, m/s
U_i	Cyclone inlet gas velocity, m/s
U_o	Gas velocity in cyclone outlet tube, m/s
U_{pi}	Particle velocity at solids inlet, m/s
U_{pf}	Particle velocity in freeboard of fluidized bed, m/s
V	Volume of a Fluid Coker zone, m^3
W_{VR}	Concentration of vacuum residue, kg/m^3

Chapter 1

1 Introduction

1.1 Synthetic crude oil production via bitumen upgrading in Canada

Global energy demand is projected to increase 30% by 2040 to meet the needs of a growing and increasingly urbanized world (International Energy Agency, 2017). This will require increased production from a mix of energy sources, including oil, coal, natural gas, hydro, nuclear and renewables. Oil demand is projected to increase 10% by 2040, particularly for petrochemicals, road freight, aviation and shipping (International Energy Agency, 2017). Canada has the third-largest proven oil reserve in the world, estimated at 171 billion barrels that are economically recoverable using current technology (CAPP, 2018). The oil sands represent 97% of this reserve and are located in three deposits within the provinces of Alberta and Saskatchewan: Athabasca, Cold Lake, and Peace River. Bitumen is recovered using surface mining technologies when the oil sands are located within 70 meters of the surface or using in-situ recovery technologies when the oil sands are located 70 meters or more below the surface. Extracted bitumen is a highly viscous substance containing 50 – 60 wt.% of vacuum residue, i.e., components which must be converted to distillable fractions by upgrading processes in order to be blended into crude oils.

The Syncrude Project is a joint venture among Imperial Oil Resources Limited; Nexen Oil Sands Partnership; Sinopec Oil Sands Partnership; and Suncor Energy Inc. (with the Suncor interest held by Canadian Oil Sands Partnership #1 and Suncor Energy Ventures Partnership, both wholly owned affiliates of Suncor Energy Inc.), as the project owners, and Syncrude as the project operator. Syncrude's Mildred Lake facility is located 40 kilometers north of Fort McMurray, Alberta, and produces Syncrude Crude Oil (SCO) at a current capacity of 350,000 barrels per day from the Athabasca oil sand deposit. The Syncrude operation involves surfacing mining the oil sand, extracting raw bitumen from the sand, and upgrading the bitumen into SCO. During the upgrading process, bitumen is extracted and separated from the oil sand and then distilled at near atmospheric pressure into Light Gas Oil and Atmospheric Tower Bottoms (ATB). A portion of the ATB is distilled a second time at vacuum pressure into Heavy Gas Oil and Vacuum Tower Bottoms (VTB). The ATB and VTB are then upgraded via the LC-Finer hydroprocessor (hydrogen addition) or the Fluid Coker reactor (carbon removal). Products from these units are then sent to fixed bed hydrotreators for nitrogen and sulfur removal prior to blending.

1.2 The Fluid Coker

This thesis focuses on the Fluid Coker reactor, shown in Figure 1. Fluid coking technology was developed by Exxon Mobil Research the mid-1950s. In this process, the liquid feed, mainly VTB, is sprayed through nozzles driven by injection steam into a fluidized bed of hot coke particles. In Syncrude’s original Fluid Cokers, these nozzles are arranged in a series of six rings along the height of each unit (Gray, 2015). The combination of steam and evolved vapours from the cracked liquid feed provide the necessary mixing to maintain fluidization of the coke particles. At operating temperatures of 510-550 ˚C, coking occurs on the surface of these particles (Gray, 2015). Jets of steam are injected above the stripper section to crush a portion of the particles, which increase in size throughout a run, by attrition. The coke particles are heated by burning a portion of the coke in a separate fluidized bed burner and returning it to the Fluid Coker unit (Figure 2). The cracked vapours rise from the dense phase zone to the dilute phase zone of the unit, pass through cyclones that separate entrained coke particles, and enter the scrubber in the top of the unit. Cyclones foul during operation due to the formation of a coke layer on the internal surfaces of the unit. A stream of hot coke particles from the burner unit, referred as scouring coke, is therefore fed into the horn chamber to "scour" the surfaces. The vapours are quenched in the scrubber by contacting with condensed liquid or fresh feed, and the scrubber overhead is finally sent to a fractionator for separation.

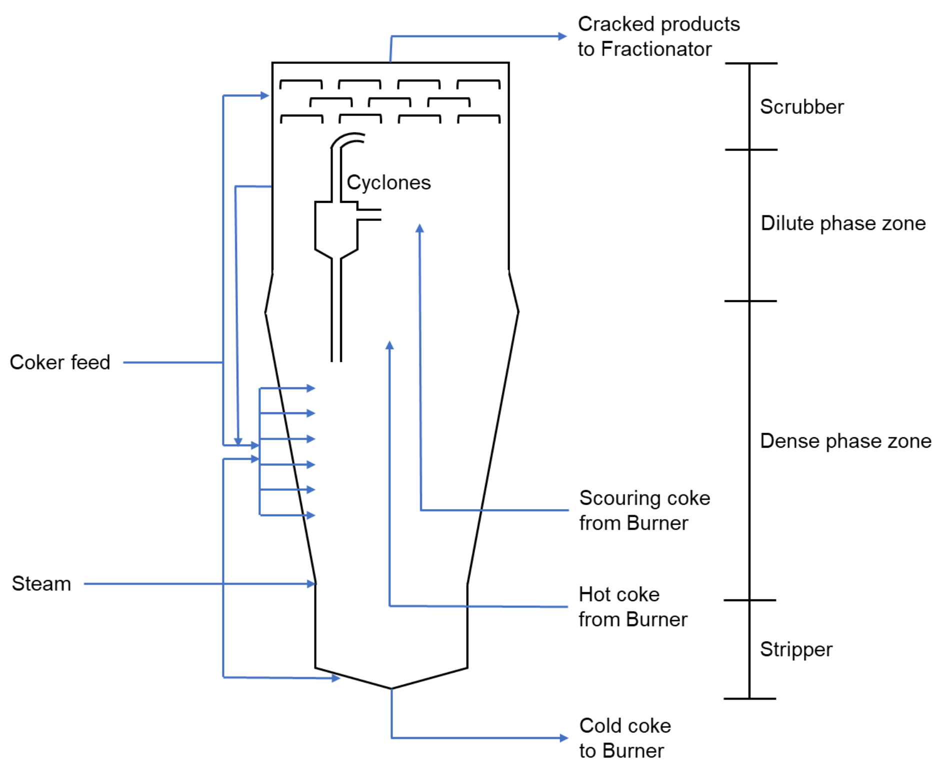


Figure 1 Schematic of a Fluid Coker (Modified from Gray, 2015)

The yields of fluid coking are mainly determined by the feed properties, the temperature of the fluid bed, the liquid distribution on the solids, and the vapour residence time in the bed. One significant disadvantage of the fluid coking process is the high rate of coke deposition inside the unit which compromises its efficient operation. Typically, Fluid Cokers must be shut down for one month every two to three years in order to remove the layers of deposited coke from internal surfaces of the unit, which can grow to a thickness of one meter during a run (Gray, 2015).

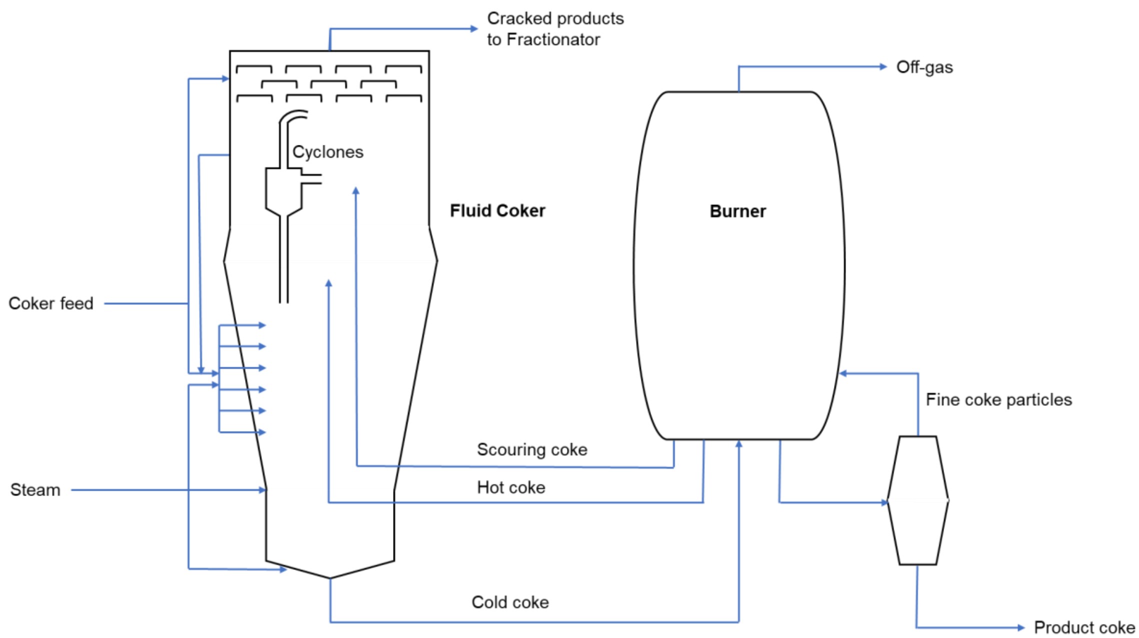


Figure 2 Schematic of the fluid coking process (Modified from Gray, 2015)

1.2.1 Fluid Coker operating conditions

Syncrude's commercial Fluid Cokers operate at a temperature range of 510 to 540 ˚C and a pressure of approximately 360 kPa (X. Song et al., 2004). The fluidized coke particles have a particle density and a mean particle diameter of approximately 1600 kg/m^3 and 145 µm, respectively (X. Song et al., 2004). These coke particles circulate to the burner, which operates at a temperature around 630 ˚C (Gray, 2015). The evolved hydrocarbon vapours have a gas density of approximately 2.28 kg/m^3 (X. Song et al., 2004) and exit the unit via gas outlet tubes at a temperature around 550 ˚C (Fan & Watkinson, 2006).

1.3 Fluid Coker cyclone fouling

The cyclone section of a Fluid Coker generally consists of 6 parallel cyclones positioned internally above the freeboard, each with individual inlet ducts, gas outlet tubes, and diplegs, illustrated in Figure 3. Evolved hydrocarbon vapours and entrained coke particles rising from the dense phase zone of the fluidized bed are accelerated through a contraction into the horn chamber, where they are provided with superheat from the scouring coke stream. This mixture in the horn chamber then enters the cyclone inlets. The cyclones separate particulate solids from the hydrocarbon vapour by exerting a radial centrifugal force on the particles, which return to the bed via the diplegs. Based on cyclone separation efficiency, a small portion of the entrained solids (and liquid droplets, if present) that enter the cyclones will exit via the gas outlet tubes an enter the scrubber section with the hydrocarbon vapour.

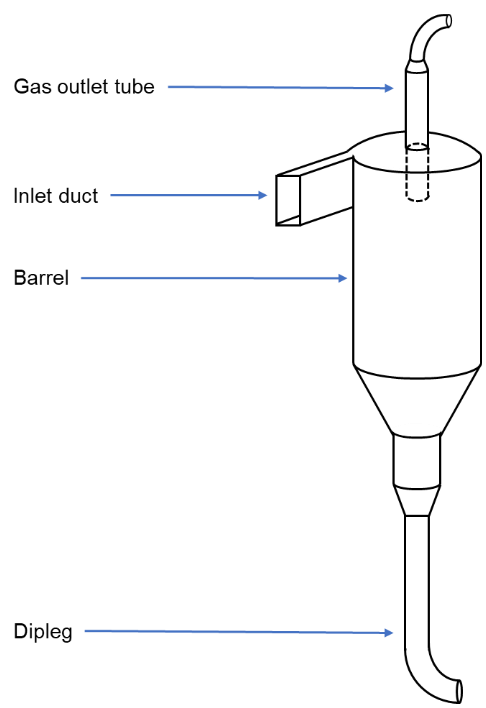


Figure 3 Schematic of a typical cyclone

Run lengths for commercial fluid cokers are generally dependent on the rate of cyclone fouling (Mallory, Mehta, Moore, & Richardson, 2000). The cyclone sections of commercial Fluid Cokers have been observed to experience significant coke deposition throughout typical runs, particularly in the gas outlet tubes as shown in Figure 4. This fouling reduces the available flow area in the gas outlet tubes, increasing pressure drop through the cyclones and subsequently increasing the reactor pressures. This pressure buildup leads to a reduction in the overall unit feed rate since the burner air blower has a maximum output, limiting the available heat for the endothermic cracking reactions. Eventually, the heavy hydrocarbon feed rates become too low, necessitating a unit shutdown.

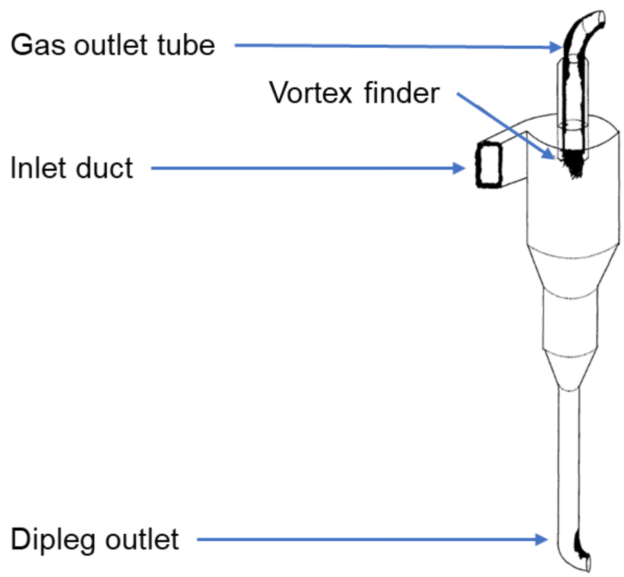


Figure 4 Primary coke deposit locations in the cyclones (Modified from Mallory et al., 2000)

1.3.1 Cyclone fouling mechanisms

Based on internal investigations, Syncrude Canada Ltd. has identified three mechanisms that impact cyclone fouling: feed droplet entrainment, chemical reaction forming condensable species, and simple condensation of heavy ends.

1.3.1.1 Feed droplet entrainment

When atomized feed is injected into the fluidized bed, it is possible that some unconverted feed droplets become entrained into the freeboard region of the Fluid Coker, resulting in deposition and subsequent coking. Experimental work at the University of British Colombia (UBC) studied feed entrainment by varying the filter characteristics between the system's feed section and an exit tube used for deposition measurements (Zhang & Watkinson, 2005a). Based on an increase in the filter pore size from 10 µm to 3 mm, the authors concluded that feed droplet entrainment was not the main contributor to cyclone fouling.

1.3.1.2 Chemical reaction forming condensable species

When atomized feed is injected into the fluidized bed, the relatively light species flash into vapour. The unreacted liquid species will contact the fluidized coke particles and react to form evolved hydrocarbon vapour. It is possible that the vapour could continue to react to form heavier species that eventually condense, resulting in deposition and subsequent coking. Experimental work at UBC studied the effects of heating or cooling the vapours obtained when atomizing heavy hydrocarbons at approximately 535 °C (Zhang & Watkinson, 2005a). The authors observed that raising the temperature above 535 °C did not increase deposition rate, up to a studied temperature of 680 °C. Deposition rate increased when cooling the vapour below 510 °C. Further experimental work studied the impact of vapour residence time but did not observe any significant impact on deposition rate, even with an eightfold reduction in residence time. Theoretical work at the University of Alberta investigated the operating conditions that would favor chemical reactions in the vapor phase leading to condensable hydrocarbon species and aerosols (Gonzalez, 2004). The author concluded that cracking reactions leading to condensable hydrocarbons were unlikely to occur at typical fluid coker operating conditions. Experimental work at the University of Calgary showed minimal coke deposition at temperatures of 490 – 560 °C when operating within residence times that approach those of fluid coker cyclones (Mallory et al., 2000). The results of these three studies suggest that chemical reaction forming condensable species is not the dominant mechanism contributing to cyclone fouling.

1.3.1.3 Condensation of heavy ends

When hydrocarbon vapours are released from the dense phase zone of the fluidized bed, they are operating in vapour-liquid equilibrium above or close to their hydrocarbon dew point. It is possible that downstream temperature, pressure, or compositional changes could lead to condensation, particularly of the relatively heavy hydrocarbon vapours. This condensation of heavy ends may result in deposition and subsequent coking within the Fluid Coker. Experimental work at UBC studied the effect of vapour dilution on deposition rate (Zhang & Watkinson, 2005a). The authors observed a strong correlation between vapour dilution and reduced deposition due to physical dilution of the vapour phase. A study by Kim et al. (2012) used an analytical approach to characterize deposits in the cyclone dipleg of a commercial residue fluid catalytic cracking reactor (RFCC). The authors identified that possible mechanisms of deposit formation are related to a variety of factors, including the condensation and polymerization of heavy oil droplets. Based on these results and those summarized in Sections 1.3.1.1 and 1.3.1.2, the condensation of heavy ends fouling mechanism will be the focus of this thesis.

1.3.2 Previous fouling models

1.3.2.1 Mathematical models

Physical condensation is considered to be a primary contributor to the fouling mechanisms in industrial transfer line exchangers (TLEs) downstream of heavy hydrocarbon cracking reactors. A study published by Zhang and Watkinson (2005b) developed a two-dimensional mathematical model based on the physical condensation fouling mechanism to simulate the deposition rate of condensed heavy hydrocarbons in a straight TLE tube with either a constant and uniform wall heat flux or a constant and uniform outside wall temperature. The simulation was validated with lab-scale experimental data and showed that decreased vapour temperature resulted in more carbonaceous deposit formation. Both the simulation and experimental results also showed that vapour dilution with steam or nitrogen resulted in lower deposition rates, and that increased vapour-phase residence time did not contribute to the deposition rate.

1.3.2.2 Computational Fluid Dynamics models

Cyclone fouling in Fluid Cokers is believed to be affected by variations in the distribution of coke particles between the six parallel cyclones. To investigate coke flow in the freeboard and horn chamber of a Fluid Coker, Syncrude commissioned Particulate Solid Research Inc. (PSRI) to develop a lab-scale room temperature air and coke model of the fluid coking process. A computational fluid dynamics (CFD) model of the experimental setup was developed and validated with experimental data (Solnordal, Reid, Hackman, Cocco, & Findlay, 2012). The results showed that CFD models can be used to qualitatively predict coke distributions in air-coke systems.

To investigate the deposition of heavy hydrocarbons droplets in Fluid Cokers, a study by Lakghomi et al. (2011) developed a CFD model of heavy hydrocarbon droplets in a gas-vapour flow normal to a circular disk at different conditions. The model was validated with room-temperature experimental data and was found to have a good capability in predicting the effects of temperature on heavy oil deposition rates. The model showed that the effect of high temperature on physical properties contributing to droplet deposition was small. To further develop the model, the authors recommended including the effects of droplet re-entrainment and droplet side distribution based on experimental results.

1.3.2.3 Process simulation models

A study by Song et al. (2014) investigated the effects of feed composition, temperature, feed flow rate, and nitrogen flow rate on the deposition rate of heavy oil. A heavy oil-diluent feed mixture was atomized with nitrogen and introduced via vertical flow to a normal circular disk. A CFD-HYSYS model was developed to predict experimental deposition rates for the system. HYSYS was used to determine droplet concentration under given conditions, while CFD was used to determine mass deposition on each side of the disk. The CFD-HYSYS model was found to be capable of determining the effects of hydrocarbon properties, temperature, and fluid flow on deposition ratees. The authors recommended that the model could be applied to the simulation of other systems, or the optimization of similar systems.

A thesis published by Jankovic (2005) developed a simulation of the scrubber section of a Syncrude Fluid Coker in Aspen HYSYS. The simulation was used to investigate the effects of operation and design parameters on scrubber performance. Jankovic simulated the scrubber feed stream as a mixture of water, light ends, and two pseudo-component streams of heavy ends. These pseudo-component streams were based on two Assays provided by Syncrude from a 1980 Fluid Coker performance study. Jankovic found that Aspen HYSYS was able to effectively simulate the scrubber section of a Fluid Coker, with simulation results matching Syncrude operating data very well, and concluded that the simulation could be used to perform additional case studies on scrubber performance.

1.4 Research Objectives

The main objective of this work is to improve Fluid Coker unit reliability by proposing fouling mitigation strategies in the reactor cyclones. The work will advance previous modeling efforts for Syncrude's Fluid Coker cyclone fouling based on the condensation of heavy ends fouling mechanism. The new modeling approach will incorporate vapor-liquid thermodynamic properties, thermal cracking reactions, and overall fluid dynamic considerations throughout zones of interest in the Fluid Coker. The following provides the scope of the present work:

1. Develop a phenomenological model for zones of interest in the Syncrude Fluid Coker that incorporates the impact of vapor-liquid thermodynamic properties, thermal cracking reactions, and overall fluid dynamics.

2. Perform case studies to investigate the impact of various operating parameters on the temperature and liquid fraction of the evolved hydrocarbon vapour throughout the Fluid Coker. Temperature and liquid flow rate will be interpreted as key performance indicators for the condensation of heavy ends fouling mechanism.

3. Identify potential process levers for mitigating Fluid Coker cyclone fouling based on the results of the case studies. Parameters that can be varied to increase temperature and decrease liquid flow rate in the cyclones and gas outlet tubes will be characterized as process levers.

1.4.1 Thesis structure

A Fluid Coker process simulation model is first developed in Chapter 2. Aspen Plus was selected as the process simulation software for this model. Chapter 2 defines the six zones of interest within the Fluid Coker that are relevant to this work and describes the model setup, involving component specification, method specification, and flowsheet setup in both Aspen Plus and Aspen Plus Simulation Workbook. The Aspen Plus Simulation Workbook is used to mathematically model the effects of endothermic reactions and pressures losses within the model. The model flowsheet and base case conditions are defined for their subsequent application in Chapter 3.

Case studies are presented in Chapter 3. To investigate the condensation of heavy ends fouling mechanism, four case studies were performed to study the impact of transfer line temperature, hot coke flow rate, hot coke entrainment and scouring coke flow rate on the temperature and liquid flow rates in the cyclones and gas outlet tubes. For each case study, two of the four parameters were varied, and the results are presented in three-dimensional surface plots.

A discussion of the results of the case studies is presented in Chapter 4. Scouring coke was identified as a potential process lever for mitigating Fluid Coker cyclone fouling. Sensitivity analyses for horn chamber diameter, thermal cracking fraction and transfer line steam flow rate were performed, and transfer line steam flow rate was found to have some impact on liquid flow in the cyclones and gas outlet tubes. Conclusions for this thesis are presented in Chapter 5.

Chapter 2

2 Process simulation in Aspen Plus

2.1 Introduction to Aspen Plus

AspenTech software is widely used across chemical process industries for process modeling, simulation and optimization. The original Advanced System for Process Engineering (ASPEN) Project began in 1977 as a collaboration between the United States Department of Energy and the Massachusetts Institute of Technology. AspenTech was founded in 1981 to commercialize the ASPEN technology, and in 1982 the Aspen Plus commercial process simulation software was released. Today, AspenTech supports a wide range of software. Aspen Plus simulation software includes a large database of pure component and phase equilibrium data for common chemicals, electrolytes, solids and polymers. Its applications include operations decisions support, process safety analysis, project cost estimation and solid process optimization (Aspen Technology Inc., 2018).

Aspen HYSYS and Aspen Plus are simulation software products developed by AspenTech for chemical process modeling, simulation and optimization. Both products are widely used across chemical process industries and overlap slightly in their capabilities such that they are occasionally considered interchangeable. However, AspenTech markets Aspen HYSYS as ‘Process Simulation for Energy’ and Aspen Plus as ‘Process Simulation for Chemicals’ (Aspen Technology Inc., 2018). More specifically, Aspen HYSYS is developed primarily for application in the Oil and Energy industry, while Aspen Plus is developed for application in the Chemicals industry.

Aspen Plus simulation software was selected for this project primarily for its solids modeling capabilities, which are unique among AspenTech products. The accurate simulation of heat and mass balances of solids is essential even for inert solids systems, and accurate representation of particle size distributions is required for many processes, including cyclone systems. Although the model developed in this work does not currently include a rigorous simulation of cyclone performance, Aspen Plus simulation software is sufficiently robust that this could be incorporated in future work.

2.2 Model setup

2.2.1 Model basis

Aspen Plus V9.0 simulation software was used to develop a steady-state model of six zones within the Syncrude Fluid Coker, hereafter referred to as the Model. Aspen Plus simulation software performs sequential modular process simulation to solve equations. In this method, the process being simulated is represented by a collection of modules that are solved sequentially and iteratively in a forward direction until convergence is achieved. The six Fluid Coker zones were represented by one or more modules, connected sequentially by material streams in the Aspen Plus Flowsheet. The zones (Figure 5) are defined as follows:

- BD1 – Identified as the region beginning from the level of the fluidized bed to immediately below the HCTL outlet. The process stream in this zone is a combination of steam, hydrocarbons, and fluidized bed coke.

- BD2 – Identified as the region beginning from immediately below the HCTL to immediately below the Fluid Coker vessel contraction. The process stream in this zone is a combination of the BD1 process stream, and hot coke and steam from the HCTL.

- CTR – Identified as the region beginning from immediately below the vessel contraction to immediately below the horn chamber. The process stream in this zone has the same composition as the BD2 process stream.

- HRN – Identified as the region beginning from immediately below the horn chamber to the vertical halfway point of the cross section of the cyclone inlet section. The process stream in this zone is a combination of the CTR process stream and hot coke and steam from the SCTL.

- CYC – Identified as the region beginning from the vertical halfway point of the cross section of the cyclone inlet section to the cyclone gas outlet tube inlet. The process stream in this zone has the same composition as the HRN process stream.

- GOT – Identified as the region beginning from the inlet of the cyclone gas outlet tube to outlet of the gas outlet tube snout. The process stream in this zone has the same composition as the HRN process stream.

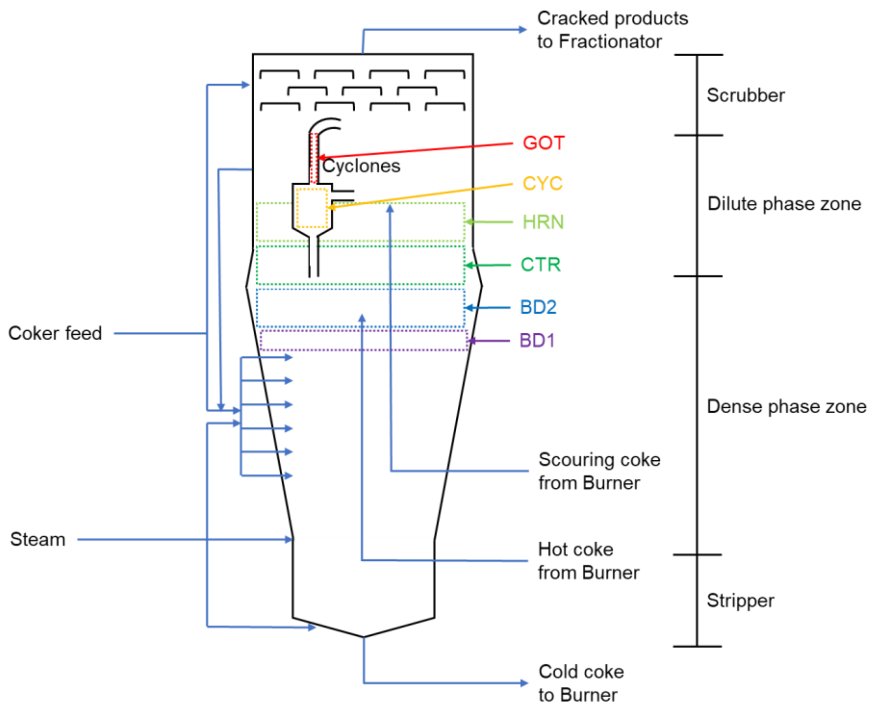


Figure 5 Schematic of Fluid Coker zones (Modified from Gray, 2015)

2.2.2 Component specification

The Fluid Coker process stream is a complex mixture of many hydrocarbons, most of which are not defined in the Aspen Simulation software database. Distillation curves for heavy hydrocarbon mixtures are typically presented in terms of the fraction (by weight or volume) that can be distilled in standard equipment as a function of temperature. The methods for testing petroleum samples are standardized by ASTM International as numbered standards (ASTM, 2018). The true boiling point (TBP) method (ASTM 2892) provides the most comprehensive data for distillation of crude oils and is used to collect accurate distillation curve data as well as samples for further characterization and study. In the Aspen Plus simulation software, TBP distillation data can be entered into the Assay and used to generate working curves of TBP, molecular weight, density and viscosity for a hydrocarbon mixture.

An Aspen Plus V9 simulation was created using a Solids template. In the Components – Specifications | Selection sheet, water and light ends (C1 – C4) were selected as Conventional components, and Coke was manually entered as a Nonconventional component. In Aspen Plus, Conventional components participate in phase equilibrium calculations, while Nonconventional components do not. The composition of light ends is provided in Table 1. In the Components – Assay/Blend tab, the heavy components (C5+) were entered as two Assays: Coker Gas Oil (CGO) and Once Through Scrubber Bottoms (OTSB). The Assay input data for CGO and OSTB are provided in Table 2 and Table 3, respectively. These compositions are based on a study performed by Syncrude in the 1980s, as reported by Jankovic (2005). With this approach, hydrocarbons heavier than light ends and lighter than CGO are not included in the component list. Improving the Assay data by incorporation this fraction of hydrocarbons in future work would improve the accuracy of this model stream.

Table 1 Composition of light ends (Jankovic, 2005)

Light ends components	wt%
Hydrogen	1
Hydrogen sulfide	6
Methane	21
Ethane	16
Ethylene	8
Propane	12
Propylene	13
Butadiene	2
Butenes	12
i-Butane	1
n-Butane	6

Table 2 CGO assay input (Jankovic, 2005)

CGO			
vol%	NBP (˚C)	vol%	NBP (˚C)
0	221	55	403
5	266	60	414
10	287	65	426
15	304	70	438
20	319	75	450
25	333	80	464
30	345	85	479
35	357	90	496
40	368	95	521
45	380	100	572
50	391		

Table 3 OTSB assay input (Jankovic, 2005)

OTSB			
vol%	NBP (˚C)	vol%	NBP (˚C)
0	315.7	50	492.1
1	318.7	55	499.3
2	327.4	60	506.3
3.5	343.7	65	512.9
5	360.7	70	518.5
7.5	383.8	75	522.5
10	400.7	80	526.0
12.5	413.6	85	529.2
15	423.7	90	532.4
17.5	432.0	92.5	534.0
20	439.0	95	535.7
25	450.5	96.5	536.6
30	459.6	98	537.9
35	468.7	99	538.6
40	477.1	100	539.4
45	484.7		

2.2.3 Method specification

The Peng-Robinson equation of state (EOS) is typically appropriate for vapour-liquid equilibrium calculations pertaining to refinery, petrochemical and gas processing. Jankovic (2005) applied the Peng-Robinson EOS property package in an Aspen HYSYS simulation of the scrubber section of a Fluid Coker with a model stream based on the light ends, CGO and OTSB compositions provided in Section 2.2.2. Jankovic found that Aspen HYSYS was able to effectively simulate the scrubber section of a Fluid Coker. Based on these findings, the Peng-Robinson EOS property package was selected for this simulation.

In the Properties | Methods – Specifications | Global sheet, Peng-Robinson was selected as the simulation property package. The property package impacts transport properties (viscosity, thermal conductivity, diffusivity), thermodynamic properties (enthalpy, fugacity, K-factors, critical constants), and physical properties (density, molecular weight, surface tension).

In the Properties | Methods – NC Props | Property Methods sheet, ENTHGEN (general enthalpy) and DNSTYGEN (general density) models were selected to calculate the enthalpy and density of the component Coke. For the purpose of this work, Coke was assumed to be a heterogeneous solid that did not participate in chemical or phase equilibrium, therefore enthalpy and density were the only physical properties that required specification. The GENANAL component attribute was used to specify that Coke was composed of 100% Constituent 1, which implied a single-constituent component.

In the Properties | Methods – Parameters | Pure Components sheet, HCGEN (heat capacity) and DENGEN (density) for Coke were specified. The ENTHGEN model calculates enthalpy from specified heat capacity and heat of formation parameters, although the latter is not required for components that do not participate in chemical reactions. For this simulation, Coke was assumed to have a constant heat capacity.

2.2.4 Flowsheet setup in Aspen Plus

In the Simulation | Setup | Global sheet, the input mode was set to Steady-State and the stream class was set to MIXNCPSD. Stream classes are used to define the structure of simulation streams that contain inert solids. The MIXNCPSD stream class contains a combination of two substreams: the MIXED substream and the NCPSD substream. All components in the MIXED substream participate in phase equilibrium flash calculations. The NCPSD substream is a Nonconventional (NC) substream used for heterogeneous solids that have no defined molecular weight and have an enabled option to specify a Particle Size Distribution (PSD).

In the Simulation |Main Flowsheet sheet, modules were arranged and specified. First, seven process streams were specified. To specify a stream, Aspen Plus requires two thermodynamic specifications and enough information to calculate the flow rate of each component. Each of the seven process input streams were specified with temperature, pressure, composition and mass flow rate. A description of these streams is listed in Table 4.

Table 4 Process input streams

Name	**Description**
STEAM	Plant saturated steam
LIGHTS	Light components (C1-C4)
CGO	Coker Gas Oil, containing heavy components
OTSB	Once Through Scrubber Bottoms, containing heavy components
ENTRAIN1	The portion of fluidized bed coke that is entrained out of the dense phase zone
HCTL	The portion of hot coke that is introduced to the Fluid Coker via the Hot Coke Transfer Line (HCTL)
SCTL	The portion of hot coke that is introduced to the Fluid Coker via the Scouring Coke Transfer Line (SCTL)

Next, a combination of Mixers, Stream Splitters, Substream Splitters, and Heaters were used to model the six zones of the Fluid Coker. The completed flowsheet is presented in Figure 6.

- The BD1 zone was modeled by mixing LIGHTS, CGO, OTSB, ENTRAIN1 and a fraction of STEAM in Mixer M-2. Heater H-0 was used to bring the mixture to fluidized bed temperature and pressure, and Heater H-1 was used to remove heat associated with endothermic cracking reactions in that zone. Internal process stream CV1 represents the average operating conditions of the Fluid Coker process stream in zone BD1.

- The BD2 zone was modeled by mixing CV1 with a fraction of the HCTL stream and a fraction of STEAM in Mixer M-3. Heater H-2 was used to remove heat associated with endothermic cracking reactions in that zone. Internal process stream CV2 represents the average operating conditions of the Fluid Coker process stream in zone BD2.

- The CTR zone was modeled by using Heater H-3 to remove heat associated with endothermic cracking reactions in that zone, and apply a pressure drop associated with the Fluid Coker vessel contraction in that zone. Internal process stream CV3 represents the average operating conditions of the Fluid Coker process stream in zone CTR.

- The HRN zone was modeled by mixing CV3 with a fraction of SCTL and a fraction of STEAM in Mixer M-4. Heater H-4 was used to remove heat associated with endothermic cracking reactions in that zone. Internal process stream CV4 represents the average operating conditions of the Fluid Coker process stream in zone HRN.

- The CYC zone was modeled by splitting CV4 into a separate SOLID and FLUID stream with Substream Splitter S-4. Stream Splitters S-5 and S-6 were used to distribute the SOLID and FLUID streams respectively to Mixers CYC-1 through to CYC-6. This allows liquid, gas, and solids distributions among the six Fluid Coker cyclones to be varied. In this project, the SOLID and FLUID streams were distributed evenly among the six cyclones. Heater H-5 was used to remove heat associated with endothermic cracking reactions from the mixture produced by Mixer CYC-1, and apply a pressure drop associated with the Fluid Coker cyclone in that zone. Internal process stream CV5 represents the average operating conditions of the Fluid Coker process stream in zone CYC.

- The GOT zone was modeled by splitting a fraction of the solids in CV5 away from the process stream in Substream Splitter CYCLONE1. Heater H-6 was used to remove heat associated with endothermic cracking reactions in that zone, and apply a pressure drop associated with the Fluid Coker gas outlet tube in that zone.

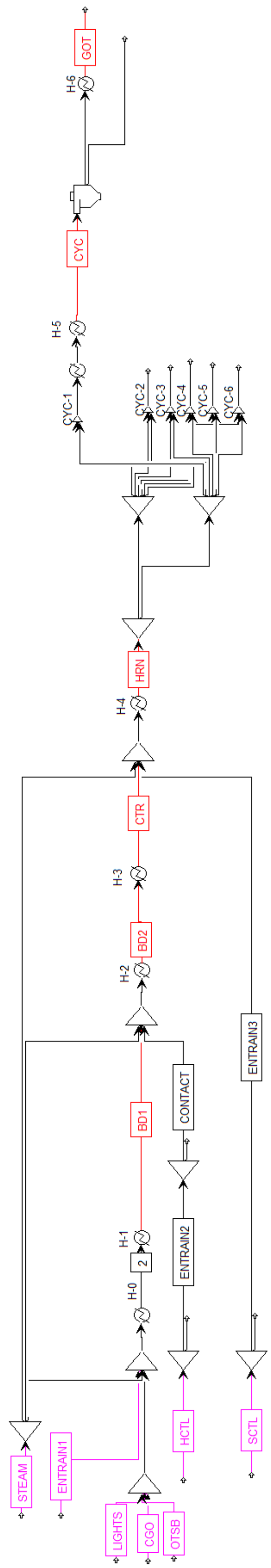


Figure 6 Simulation flowsheet

2.2.5 Flowsheet setup in Aspen Simulation Workbook

The Aspen Simulation Workbook (ASW) Add-in for Microsoft Excel is a tool for creating user interfaces to Aspen Tech. This enables case studies, troubleshooting, external calculations and analyses to be performed with simulation variables in Microsoft Excel. Simulation variables designated as ‘Calculated’ can be imported to an Excel workbook, stored in tables and referenced in calculations. Simulations variables designated as ‘Specified’ can be imported, stored in tables, referenced in calculations, and modified within the workbook. Any modifications made to Specified variables in an Excel workbook with an enabled ASW Add-in will be immediately made to the same variables in the connected Aspen Plus simulation. In this project, the ASW Add-in was used to calculate the heat loss associated with endothermic cracking reactions in the Fluid Coker, and the pressure drops associated with the contraction (CTR) zone, cyclone (CYC) zone and gas outlet tube (GOT) zone. Mach numbers calculated for flow in the CTR, CYC and GOT zones were all below 0.3, so flow was assumed to be incompressible and therefore the impact of pressure drop on fluid temperature was assumed to be negligible.

2.2.5.1 Endothermic cracking reactions

In Aspen Plus simulation software, streams defined by Assays cannot participate in conventional reactions, so the heat loss associated with endothermic cracking reactions in the Fluid Coker was calculated in Excel and applied to The Model using the ASW Add-in.

The thermal cracking of bitumen follows apparent first-order kinetics (Gray, 2015). With a mass-based approach, first-order kinetics were used to relate the rate of conversion of vacuum residue to the initial mass of residue (Equation 2.1), with the temperature dependence of the rate constant modeled by the Arrhenius equation (Equation 2.2). It was assumed that 10 mass% of the total condensed liquid flow would participate in thermal cracking. This assumption will be discussed further in Chapter 4.

$$-r_{VR} = k_{VR} f_{tc} W_{VR} \tag{2.1}$$

$$k_{VR} = A \exp\left[\frac{-E_a}{RT}\right] \tag{2.2}$$

Thermal conversion kinetic data from a non-isothermal Thermogravimetric Analysis of Cold Lake petroleum residue obtained by Olmstead and Freund (1998) was used to calculate the rate constant. The heat loss associated with thermal cracking was calculated by relating the heat of reaction to the rate of reaction and reaction volume (Equation 2.3). This heat loss calculated for each Fluid Coker zone was applied to the Model via Heater modules. Relevant thermal cracking parameters are provided in Table 5.

$$Q_{VR} = -\Delta H_r r_{VR} V \tag{2.3}$$

Table 5 Thermal cracking parameters

Parameter	Value	Unit	Source
log A	13.21	s^{-1}	(Olmstead & Freund, 1998)
E_a	212.8	kJ/mol	(Olmstead & Freund, 1998)
f_{tc}	0.1		Assumed
R	0.008314	kJ/mol·K	

2.2.5.2 Pressure drops

Pressure drops in a piping system result from four possible system characteristics: pipe friction, changes to flow path direction, obstructions to flow path, and changes to the cross-section and shape of flow path. The pressure drops associated with the CTR, CYC and GOT zones were calculated in Excel and applied to The Model using the ASW Add-in. The geometry values used in these calculations were provided confidentially by Syncrude and will therefore not be reported in this thesis.

From Crane Technical Paper 410 (CRANE Co., 1982), the resistance coefficient ‘K’ for resistance to pipe flow is defined as the velocity head loss due to a valve or fitting, independent of friction factor or Reynold’s number and may be treated as a constant for all conditions of flow. The resistance to flow due to a sudden contraction is expressed by Equation 2.4, where subscripts 1 and 2 define the internal diameters of the large and small pipes, respectively (CRANE Co., 1982).

$$K = 0.5\left(1 - \frac{d_1^2}{d_2^2}\right) \qquad 2.4$$

This equation is derived from the Bernoulli equation, continuity equation, and an approximation of the contraction coefficients determined by Julius Weisbach. However, this does not accurately represent the pressure drop resulting from geometry in the CTR. For a more gradual contraction, the resistance coefficient is expressed by Equation 2.5, where theta represents the angle of contraction relative to the direction of fluid flow, and $\beta = d_1^2 / d_2^2$ (CRANE Co., 1982).

$$K = \frac{0.5\sqrt{\sin\frac{\theta}{2}}(1-\beta^2)}{\beta^4}, 45° < \theta < 180°$$

2.5

$$\beta = \frac{d_1^2}{d_2^2}$$

This resistance coefficient can then be related to the change in velocity head using Equation 2.6 and applied to pressure drop calculations via a working form of the Bernoulli equation. The calculated pressure drops associated with geometric contractions in the CTR and GOT were applied to the Model via Heater modules by specifying a change in pressure with no change in temperature.

$$h_L = K\frac{v^2}{2g_n} \quad 2.6$$

Pressure drops in cyclones are typically calculated by summing individual pressure drop terms. From The Handbook of Fluidization and Fluid-Particle Systems (Knowlton, 2003), these pressure drop terms represent the effects of: contraction, acceleration of solids, barrel friction, gas reversal, and outlet exit contraction. These five pressure drop terms are shown in Equation 2.7. The calculated pressure drops associated with the CYC were applied to the Model via Heater modules by specifying a change in pressure with no temperature change.

$$\Delta P_{(f-i)g} = 0.5\rho_g\left(U_i^2 - U_f^2 + K_{fi}U_i^2\right)$$

2.7

$$\Delta P = LU_{pi}\left(U_{pi} - U_{pf}\right)$$

$$\Delta P_{bf} = \frac{2f\rho_g U_i^2 \pi D_b N_s}{d_{hi}}$$

$$\Delta P_r = \frac{\rho_g U_i^2}{\mu}$$

$$\Delta P_o = 0.5\rho_g(U_o^2 - U_b^2 + K_o U_o^2)$$

For internal cyclones such as those within the Fluid Coker, the contraction pressure drop applies to the contraction from the freeboard to the cyclone inlet. The contraction coefficient is a function of the ratio of the cyclone inlet diameter to the freeboard diameter. The acceleration of solids pressure drop applies to the velocity increase of entrained solids from the freeboard to the cyclone inlet. The barrel friction pressure drop applies to solids flowing along the internal barrel wall of the cyclone. The Fanning friction factor generally ranges between 0.003 and 0.008 (Knowlton, 2003), and the hydraulic diameter is based on the Reynolds number. The gas reversal pressure drop applies to the gas reversing direction within the cyclone vortex. The outlet exit contraction pressure drop applies to the contraction from the barrel of the cyclone to the gas outlet tube. The contraction coefficient is a function of the ratio of the gas outlet tube diameter to the cyclone barrel diameter.

The Ranque-Hilsche effect refers to the separation of one gas stream into separate hot and cold streams by a vortex. In an effort to conservatively simulate a Ranque-Hilsch cooling effect within the CYC zone, pressure and temperature losses were applied to the Model via one Heater module by specifying a change in pressure and temperature.

2.3 Model base case

After the Aspen Plus Flowsheet and Aspen Plus Simulation workbook were set up, the Model was run and converged. A series of sensitivity analyses were performed to identify a set of operating conditions within which the Model would predict liquid flow in most of the Fluid Coker zones. These operating conditions were separated into two groups: the base case set points, and the base case operating envelope. The base case set points are Model input parameters that are not varied in any case studies, presented in Table 6. Total steam flow light ends flow, CGO flow and OTSB flow are provided as wt% of their combined flow.

Table 6 Base case set points

Variable	Value	Units
Total steam flow	10	wt%
Light ends flow	12	wt%
CGO flow	61	wt%
OTSB flow	17	wt%
Bed temperature	524	˚C
Bed pressure	222	kPa
Scouring coke entrainment	1	wt. frac.

The base case operating envelope is a set of Model input parameters that were selected to be varied in case studies, presented in Table 7. In the aforementioned sensitivity analyses, these parameters most significantly impacted liquid flow rates throughout the Fluid Coker and were identified as potential process levers for mitigating cyclone fouling. Transfer line temperature refers to the temperature of the hot coke and scouring coke supplied to the Fluid Coker from the burner unit. Hot coke entrainment refers to the portion of hot coke introduced to the BD2 zone of the Fluid Coker that is transported to downstream zones via the flow of hydrocarbon vapours. Together with hot coke flow rate and scouring coke flow rate, these four parameters impact the temperature and liquid flow rate of the six Fluid Coke zones defined in Section 2.2.1. Further investigation of these parameters is presented in Chapter 3.

Table 7 Case study operating envelope

Variable	**Value**	**Units**
Transfer line temperature	590 – 610	˚C
Hot coke flow rate	40 – 60 3628 – 5443	tons/min kg/s
Hot coke entrainment	0.1 – 0.5	wt. frac.
Scouring coke flow rate	2 – 12 181 – 1088	tons/min kg/s

Chapter 3

3 Case studies

As previously described in Section 1.3.1.3, the condensation of heavy ends fouling mechanism is driven by operating conditions that cause temperature, pressure or compositional changes to the evolved hydrocarbon vapours released from the dense phase zone of the fluidized bed. To investigate this mechanism, four case studies were performed to study the impact of transfer line temperature, hot coke flow rate, hot coke entrainment and scouring coke flow rate on the temperature and liquid flow rates in the CYC and GOT zones. The case studies and their varied parameters are as follows:

- Case 1: Transfer line temperature and hot coke flow rate
- Case 2: Transfer line temperature and hot coke entrainment
- Case 3: Hot coke flow rate and hot coke entrainment
- Case 4: Hot coke flow rate and scouring coke flow rate

The Model was used to estimate the temperature and liquid flow rate in the CYC and GOT for each case study. These two variables can be considered as indicators of fouling via the condensation of heavy ends mechanism. Case studies were performed by creating a Scenario Table in Excel using the ASW Add-in and using it to converge the Model with different combinations of operating parameters. The results of these case studies are shown in three-dimensional surface plots.

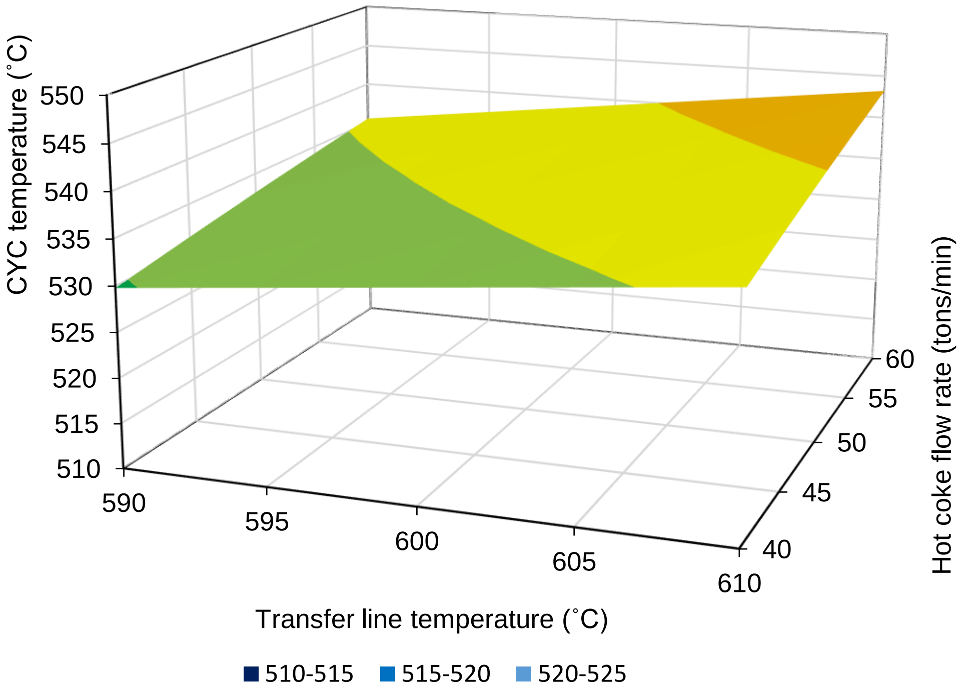
3.1 Case 1

The operating envelope for Case 1 is provided in Table 8. Transfer line temperature was varied from 590 to 610˚C, while hot coke flow rate was varied from 40 to 60 tons/min.

Table 8 Case 1 operating envelope

Variable	Value	Units
Bed temperature	524	˚C
Transfer line temperature	590 – 610	˚C
Hot coke flow rate	40 – 60	tons/min
Hot coke entrainment	0.5	wt. frac.
Scouring coke flow rate	6	tons/min

CYC and GOT temperatures are presented in Figure 7. The temperature of the transfer line from the burner was varied from 590 to 610˚C while the hot coke flow rate was varied from 40 to 60 tons/min. Figure 7 shows that zone temperatures in the CYC and GOT were comparable for this operating envelope, both increasing at higher transfer line temperatures and increased hot coke flow rate. Liquid flow rates were not predicted in the CYC and GOT for the studied ranges.



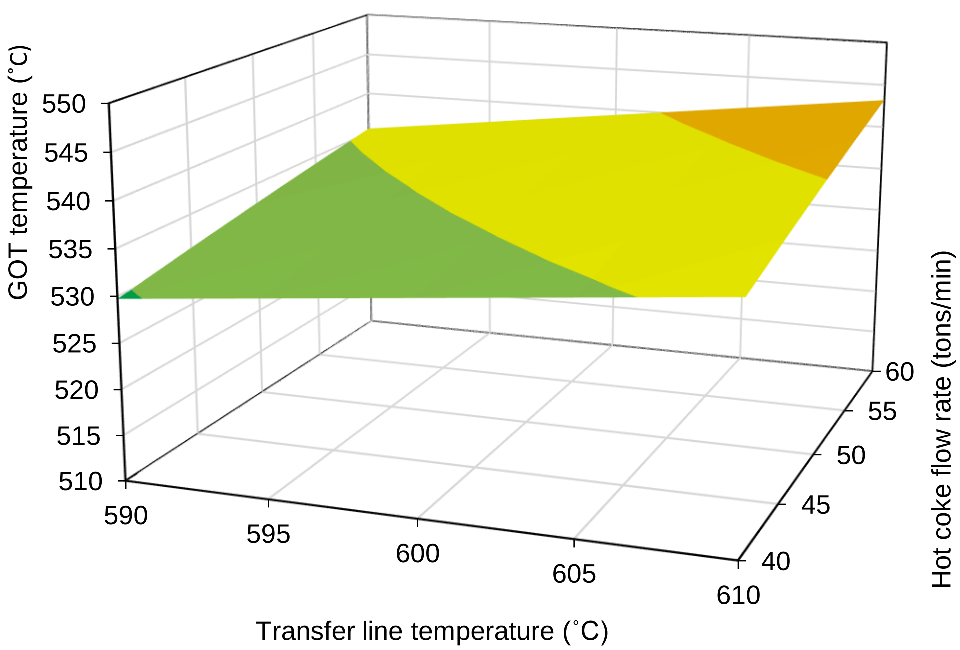


Figure 7 CYC and GOT temperature for varied hot coke/scouring coke temperature and hot coke flow rate

3.2 Case 2

The operating envelope for Case 2 is provided in Table 9. Transfer line temperature was varied from 590 to 610 ˚C while hot coke entrainment was varied from 0.1 to 0.5 wt. frac.

Table 9 Case 2 operating envelope

Variable	Value	Units
Bed temperature	524	˚C
Transfer line temperature	590 – 610	˚C
Hot coke flow rate	45	tons/min
Hot coke entrainment	0.1 – 0.5	wt. frac.
Scouring coke flow rate	6	tons/min

CYC and GOT temperatures are presented in Figure 8. CYC and GOT liquid flow rates are presented in Figure 9. The temperature of the transfer line from the burner was varied from 590 to 610 ˚C while the hot coke entrainment from the transfer line to the horn chamber was varied from 0.1 to 0.5 wt. fraction. Figure 8 shows that the zone temperatures in the CYC and GOT were comparable for this operating envelope, both increasing at higher transfer line temperatures and greater hot coke entrainment. Figure 9 shows that liquid flow rates in the CYC and GOT zones were similar, increasing both with reduced hot coke entrainment and lower transfer line temperatures.

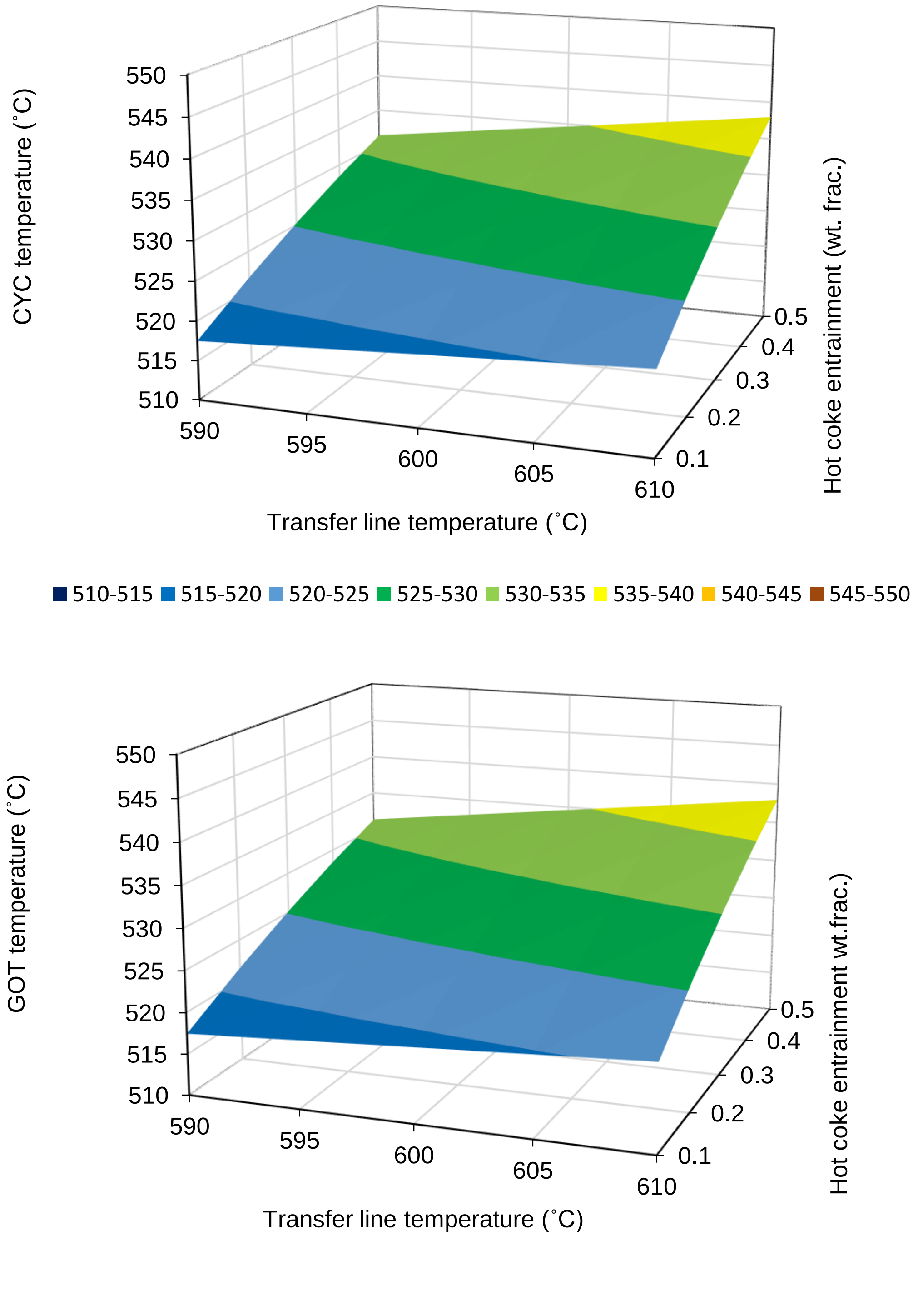


Figure 8 CYC and GOT temperatures for varied transfer line temperature and hot coke entrainment

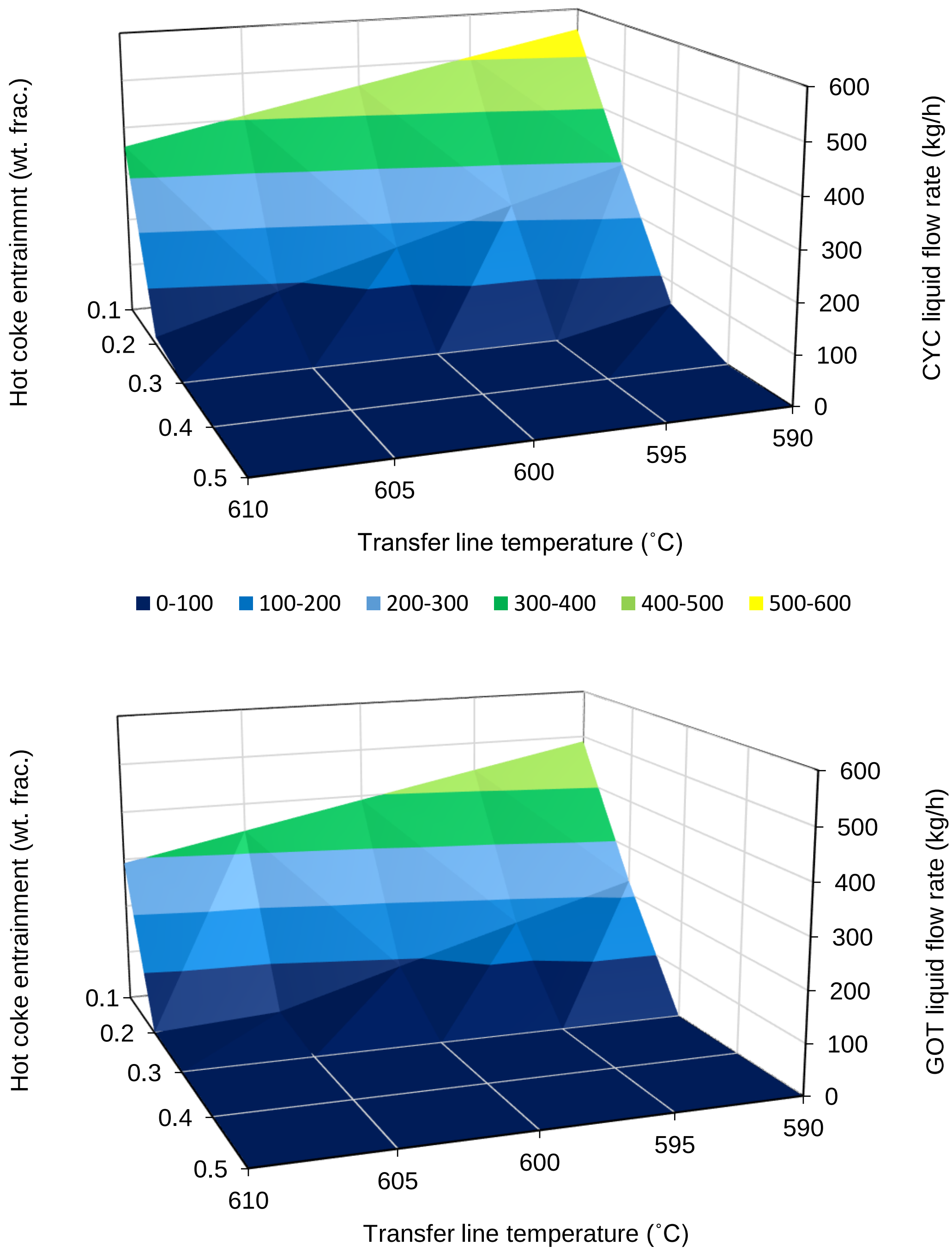


Figure 9 CYC and GOT liquid flow rates for varied transfer line temperature and hot coke flow rate

3.3 Case 3

The operating envelope for Case 3 is provided in Table 10. Hot coke flow rate was varied from 40 to 60 tons/min while hot coke entrainment was varied from 0.1 to 0.5 wt. frac.

Table 10 Case 3 operating envelope

Variable	Value	Units
Bed temperature	524	˚C
Transfer line temperature	595	˚C
Hot coke flow rate	40 – 60	tons/min
Hot coke entrainment	0.1 – 0.5	wt. frac.
Scouring coke flow rate	6	tons/min

CYC and GOT temperatures are presented in Figure 10. CYC and GOT liquid flow rates are presented in Figure 11. In Case 3, the hot coke flow rate was varied from 40 to 60 ton/min while hot coke entrainment was varied from 0.1 to 0.5 wt. fraction. Figure 10 shows that the zone temperatures in the CYC and GOT were comparable for this operating envelope, increasing both with increased hot coke flow rate and hot coke entrainment. Figure 11 shows that liquid flow rates in the CYC and GOT zones were similar, increasing both with decreased hot coke flow rate and decreased hot coke entrainment.

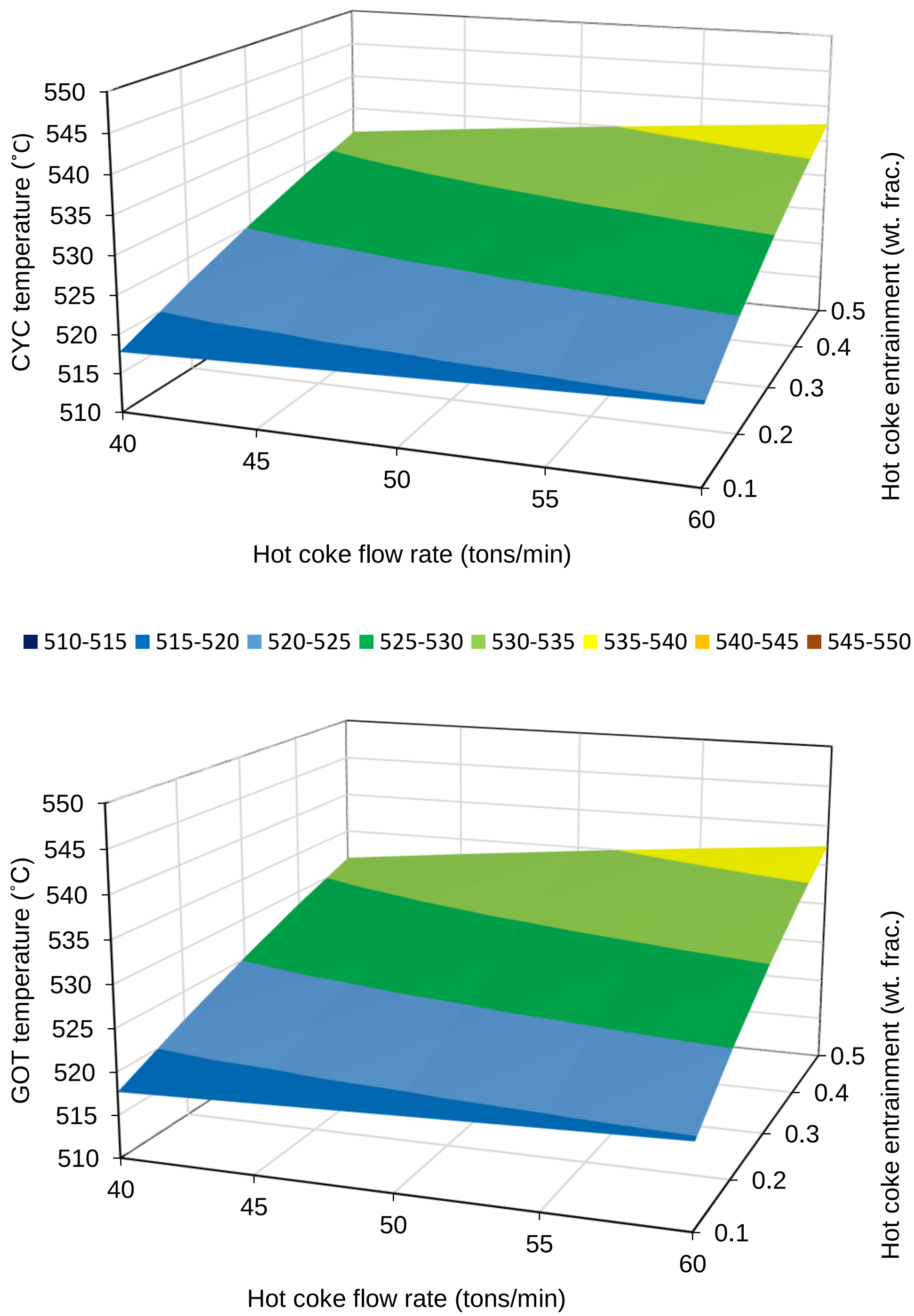


Figure 10 CYC and GOT temperatures for varied hot coke flow rate and hot coke entrainment

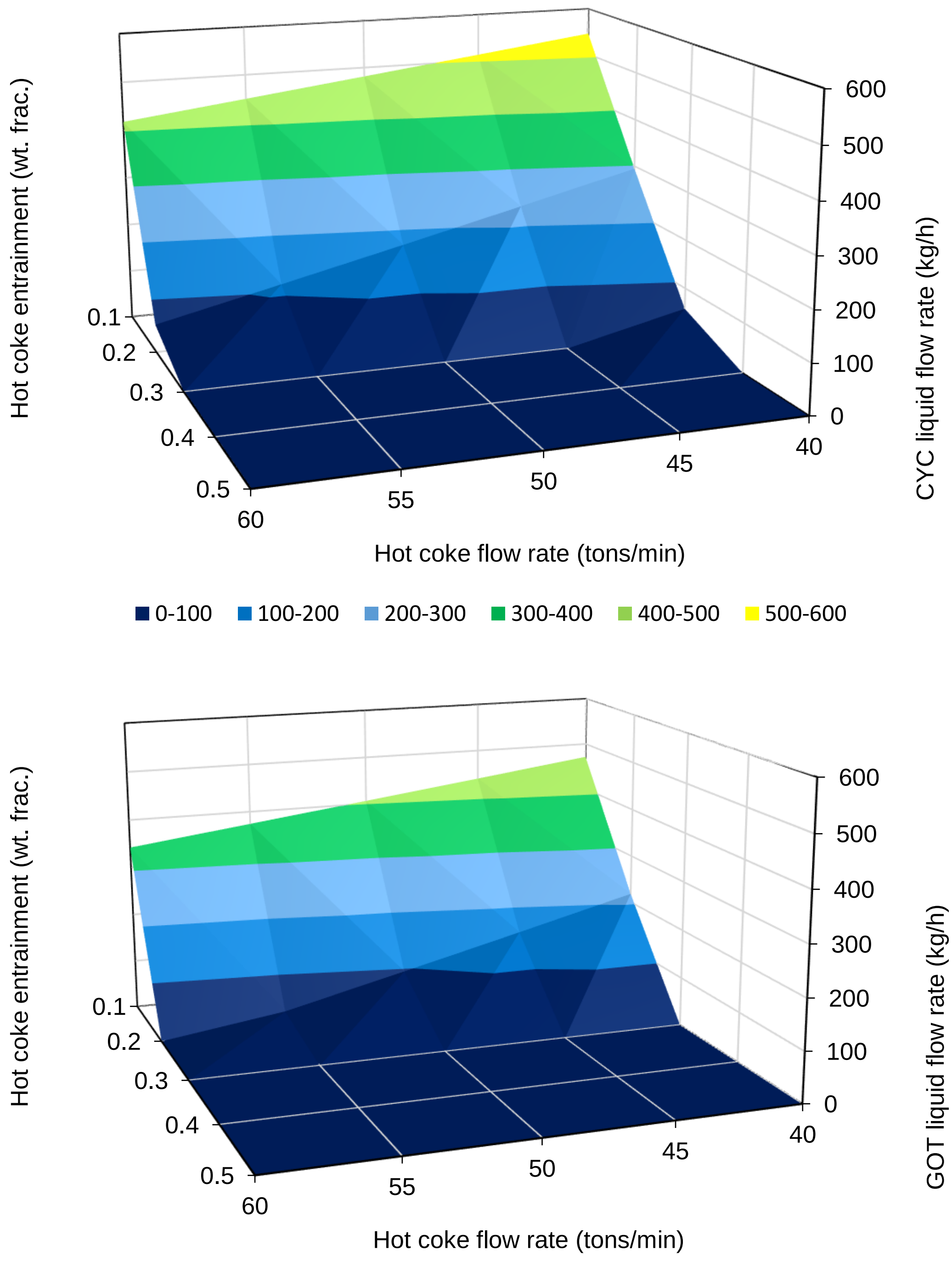


Figure 11 CYC and GOT liquid flow rates for varied hot coke flow rate and hot coke entrainment

3.4 Case 4

The operating envelope for Case 4 is provided in Table 11. Hot coke flow rate was varied from 40 to 60 tons/min while scouring coke flow rate was varied from 4 to 12 tons/min.

Table 11 Case 4 operating envelope

Variable	Value	Units
Bed temperature	524	˚C
Transfer line temperature	590	˚C
Hot coke flow rate	40 – 60	tons/min
Hot coke entrainment	0.2	wt. frac.
Scouring coke flow rate	4 – 12	tons/min

CYC and GOT temperatures are presented in Figure 12. CYC and GOT liquid flow rates are presented in Figure 13. In Case 4, hot coke flow rate was varied from 40 to 60 ton/min while scouring coke flow rate was varied from 2 to 10 ton/min. Figure 12 shows that zone temperatures in the CYC and GOT were comparable for this operating envelope, increasing with both increased hot coke flow rate and increased scouring coke flow rate. Figure 13 shows that liquid flow rates in the CYC and GOT zones were similar, increasing both with decreased hot coke flow rate and decreased flow rate.

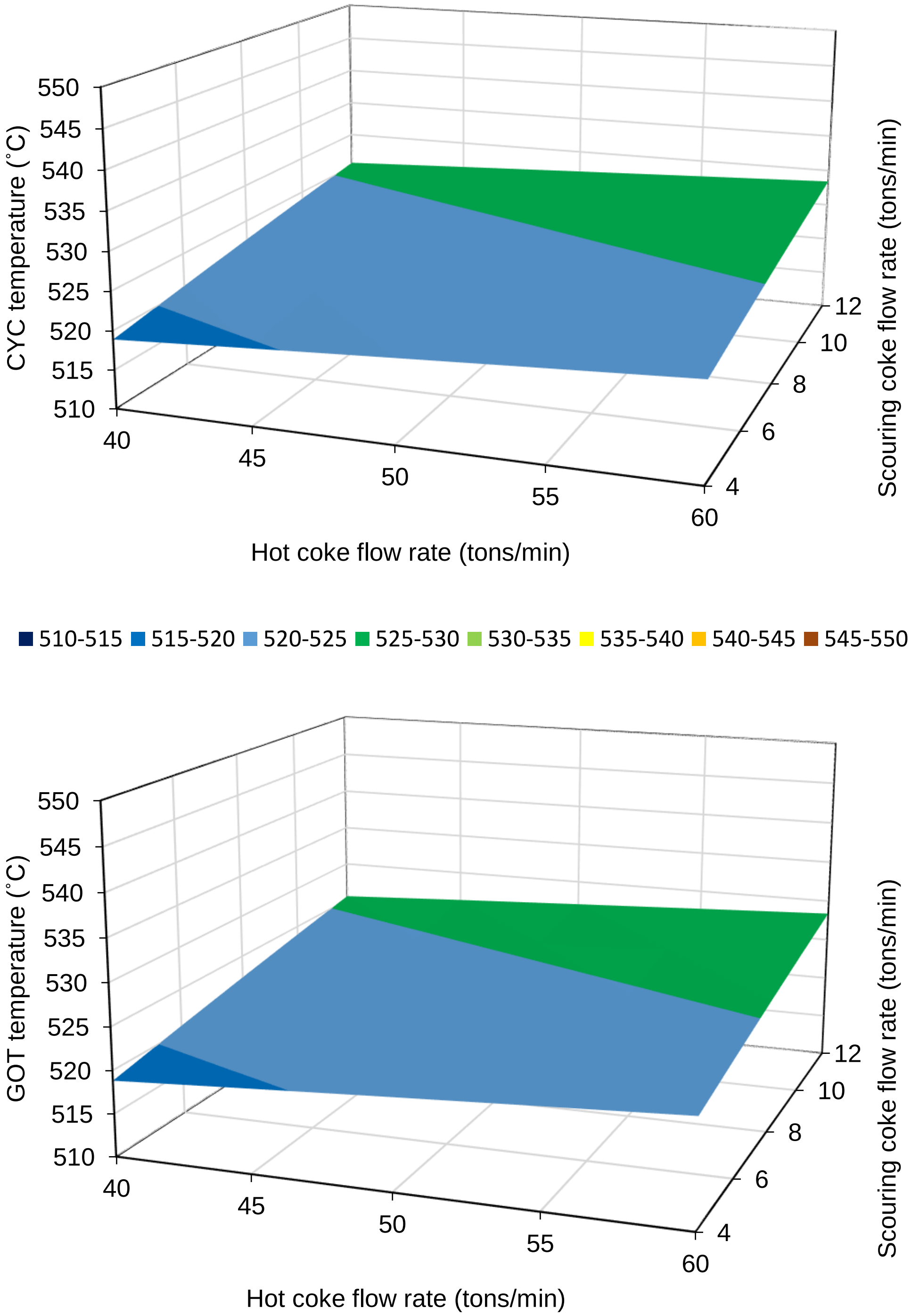


Figure 12 CYC and GOT temperatures for varied hot coke flow rate and scouring coke flow rate

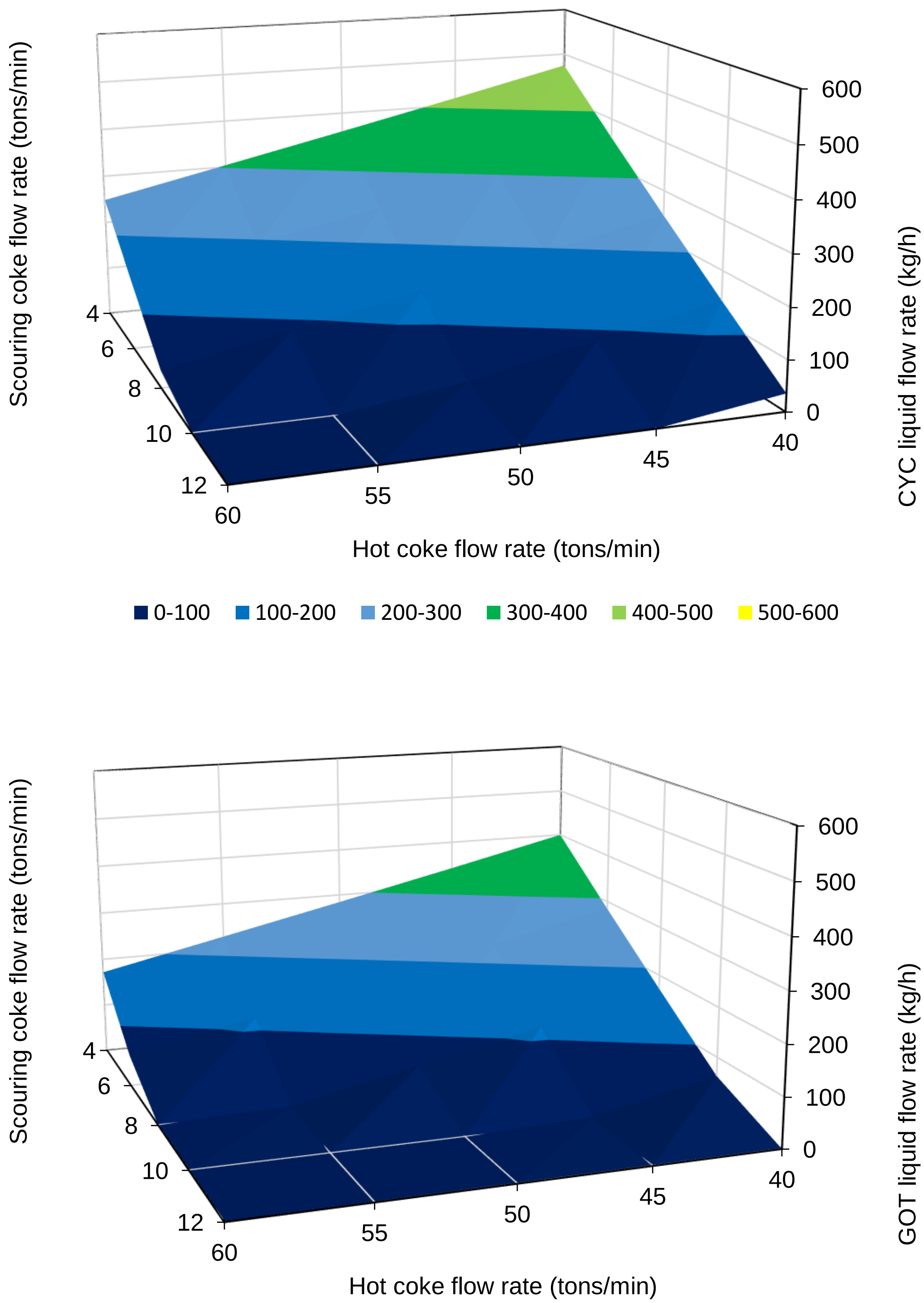


Figure 13 CYC and GOT liquid flow rates for varied hot coke flow rate and scouring coke flow rate

Chapter 4

4 Discussion

An Aspen Plus simulation model of a Syncrude Fluid Coker was developed to investigate the impact of transfer line temperature, hot coke entrainment, hot coke flow rate and scouring coke flow rate on temperature and liquid flow rate in the cyclone and gas outlet tube zones of the unit. Case studies were designed to facilitate the identification of process levers that can be used to mitigate cyclone fouling in commercial Fluid Coker operation. In this thesis, the temperature and liquid flow rate in these zones are considered to be key performance indicators for the condensation of heavy ends fouling mechanism. Therefore, for the purposes of this thesis, parameters that can be varied to increase temperature and decrease liquid flow rate in the cyclone and gas outlet tube zones will be characterized as promising process levers that require further investigation in future work.

Comparing the cyclone and gas outlet tube temperatures for each case study, both zones are impacted similarly by the studied parameters. This is due to the structure of the Model and the order of calculations performed to reach convergence. For the cyclone zone, temperature changes and pressure drops are applied immediately upstream of the point where the Model measures the temperature and liquid flow rate in that zone. Similarly, for the gas outlet tube zone, temperature changes and pressure drops are applied immediately upstream of the measuring point. This structure ensures relatively conservative convergence results but requires careful discernment when interpreting Model results. For example, although it may appear as though the cyclone and gas outlet tubes zones have comparable operating conditions, this is not the case. The gas outlet tube zone experiences pressure drops due to the geometry of the tube exit. These pressure drops are sufficient to allow some liquid from the cyclone zone to vaporize in the gas outlet tube zone. The effects of this vaporization can be seen in the liquid flow rate results for all case studies. Comparing the cyclone and gas outlet tube liquid flow rates for each case study, the cyclone zone is consistently predicted to have a slightly higher flow rate than the gas outlet tube.

The Model was also used to investigate the impact of secondary parameters on temperature and liquid flow rate in the cyclone and gas outlet tube zones. Sensitivity analyses were performed on horn chamber diameter, thermal cracking reactions fraction, and transfer line steam. The horn chamber diameter impacts the effects the contraction geometry in the dilute phase zone of the Fluid Coker, and therefore impacts the pressure drops in that zone. The thermal cracking reactions fraction is the mass fraction of liquid flow that is assumed to participate in thermal cracking reactions in the Model, and therefore impacts the temperature in all zones with liquid flow. The transfer line steam affects the composition, temperature, and flow rate in all zones of the Fluid Coker downstream of the dense phase zone.

4.1 Transfer line temperature

The burner transfer line transports hot coke particles from the burner unit to the Fluid Coker. One stream of hot coke particles from the burner unit, referred to as hot coke, is fed into the dilute phase zone to provide the heat required for endothermic cracking reactions. Another stream of hot coke particles, referred to as scouring coke, is fed into the horn chamber to scour any coke deposits by attrition. Transfer line temperature therefore impacts the heat supplied to the Fluid Coker via both the hot coke and scouring coke streams. In Cases 1 and 2, transfer line temperature was varied from 590 to 610 ˚C.

In Case 1, The CYC and GOT temperatures ranged from 529 to 543 ˚C (Figure **7**). Figure 14 shows the impact of transfer line temperature on the Fluid Coker at a hot coke flow rate of 40 tons/min. The impact of transfer line temperature is particularly noticeable in the BD2 and HRN zones, where hot coke and scouring coke, respectively, are introduced to the Model. In a commercial Fluid Coker, transfer line temperature should impact all zones of the Fluid Coker, including BD1. In the Model, the portion of hot coke that is not entrained downstream from BD2 is not mixed back into the bed, so transfer line temperature does not impact the BD1 zone. Instead, bed temperature is set to 524 ˚C for all case studies. Figure 14 also shows that the HRN zone has the highest operating temperature of all Fluid Coker zones in the Model. This is due to the addition of scouring coke in this zone from the transfer line.

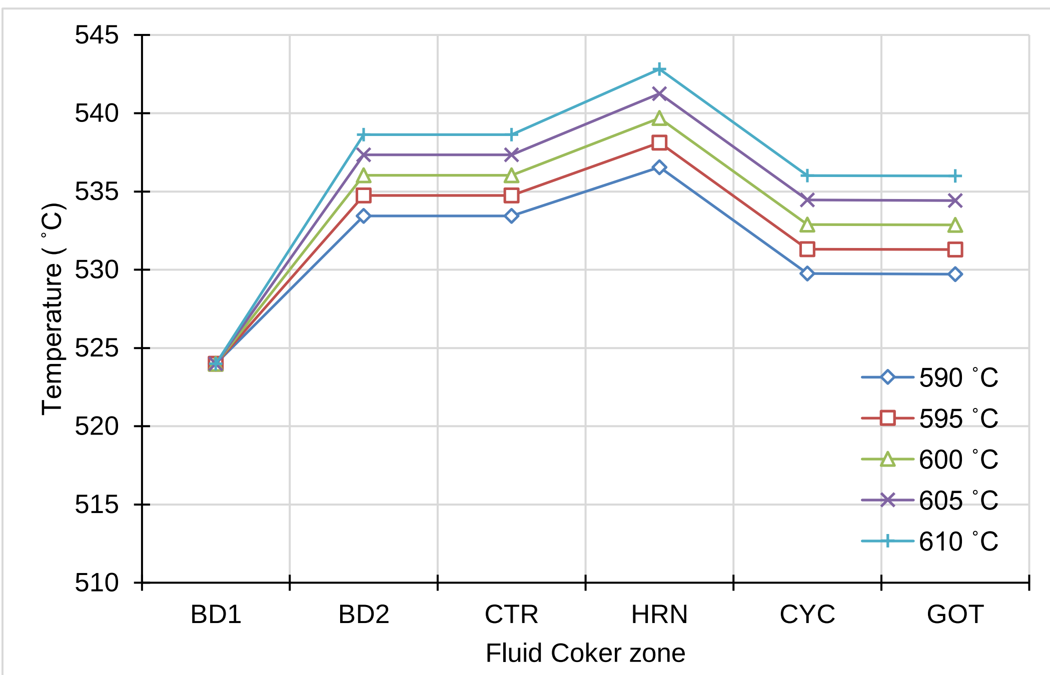


Figure 14 Fluid coker zone temperature for varied transfer line temperature with a hot coke flow of 40 tons/min (Case 1)

In Case 2, the CYC and GOT temperatures ranged from 517 to 537 ˚C (Figure 8). Liquid flow was predicted in the CYC and GOT within temperature ranges of 517 to 525 ˚C (Figure 9). Figure 9 shows a slightly higher liquid flow rate in the CYC compare to the GOT, which is due to pressure drops in the GOT as explained above. This effect is particularly noticeable when comparing the liquid flow in the CYC and GOT within the hot coke entrainment range of 0.2 to 0.4 wt. frac.

The impact of transfer line temperature on liquid flow throughout the Fluid Coker is shown in Figure 15. It is clear that transfer line temperature impacts the liquid flow rate of BD2, where hot coke is introduced to the Fluid Coker. Figure 15 also highlights the significance of scouring coke in the HRN zone, where no liquid flow rate is predicted for any of the studied transfer line temperatures. In Case 2, the scouring coke provides sufficient heat to vaporize all the liquid flow from the CTR zone, which was as high as 2017 kg/h for the transfer line temperature of 590 ˚C. This suggests that scouring coke could be used as a process lever to mitigate fouling in commercial Fluid Coker operation.

Figure 15 also shows some liquid flow in the CYC and GOT despite the prediction of no liquid flow in the HRN. This condensation is the result of a temperature change in the CYC zone, which is predominantly due to the Ranque-Hilsch effect. Although the Model does not rigorously simulate the fluid dynamics of this effect, a temperature drop and pressure drop are applied to the CYC zone to conservatively simulate the potential impact of this effect. This result emphasizes how temperature and pressure changes may result in the condensation of heavy ends throughout the Fluid Coker.

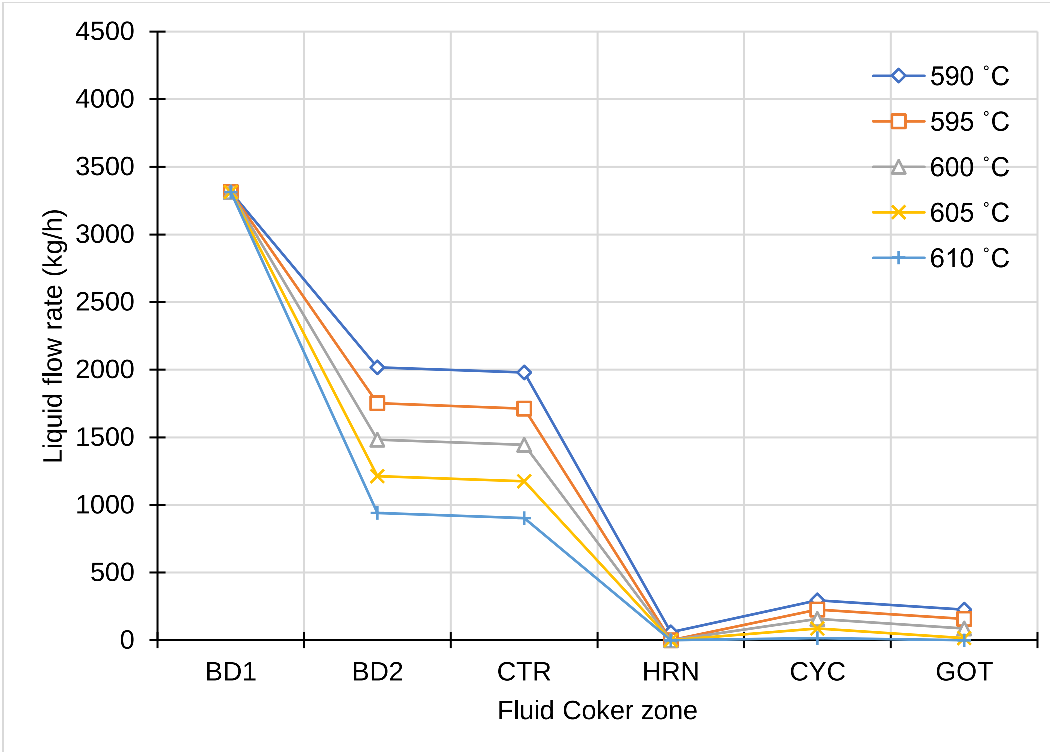


Figure 15 Fluid Coker zones liquid flow rate for varied transfer line temperature with a hot coke entrainment of 0.2 wt. frac. (Case 2)

Local liquid flow rate in the BD1 zone is shown to be 3313 kg/h in Figure 15, which represents a liquid fraction of 0.00044 in that zone. This liquid presence in the BD1 zone is due to the operating conditions of the dense phase zone of the fluidized bed. In this zone, evolved hydrocarbon vapours are operating in vapour-liquid equilibrium above or around their hydrocarbon dew point. Downstream of BD1, hot coke and scouring coke provide heat to the hydrocarbon vapours so that they operate farther above their hydrocarbon dew point. As a result, the BD1 zone has the highest liquid flow rate of all Fluid Coker zones.

4.2 Hot coke and scouring coke flow rates

The burner transfer line transports hot coke particles from the burner unit to the Fluid Coker. One stream of hot coke particles from the burner unit, referred to as hot coke, is fed into the dilute phase zone to provide the heat required for endothermic cracking reactions. Another stream of hot coke particles, referred to as scouring coke, is fed into the horn chamber to scour any coke deposits by attrition. Hot coke flow rate and scouring coke flow rate therefore impact the heat supplied to the Fluid Coker. In Cases 1, 3 and 4, hot coke flow rate was varied from 40 to 60 tons/min. In Case 4, scouring coke flow rate was varied from 2 to 10 tons/min.

In Case 1, the CYC and GOT temperatures ranged from 529 to 543 ˚C (Figure 7). No liquid flow was predicted in the CYC or GOT. Figure 16 shows the impact of hot coke flow rate on the Fluid Coker at a transfer line temperature of 590 ˚C. The impact of heat provided by hot coke and scouring coke can be seen in the BD2 and HRN zones, respectively. A 50% increase in hot coke flow rate, from 40 to 60 tons/min, results in a temperature increase of 6 ˚C on average for all zones.

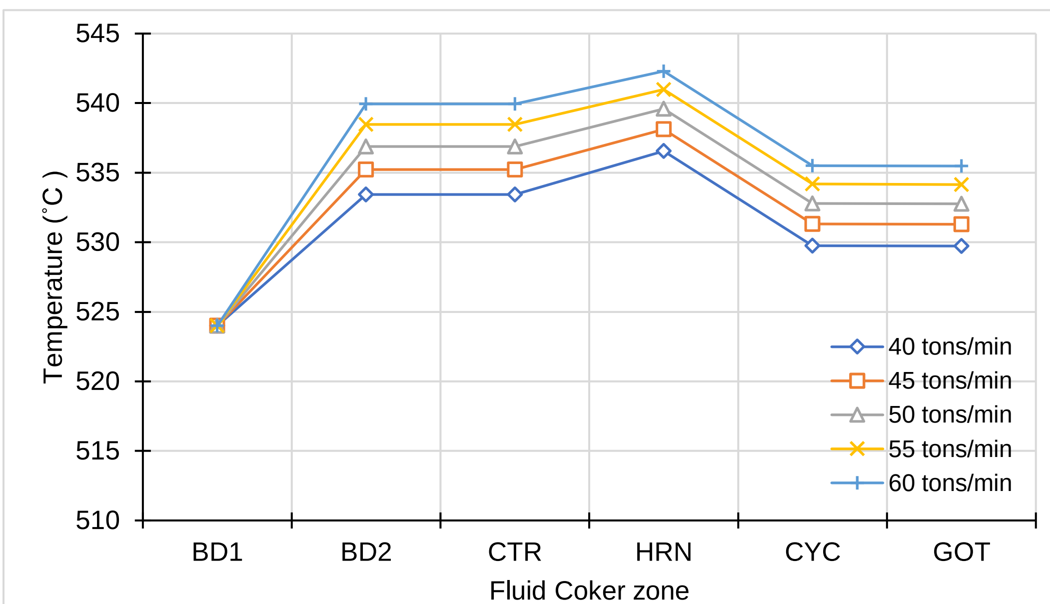


Figure 16 Fluid coker zone temperature for varied hot coke flow rate at transfer line temperature of 590 ˚C (Case 1)

In Case 3, the CYC and GOT temperatures ranged from 517 to 537 ˚C (Figure 10). Liquid flow was predicted in the CYC and GOT within temperature ranges of 517 to 525 ˚C (Figure 11). Figure 11 shows a slightly higher liquid flow rate in the CYC compare to the GOT, which is due to pressure drops in the GOT as explained above. This effect is particularly noticeable when comparing the liquid flow in the CYC and GOT within the hot coke entrainment range of 0.2 to 0.4 wt. frac. The impact of hot coke flow rate on liquid flow throughout the Fluid Coker is shown in Figure 17. A 50% increase in hot coke flow rate, from 40 to 60 tons/min, results in a liquid flow rate decrease of 76% on average in the BD2 and CTR zones, 81% in the CYC zone, and 100% in the GOT zone.

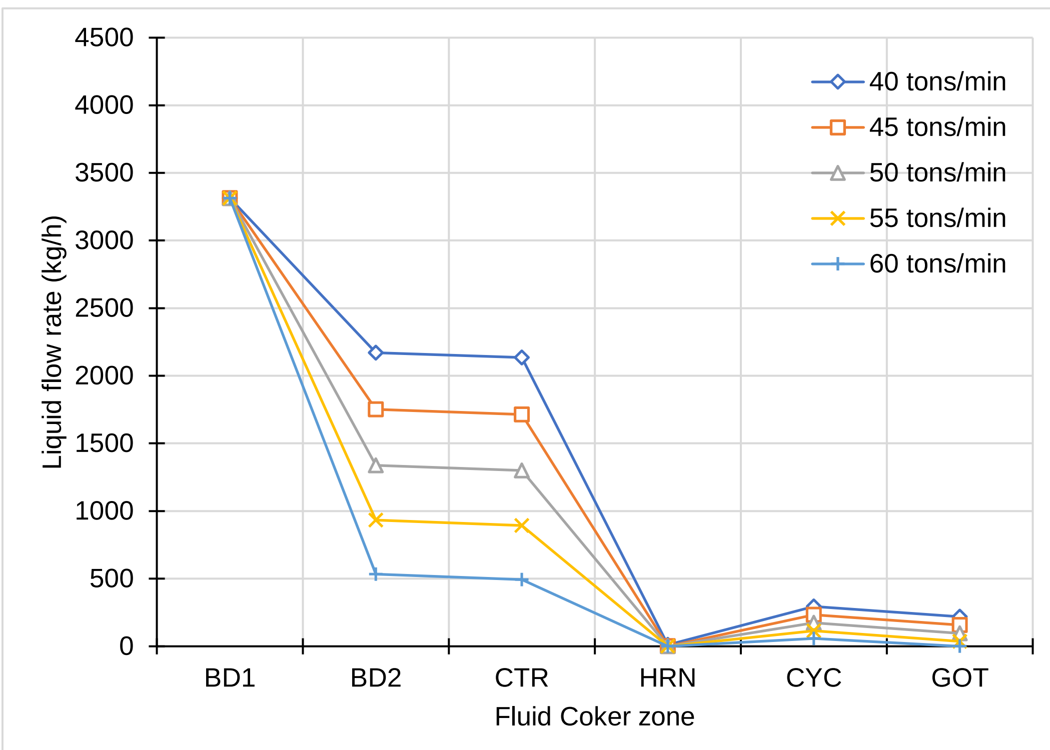


Figure 17 Fluid Coker zones liquid flow rate for varied hot coke flow rate with a hot coke entrainment of 0.2 wt. frac. (Case 3)

In Case 4, the CYC and GOT temperatures ranged from 518 to 528 ˚C (Figure 12). Liquid flow was predicted in the CYC and GOT within temperature ranges of 518 to 525 ˚C (Figure 13). Figure 13 shows a slightly higher liquid flow rate in the CYC compare to the GOT, which is due to pressure drops in the GOT as explained above. This effect is particularly noticeable when comparing the liquid flow in the CYC and GOT within the scouring coke flow rate range of 8 to 12 tons/min. The impact of hot coke flow rate on liquid flow throughout the Fluid Coker is shown in Figure 18. A 50% increase in hot coke flow rate, from 40 to 60 tons/min, results in a liquid flow rate decrease of 63% on average in the BD2, CTR and CYC zones, and 78% in the GOT zone. Figure 18 also shows some liquid flow in the HRN at hot coke flow rates of 40 and 45 tons/min. A 25% increase in hot coke flow rate, from 40 to 50 tons/min, is required to eliminate liquid flow in the HRN.

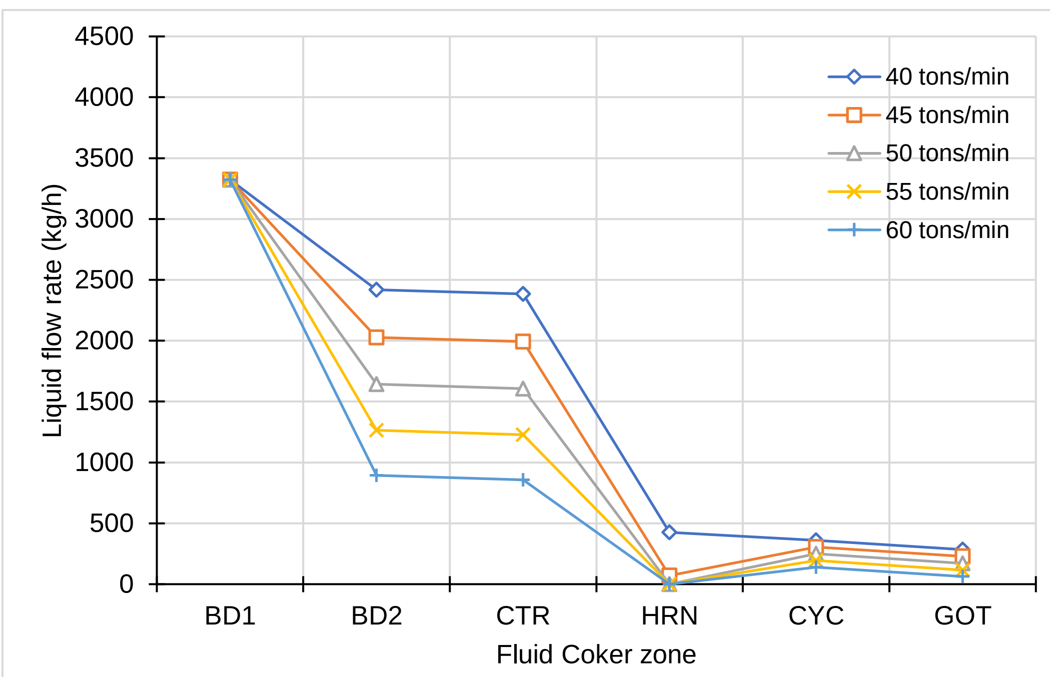


Figure 18 Fluid Coker liquid flow rate for varied hot coke flow rate with a scouring coke flow rate of 4 tons/min (Case 4)

The impact of scouring coke flow rate on liquid flow throughout the Fluid Coker is shown in Figure 19. Because the Model assumed 100 wt% entrainment of scouring coke into the CYC zone, scouring coke only impacts the HRN, CYC and GOT zones of the Fluid Coker. This effect is shown in Figure 19. A 100% increase in in scouring coke flow rate, from 4 to 8 tons/min, is required to eliminate liquid flow in the HRN. However, this does not eliminate liquid flow in the CYC or GOT. A 200% increase in scouring coke flow rate, from 4 to 12 tons/min, results in a liquid flow rate decrease of 48% in the CYC and 57% in the GOT.

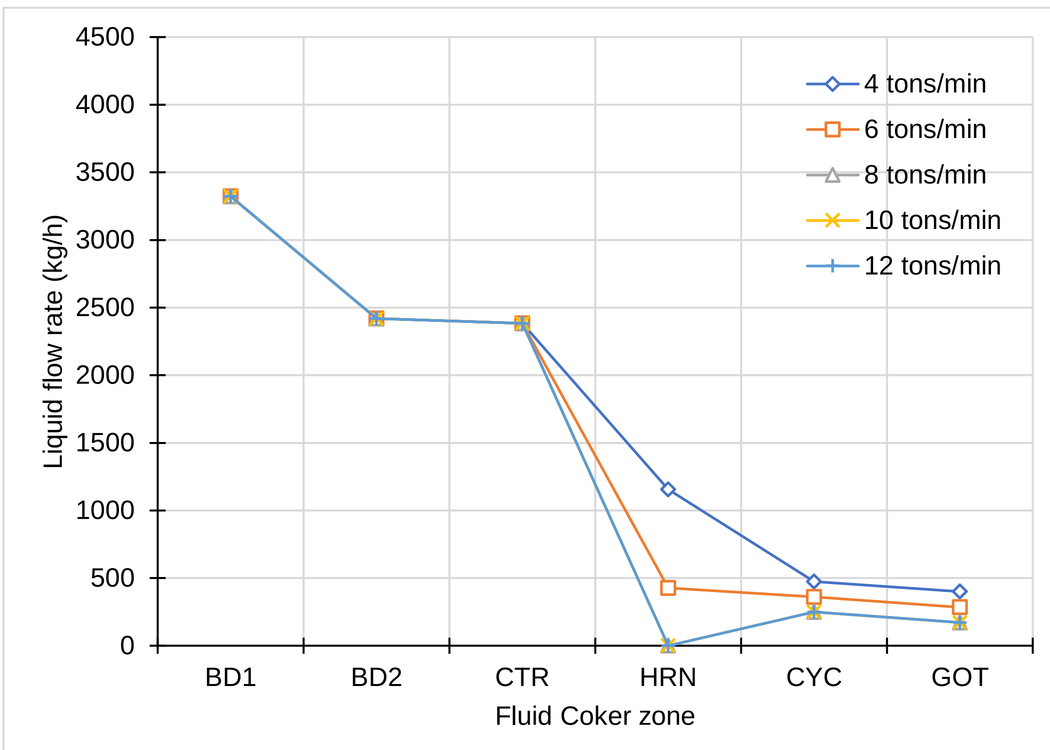


Figure 19 Fluid Coker liquid flow rate for varied scouring coke flow rate with a hot coke flow rate of 40 tons/min (Case 4)

4.3 Hot coke entrainment

One stream of hot coke particles from the burner unit, referred to as hot coke, is fed into the dilute phase zone to provide the heat required for endothermic cracking reactions. A portion of this stream of hot coke will become entrained with the hydrocarbon vapours rising from the top of the fluidized bed. Hot coke entrainment therefore impacts the heat supplied to the Fluid Coker. In Cases 2 and 3, hot coke entrainment was varied from 0.1 to 0.5 wt frac.

In Case 2, the CYC and GOT temperatures ranged from 517 to 537 ˚C (Figure 8). Liquid flow was predicted in the CYC and GOT within temperature ranges of 517 to 525 ˚C (Figure 9). Figure 9 shows a slightly higher liquid flow rate in the CYC compare to the GOT, which is due to pressure drops in the GOT as explained above. This effect is particularly noticeable when comparing the liquid flow in the CYC and GOT within the hot coke entrainment range of 0.2 to 0.4 wt. frac. The impact of hot coke entrainment on liquid flow throughout the Fluid Coker is shown in Figure 20. It is clear that hot coke entrainment impacts the liquid flow rate of BD2, where hot coke is introduced to the Fluid Coker. In the Model, the portion of hot coke that is not entrained downstream from BD2 is not mixed back into the bed, so hot coke entrainment does not impact the BD1 zone. The effects of hot coke entrainment are particularly interesting in BD2, where liquid flow is predicted to increase at a hot coke entrainment of 0.1 wt. frac. This is due to the Model's heat balance calculation for the hot coke transfer line. In the Model, hot coke is introduced to BD2 with a portion of saturated steam. While burner line temperature, hot coke flow rate, and hot coke entrainment can be varied, the flow of saturated steam remains constant. At low hot coke entrainment, there is insufficient heat supplied to the BD2 zone to mitigate the effects of the relatively cool saturated steam on the temperature of the zone. As a result, the Model predicts increasing condensation in BD2 at low hot coke entrainment. A 30 wt% increase in hot coke entrainment, from 0.1 to 0.4 wt. frac., is required to eliminate liquid flow in the BD2 zone.

Figure 20 also shows some liquid flow in the HRN at a hot coke entrainment of 0.1 and 0.2 wt. frac. A 20 wt% increase in hot coke entrainment, from 0.1 to 0.3 ft. frac. Is required to eliminate liquid flow in the HRN. However, this does not eliminate liquid flow in the CYC or GOT. A 30 wt% increase in hot coke entrainment, from 0.1 to 0.4 wt. frac., is required to eliminate liquid flow in the CYC. A 20% increase in hot coke entrainment, from 0.1 to 0.3 wt. frac., is required to eliminate liquid flow in the GOT.

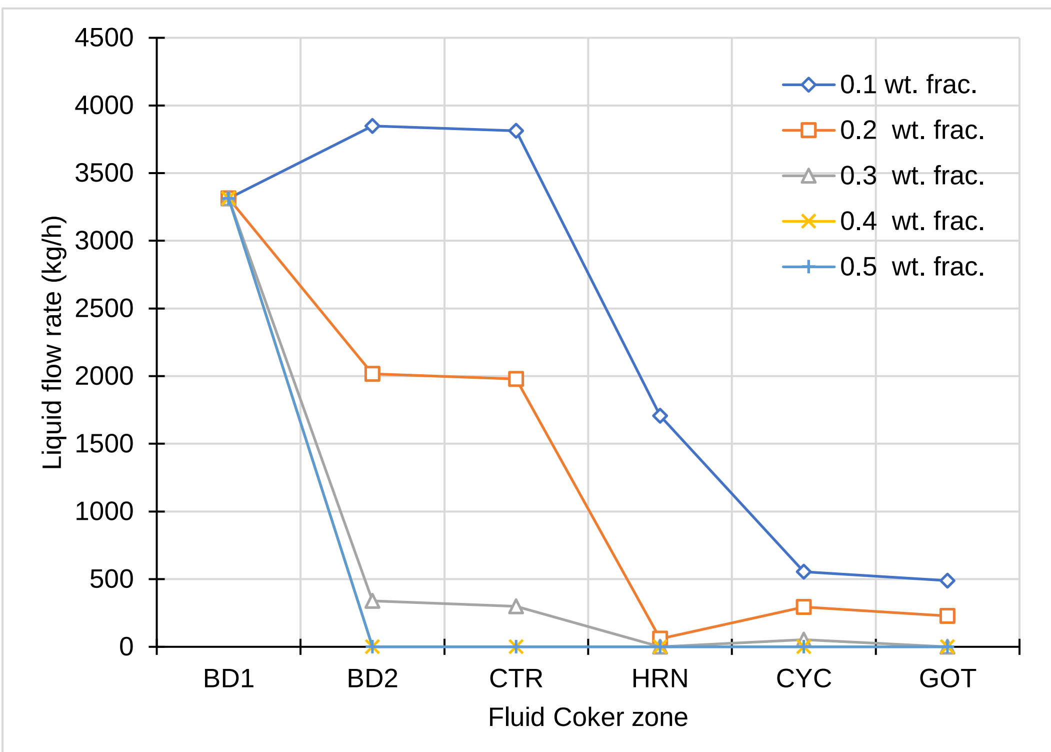


Figure 20 Fluid Coker liquid flow rate for varied hot coke entrainment, with a transfer line temperature of 590 ˚C (Case 2)

In Case 3, the CYC and GOT temperatures ranged from 517 to 537 ˚C (Figure 10). Liquid flow was predicted in the CYC and GOT within temperature ranges of 517 to 525 ˚C (Figure 10). The effects of hot coke entrainment were comparable to those described for Case 2.

4.4 Secondary parameters

The Model was also used to investigate the impact of secondary parameters on temperature and liquid flow rate in the cyclone and gas outlet tube zones. Sensitivity analyses were performed on horn chamber diameter, thermal cracking fraction, and transfer line steam flow rate. The horn chamber diameter impacts the contraction geometry in the dilute phase zone of the Fluid Coker, and therefore impacts the pressure drops in that zone. The thermal cracking fraction is the mass fraction of liquid that is assumed to participate in thermal cracking reactions in the Model, and therefore impacts the temperature in all zones with liquid flow. The transfer line steam flow rate affects the composition, temperature, and flow rate in the Fluid Coker from BD2 through to the GOT.

4.4.1 Horn chamber diameter

In a commercial Fluid Coker, the horn chamber diameter impacts the velocity, residence time and gas-solid mixing in the horn chamber and the downstream cyclones and gas outlet tubes. Although the Model assumes ideal mixing and therefore does not currently account for variations in gas-solid mixing, it does account for the effects of Fluid Coker geometry on velocity and vapour residence time in each of the six modeled zones. To investigate whether horn chamber geometry significantly impacts liquid flow in the GOT, horn chamber diameter was varied from 6 to 12 feet for the operating envelope presented in Table 12. Sensitivity analysis results are presented in Figure 21.

Table 12 Operating envelope for horn chamber diameter sensitivity analysis

Variable	**Value**	**Units**
Bed temperatur	524	˚C
Transfer line temperature	590	˚C
Hot coke flow rate	45	tons/min
Hot coke entrainment	0.2	wt. frac.
Scouring coke flow rate	6	tons/min
Horn chamber diameter	6 – 12	feet

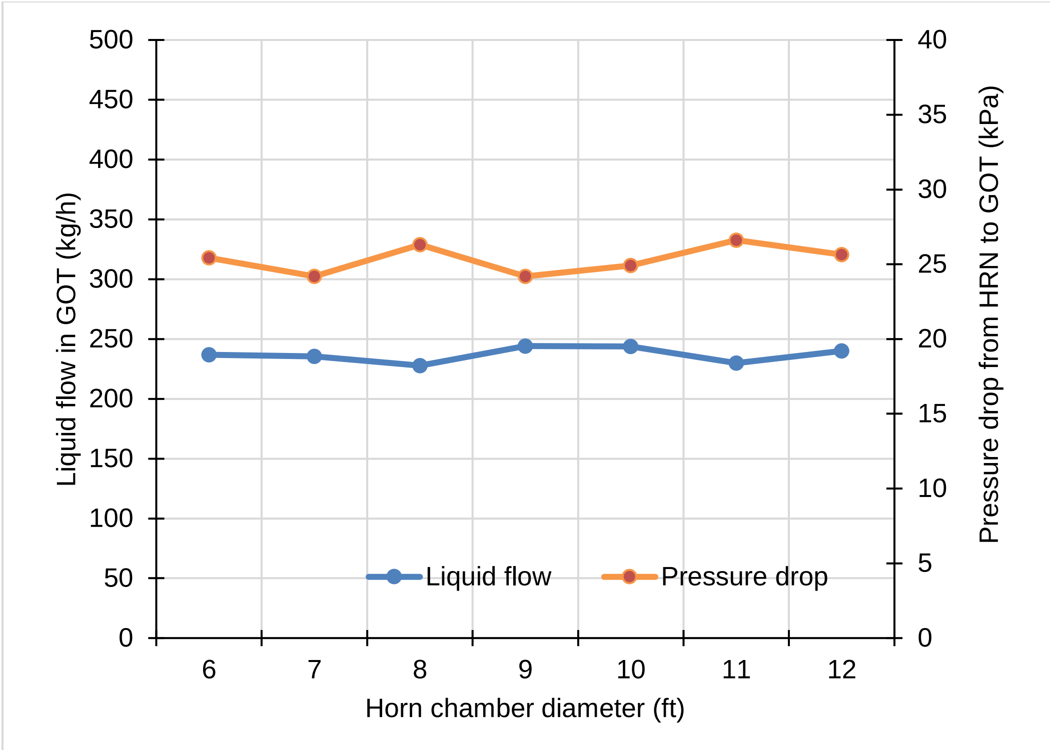


Figure 21 Impact of horn chamber diameter of liquid flow in the GOT

Sufficiently-high pressure drops can promote vaporization of condensed heavy hydrocarbons. However, variation in horn chamber diameter did not result in significant variation in pressure drop between the HRN and GOT, and consequently did not significantly impact liquid flow in the GOT. This suggests that horn chamber diameter may not be an adequate design lever for mitigating cyclone fouling.

4.4.2 Thermal cracking fraction

In a commercial Fluid Coker, endothermic thermal cracking reactions impact the stream composition and temperature wherever they take place throughout the unit. Although the Model does not account for the compositional changes affected by thermal cracking, it does account of the effects of thermal cracking on the temperature of each of the six modeled zones. To investigate whether the thermal cracking fraction (i.e., the mass fraction of liquid that is assumed to participate in thermal cracking reactions in the Model) significantly impacts liquid flow in the GOT, thermal cracking fraction was varied from 0.1 to 0.5 wt. frac. for the operating envelope presents in Table 13. Sensitivity analysis results are presented in Figure 22.

Table 13 Operating envelope for thermal cracking fraction sensitivity analysis

Variable	Value	Units
Bed temperature	524	(˚C)
Transfer line temperature	590	(˚C)
Hot coke flow rate	40	tons/min
Hot coke entrainment	0.3	wt. frac.
Scouring coke flow rate	6	tons/min
Thermal cracking fraction	0.1 – 0.5	wt. frac.

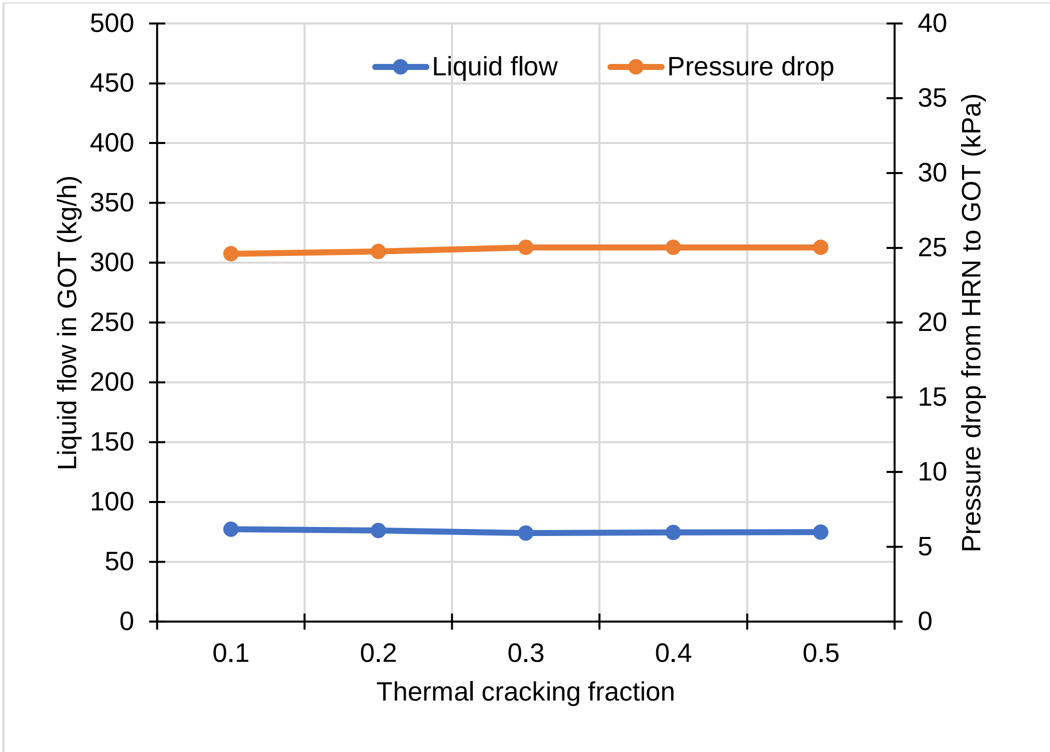


Figure 22 Impact of thermal cracking fraction on liquid flow in the GOT

Sufficiently-high temperature drops can promote condensation of heavy hydrocarbons. In the Model, an increase in the thermal cracking fraction should slightly decrease the temperature of each Fluid Coker zone that has liquid flow. However, variation in thermal cracking fraction did not result in significant variation in liquid flow rate in the GOT and did not significantly impact pressure drop between the HRN and GOT. This suggests that thermal cracking reactions may not significantly impact Fluid Coker cyclone fouling.

4.4.3 Transfer line steam flow rate

In a commercial Fluid Coker, the burner transfer line transports hot coke particles from the burner unit with steam to the Fluid Coker. The hot coke and scouring coke stream both contain steam from the burner transfer line. Transfer line steam flow rate therefore impacts the temperature of the hot coke and scouring coke streams, subsequently impacting the temperature, composition and flow rates at the hot coke outlet and all downstream zones. To investigate whether transfer line steam flow rate significantly impacts liquid flow in the GOT, transfer line steam flow rate was varied from 1 to 10 kg/h for the operating envelope presented in Table 14. Sensitivity analysis results are presented in Figure 23 and Figure 24.

Table 14 Operating envelope for transfer line steam flow rate sensitivity analysis

Variable	**Value**	**Units**
Bed temperature	524	˚C
Transfer line temperature	590	˚C
Hot coke flow rate	45	tons/min
Hot coke entrainment	0.2	wt. frac.
Scouring coke flow rate	6	tons/min
Transfer line steam flow rate	1 – 10	kg/s

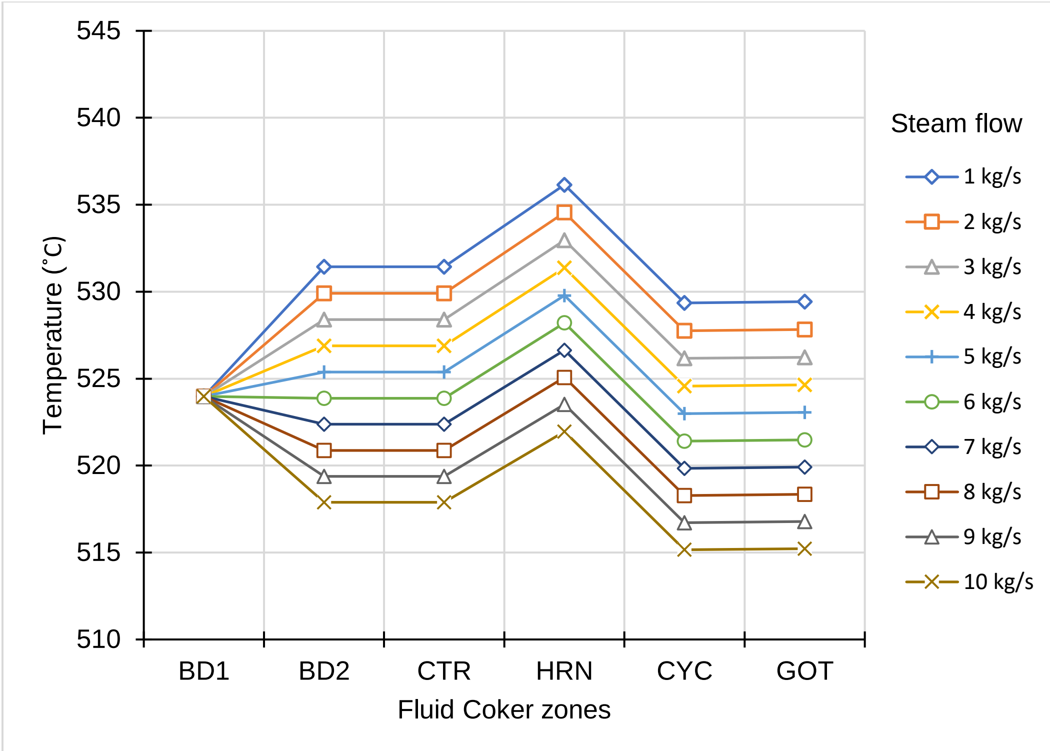


Figure 23 Effect of transfer line steam flow on temperature in the Fluid Coker zones

The impact of transfer line steam flow rate on Fluid Coker zone temperatures is shown in Figure 23. Increasing transfer line steam flow rate results in decreased temperature for all Fluid Coker zones downstream of BD1. This may be partly due to the transfer line steam temperature, which is relatively low (185 ˚C) compared to the transfer line temperature (590 ˚C). Figure 23 shows that a variation from 1 to 10 kg/s of transfer line steam results in a temperature decrease of 14 ˚C on average for all zones. A transfer line steam flow rate of 10 kg/s represents 1 mass% of the transfer line burner coke flow rate. Based on these results, it is expected that decreasing transfer line steam flow rate results in decreased liquid flow for all Fluid Coker zones.

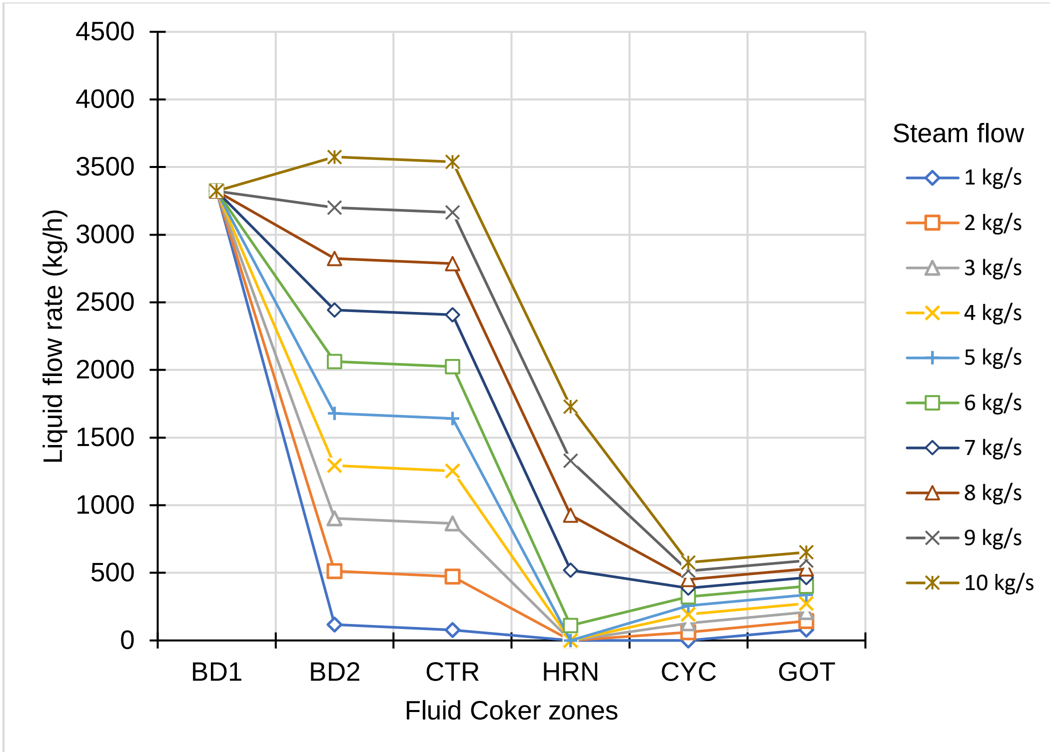


Figure 24 Effect of transfer line steam flow on liquid flow in the Fluid Coker zones

The impact of transfer line steam flow rate on Fluid Coker zone temperatures is shown in Figure 24. Decreasing transfer line steam flow rate results in decreased liquid flow rate for all Fluid Coker zones. This suggests that transfer line steam flow rate could be a process lever for mitigating cyclone fouling.

Chapter 5

5 Conclusions and recommendations

The main objective of this thesis was to advance modeling efforts for Syncrude's Fluid Coker cyclone fouling based on the condensation of heavy ends fouling mechanism and improve Fluid Coker unit reliability by proposing fouling mitigation strategies in the reactor cyclones. A phenomenological Model of six zones in the Syncrude Fluid Coker was developed in Aspen Plus and incorporated the impact of vapor-liquid thermodynamic properties, thermal cracking reactions, and overall fluid dynamics.

Four case studies were performed to investigate the impact of burner transfer line temperature, hot coke flow rate, hot coke entrainment from the bed to the horn chamber and scouring coke flow rate on the temperatures and liquid flow rates in the Fluid Coker cyclones and gas outlet tubes. Three sensitivity analyses were performed to study the impact of horn chamber diameter, thermal cracking fraction, and transfer line steam flow rate on liquid flow rate in the gas outlet tubes.

Case study results indicated that the temperatures and liquid flow rates in all Fluid Coker zones simulated by the model were considerably impacted by the studied parameters. The effects of these parameters were particularly relevant in the zones where hot coke and scouring coke were introduced to the Fluid Coker, i.e., near the top of the dense phase zone and in the horn chamber, respectively. The horn chamber was consistently predicted to operate at the highest temperature of all studied Fluid Coker zones due to the introduction of scouring coke. It was found that the absence of liquid flow in the horn chamber did not preclude liquid flow in the cyclones and gas outlet tubes, which can experience condensation driven by pressure drops due to the geometry of the gas outlet tube exit.

The following case study and sensitivity analyses results were obtained:

- Heat provided by hot coke in the dense phase zone was shown to significantly decrease liquid flow rate in all downstream zones under Case 3 operating conditions.

- Heat provided by scouring coke in the horn chamber was shown to significantly decrease liquid flow rate in all downstream zones under Case 4 operating conditions.

- Heat provided by scouring coke in the horn chamber was shown to provide sufficient heat to vaporize all liquid flow to that zone under Case 2 operating conditions.

- Heat provided by an increase in hot coke entrainment was shown to decrease liquid flow rate in all downstream zones under Case 1 operating conditions, except at very low entrainment. In the case of very low entrainment (0.1 wt. frac.), liquid flow rate was shown to increase from the bed to the top of the dense phase zone. This is likely due to insufficient heat being provided to mitigate the cooling effects of transfer line saturated steam.

- Decreased transfer line steam flow rate in the dense phase zone and horn chamber was shown to decrease liquid flow rate in all downstream zones under base case operating conditions.

While the entire complexity of the commercial operation of a Syncrude Fluid Coker is not fully simulated by the Aspen Plus model, these results have identified potential process levers and can provide some guidance on future work for cyclone fouling mitigation. Transfer line temperature and hot coke flow rate may have considerable effects on the overall operation of a commercial Fluid Coker. However, the scouring coke flow rate may be varied commercially without a significant impact on upstream bed operation. Based on the results of the case studies, scouring coke has been identified as the most promising process lever for mitigating Fluid Coker cyclone fouling. In the case of low burner operating temperature, increasing scouring coke flow rate may provide sufficient heat to the horn chamber to vaporize liquid flow in that zone.

Recommendations and future work

This thesis has developed a steady-state process simulation of the Syncrude Fluid Coker which can be used to continue studying the impact of various process and design parameters on Fluid Coker performance. The sequential modular process simulation strategy of Aspen Plus allows for straightforward modifications in the Flowsheet environment, so additional layers of complexity can be incorporated into the Model in future work.

A rigorous simulation of cyclone separation can be performed in Aspen Plus, and this may provide a more accurate simulation of pressure drops in the Fluid Coker cyclones. Similarly, a rigorous simulation of a pipe segment can be performed in Aspen Plus, and this may provide a more accurate simulation of pressure drops in the Fluid Coker gas outlet tubes. It is possible that pressure drops due to horn chamber contraction could be rigorously simulated with a pipe segment as well.

Further simulation efforts in Aspen Plus to better understand the effects of thermal cracking throughout the Fluid Coker would not be trivial. One limitation of the Assay-based model stream is that its composition of pseudocomponents is based on boiling point ranges. These pseudocomponents can be simulated to undergo chemical reactions, however this would be a difficult approach for a model stream with the complexity of Fluid Coker feed. An experimental study that categorizes the reacting fractions of the Fluid Coker (or comparable) feed by boiling point may provide sufficient data to approximate the compositional changes resulting from chemical reactions in Aspen Plus.

Unideal gas-solid mixing cannot be simulated in Aspen Plus, however gas and solids streams can be split and re-mixed in different fractions to approximate unideal mixing. However, this will not provide sufficient flexibility to simulate the effects of any varied parameters on the fluidized bed. Further investigation into the effects on hot coke entrainment on all Fluid Coker zones should be first done experimentally, and approximations may then be applied to the Aspen Plus model.

While the current model has been developed to simulate the global behaviour of the Fluid Coker, further modeling efforts could continue to study local behaviour in individual Fluid Coker zones. Future study on deposition rate in the cyclones and gas outlet tubes would be a natural progression to this work. Specifically, the temperature and bulk liquid concentration predicted by the Model could be combined with mathematical mass transfer models to calculate deposition rate, and this could be subsequently related to upstream burner pressure leading to unit shutdowns.

Furthermore, a combined Aspen Plus-CFD approach could be used to related global parameters such as gas and liquid flow rates and temperatures to local phenomena such as deposition. This approach would be best applied first to the gas outlet tubes, where the operating conditions can be compared to Syncrude operating data and the deposition can be directly related to operating pressure.

Experimental pilot-scale work is recommended to further investigate scouring coke as a process lever for fouling mitigation, and to further investigate the effects.

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