CFD simulation of an industrial FCC regenerator

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Bioprocesos y flujos reactivos
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“The Lord is my shepherd, I shall not want”
Through a Computational Fluid Dynamics (CFD) simulation of the particle-laden flow of the two stages of a Fluid Catalytic Cracking (FCC) High Temperature Regenerator (HTR), new designs for the particle distributor in the combustor stage and the arm disengagers in the regenerator stage that improved the HTR performance were proposed. The simulations involved 580 thousand cells for the combustor and 1.5 million cells for the regenerator and were conducted with the commercial CFD software package Fluent 15.0 using an Euler-Euler model and a phase-coupled SIMPLE algorithm. A thorough analysis of a 298-hole air distributor conducted prior to the combustor simulation, set the air flow boundary conditions of the 22 m high and 3.2 m diameter combustor. After the evaluation of several drag models available in the literature, the Modified model ([1]) with cluster diameters of 400 m and 200 m for the dense and dilute phases, respectively, reproduced the theoretical characteristics of the turbulent bed that is typical of HTR combustors. The same drag model also reproduced the bubbling bed that is reported for the regenerator stage of HTRs. An analysis of the solid distribution showed that when solids enter the reactor through simple inlets located at opposite locations, the solid distribution is poor. However, when a two-arm, solid distributor that includes six lateral and a central inlet is implemented, the solid distribution improves, as the mal-distribution coefficient ($M_f$) decreases from 0.31 to 0.22 in the most critical region of the dense phase. Improvements in the characteristics of the Residence Time Distribution (RTD) and the size of the bed are also evidence of the benefits that the new proposed combustor design gives to the HTR performance.

For the regenerator stage of the HTR the CFD simulation revealed the existence of a high-velocity field surrounding the solid disengangers that transport the solid from the combustor. This high velocity contributed to a relatively high solid flow through the cyclones, 42%, when compared to the recommended range of 20% to 30%. By increasing the length of the disengager shroud, the gas velocity decreased and the solid flow through cyclones was reduced to 34%. The two simulations illustrate the ability of CFD to improve the performance of complex industrial equipment.
I want to thank my supervisor, Professor Alejandro Molina.

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<tr>
<td>CFD</td>
<td>Computational Fluid Dynamic</td>
</tr>
<tr>
<td>FCC</td>
<td>Fluid Catalytic Cracking</td>
</tr>
<tr>
<td>HTR</td>
<td>High Temperature Regenerator</td>
</tr>
<tr>
<td>UDF</td>
<td>User Define Function</td>
</tr>
<tr>
<td>BC</td>
<td>Boundary Condition</td>
</tr>
<tr>
<td>PFR</td>
<td>Plug Flow Reactor</td>
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<tr>
<td>CSTR</td>
<td>Continuous Stirred Tank Reactor</td>
</tr>
<tr>
<td>RTD</td>
<td>Residence Time Distribution</td>
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<table>
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<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tbody>
<tr>
<td>$\beta$</td>
<td>Drag coefficient</td>
<td>$kg/m^3 \cdot s$</td>
</tr>
<tr>
<td>$\rho_q$</td>
<td>Density $q^{th}$ phase</td>
<td>$kg/m^3$</td>
</tr>
<tr>
<td>$\alpha_q$</td>
<td>Volume fraction $q^{th}$ phase</td>
<td></td>
</tr>
<tr>
<td>$g$</td>
<td>Gravity</td>
<td>$m/s^2$</td>
</tr>
<tr>
<td>$Y_{iq}$</td>
<td>Mass fraction $i^{th}$ specie, $q^{th}$ phase</td>
<td></td>
</tr>
<tr>
<td>$v_q$</td>
<td>Velocity $q^{th}$ phase</td>
<td>$m/s$</td>
</tr>
<tr>
<td>$m_{pq}$</td>
<td>Mass transfer from $p^{th}$ phase to $q^{th}$ phase</td>
<td>$kg/s$</td>
</tr>
<tr>
<td>$\beta_c$</td>
<td>CO/CO2 ratio</td>
<td></td>
</tr>
<tr>
<td>$k_c$</td>
<td>Carbon combustion rate</td>
<td>$1/(atm \cdot s)$</td>
</tr>
<tr>
<td>$x_{pt}$</td>
<td>Relative catalytic CO combustion rate</td>
<td></td>
</tr>
<tr>
<td>$k_{het}$</td>
<td>Heterogeneous rate constant</td>
<td>$kmol/(kgcat \cdot s \cdot atm^2)$</td>
</tr>
<tr>
<td>$k_{hom}$</td>
<td>Homogeneous rate constant</td>
<td>$kmol/(m^3 \cdot s \cdot atm^2)$</td>
</tr>
<tr>
<td>$C_{rgc}$</td>
<td>Mass of carbon on catalyst surface</td>
<td>$kg/s$</td>
</tr>
<tr>
<td>$C_{rgh}$</td>
<td>Mass of hydrogen on catalyst surface</td>
<td>$kg/s$</td>
</tr>
<tr>
<td>$MWC$</td>
<td>Molecular weigh Carbon</td>
<td>$kg/kmol$</td>
</tr>
<tr>
<td>$MWH$</td>
<td>Molecular weigh Hydrogen</td>
<td>$kg/kmol$</td>
</tr>
<tr>
<td>$E_i$</td>
<td>Activation Energy</td>
<td>$K, J/mol$</td>
</tr>
<tr>
<td>$A_i$</td>
<td>Pre-exponential factor</td>
<td></td>
</tr>
<tr>
<td>$R$</td>
<td>Universal constant of gases</td>
<td>$J/(mol \cdot K)$</td>
</tr>
<tr>
<td>$P$</td>
<td>Pressure</td>
<td>$atm$</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
<td>$K$</td>
</tr>
<tr>
<td>$h/H$</td>
<td>Dimensionless height</td>
<td></td>
</tr>
<tr>
<td>$M_f$</td>
<td>Mal-distribution factor</td>
<td></td>
</tr>
<tr>
<td>$d^*_p$</td>
<td>Mean cluster diameter, dense zone</td>
<td>$\mu m$</td>
</tr>
<tr>
<td>$d_p$</td>
<td>Mean cluster diameter, diluted zone</td>
<td>$\mu m$</td>
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To my Grandmother...
Chapter 1

Introduction

1.1 Background

Fluid Catalytic Cracking is the process used by petroleum industry to transform feedstock with low-value, high molecular weight and high boiling point in more valuable products, through catalytic reactions. A riser reactor, catalyst separators and a regenerator normally compose the FCC unit. In the reactor the endothermic cracking reactions of the gas oil occur. Coke formation is unavoidable in the catalytic cracking process. Fast deactivation by blocking of the active pores of the catalyst is a consequence of coke deposition. To burn the coke deposited on the catalyst surface. The FCC regenerators are employed.

The FCC regenerator is as important as the riser reactor. First, because in it the activity of the catalyst is reestablished and second, because the exothermic reactions of coke combustion provide a large fraction of the energy used in the riser. The phenomena inside the FCC regenerator are complex as it involves gas-solid mixing and the heterogeneous, as well as some homogeneous reactions of coke combustion. This complexity increases the difficulty of predicting its performance. Computational fluid dynamics (CFD) is a tool that has proved to be a useful approach for understanding hydrodynamics and reactive behavior in multiphase flow.

1.2 Literature Review

In a typical FCC unit, catalytic cracking reactions take place in a vertical riser reactor. With the help of steam, the liquid oil is atomized. Smaller oil droplets increase the availability of feed at the reactive acid sites on the catalyst-vaporized oil. Hot catalyst allows breaking the vaporized oil into smaller molecules. This phenomenon causes a gas expansion, which drags the catalyst to the top of the reactor [2]. The reactions are rapid, and a few seconds of contact time is necessary. Cracking reactions take place in 3 seconds or less [3]. Coke formation is unavoidable in FCC process due to dehydrogenation and condensation of poly-aromatics and olefins [4]. Coke deposition blocks the active pores of the catalyst lowering its activity. The spent catalyst contains carbon in an amount from 0.2 to 2 wt-%, which is
Chapter 1. Introduction

present in the form of coke. Afterwards, catalyst particles and light products enter the stripper section. Stripping steam primarily removes the entrained hydrocarbons from catalyst surface. Afterwards, the cracking products and the spent catalyst leave the stripping section to the fractionation tower and the regenerator respectively.

Fluidized beds are widely used in a variety of processes with gas-solid multiphase flows, such as coal combustion [5] and FCC regenerators [6]. This is due to good gas-solid mixing and high heat and mass transfer rates [7]. In these reactors, a gas is passed through solid particles at high enough velocities to suspend the solids and cause them to behave as a fluid [8]. The particles used in FCC belong to group A of the Geldart classification of powders. In Gerdart’s classification the solid particles are organized in groups characterized by density difference between solid and air, and the mean particle size [9]. Geldart A particles have a small mean particle size and/or a low particle density, typical example FCC catalysts ($d_p = 75 \mu m$ and $\rho_p = 1500 kg/m^3$) [10].

FCC regenerators usually operate in turbulent fluidization regimen and are characterized by two zones, a ”dense zone” in the lower part of the regenerator with high solid concentration and where almost all coke is burned [11], and a ”dilute zone” with lower concentration of solids which have been dragged by the gas to the top. Two-stage cyclones separate the solid particles from the gas in top of the regenerator. To fluidize the particles and to burn the coke, air enters the regenerator through a gas distributor. The turbulent fluidization regimen is commonly considered to occur between bubbling fluidization and the fast fluidization regimes [12]. A gas velocity higher than in blubbing fluidization regimen, no distinct bubbles, much churning, and violent solid movement are characteristics of this regimen. The surface of the dense bed fades and there are increase of the solids concentration in the region above the dense bed [13]. In extremely high gas velocities, the fluidized bed transits to pneumatic conveying flow, and the most solid particles leave the dense bed.

To remove the coke is the main function of the FCC regenerator. Coke is primarily composed of carbon, it may contain from 3 to 12 wt-% hydrogen and a small amount of sulfur and organic nitrogen molecules [14]. A fraction of hydrocarbon vapors that cannot be removed from the catalyst pores in the stripping section are also carried with the spent catalyst to the regenerator [3]. Air provides oxygen for the combustion of coke. The oxidation of carbon and hydrogen are the main reactions that are usually used to describe the coke combustion process that takes place in the regenerator [15], [16]. The main components in the gas phase are oxygen, nitrogen, carbon monoxide, carbon dioxide and water vapor. Depending upon the feed nitrogen levels and the regenerator conditions $NO_X$ concentrations are typically in the range of 50–500 ppm [17]. $NO$ is the primary component of $NO_X$ in the FCC regenerator. Its consist of 90% $NO$ and 10% $NO_2$ [18]. The fluid catalytic cracking unit contributes with about 50% of the $NO_X$ emissions in the refinery [19]. Refining industry must use additives...
or platinum-based zeolite catalysts for \( CO \) oxidation and minimize its emission. It has been proven that platinum presence decreases the \( CO \) to \( CO_2 \) ratio at the reactor effluent [20].

Various studies at laboratory scale have been carried out to obtain mechanisms and kinetics for coke combustion on a cracking catalyst. Weisz and Goodwin [21], studied the intrinsic burning of coke finding that the burning kinetics are largely independent of source and method of coke deposition. Furthermore, they found that the carbon oxidation rates are normally proportional to the amount of carbon present, indicating the degree of dispersion is high enough to make the carbon atoms fully accessible to oxygen. The carbon and hydrogen burning rates have been reported as first order with regard to the carbon and hydrogen on catalyst surface and on the partial pressure of oxygen [22]. De Lasa [23], found that the coke burning rate value is independent of the rate equation chosen for the carbon monoxide post-combustion reaction. Arbel et al. [24] proposed an improved and updated model for modern FCC units. Based on a more detailed kinetic description of the chemistry in the regenerator using the full range of published data. Unlike of Weisz [25], who used a correlation for the \( CO_2 \) to \( CO \) ratio dependent of the on temperature, Arbel et al. included a complete description of \( CO \) to \( CO_2 \) combustion kinetics considering the effect of catalytic combustion promoters. The model realistically described the transition of operating conditions from partial to full combustion.

First studies of the FCC regeneration process used different ways and models to integrate both hydrodynamic and chemistry phenomena into regenerator. One example is the two-fluid model [26], where the dense zone of the fluidized bed is divided in bubble and emulsion phases. The bubble phase does not contain any solids and gas flows following a plug flow behavior. In the emulsion phase, gas and solid components are fully mixed. The freeboard is modeled as an ideal plug flow reactor [27]. The kinetic parameters are taken from different sources [28], temperature profiles, gas and solid conversions obtained are in good agreement with industrial data. The grid model was also developed to incorporate the influence of the grid jets in the two-fluid model [29]. The grid model including thermal effects, gives better results than the two-fluid model for industrial scale temperature [30]. A third model, the bubbling bed model [31], assumes that the catalyst underneath a bubble is carried up by the bubble until it reaches the emulsion phase and becomes mixed into it. A comparison of the above models concluded that the bubbling-bed model of the fluidized-bed catalyst reactor, with the proposed two thermally uniform stages to account for the heat balance, is able to describe a regenerator with the smallest error [11]. Other studies [32], [33] have also addressed the interaction between hydrodynamics and kinetics with simplified approaches such as combinations of PFRs and CSTRs in series.

Although the above models showed comparable predictions with industrial data for the regeneration process, a deep understanding of the hydrodynamic and chemical phenomena, combined with an evaluation of
the physical configuration, is necessary to improve the regenerator performance. Computational Fluid Dynamics (CFD) is considered a powerful tool for predicting the hydrodynamic properties and other characteristics of fluidized beds and other dense multiphase flows [34]. CFD models have been used to study several variables associated to regenerator performance: spent catalyst distribution in order to obtain better mixing and hence significantly reduced breakthrough of oxygen and CO into the freeboard compared with the existing design to reduce after-burning phenomenon [35]; the effect of changing the operations conditions to improve the regenerator behavior without physical modifications [6], and the effect of a complex geometry on the performance of of an industrial FCC regenerator [36].

1.3 Objectives

1.3.1 Overall objective

To propose design alternatives to improve the operation of an industrial fluid catalytic cracking regenerator.

1.3.2 Specific objectives

- To develop CFD simulations to better understand the behavior of an industrial FCC regenerator.

- To identify the main bottlenecks in the catalyst regeneration in a FCC unit.

- To evaluate design alternatives to improve operation of a FCC regenerator

1.4 Problems associated to FCC regenerators

The FCC regenerator must behave as a CSTR, at least in the dense zone with spent catalyst and air perfectly mixed without temperature and density variations. However, in the industrial application is not easy obtain this behavior. The FCC regenerators can suffer different operational problems, such as afterburn, non-homogenous regenerated catalyst, emissions (NOX, SOX, CO) and severe catalyst attrition. Typical pollutant concentration ranges in fluid catalytic cracking units are 50-200 vppm for NOX; 300-600 vppm for SOX and 0-5 vol% for CO. Particulate emissions due to
catalyst attrition and cyclone efficiency are approximately 1 pound of catalyst fines per 1000 pounds of coke burned in the regenerator [37].

### 1.4.1 Afterburn

Afterburn is an abnormal temperature difference between the dense and dilute zones of a FCC regenerator. This phenomenon is the result of combustion of the CO in the flue gas leaving the dense bed with excess of O$_2$. Ideally, all the carbon in coke is burned essentially completely to CO$_2$, with only a trace of CO remaining in the flue gas. The mixture between solid particles and combustion air in the regeneration process is critical since most of the catalyst in the bed has very little coke on it, about 1%w. If an area of the regenerator no contains coke, the combustion air escapes from the regenerator with most of its oxygen intact. At the same time, the CO content in the flue gases is high due to inefficient mix between the air and the particles. Afterburn results when the CO content in the flue gases mix with the high oxygen content gases in the regenerator vessel. Low temperature can promote the occurrence of afterburn. Other factor is low residence time. Afterburn usually take place between the dilute phase and the cyclone outlets. The oxidation of CO to CO$_2$ releases twice as much heat as does the burning of C to CO. The large heat release coupled with the relatively small amount of mass in the dilute-phase produces a large delta of temperature between the dilute and dense phases in the regenerator [38]. The afterburn causes thermal deactivation of the FCC catalyst and damage on cyclones due to hot spots. Although a certain amount of afterburn is normal in most FCC regenerators, it can become critical if the temperatures approach or exceed the mechanical or metallurgical design conditions of regenerator components, such as cyclones.

### 1.4.2 Emissions

The flue gas stream at the exit of a FCC regenerator consists of oxygen, carbon monoxide, carbon dioxide, water, nitrogen, NO$_X$ and SO$_X$. The NO$_X$ emissions of a FCC regenerator can contribute up to 50% of the total NO$_X$ emissions in a refinery [39]. The NO$_X$ could be formed by two mechanism. Thermal NO$_X$ produced from the reaction of molecular nitrogen with oxygen and fuel NO$_X$ produced from the oxidation of nitrogen in the coke. The major component, more than 95%, of NO$_X$ is NO. Formation of N$_2$O and NO$_2$ is negligible under FCC regenerator conditions [19].

Feed quality is the most significant factor affecting SO$_X$ emissions from an FCC unit. The SO$_X$ in the FCC regenerator is formed from the combustion of sulfur containing molecules bound in coke. Although only a small percentage of the feed sulfur ends up in coke, typically <10%, all of the sulfur in coke is oxidized to SO$_X$ [40].
Different commercial additives have been used in the industry for the reduction of $NO_X$ and $SO_X$ emissions. Additives for $NO_X$ are used to catalyze its reaction with $CO$ or coke in the dense phase bed of the regenerator. The reduction of emissions of $SO_X$ involve three steps. The $SO_2$ oxidation to $SO_3$, after the chemisorption and storage of $SO_3$ as a sulfate and finally released as $H_2S$ in the reactor [41].

The mixing between spent catalyst and air is a key parameter in the performance of an industrial FCC regenerator. This may exhibit no uniform catalyst flow patterns, which produce no uniform coke and oxygen profiles. These non-uniformities can result in increased afterburn, as was already discussed. Carbon monoxide from oxygen deficient regions of the bed mixes with excess oxygen from other regions. In partial combustion operation, this requires reduction in air rate leading to poor combustion efficiency. In complete combustion, it requires higher excess oxygen, which increases $NO_X$ emissions [42]. Modern refineries add $CO$ promoters, Pt-based compounds that accelerate the oxidation of $CO$. Unfortunately, $CO$ promoters increase $NO_X$ emissions [43]. This is due to the fact that $CO$ reacts with $NO_X$ to produce $N_2$ and $CO_2$.

1.4.3 Catalyst Attrition

The formation of fines in a fluidized catalytic cracker unit (FCCU) due to catalyst attrition is a major source of catalyst loss [44]. In a FCC unit, the catalyst is continuously being lost through both the reactor and regenerator. Minimizing these losses is essential to maintain optimum unit operation as well as environmental compliance and to reduce catalyst costs. In FCC regenerators two attrition mechanisms are generally recognized: particle shattering and surface abrasion of particles. The abrasion mechanism generates fines of much smaller average size [38]. In fluidized beds have been identified three regions as main attrition sources, namely the grid jets, the bubbling bed itself, and the cyclone section [45]. The high air velocity within the regenerator promotes particle to particle and particle to wall collisions. The inter-particle collisions cause abrasion of the particle surfaces [46]. In the bubbling bed zone, the particle attrition is proportional to the difference between the superficial gas velocity and the minimum fluidization velocity [47]. The particle collisions in the bed in movement cause particle attrition. Cyclones for removing small particles from a gas stream also give rise to attrition due to the particles impact on walls of the cyclones [48]. During normal operation, an average FCC unit may replace 1% of its catalyst inventory to make up for particle attrition. The physical properties of FCC catalysts are designed for optimum fluidization and low attrition [40].

The design of gas and solids distributor are the key to minimize the operational troubles of a FCC regenerator. Low jet velocities in the gas distributor can decrease the catalyst attrition phenomenon. “Perfect” mixing in dense bed of solid particles and air allows to decrease the use of $CO$
1.4. Problems associated to FCC regenerators

combustion promoters, minimize the afterburn phenomenon and reduce the operational cost. In this study a gas distributor and two different configurations of distributor of solids were evaluated in order improve the performance of an industrial FCC regenerator.
Chapter 2

Methodology

A High-Temperature Regenerator (HTR) was simulated in this study. This model of regenerator was originally patented by Universal Oil Company (UOP) [3]. The CFD simulation of this industrial equipment is complex due to its large dimensions, which increases the computational cost. For this reason, the CFD simulation of the HTR FCC regenerator was divided in three parts: air distributor, combustor and regenerator vessel. These simulations share boundary conditions to relate each of them with the others to obtain the general behavior of the HTR regenerator. The geometries and dimensions of the air distributor for both stages of the HTR regenerator, solid inlets and cyclones are improvements from this work based on the literature and industrial recommendations. Geometries, process description, operating conditions, mathematical model, boundary conditions and models used in the simulations of this industrial FCC regenerator are listed in this section.

2.1 Geometry and process description

Figure 2.1 shows the main components of a high Temperature Regenerator (HTR). It is divided in two zones: a combustor where large portion of the coke is burned and a regenerator vessel where, depending on the needs, air can be used only for fluidization if complete combustion has occurred in the combustor. Otherwise air is use for coke combustion.

The catalyst with coke on its surface enters to the combustor through the spent catalyst inlet. The spent catalyst from the riser reactor usually contains coke in an amount varying from 0.2 to 2 wt-%. It is primarily composed of carbon, 3 to 12 wt-% hydrogen and small amounts of sulfur, nitrogen and other materials [14].

The air used to fluidize the spent catalyst and for the combustion of coke is fed to the combustor stage through of the air distributor. The catalyst is dragged to the top of the combustor by the air and the flue gas. The mixture of catalyst particles and flue gas is discharged in the second zone of the
regenerator. Arms disengagers provide the first stage of separation of catalyst from the combustion products. Air fed to the regenerator vessel, flue gas and catalyst fines enter the two-stage of cyclones. Flue gas is collected in the plenum chamber and withdrawn from the combustor regenerator vessel through an exit conduit. Catalyst particles are returned to the dense bed of the regenerator vessel through cyclone diplegs. Catalyst from the dense bed of the regenerator vessel is transferred through the regenerated catalyst standpipe back to the riser reactor, where it again contacts feed as the FCC process continues. In order to accelerate coke combustion, hot regenerated catalyst is recycles to the combuster through an external standpipe.

The most important dimensions in Figure 2.1 are listed in Table 2.1. They agree with data in different patents [14], [49], [50] and handbook [3] of FCC regenerators.

<table>
<thead>
<tr>
<th>Height</th>
<th>Value (m)</th>
<th>Diameter</th>
<th>Value (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H1</td>
<td>10.5</td>
<td>D1</td>
<td>3.2</td>
</tr>
<tr>
<td>H2</td>
<td>3.5</td>
<td>D2</td>
<td>1.4</td>
</tr>
<tr>
<td>H3</td>
<td>8.1</td>
<td>D3</td>
<td>4.75</td>
</tr>
<tr>
<td>H4</td>
<td>20.1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
2.2 Operating conditions

Operating conditions used in this study were obtained from typical values reported in patents [14], [49]–[51] and in the literature [6], [11], [15], [16], [28], [32], [36] and are listed in, Table 2.2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Literature</th>
<th>CFD simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure, kPa</td>
<td>173-414</td>
<td>289</td>
</tr>
<tr>
<td>Temperature, K</td>
<td>800-1020</td>
<td>800-930</td>
</tr>
<tr>
<td>Coke on catalyst, w%</td>
<td>0.2-2.0</td>
<td>0.96</td>
</tr>
<tr>
<td>C/H mass ratio, w%</td>
<td>8.0-15.0</td>
<td>8.0</td>
</tr>
<tr>
<td>Air/coke mass ratio, kg/kg</td>
<td>13-15</td>
<td>14</td>
</tr>
<tr>
<td>Air Temperature, K</td>
<td>433-727</td>
<td>600</td>
</tr>
<tr>
<td>Spent catalyst, kg/s</td>
<td>376-501</td>
<td>466.6</td>
</tr>
<tr>
<td>Solid volume fraction, spent catalyst</td>
<td>0.15-0.25</td>
<td>0.2</td>
</tr>
<tr>
<td>Temperature spent catalyst, K</td>
<td>753-810</td>
<td>800</td>
</tr>
<tr>
<td>Recirculated/spent catalyst mass ratio, kg/kg</td>
<td>1.1-1.3</td>
<td>1.2</td>
</tr>
<tr>
<td>Solid volume fraction, recirculated catalyst</td>
<td>0.15-0.25</td>
<td>0.2</td>
</tr>
<tr>
<td>Temperature recirculated catalyst, K</td>
<td>800-1012</td>
<td>850</td>
</tr>
</tbody>
</table>

2.3 Mathematical model

The three-dimensional simulation of an industrial FCC regenerator was conducted using the Euler-Euler approach. In this model both, the gas phase and the solid phase, are modeled as interpenetrating continua with similar conservation equations. The interactions between the two phases are expressed as additional source terms added to the conservation equations. Moreover, the solid phase has similar properties to a continuous fluid. Using the kinetic theory of granular flows, the viscous forces and the solid pressure of the solid phase can be described as a function of the granular temperature [52], [53]. The commercial CFD package Fluent V15.0 was used to carry out the simulation, which allows the discretization of the Navier Stokes equations of continuity, momentum, species transport, mass and energy transfer, by the method of finite volumes. User define functions (UDFs) were employed for the momentum exchange between gas and solid phases (more detail Chapter 3) and the kinetic mechanism for coke combustion (more detail Chapter 6). The chapter only describes the equations of momentum and species transport, because in these UDFs were used. The
equations of the conservation, of mass and heat transfer can be consulted in the Fluent user guide [54].

2.3.1 Momentum equation

The equation for momentum conservation of phase $q$ is

$$\frac{\partial}{\partial t} \left( \rho_q \alpha_q \vec{v}_q \right) + \nabla \cdot \left( \rho_q \alpha_q \vec{v}_q \vec{v}_q \right) = -\alpha_q \nabla p + \nabla \cdot \tau_q + \rho_q \alpha_q \vec{g} + \beta \left( \vec{v}_p - \vec{v}_q \right) + \vec{v}_p \dot{m}_{pq} + \vec{v}_g \dot{m}_{gp} \tag{2.1}$$

where $\tau_q$ is the $q^{th}$ phase stress-strain tensor and $\beta$ is the interphase momentum exchange coefficient. Equation 2.1 must be closed with appropriate expressions for the interphase momentum exchange coefficient. For this purpose a User Define Function (UDF) was used (See Appendix B). In Chapter 3, more detail is given about the interphase momentum exchange coefficient.

2.3.2 Species transport model

Equation 2.2 represents the species balance model for the specie $i$ in the phase $q$.

$$\frac{\partial}{\partial t} \left( \rho_q \alpha_q Y_{iq} \right) + \nabla \cdot \left( \rho_q \alpha_q Y_{iq} \vec{v}_q \right) = -\nabla \cdot \alpha_q \vec{J}_{iq} + \alpha_q S_{iq} + \alpha_q R_{iq} + \sum_{p=1}^{n} \left( \dot{m}_{q'p} - \dot{m}_{p'q'} \right) + \text{Rate} \tag{2.2}$$

where $S_{iq}$ is the rate of creation by addition from the dispersed phase plus any user-defined sources, $R_{iq}$ is the net rate of production of homogeneous species by chemical reaction for phase $q$, $\dot{m}_{q'p}$ is the mass transfer source between species and from phase $q$ to $p$ and Rate is the heterogeneous reaction rate. An UDF was used for calculating the heterogeneous reaction rate (See Appendix C).

2.3.3 Residence time distribution (RTD)

The residence time distribution (RTD) is an indirect way to characterize and understand the mixing in a reactor. CFD is an economical and practical tool when compared to experimental methods to carry this analysis. In this study, to compare the mixing between solid particles and the gas in the combustor stage a CFD study was conducted. To obtain the RTD for both combustor stage designs (more details later). The species transport equation for a new species called tracer was resolved. In a time step, the
2.3. Mathematical model

tracer is injected through the gas inlet boundary and the concentration of the tracer at the outlet was monitored to obtain the RTD.

Equation 2.3, describes the residence time distribution function. This function can be used to calculate the time spent by the tracer within the reactor. The amount \( \int_t^{t+\Delta t} E(t)dt \) is the fraction of material leaving the reactor that has resided in the reactor between \( t \) and \( t+\Delta t \).

\[
E(t) = \frac{C(t)}{\int_t^{t+\Delta t} C(t)dt}
\]  
(2.3)

The fraction of all the material that has resided for a time \( t \) in the reactor between \( t = 0 \) and \( t = \infty \) is 1, equation 2.4.

\[
\int_0^{\infty} E(t)dt = 1
\]  
(2.4)

Because the residence time distribution is a probability density function, it may be characterized using statistical moments. Usually only the first two moments are considered [55]. As is the case with other variables described by distribution functions, the mean value of the variable is equal to the first moment of the RTD function. Thus the mean residence time is defined by equation 2.5.

\[
t_m = \frac{\int_0^{\infty} tE(t)dt}{\int_0^{\infty} E(t)dt} = \int_0^{\infty} tE(t)dt
\]  
(2.5)

The second moment commonly used is taken about the mean and is called the variance, or square of the standard deviation. It is defined by equation 2.6.

\[
\sigma^2 = \int_0^{\infty} (t - t_m)^2 E(t)dt
\]  
(2.6)

In reference [56] a more detailed description of applications of the RTD functions and of its mathematical derivation can be consulted.

2.3.4 Mal-distribution coefficient

To measure the radial distribution of solid at different levels of the both combustor designs a mal-distribution coefficient \( (M_f) \) was used. This coefficient has been used to quantify the radial distribution of liquid and gas in Trickle bed reactors (TBRs) [57] and is defined by equation 2.7.
Chapter 2. Methodology

\[ M_f = \sqrt{\frac{1}{N(N-1)} \sum \frac{(Q_{si} - Q_{mean})^2}{Q_{mean}}} \]  

(2.7)

where \( Q_{si} \) is the solid flow rate through zone \( i \), \( N \) the number of zones (8 for each level, in this case) and \( Q_{mean} \) the mean flow rate through all zones (\( = Q_{s}/N \)). The mal-distribution coefficient was calculated in four different levels for each design of combustor. More detail of the location of these levels is available in Chapter 3. During 40 seconds after reaching the quasi-steady state, the data sampling for mal-distribution analysis were taken.

2.4 Mesh and Boundary conditions

2.4.1 Combustor Design A

Due to the complexity of the geometry a hybrid mesh was constructed for the CFD simulation of the first stage (combustor). Figure 2.2 shows the combination of tetrahedral and hexahedral cells used to obtain a mesh similar to the industrial prototype. The output of the air distribution simulation was imposed as a velocity inlet BC for the combustor simulation (See Appendix A) for a detailed description. For both spent catalyst inlet and recycle inlet a BC of mass flow inlet was selected. Pressure outlet was imposed as BC in the solids and flue gases outlet. Finally no slip for gas and partial slip for solid phase conditions were selected for the wall. Temperatures of 600 K, 800 K and 850 K as boundary conditions for the air, spent catalyst and catalyst recirculated respectively were imposed.

![Figure 2.2: Mesh Design A](image)
2.4.2 Regenerator vessel

The regenerator vessel is the second stage of the HTR regenerator. This part of the regenerator is geometrically more complex than the combustor, as it includes two stages to separate the solid particles from the gas. The first stage of separation are the arm disengagers where large portion of solid particles are returned to the dense bed zone. In the second stage the separation is made up of seven pairs of cyclones where the rest of the solid particles are separated of the gas and returned to the dense bed. Figure 2.3 shows the tetrahedral mesh of the regenerator vessel. The boundary conditions for the CFD simulation of the regenerator vessel were the following: mass flow inlet for the particles and the gas coming from combustor; velocity inlet for the air inlet (less 2% of total stoichiometric air [14]); pressure outlet for the cyclones inlet; mass flow inlet for the mass flow of solids that are returned to the dense bed through the cyclones and partial slip for the solid and not slip for the gas for the rest of the regenerator vessel that were defined as walls.

This study did not simulate the flow inside the seven pair of cyclones. Instead, an UDF (See AppendixD) imposed an efficiency of separation of solid particles from gas of 99.9%. That is to say, 99.9% of the solid mass flow that leaves the regenerator vessel through cyclone inlets was returned to the dense bed.
2.4.3 Distributor of solids

The mixing between solid particles and gas is a key parameter in the FCC regenerator performance. For this reason, in this study a second design (Design B) of distributor of solids was proposed. Figure 2.4 shows the geometry and the tetrahedral mesh of this distributor of solids. A CFD simulation of the distributor of solids was carried out to optimize the computational costs and to define the boundary conditions of spent catalyst and of recirculated catalyst that enter the combustor in the Design B. The modification of the distributor of solids is the same for both spent and hot recirculated catalyst. The boundary conditions used in the CFD simulation were the following: mass flow inlet for the catalyst inlet (spent and recirculated), pressure outlet for the outlets and partial slip for solids and no slip for gas in the wall.

![Figure 2.4: Mesh distributor of solids](image)

2.4.4 Combustor Design B

Figure 2.5 shows the mesh of Design B. This mesh, like Design A, is composed of tetrahedral and hexahedral cells. As boundary conditions, the outputs of the air distributor (velocity inlet) and the distributor of solids (mass flow inlet) were imposed. Pressure outlet BC in the solids and gas outlets were imposed. No slip for gas and partial slip for solids conditions for the wall were selected. The same temperature boundary conditions of Design A were used.
2.5 Physical properties

For the CFD simulations the physical properties taken from Ansys Fluent v.15.0 database for the components of the gas and solid phases were used. The molecular weight of carbon, $12 \text{ kg/kmol}$, was assigned as molecular weight of coke. Equation 2.8 to calculate the heat capacity $C_p (\text{J/kg \cdot K})$, as a function of temperature of the gas components and for the carbon and hydrogen in the coke. For catalyst was used a constant heat capacity. Table 2.3 lists the coefficients for equation 2.8.

$$C_p(T) = A_1 + A_2 T + A_3 T^2 + A_4 T^3 + A_5 T^4 \quad (2.8)$$

<table>
<thead>
<tr>
<th>Species</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$A_4$</th>
<th>$A_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_2$</td>
<td>834.82</td>
<td>0.293</td>
<td>$-1.50 \times 10^{-4}$</td>
<td>$3.41 \times 10^{-7}$</td>
<td>$-2.28 \times 10^{-10}$</td>
</tr>
<tr>
<td>$CO$</td>
<td>968.38</td>
<td>0.448</td>
<td>$-1.15 \times 10^{-3}$</td>
<td>$1.65 \times 10^{-6}$</td>
<td>$-7.35 \times 10^{-10}$</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>429.93</td>
<td>1.87</td>
<td>$-2.0 \times 10^{-3}$</td>
<td>$1.29 \times 10^{-6}$</td>
<td>$-4.0 \times 10^{-10}$</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>1563.07</td>
<td>1.60</td>
<td>$-3.20 \times 10^{-3}$</td>
<td>$3.21 \times 10^{-6}$</td>
<td>$-1.16 \times 10^{-9}$</td>
</tr>
<tr>
<td>$N_2$</td>
<td>979.04</td>
<td>0.42</td>
<td>$-1.20 \times 10^{-3}$</td>
<td>$1.67 \times 10^{-6}$</td>
<td>$-7.26 \times 10^{-10}$</td>
</tr>
<tr>
<td>$C$</td>
<td>1729.57</td>
<td>0.056</td>
<td>$-2.0 \times 10^{-4}$</td>
<td>$2.10 \times 10^{-7}$</td>
<td>$-7.66 \times 10^{-11}$</td>
</tr>
<tr>
<td>$H_2$</td>
<td>13602.45</td>
<td>3.40</td>
<td>$-3.4 \times 10^{-3}$</td>
<td>$3.90 \times 10^{-7}$</td>
<td>$-1.70 \times 10^{-9}$</td>
</tr>
<tr>
<td>Catalyst</td>
<td>1290</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>


2.6 Simulation parameters

The models used and detailed parameters for all simulation are listed in Table 2.4.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Models/Methods/Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Two phase flow</td>
<td>Gas-Solid Euler-Euler, kinetic theory of granular flow</td>
</tr>
<tr>
<td>Model</td>
<td>Granular</td>
</tr>
<tr>
<td>Granular temperature</td>
<td>Algebraic formulation</td>
</tr>
<tr>
<td>Solver</td>
<td>Pressure-Based transient</td>
</tr>
<tr>
<td>Pressure velocity coupling scheme</td>
<td>Phase-coupled SIMPLE</td>
</tr>
<tr>
<td>Time step</td>
<td>0.01 seconds</td>
</tr>
<tr>
<td>Maximum number of iterations per time step</td>
<td>40</td>
</tr>
<tr>
<td>Residual convergence criteria</td>
<td>$1 \times 10^{-3}$</td>
</tr>
<tr>
<td>Discretization Scheme</td>
<td>First-order upwind</td>
</tr>
<tr>
<td>Maximum solid packing volume fraction</td>
<td>0.6</td>
</tr>
<tr>
<td>FCC particle density</td>
<td>1500 kg/m$^3$</td>
</tr>
<tr>
<td>FCC particle mean diameter</td>
<td>70 $\mu$m</td>
</tr>
<tr>
<td>Restitution coefficient</td>
<td>0.95</td>
</tr>
<tr>
<td>Gas density</td>
<td>Incompressible ideal gas</td>
</tr>
<tr>
<td>Turbulence</td>
<td>$k-\varepsilon$ model</td>
</tr>
<tr>
<td>Heat transfer</td>
<td>Gunn model</td>
</tr>
</tbody>
</table>

**Combustor**

Under-relaxation Factors | Pressure 0.3, density 0.2, momentum 0.5, energy 0.6, species 0.6, volume fraction 0.6, granular temperature 0.2 |

**Regenerator vessel**

Under-relaxation Factors | Pressure 0.3, density 0.8, momentum 0.2, energy 0.6, species 1.0, volume fraction 0.6, granular temperature 0.2 |
2.7 Mesh independence study

To guarantee that the results were independent of mesh size, a study of mesh independence for both combustor designs and for the regenerator vessel was conducted. The profile of volume fraction of solids was the parameter selected for the mesh independence study.

2.7.1 Mesh independence Design A

For Design A three different meshes with a cells number of 420k, 580k and 850k were constructed. The figure 2.6 shows the solid volume fraction profile along to combustor for the three meshes. All cases predict the existence a turbulent bed. The results obtained were similar for the 580k and 850k meshes, therefore the 580k mesh was selected as it imposed a lower computational cost.

![Figure 2.6: Analysis mesh independence for Design A](image)

2.7.2 Mesh independence regenerator vessel

The geometry of the regenerator vessel is more complex that of the two combustor designs. Two different meshes were constructed. The size of these were 1.5M and 2.2M respectively. Figure 2.7 shows the profile of the average volume fraction of solids along the combustor. The results were similar in both meshes. In order to minimize the computational costs the mesh with 1.5M was selected to obtain the results from here onwards.
2.7.3 Mesh independence Design B

For design B three different meshes with 450k, 650k and 900k cells were constructed. Figure 2.8 shows the results. Based on the same analysis conducted for "Design A", the 650k was selected to obtain the results shown in this thesis.
Chapter 3

Hydrodynamics

The study in detail of the hydrodynamic behavior of HTR is an objective of this thesis. The two-phase flow gas-solid inside the FCC regenerator adds complexity to better understanding of its behavior. In this Chapter, a hydrodynamic study for the combustor and regenerator vessel is shown.

3.1 Drag Force

The drag force is a key parameter for the successful simulation of the hydrodynamics in a turbulent fluidized bed. Several drag models have been developed for the gas-solid two-phase interaction, such as Syamlal O’Brien [58], Gidaspow [59] and McKeen [60] drag models. A comparison between experimental data and simulation results obtained with the use of these models was conducted by Li et al.[1]. In that study, the Syamlal O’Brien and Gidaspow drag models overestimated the gas–solid momentum exchange and could not predict the formation of a dense zone in the fluidized bed, while the McKeen drag model could not capture the diluted zone characteristics due to underestimation of the drag force. For this reason, Li et al.[1] proposed a modified drag model that showed satisfactory agreement between predictions and experimental results. The modified drag model is shown below in Table 3.1.
### Table 3.1: Modified drag model [1]

<table>
<thead>
<tr>
<th>Void fraction</th>
<th>Drag force model</th>
<th>Drag force coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>≤ 0.8</td>
<td>Ergun</td>
<td>( \beta_1 = 150 \alpha_g (1-\alpha_g) \mu_g + 1.75 \rho_g \alpha_g \frac{u_p - u_g}{d_p} )</td>
</tr>
<tr>
<td>0.8 − 0.933</td>
<td>ZP</td>
<td>( \beta_2 = \frac{5}{12} C_D \frac{\alpha_g\rho_g}{d_p} \frac{u_p - u_g}{\mu_g} )</td>
</tr>
</tbody>
</table>
| 0.933 − 0.990 | Wen and Yu       | \( C_D = \left\{ \begin{array}{ll} \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}) & \text{if } (Re_p^* \leq 1000) \\
                                   44 & \text{if } (Re_p^* > 1000) \end{array} \right. \) |
| 0.990 − 1.00  | Schiller and Naumann | \( \beta_3 = \frac{2}{3} C_D \frac{\alpha_g\rho_g}{d_p} \frac{u_p - u_g}{\mu_g} \alpha_g^{-2.65} \) |

The modified drag model considered four ranges of void fraction: \( \alpha_g \leq 0.8, 0.8 < \alpha_g < 0.933, 0.933 < \alpha_g < 0.990 \) and \( 0.990 < \alpha_g < 1.00 \) and described the drag force coefficient according to the void fraction of each zone. The step changes in the drag coefficient at the void fractions of 0.8, 0.933, and 0.99, possibly lead to difficulties in numerical convergence. To avoid the discontinuous behavior, four drag correlations were stitched together by Equation 3.1.

\[
\beta = (1 - \varphi_1)\beta_1 + \varphi_1 \{(1 - \varphi_2)\beta_2 + \varphi_2 [(1 - \varphi_3)\beta_3 + \varphi_3\beta_4] \} \tag{3.1}
\]

\( \varphi_1, \varphi_2, \varphi_3 \), are the stitching functions, which are calculate by Equation 3.2 proposed by Lu and Gidaspow [61].

\[
\varphi_i = \frac{\arctan[150 \times 1.75(\alpha_g - \alpha_i)]}{\pi} + 0.5 \tag{3.2}
\]

\( \alpha_1 = 0.8, \alpha_2 = 0.933 \) and \( \alpha_3 = 0.99 \) are the transition points.
3.2 Hydrodynamic study for combustor

The change over time of the average volume fraction of the solid phase at different levels (h/H=0.02, 0.09, 0.20, 0.30, 0.34) of the combustor with the modified drag model is shown on the Figure 3.1. The quasi-steady state was reached after the 40 seconds. The sampling data to obtain the average solid volume fraction in each level were taken between the 40-80 seconds. The levels h/H=0.09 and h/H=0.20 are located in the dense bed. For this reason, significant changes, in the average solid volume fraction profiles take place in these levels. In the diluted zone, h/H=0.30 and h/H=0.34, not significant changes over time were observed. This behavior is due to the small amount of solid particles that escapes the dense bed. In the particular case of the level h/H=0.02, this is located bellow the air distributor where a high solid particles concentration takes place and the average solid volume fraction does not evidence any significant change.

![Figure 3.1: Analysis of the variation with time of the convergence, average solid volume fractions, combustor Design A](image)

Given the importance that drag models have on the CFD modeling of solid-gas systems, a detailed analysis of the results with three well-known drag models, was undertaken. Particularly Syamlal-O’Brien drag model, Gidaspow drag model and modified drag model were used to capture the hydrodynamic behavior in the combustor stage of a HTR. The profiles of the average solid volume fraction along the combustor by using the three drag models are shown in the Figure 3.2. It is important to note that the modified model in Figure 3.1 considered a mean cluster diameter \( d_p^* = 400\mu m \) in the dense zone and of 200\(\mu m \) in the diluted zone. These value are different from those originally proposed in references [1], [62], that was 300\(\mu m \) for the dense zone. A simple parametric analysis showed that the lower values of cluster diameter do not guarantee bed expansion, as illustrated below. Mean cluster diameter in the range 200 to 400 \(\mu m \) for FCC catalyst,
with Sauter mean diameter from 49 to 71 \( \mu m \) have been reported [63]. The modified drag model was coupled to Euler-Euler model through an UDF.

As experimental data on the variation of the solid fraction along the combustor is scarce, but is widely known that HTR combustors operate in a turbulent fluidization regimen [14], [64], to evaluate the results obtained with the three drag models, a theoretical profile for turbulent fluidization regimen suggested by Levenspiel [13] (blue line) in the Figure 3.2 was used. In the theoretical profile two dense and diluted zones, are evident. The results show a similar solid volume fraction profile with the Syamlal-O’Brien and Gidaspow drag models. These models underestimated the bed expansion, as was evidenced in the study of Li et al.[1]. Contrary, the modified drag model predicted a profile of solid volume fraction similar to the theoretical profile. The dense and diluted zones of a turbulent fluidized bed were clearly captured with the use of this model.

The difference between the modified drag model and the other drag models is the consideration of grouping phenomena in the gas-solid two-phase flow. The existence of cohesive inter-particle forces leads to grouping of particles, resulting in larger effective particle sizes, and hence reduced fluid-particle drag forces [62]. As shown in Figure 3.2 the influential cluster diameter in the FCC regenerator directly determines the solid volume fraction profile.

Figure 3.3 shows the volume rendering of the solid volume fraction in the combustor obtained with the drag models. The results obtained in Figure 3.3 confirms those above as only the modified drag model renders the expected turbulent and disorderly behavior in the dense zone, as well as the bed expansion.
3.2. Hydrodynamic study for combustor

3.2.1 Mal-distribution

As mentioned in the methodology section, a mal-distribution coefficient ($M_f$) was used to evaluate the radial distribution of solids. Figure 3.4 shows the four planes along the combustor where ($M_f$) was calculated. The figure also shows eight sections in which each plane is divided. Each section has the same area. ($M_f$) can vary from zero (ideal distribution) to one (all the solid goes through one single of the 8 zones). The analysis of ($M_f$) was undertaken at $h/H=0.20$, 0.30, 0.55, 0.85. The first levels ($h/H=0.20$ and 0.30), are located in the dense zone.

![Figure 3.4: Planes (a) and sections (b) used to define ($M_f$)](image-url)
Figure 3.5 shows the radial distribution of the solid phase in the levels $h/H=0.20$, 0.30, 0.55, 0.85. For the HTR combustor, Design A. Level $h/H=0.20$ has a value of $M_f$ of 0.31. This high value of $M_f$ is explained because at this height level the two lateral inlets of solids are located. In fact, Figure 3.5 a. shows a higher value of volume fraction where the solids enter the reactor. The solids show a significant heterogeneity in the radial direction. In level $h/H=0.30$, Figure 3.5 b., $M_f$ is 0.29. Due to the turbulent movement of the solid particles and the gas, the solids have a better distribution in the radial direction. Level $h/H=0.55$ is located in the dilute zone, Figure 3.5 c. There are few solids in this zone, and some reduction of the cross sectional area. These two factors facilitate the radial distribution of solids. This same analysis is also valid for Figure 3.5 d., at $h/H=0.85$.

![Figure 3.5: Analysis of $M_f$ at different planes along the combustor, Design A. $h/H = (a) 0.20$, (b) 0.30, (c) 0.55, (d) 0.85. Note the different scale in the color bar between planes a and b and planes c and d.](image-url)
3.3 Hydrodynamic study for Regenerator vessel

Figure 3.6 shows the variation of the average volume fraction of the solid phase with time in the regenerator vessel at four heights (h/H=0.13, 0.21, 0.25, 0.80). After 30 seconds the quasi-steady state for each height was reached. The sampling data to obtain the average solid volume fraction in each level were taken between 30 and 100 seconds.

The bubbling bed is the regimen of fluidization in the regenerator vessel [14], [64]. Figure 3.7 shows the profile of volume fraction of solid phase, as well as, the theoretical profile published by Levenspiel [13] (blue line) for a bubbling bed. This simulation is without any chemistry and at constant temperature of 920 K. For consistency with the previous simulation, the modified drag model was used with a particle cluster diameter of 400µm and 200µm. The results agree with the theoretical profile.
Chapter 3. Hydrodynamics

Figure 3.7: Profile solid volume fraction in the regenerator vessel with modified drag model

Figure 3.8 shows the volume fraction of solid phase in the regenerator vessel. The high density of solid particles in the dense zone of the regenerator vessel is explain by factors such as low superficial velocity of the gas, small amount of solids escaping from the dense bed to the diluted zone and the re-entering of solids to the dense bed through arm disengagers and cyclones.

Figure 3.8: Solid volume fraction in the regenerator vessel

The mixture of catalyst particles and flue gas is discharged from the upper section of the combustor into the regenerator vessel. The regenerator vessel has two pieces to separate the solid particles from the gas. The
3.3. Hydrodynamic study for Regenerator vessel

arm disengagers and the cyclones. The arm disengagers provide the first-stage of separation. The recommended solid mass flow through the cyclones is between 20-30% of solid mass flow that enters to regenerator vessel [64]. Figure 3.9 shows the solid mass flow through each cyclone inlet. The point in the middle of the box represents the average flow and the vertical bars one standard deviation. In the quasi-steady state, the solid mass flow changes over time. Although fluctuations in the solid mass flow from cyclone to cyclone are evident, the mean value of the seven cyclones remains stable in a range of 61 to 63.5 kg/s. The total flow through the seven cyclones indicates that with the actual arm disengagers configuration, 42% of the solid mass flow that enters the regenerator vessel arrives to the cyclones.

![Solid mass flow through the cyclones](image)

**Figure 3.9:** Solid mass flow through the cyclones. Results from a 60 s period of quasi-steady state. Points represent the average while vertical lines one standard deviation.

As previously mentioned, the solid mass flow through cyclones must be on a range between 20-30% of solid mass flow that enter to regenerator vessel [64]. With the current arm disengager configuration, the value of solid mass flow through cyclones is 42.23%. The configuration of the arm disengager must facilitate the inertial separation of the solid particles from the gas, without increasing the attrition phenomenon. Figure 3.10 shows the velocity vectors of the gas phase in the arm disengagers. The value of the velocity is between 7 m/s and 12 m/s for the current configuration. This high velocity causes the drag of solid particles to the upper section where the cyclone inlets are located. Furthermore, it may also lead to re-entrainment of the particles to the cyclones discharge in bottom. To reduce the velocity in the arm disengager exit and to reduce the solid mass flow through cyclones inlet, a modification of the arm disengager is necessary. In Chapter 5 a modification for this purpose is presented.
In this chapter, the hydrodynamics behavior of an industrial HTR was studied. Three different drag models were tested. Modified drag model with a cluster diameters of 400 $\mu m$ and 200 $\mu m$ for the dense zone a diluted zone, selected on base a literature review, give the best prediction in the profiles of solid volume fraction in both combustor and regenerator vessel.

An analysis of the distribution of solids showed the need to improve the way in that solid particles enter the combustor. Furthermore, the velocity field in the arm disengagers showed a high velocity in this part of the regenerator vessel, which lead to increases of the solid particles dragged to the cyclone inlets. In the next chapter modifications were proposed and evaluated to improve this problems.
Chapter 4

Improvement of the hydrodynamic behavior of regenerator

One of the essential objectives of this work is to improve the performance of the FCC regenerator. Mal-distribution of air and solids is an important bottleneck of a FCC regenerator. The amount of coke on catalyst surface is less than 1.0w%. The mixing between gas and the solid is a critical parameter for catalyst regeneration. Good mixing of air and solid can reduce the use of CO combustion promoters. To reduce the thermal damage of cyclones and catalyst deactivation, the good mixing is a key parameter.

Even though the discussion in Chapter 3 involved a geometry defined based on the current state of the art for HTR systems, the analysis of mixing with CFD showed the possibility of improving solid distribution in the combustor and the velocity profile out of the arm disenganger in the regeneration stage. In this chapter, therefore a new configuration for the solids distributor was proposed to improve the gas and solid mixing in the regenerator. At the same time, in order to reduce the solid mass flow through cyclones, the upper section of the combustor was modified in the region of the arm disengagers.

4.1 Combustor

Figure 4.1 shows the geometry proposed modification to the geometry of the combustor, named Design B. In order to improve the mixing between solid particles and gas in the radial direction, a new design for the distributor of solids of spent and recirculated hot catalyst recirculated was proposed. Sections 2.4.3 and 2.4.4, in the methodology Chapter, described in detail the modified solid distributor, Figure 2.4. Previous to the simulation of the combustor with this new solid distributor, the flow inside the distributor was modeled with CFD.
Chapter 4. Improvement of the hydrodynamic behavior of regenerator

The boundary conditions for the mass flow of solids through the seven exits of the distributor were taken from the aforementioned CFD simulation of the distributor of solids as described in Table 4.1.

Table 4.1: Distribution of solids flow through the seven exits of the solid distributor used in Design B. See Figure 2.4 for the location of the inlets.

<table>
<thead>
<tr>
<th>Inlet</th>
<th>Mass flow of solids (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 and 2</td>
<td>5.60</td>
</tr>
<tr>
<td>3 and 4</td>
<td>8.17</td>
</tr>
<tr>
<td>5 and 6</td>
<td>6.23</td>
</tr>
<tr>
<td>7</td>
<td>60.00</td>
</tr>
</tbody>
</table>

Figure 4.1: Geometry of the combustor with the Design B. a. Isometric view. b. Top view of the air distributor.

Figure 4.2 shows the profiles of solid volume fraction for both combustor designs. In both cases, the same cluster diameters were used. The results obtained for the Design B show more bed expansion, and therefore, are more similar to theoretical values (blue line) [13]. Both Designs A and B show two zones of typical turbulent fluidized beds; however, Design B shows evidence of better bed expansion. The solid particles do not easily escape the dense bed, this guarantees a longer contact time that should promote better coke combustion. Even though Figure 4.2 gives evidence of the advantage of Design B when compared to Design A, further analysis was
undertaken by the analysis of the residence time distribution coming out of the reactor and the mal-distribution coefficient along the combustor.

\[ \text{Figure 4.2: Comparison of the predicted solid volume fraction profile along the HTR, combustor designs A and B} \]

4.1.1 Residence time distribution (RTD)

Figure 4.3 shows the RTD functions for both combustor designs. Additionally, this figure shows the theoretical RTD for both CSTR and PFR reactors with the same volume that the combustor. Figure 4.3 shows a delay in the RTD, around 2 seconds. This suggest that the combustor could be represented by two reactors in series: PFR and CSTR\cite{13}. The fact that multiple decaying peaks at regular intervals, sharp early peaks and early curve are not present suggest that the combustor does not present internal recirculation, dead zones or short-circuiting.
Chapter 4. Improvement of the hydrodynamic behavior of regenerator

The average residence time and variance obtained from the RTDs in Figure 4.3 are listed in Table 4.2. The theoretical residence time for an ideal reactor, defined as the ratio of the reactor volume and the volumetric flow, was also calculated. The value of average residence time of the Design B is closer to that of an ideal reactor than that of the Design A. For the Design B, its RTD and average residence time are closer to those of a PFR reactor which suggests that Design B presents a better mixing in the radial direction than Design A. A lower variance for Design B than for the Design A, rectifies this conclusion.

<table>
<thead>
<tr>
<th></th>
<th>$\tau$ (s)</th>
<th>$t_m$ (s)</th>
<th>$\sigma^2$ ($s^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CSTR-PFR</td>
<td>9.28</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Design A</td>
<td>7.82</td>
<td>19.93</td>
<td></td>
</tr>
<tr>
<td>Design B</td>
<td>8.67</td>
<td>18.26</td>
<td></td>
</tr>
</tbody>
</table>

4.1.2 Mal-distribution

In Design A, the solid phase enters to the combustor through a simple inlet. Design B, considered a distributor of solids where the 40% of solids enters the combustor through six laterals inlets, (see Figure 2.4 for details of the geometry). Figures 4.4 and 4.5 compare the mal-distribution factor at different horizontal planes along the combustor for both designs. Figure 4.4 shows results for planes at $h/H=0.20$ and $h/H=0.30$, located in the dense zone. A better distribution of the solid particles is evident for Design B. As
4.1. Combustor

As expected, the radial distribution in the dense bed with the implementation of distributor of solids was improved. Figure 4.5 shows planes in the diluted zone (h/H=0.55, 0.85). A better radial distribution of solids with the Design B is again readily noticeable.

**Figure 4.4:** Comparison of the solid distribution in the dense zone of the HTR combustor for designs A and B at two different heights, planes h/H=0.20, 0.30. The figure also includes values of the mal-distribution coefficient, $M_f$.

**Figure 4.5:** Comparison of the solid distribution in the diluted zone of the HTR combustor for designs A and B at two different heights, planes h/H=0.55, 0.85. The figure also includes values of the mal-distribution coefficient, $M_f$.

Figure 4.6 shows the profile of $M_f$ for both combustor designs. The results obtained shown a low value of the mal-distribution factor with the
Design B in the four levels.

\[ \text{Mal-distribution factor (Mf)} \]

\[ \text{Dimensionless heigth (h/H)} \]

**Figure 4.6:** Comparison of predicted mal-distribution profiles along the HTR combustor for designs A and B.

### 4.2 Arm disengager

As explained above, in order to improve the velocity field, a modification of the arm disengagers geometry was recommended. The new design should improve gas flow paths and catalyst separation efficiencies. Figure 4.7 shows the geometries of the base case and the modification. The curves of the base case is maintained equal for the modification to lower the impact of the solid particles and reduce the attrition phenomenon. To return more solid particles to the dense bed, the length of the shroud was increased. This increase in length is limited by the fact that high efficiency of separation could lead to afterburning phenomenon and high dilute phase temperatures.
The velocity vectors of the gas for both disengager cases are shown in Figure 4.8. Gas velocity decreases from a range of 7-12 m/s in the base case to 7-9 m/s in the modification. The decrease in the gas velocity is due to loss of the momentum of the gas with a more extended shroud. In addition, the velocity of the gas that goes to the cyclones also decreases, as illustrated below. Possibly dragging less catalyst to the cyclones.

According to Figure 4.9 the proposed modification decreases the solid mass flow through the cyclones. The modification reduced by 8% the average total solid mass flow through the cyclones compared with the base case.
With an extended shroud, the momentum losses of the gas and the solid particles increased. The amount of solid particles returned to the dense bed also increases and the solid particles dragged by the gas to the cyclones inlet decreases.

**Figure 4.9:** Solid mass flow through the cyclones, After Arm disengagers modification. Results from a 60 s period of quasi-steady state. Points represent the average while vertical lines one standard deviation.
Chapter 5

Conclusions

Based on literature review, afterburn, gas emissions ($NO_x$, $SO_x$ and $CO$) and catalyst attrition were the most important bottlenecks identified in the operation of an industrial FCC regenerator. All these bottlenecks are directly related to the correct operation of the gas distributor and the way that the spent catalyst esters the regenerator.

In order to understand and improve the hydrodynamic behavior inside an industrial FCC regenerator, a CFD analysis using the Euler-Euler approach was conducted. The CFD study was carried out using the commercial CFD package, Fluent V15.0. The suitability for predicting the hydrodynamics inside of the FCC regenerator was granted by a careful analysis that evaluated three different drag models: Syamlal–O’Brien [58], Gidaspow [59] and Modified [1].

The hydrodynamic behavior inside an industrial HTR was correctly represented by Modified drag model based on effective cluster diameters for the FCC particles equal to 400 $\mu m$ and 200 $\mu m$ for the dense and diluted phases, respectively.

An analysis of the CFD simulation suggested that the simple inlet of spent and recirculated catalyst, named as Design A in this thesis, did not guarantee proper radial solid distribution. A new design, Design B included a distributor of solids with six lateral and an one central inlet was proposed.

An analysis of the mal-distribution factor showed a better radial distribution of solids in the combustor with Design B. The improvement in distribution was confirmed, with Design B as a more expanded dense bed was obtained. Furthermore, a residence time distribution study showed an increase in the mean residence time for the gas phase with the Design B. The results obtained were a mean residence time of 7.82 s for Design A and 8.67 s for Design B. The value of the mean residence time for Design B is closer to the theoretical value for an ideal PFR reactor 9.2 s. The proposed solid distributor clearly improves the performance of the HTR combustor.
In addition to the analysis of the combustor, a CFD simulation of the regenerator vessel of the HTR correctly showed the existence of a bubbling bed just below the cyclones. This simulation indicated that the velocity field around the arm disengangers, where the solids transition from the combustor to the regenerator vessel, was too high. Therefore, a modification to the geometry of the arm disengangers in order to separate the solid particles from the gas in the regenerator vessel was proposed. By increasing the length of the shroud of the disenganger, the solid mass flow through cyclones decreased from 42\% for a base case, to 34\% with the modification. This value is closed to that recommended of 20-30\% by [64].

These two examples, the variation of the geometry of the solid distributor in the combustor and that of the arm disenganger, illustrate the ability of CFD to positively affect the hydrodynamics of a HTR system.
Chapter 6

Future work

Clearly the next step would be to quantify the effect of the proposed geometry changes on the chemistry of the process. While computational limitations prevented accomplishing this task during this thesis, the following sections suggest a path to include chemistry in the simulations. Particularly, the reaction mechanism that needs to be used and a UDF that includes that mechanism in the CFD simulation are presented and validated.

6.1 Kinetic mechanism

From the different kinetic mechanisms available in the literature to represent the chemical reactions that happen in the regeneration process, the kinetic mechanisms proposed by Arbel et al.[24] and Tang et al. [36] were selected due to the complete description of the mechanisms and the kinetic parameters availability. Both mechanisms consider four reactions for coke combustion. These reactions are listed below. The Arbel’s mechanism is an improve and update mechanism based on a more detailed kinetic description of the kinetics in the regenerator using the full range of published data both on FCC performance and kinetic rates, describes the transition of operating conditions from partial to full combustion with a complete description of CO to CO$_2$ combustion kinetics including the effect of catalytic combustion promoters such as platinum. This phenomenon is not considered by Tang’s mechanism and the CO oxidation is only dependent on the temperature and does not include promoters.

The reaction rate expressions are the same for both Arbel’s and Tang’s mechanisms and are listed in Table 6.1. All the hydrogen in the coke is converted to steam. The carbon can be converted to either CO or CO$_2$. As the heat of combustion to CO$_2$ is almost 3 times the heat of combustion to CO, it is very important to simulate the impact of operating conditions on the ratio of CO$_2$ to CO as this controls the heat balance. The Arbel’s mechanism provided the $\beta_c$ parameter for estimating of this ratio, which is calculated with an Arrhenius expression and is involved in the pre-exponential factor
of the kinetic constants of the carbon consumption for the \( CO \) and \( CO_2 \) production as shown in Table 6.1. The kinetic parameter for Arbel’s and Tang’s mechanisms are listed in Tables 6.2 and 6.3, respectively.

Heterogeneous reactions: \( C + O_2 \rightarrow CO_2 \) \( R_1 \)
\( C + 0.5O_2 \rightarrow CO \) \( R_2 \)
\( 2H + 0.5O_2 \rightarrow H_2O \) \( R_3 \)
\( CO + 0.5O_2 \text{het} \rightarrow CO_2 \) \( R_4 \)

Homogeneous Reaction: \( CO + 0.5O_2 \text{hom} \rightarrow CO_2 \) \( R_4 \)

Table 6.1: Reaction rate expressions Arbel et al. [24]

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Reaction rate</th>
<th>( k_i ) expression Arbel’s mechanism</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>( k_1(1 - \alpha_s) \rho_p \frac{C_{rgc}}{MWC} P_{O_2} )</td>
<td>( k_1 = \frac{\beta_c k_i}{\beta_c + 1} )</td>
</tr>
<tr>
<td>R2</td>
<td>( k_2(1 - \alpha_s) \rho_p \frac{C_{rgc}}{MWC} P_{O_2} )</td>
<td>( k_2 = \frac{k_i}{\beta_c + 1} )</td>
</tr>
<tr>
<td>R3</td>
<td>( k_3(1 - \alpha_s) \rho_p \frac{C_{reh}}{MWH} P_{O_2} )</td>
<td>Not apply</td>
</tr>
<tr>
<td>R4</td>
<td>( k_4 P_{O_2} P_{CO} )</td>
<td>( k_4 = x_p(1 - \alpha_s) \rho_p k_{het} + \alpha_s k_{hom} )</td>
</tr>
</tbody>
</table>

Table 6.2: Kinetic parameters Arbel et al. [24]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Pre-exponential ( (A_i) )</th>
<th>Activation energy ( (E_i/R) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>Units</td>
<td>( (K) )</td>
</tr>
<tr>
<td>( \beta_c )</td>
<td>2.51</td>
<td>Dimensionless</td>
</tr>
<tr>
<td>( k_c )</td>
<td>( 1.069 \times 10^8 )</td>
<td>( s^{-1}atm^{-1} )</td>
</tr>
<tr>
<td>( k_3 )</td>
<td>( 3.301 \times 10^8 )</td>
<td>( s^{-1}atm^{-1} )</td>
</tr>
<tr>
<td>( k_{het} )</td>
<td>1560.62</td>
<td>( kmolkg_{cat}^{-1}s^{-1}atm^{-2} )</td>
</tr>
<tr>
<td>( k_{hom} )</td>
<td>( 5.068 \times 10^{14} )</td>
<td>( kmolm^{-3}s^{-1}atm^{-2} )</td>
</tr>
</tbody>
</table>

Table 6.3: Kinetic parameters Tang et al.[36]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Pre-exponential ( (A_i) )</th>
<th>Activation energy ( (E_i) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>Units</td>
<td>( (j/mol) )</td>
</tr>
<tr>
<td>( k_1 )</td>
<td>( 0.3766 \times 10^8 )</td>
<td>( s^{-1}atm^{-1} )</td>
</tr>
<tr>
<td>( k_2 )</td>
<td>( 0.155 \times 10^8 )</td>
<td>( s^{-1}atm^{-1} )</td>
</tr>
<tr>
<td>( k_3 )</td>
<td>( 3.13 \times 10^7 )</td>
<td>( s^{-1}atm^{-1} )</td>
</tr>
<tr>
<td>( k_4 )</td>
<td>( 0.149 \times 10^{12} )</td>
<td>( kmolkg_{cat}^{-1}s^{-1}atm^{-2} )</td>
</tr>
</tbody>
</table>
6.2 1-D combustor model

A 1-D model of the combustor stage was used to evaluated the behavior of
the two kinetic mechanism for coke combustion mentioned above. Dasila
et al. [65] simulated a FCC regenerator as PFR reactor. The key assumption
is that the fluid is perfectly mixed in the radial direction but not in the ax-
ial direction. The PFR model also was implemented in this work to obtain
the axial profiles of the species concentration and temperature inside of the
combustor stage. The following assumptions are made in the development
of the PFR model: the gases are in the plug flow through bed and in ther-
mal equilibrium with surrounding bed; catalyst in dense bed is well mixed
and isothermal with uniform carbon on catalyst; resistance to mass transfer
from gas to catalyst phase is negligible; mean heat capacities of gases and
catalyst are assumed to remain constant over the temperature range en-
countered. Two ordinary differential equations 6.2; 6.3 were implemented
to describe the steady state behavior of the gas species and temperature in
the regenerator.

Equation 6.2, was proposed to obtain the species profile in axial direc-
tion of the combustor.

\[
\frac{df_i}{dz} = A_{r\text{gn}} r_i
\]  

(6.2)

\( f_i \) represents the molar flow of each species \( i \); \( A_{r\text{gn}} \) is the cross sectional
area and \( r_i \) is the consumption or production rate of the specie \( i \). The
species considered were \( O_2, CO, CO_2, H_2O, N_2, C \) and \( H_2 \).

Equation 6.3 was used to calculate the temperature profile in axial di-
rection of the combustor.

\[
\frac{dT}{dz} = \frac{A_{r\text{gn}}}{C_{p\text{tot}}} (H_{CO} r_{CO} + H_{CO_2} r_{CO_2} + H_{H_2O} r_{H_2O})
\]  

(6.3)

\( C_{p\text{tot}} \) is calculated with a mixing law and \( H_{CO}, H_{CO_2}, H_{H_2O} \) are the
heat of formation of carbon monoxide, carbon dioxide and water re-
spectively.

the rate constants \( \beta_c, k_c, k_3, k_{\text{hot}} \) and \( k_{\text{hom}} \) for Arbel et al. (1995), and \( k_1, k_2, k_3, k_4 \) for Tang et al. (2015) are Arrhenius-type, as expressed in equation 6.1.

\[ k_i = A_i \exp \left( -\frac{E_i}{RT} \right) \]  

(6.1)
Figure 6.1 shows the axial profiles of the gas species obtained with the Arbel mechanism (continuous line) and Tang mechanism (dotted line). The values of oxygen consumption and water production are the same values for both mechanisms. The difference between the two mechanisms is in the prediction of carbon monoxide and carbon dioxide. In Arbel’s mechanism the production and consumption of $CO$ can be seen. In the Tang’s mechanism, this phenomenon is not considered. When this mechanism is used, all carbon is converted into carbon dioxide.

![Figure 6.1: Gas species profile 1-D model](image)

Although the general behavior of an industrial FCC regenerator can be captured with both kinetic mechanisms. With the Arbel’s mechanism can be captured the transition from partial to full combustion. Furthermore, the effect of the use the promoters for the $CO$ oxidation can be assessed with this mechanism. Due to this was selected the Arbel’s mechanism for a 2-D validation.

### 6.3 2-D Validation

A 2D simulation was carried out to validate the kinetic mechanism of Arbel et al.[24]. The geometry and boundary conditions shown in Figure 6.2 and operating conditions listed in Table 6.4, were taken from Cao et al. (2008) [15]. The Figure 6.2 also shows the volume fraction of the solid phase. The two characteristic zones of a turbulent fluidized bed: dense zone and diluted zone are captured with the use of the modified drag model with the same cluster diameter used for the combustor and regenerator vessel in Chapter 3.
6.3. 2-D Validation

There are differences between the results obtained with 2-D validation and the industrial data reported by [15] as can be seen in Table 6.5. However, is obtained a low relative error in the temperature value for both dense and diluted zones. Furthermore, the values of the species concentration obtained with the 2-D validation are in the range reported in the literature for others industrial FCC regenerators. This allow concluding that can be used the Arbel’s mechanism to simulate the HTR regenerator with certainty of its results. The Arbel’s kinetic mechanism for coke combustion has been validated and can be use subsequently in the chemical evaluation of the HTR.

![Image of mesh and boundary conditions](image)

**FIGURE 6.2:** 2D validation. a) mesh and boundary conditions. b) volume fraction solid phase

**TABLE 6.4:** Operating conditions from Cao et al. (2008) [15]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Catalyst density</td>
<td>kg/m³</td>
<td>1500</td>
</tr>
<tr>
<td>Catalyst mean diameter</td>
<td>µm</td>
<td>70</td>
</tr>
<tr>
<td>Superficial gas velocity</td>
<td>m/s</td>
<td>0.788</td>
</tr>
<tr>
<td>Temperature gas inlet</td>
<td>K</td>
<td>573</td>
</tr>
<tr>
<td>Spent catalyst mass flow</td>
<td>kg/s</td>
<td>22.7</td>
</tr>
<tr>
<td>Temperature catalyst inlet</td>
<td>K</td>
<td>753</td>
</tr>
<tr>
<td>Carbon content of catalyst</td>
<td>wt%</td>
<td>0.9</td>
</tr>
<tr>
<td>H/C ratio</td>
<td>wt/wt</td>
<td>0.08</td>
</tr>
</tbody>
</table>
Chapter 6. Future work

![2D species profile]

**Figure 6.3:** 2D species profile

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Industrial data</th>
<th>2-D validation</th>
<th>Relative error (%)</th>
<th>Literature [27]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dilute phase temperature, ( K )</td>
<td>932 (gas)</td>
<td>930</td>
<td>2.1</td>
<td>–</td>
</tr>
<tr>
<td>Dense phase temperature, ( K )</td>
<td>907 (gas)</td>
<td>910</td>
<td>0.3</td>
<td>–</td>
</tr>
<tr>
<td>Content of ( CO_2 ) in flue gas, mol%</td>
<td>17.8</td>
<td>16.3</td>
<td>8.5</td>
<td>16.24</td>
</tr>
<tr>
<td>Content of ( O_2 ) in flue gas, mol%</td>
<td>3.1</td>
<td>2.1</td>
<td>32.2</td>
<td>1.67</td>
</tr>
<tr>
<td>Content of ( CO ) in flue gas, mol%</td>
<td>0.15</td>
<td>0.01</td>
<td>93.3</td>
<td>0.03</td>
</tr>
</tbody>
</table>
Appendix A

Air distributor simulation

The FCC regenerator may suffer from different operational problems such as, afterburning, cyclone damage, non-homogeneous catalyst at the exit, emissions ($NO_X$, $SO_X$, $CO$) and severe catalyst attrition. All these problems are relate with the performance of the air and solid distributors in the reactor. There are different types of the air distributor with industrial application for FCC regenerators such as air ring distributor, plate distributor and pipe grid distributor. In this work, was selected a pipe grid distributor due to good air distribution properties and low-pressure drop. Figure A.1 shows the geometry of the air distributor constructed in the software ICEM CFD of the ANSYS package.

![Pipe grid distributor](image)

**Figure A.1:** Pipe grid distributor. a) top view b) front view

The pipe grid distributor is composed by 298 holes of 4 cm diameter orifices. Air flowed through nozzles pointing downward at 45 degrees from the vertical plane. The hole pattern guaranteed low pressure drop and relatively homogeneous air distribution in the reactor.
A.0.1 Boundary conditions and simulation models

Figure A.2 shows the mesh with 300K tetrahedral cells for the steady state CFD simulation of the air distributor, carried out in ANSYS Fluent Version 15.0. The air mass flow guaranteed a 2% air excess based on the coke entering the regenerator. For the inlet and outlet of the air distributor were imposed a mass flow inlet BC and pressure outlet BC respectively. The $K - \epsilon$ model was used to include the turbulence phenomena.

![Figure A.2: Mesh air distributor](image)

A histogram of the distribution of exit velocity at each orifices is shown in Figure A.3. The exit velocity varies from 32 to 46 m/s with an average of 42 m/s and a standard deviation of 3.32 m/s.

![Figure A.3: Histogram exit velocity air distributor](image)

Some dispersion in the velocity magnitude is evident. Higher velocities are concentrated close to distribution pipe and the lowest velocity are
at the corners where distance to the manifold is the highest. However, a relatively homogeneous air distributor was guaranteed inside the reactor. The exit velocity profile obtained with air distributor simulation was used for hydrodynamic study carried out in chapter 3.
Appendix B

UDF modified drag model

UDF modified drag model [1], used in the CFD simulations of both combustor and regenerator vessel of a HTR.

    /*UDF modified drag model*/
    /*Programada por Juan David Alzate*/
#include "udf.h"
#include "sg_mphase.h"
#include "math.h"
#define diam 70e-6 /* diameter of particle (µm) */
#define diamdense 400e-6 /* dense zone cluster (µm)*/
#define diamdiluted 200e-6 /* diluted zone cluster (µm)*/
#define alpha_1 0.80
#define alpha_2 0.933
#define alpha_3 0.99

    DEFINE_EXCHANGE_PROPERTY(drag,c,mix_thread,sec_col,first_col)
    {
        real x_vel_g, x_vel_s, y_vel_g, y_vel_s, z_vel_g, z_vel_s, slip_x, slip_y, slip_z;
        real abs_v, rho_g, rho_s, mu_g, reyp, reypdense, reypdiluted;
        real beta, beta_1, beta_2, beta_3, beta_4, phi_1, phi_2, phi_3, coeff_drag_star,coeff_drag
        real alpha_g, alpha_s, coeff_drag_star_1;

        Thread *tg = THREAD_SUB_THREAD(mix_thread,sec_col);
        Thread *ts = THREAD_SUB_THREAD(mix_thread,first_col);
        x_vel_g = C_U(c,tg);
        y_vel_g = C_V(c,tg);
        z_vel_g = C_W(c,tg);
        x_vel_s = C_U(c,ts);
        y_vel_s = C_V(c,ts);
        z_vel_s = C_W(c,ts);
        slip_x = x_vel_g - x_vel_s;
        slip_y = y_vel_g - y_vel_s;
        slip_z = z_vel_g - z_vel_s;
        rho_g = C_R(c,tg);
        rho_s = C_R(c,ts);
mu_g = C_MU_L(c,tg);
alpha_g = C_VOF(c,tg);
alpha_s = C_VOF(c,ts);

abs_v = sqrt(slip_x*slip_x + slip_y*slip_y + slip_z*slip_z);

reyp = alpha_g*rho_g*diam*abs_v/mu_g;
reypdense = alpha_g*rho_g*diamdense*abs_v/mu_g;
reypdiluted = alpha_g*rho_g*diamdiluted*abs_v/mu_g;

if(reypdense <= 0.)
coeff_drag_star = 0.;
else if (reypdense <= 1000.)
coeff_drag_star = (24./reypdense) * (1.+0.15*pow(reypdense,0.687));
else
coeff_drag_star = 0.44;
if(reypdiluted <= 0.)
coeff_drag_star_1 = 0.;
else if (reypdiluted <= 1000.)
coeff_drag_star_1 = (24./reypdiluted) * (1.+0.15*pow(reypdiluted,0.687));
else
coeff_drag_star_1 = 0.44;
if(reyp <= 0.)
coeff_drag = 0.;
else if(reyp <= 1000.)
coeff_drag = (24./reyp) * (1.+0.15*pow(reyp,0.687));
else
coeff_drag = 0.44;
if (alpha_g == 1.)
alpha_g = 0.9999;
else if (alpha_g == 0.)
alpha_g = 0.0001;
beta_1 = 150.*alpha_s*(1.-alpha_g)*mu_g/(alpha_g*pow(diamdense,2.)) +1.75*rho_g*alpha_s *abs_v/diamdense;
beta_2 = (5./72.)*coeff_drag_star*alpha_s*alpha_g*rho_g*abs_v / (diamdense* pow((1.-alpha_g),0.293));
beta_3 = (3./4.)*(coeff_drag_star_1*alpha_s*alpha_g*rho_g*abs_v / (diamdiluted)) *pow(alpha_g,2.65);
beta_4 = (3./4.)*coeff_drag*alpha_s*alpha_g*rho_g*abs_v / diamdiluted;
phi_1 = atan(150.*1.75*(alpha_g-alpha_1)) / M_PI + 0.5;
phi_2 = atan(150.*1.75*(alpha_g-alpha_2)) / M_PI + 0.5;
phi_3 = atan(150.*1.75*(alpha_g-alpha_3)) / M_PI + 0.5;
beta=(1.-phi_1)*beta_1 + phi_1 * ((1.-phi_2)*beta_2 + phi_2*(1.-phi_3)*beta_3 + phi_3)
*beta_4));
return beta;
Appendix C

UDF Chemical Reactions

UDF kinetic mechanism for coke combustion proposed by Arbel et al. [24].

/* UDF para reaccion heterogena combustor de FCC*/
/*Modelo de Arbel et al.(1995) */
/*Programada por Juan David Alzate*/

#include "udf.h"
#include <stdio.h>
#include "math.h"
/*factor pre-exponencial*/
#define kbeta0 2.51
#define kc0 1.069e8
#define k13c0 116.68
#define k13h0 5.06820e14
/*Energia de activacion*/
#define Ebeta 5795.6
#define Ec 18888.9
#define E13c 13588.9
#define E13h 35555.6
#define Eagua 17789
#define koagua 3.301e8
#define Ppa 101325.0
/* Peso molecular*/
#define mw_C 12.01115
#define mw_O2 31.9988
#define mw_CO 28.01055
#define mw_CO2 44.00995
#define mw_H2O 18.01534
#define mw_H2 2.01594
#define mw_N2 28.0134
#define rho_cat 1500
#define X_pt 0.1

static cxboolean init_flag = TRUE;
/* Search the index for each species */
Appendix C. UDF Chemical Reactions

static real mw[MAX_PHASES][MAX_SPE_EQNS];
static int INDEX_PHASE_O2 = 0, INDEX_SPECIES_O2 = 0, INDEX_PHASE_CO 
= 0, INDEX_SPECIES_CO = 0, 
INDEX_PHASE_CO2 = 0, INDEX_SPECIES_CO2 = 0, INDEX_PHASE_H2O 
= 0, INDEX_SPECIES_H2O = 0, 
INDEX_PHASE_N2 = 0, INDEX_SPECIES_N2 = 0, INDEX_PHASE_C = 0, 
INDEX_SPECIES_C = 0, 
INDEX_PHASE_H2 = 0, INDEX_SPECIES_H2 = 0;

    DEFINE_ADJUST(combustor1,domain)
    {
        #if !RP_HOST
        int n, ns;
        Domain *subdomain;
        /*int n_phases = DOMAIN_N_DOMAINS(domain);*/
        if(init_flag)
        {
            /* search all the species and saved the Molecular Weight */
            sub_domain_loop(subdomain, domain, n)
            {
                Material *m_mat, *s_mat;
                if (DOMAIN_NSPE(subdomain) > 0)
                {
                    m_mat = Pick_Material(DOMAIN_MATERIAL_NAME(subdomain),NULL);
                    mixture_species_loop(m_mat,s_mat,ns) {
                        if (0 == strcmp(MIXTURE_SPECIE_NAME(m_mat,ns),"o2"))
                        {
                            INDEX_PHASE_O2 = n;
                            INDEX_SPECIES_O2 = ns;
                        }
                        else if (0 == strcmp(MIXTURE_SPECIE_NAME(m_mat,ns),"co"))
                        {
                            INDEX_PHASE_CO = n;
                            INDEX_SPECIES_CO = ns;
                        }
                        else if (0 == strcmp(MIXTURE_SPECIE_NAME(m_mat,ns),"co2"))
                        {
                            INDEX_PHASE_CO2 = n;
                            INDEX_SPECIES_CO2 = ns;
                        }
                        else if (0 == strcmp(MIXTURE_SPECIE_NAME(m_mat,ns),"h2o"))
                        {
                            INDEX_PHASE_H2O = n;
                            INDEX_SPECIES_H2O = ns;
                        }
                        else if (0 == strcmp(MIXTURE_SPECIE_NAME(m_mat,ns),"n2"))
                        {
                            INDEX_PHASE_N2 = n;
                            INDEX_SPECIES_N2 = ns;
                        }
                    } 
                } }
    } 
}
else if (0 == strcmp(MIXTURE_SPECIE_NAME(m_mat,ns),"c"))
{
INDEX_PHASE_C = n;
INDEX_SPECIES_C = ns;
}
else if (0 == strcmp(MIXTURE_SPECIE_NAME(m_mat,ns),"h2"))
{
INDEX_PHASE_H2 = n;
INDEX_SPECIES_H2 = ns;
}
CX_Message ("—%d %d, %d %d, %d %d,%d %d,%d %d, %d %d, %d %d ",
INDEX_PHASE_O2,
INDEX_SPECIES_O2, INDEX_PHASE_CO, INDEX_SPECIES_CO,INDEX_PHASE_CO2,
INDEX_SPECIES_CO2,
INDEX_PHASE_H2O, INDEX_SPECIES_H2O, INDEX_PHASE_N2, INDEX_SPECIES_N2,
INDEX_PHASE_C,
INDEX_SPECIES_C, INDEX_PHASE_H2, INDEX_SPECIES_H2);
mw[n][ns] = MATERIAL_PROP(s_mat,PROP_mwi);
}
else
{
}
s_mat = Pick_Material(DOMAIN_MATERIAL_NAME(subdomain),NULL);
mw[n][0] = MATERIAL_PROP(s_mat,PROP_mwi);
}
}
init_flag = FALSE;
#endif

DEFINE_HET_RXN_RATE(combustorCO2,c,t,r,mw,yi,rr,rr_t)
{
#if !RP_HOST
Thread **pt = THREAD_SUB_THREADS(t);
Thread *tp = pt[0];
Thread *ts = pt[1];
int i;
real C_rgc, p_oper, kagua, T, rho, P, moles_tot, X_O2, X_CO, C_rgh, betac,
kc, k13c, k13h,
k11, k12, P_atm, moles_totales, y_o2, y_co, y_co2, y_h2o, y_c, y_n2, y_h2;
real vof_s;
p_oper = RP_Get_Real ("operating-pressure");
T = C_T(c, tp);
rho = C_R(c,tp);
P = p_oper;
vof_s= C_VOF(c,ts);
*rr = 0; moles_totales=0;
y_o2 = yi[INDEX_PHASE_O2][INDEX_SPECIES_O2]/mw_O2;
y_co = yi[INDEX_PHASE_CO][INDEX_SPECIES_CO]/mw_CO;
y_co2= yi[INDEX_PHASE_CO2][INDEX_SPECIES_CO2]/mw_CO2;
Appendix C. UDF Chemical Reactions

\[ y_{h2o} = \frac{yi[INDEX\_PHASE\_H2O][INDEX\_SPECIES\_H2O]}{mw\_H2O}; \]
\[ y_c = \frac{yi[INDEX\_PHASE\_C][INDEX\_SPECIES\_C]}{y_{h2o}}; \]
\[ y_{n2} = \frac{yi[INDEX\_PHASE\_N2][INDEX\_SPECIES\_N2]}{mw\_N2}; \]
\[ y_{h2} = \frac{yi[INDEX\_PHASE\_H2][INDEX\_SPECIES\_H2]}{mw\_H2}; \]
\[ moles\_totales = y_{o2} + y_{co} + y_{co2} + y_{h2o} + y_{n2}; \]
\[ X_{O2} = y_{o2}/moles\_totales; \]
\[ C\_rgc = y_c/F_s; \]
\[ P\_atm = P/Ppa; \]
\[ betac = kbeta0*exp(-Ebeta/T); \]
\[ kc = kc0*exp(-Ec/T); \]
\[ k13c = k13c0*exp(-E13c/T); \]
\[ k13h = k13h0*exp(-E13h/T); \]
\[ k11 = betac*kc/(betac+1); \]
\[ k12 = kc/(betac+1); \]
\[ kagua = koagua*exp(-Eagua/T); \]
\[ *rr = (1-vof_s)*rho\_cat*k12*C\_rgc*(X\_O2*P\_atm)/mw\_C; \]

#define HET_RXN_RATE(combustorCO,c,t,r,mw,yi,rr,rr_t) 
{
    if !RP\_HOST
    Thread **pt = THREAD\_SUB\_THREADS(t);
    Thread *tp = pt[0];
    Thread *ts = pt[1];
    int i;
    real C\_rgc, p\_oper, kagua, T, rho, P, moles\_tot, X\_O2, X\_CO, C\_rgh, betac,
    kc, k13c, k13h,
    k11, k12, P\_atm, moles\_totales, y\_{o2}, y\_{co}, y\_{co2}, y\_{h2o}, y\_c, y\_n2, y\_h2;
    real vof\_s;
    p\_oper = RP\_Get\_Real ("operating-pressure");
    T = C\_T(c, tp);
    rho = C\_R(c,tp);
    P = p\_oper;
    vof\_s = C\_VOF(c,ts);
    *rr = 0; moles\_totales=0;
    y\_{o2} = yi[INDEX\_PHASE\_O2][INDEX\_SPECIES\_O2]/mw\_O2;
    y\_{co} = yi[INDEX\_PHASE\_CO][INDEX\_SPECIES\_CO]/mw\_CO;
    y\_{co2} = yi[INDEX\_PHASE\_CO2][INDEX\_SPECIES\_CO2]/mw\_CO2;
    y\_{h2o} = yi[INDEX\_PHASE\_H2O][INDEX\_SPECIES\_H2O]/mw\_H2O;
    y\_c = yi[INDEX\_PHASE\_C][INDEX\_SPECIES\_C];
    y\_n2 = yi[INDEX\_PHASE\_N2][INDEX\_SPECIES\_N2]/mw\_N2;
    y\_{h2} = yi[INDEX\_PHASE\_H2][INDEX\_SPECIES\_H2]/mw\_H2;
    moles\_totales = y\_{o2} + y\_{co} + y\_{co2} + y\_{h2o} + y\_n2;
    X\_O2 = y\_{o2}/moles\_totales;
    C\_rgc = y\_c/F_s;
    P\_atm = P/Ppa;
    betac = kbeta0*exp(-Ebeta/T);
    kc = kc0*exp(-Ec/T);
    k13c = k13c0*exp(-E13c/T);
    k13h = k13h0*exp(-E13h/T);
    k11 = betac*kc/(betac+1);
    k12 = kc/(betac+1); 
}
Appendix C. UDF Chemical Reactions

kagua = koagua*exp(-Eagua/T);
*rr = (1-vof_s)*rho_cat*k11*C_rgc*(X_O2*P_atm)/mw_C;
#endif }
DEFINE_HET_RXN_RATE(combustorH2O,c,t,r,mw,yi,rr,rr_t)
{
#if !RP_HOST
Thread **pt = THREAD_SUB_THREADS(t);
Thread *tp = pt[0];
Thread *ts = pt[1];
int i;
real C_rgc, p_oper, kagua, T, rho, P, moles_tot, X_O2, X_CO, C_rgh, betac,
kc, k13c, k13h,
k11, k12, P_atm, moles_totales, y_o2, y_co, y_co2, y_h2o, y_c, y_n2, y_h2;
real vof_s;
p_oper = RP_Get_Real("operating-pressure");
T = C_T(c, tp);
rho = C_R(c,tp);
P = p_oper;
vof_s = C_VOF(c,ts);
*rr = 0; moles_totales=0;
y_o2 = yi[INDEX_PHASE_O2][INDEX_SPECIES_O2]/mw_O2;
y_co = yi[INDEX_PHASE_CO][INDEX_SPECIES_CO]/mw_CO;
y_co2 = yi[INDEX_PHASE_CO2][INDEX_SPECIES_CO2]/mw_CO2;
y_h2o = yi[INDEX_PHASE_H2O][INDEX_SPECIES_H2O]/mw_H2O;
y_c = yi[INDEX_PHASE_C][INDEX_SPECIES_C];
y_n2 = yi[INDEX_PHASE_N2][INDEX_SPECIES_N2]/mw_N2;
y_h2 = yi[INDEX_PHASE_H2][INDEX_SPECIES_H2]/mw_H2;
moles_totales=y_o2+y_co+y_co2+y_h2o+y_c+y_n2;
X_O2=y_o2/moles_totales;
C_rgh=y_h2/F_s;
P_atm = P/Ppa;
betac = kbeta0*exp(-Ebeta/T);
kc = kc0*exp(-Ec/T);
k13c = k13c0*exp(-E13c/T);
k13h = k13h0*exp(-E13h/T);
k11 = betac*kc/(betac+1);
k12 = kc/(betac+1);
kagua = koagua*exp(-Eagua/T);
*rr = (1-vof_s)*rho_cat*kagua*C_rgh*X_O2*P_atm/mw_C;
#endif }
DEFINE_HET_RXN_RATE(combustorCOaCO2,c,t,r,mw,yi,rr,rr_t)
{
#if !RP_HOST
Thread **pt = THREAD_SUB_THREADS(t);
Thread *tp = pt[0];
Thread *ts = pt[1];
int i;
real C_rgc, p_oper, kagua, T, rho, P, moles_tot, X_O2, X_CO, C_rgh, betac,
kc, k13c, k13h,
k11, k12, P_atm, moles_totales, y_o2, y_co, y_co2, y_h2o, y_c, y_n2, y_h2;
real vof_s;
p_oper = RP_Get_Real(“operating-pressure”);
T = C_T(c, tp);
rho = C_R(c, tp);
P = p_oper;
vof_s = C_VOF(c, ts);
*rr = 0; moles_totales=0;
y_o2 = yi[INDEX_PHASE_O2][INDEX_SPECIES_O2]/mw_O2;
y_co = yi[INDEX_PHASE_CO][INDEX_SPECIES_CO]/mw_CO;
y_co2= yi[INDEX_PHASE_CO2][INDEX_SPECIES_CO2]/mw_CO2;
y_h2o= yi[INDEX_PHASE_H2O][INDEX_SPECIES_H2O]/mw_H2O;
y_c = yi[INDEX_PHASE_C][INDEX_SPECIES_C];
y_n2= yi[INDEX_PHASE_N2][INDEX_SPECIES_N2]/mw_N2;
y_h2= yi[INDEX_PHASE_H2][INDEX_SPECIES_H2]/mw_H2;
moles_totales=y_o2+y_co+y_co2+y_h2o;
X_O2=y_o2/moles_totales;
X_CO=y_co/moles_totales;
C_rgh=y_h2/F_s;
P_atm = P/Ppa;
betac = kbeto*exp(-Ebeto/T);
kc = kc0*exp(-Ec/T);
k13c = k13c0*exp(-E13c/T);
k13h = k13h0*exp(-E13h/T);
k11 = betac*kc/(betac+1);
k12 = kc/(betac+1);
kagua = koagua*exp(-Eagua/T);
*rr = (X_pt*(1-vof_s)*rho_cat*k13c + vof_s*k13h)*X_O2*X_CO*pow(P_atm,2);
#endif
}
Appendix D

UDF Solid mass flow recirculation

User define function (UDF) used for the recirculation of solid mass flow from each cyclone inlet to dense bed in the regenerator vessel simulation.

```c
/*UDF recirculacion ciclones*/
/*Programada por Juan David Alzate*/
#include "udf.h"
double global_sum_massflow1=0.0;
/* Average solid mass flow is calculated and share with other CPUs */

DEFINE_EXECUTE_AT_END(massflow1)
{
#if !RP_HOST

face_t f;
int nfaces = 0, i;
int ID = 54; /*Cyclone inlet (Pressure outlet BC)* /
int ID1 = 61; /*Recirculation Inlet (Mass flow inlet BC)* /
real auxiliar1=0.0;
Domain *domain = Get_Domain(1);
Thread *mixture_thread = Lookup_Thread(domain,ID);
Thread **pt = THREAD_SUB_THREADS(mixture_thread);
Thread *tp = pt[0];
Thread *ts = pt[1];
Thread *thread1 = Lookup_Thread(domain, ID1);
begin_f_loop(f, ts)
{
 nfaces = nfaces + 1;
auxiliar1 +=F_FLUX(f,ts);
}
end_f_loop(f,ts)
global_sum_massflow1= PRF_GRSUM1(auxiliar1);
#if RP_NODE
```
```
if(I_AM_NODE_ZERO_P)
{
    compute_node_loop_not_zero(i)
    
    PRF_CSEND_REAL(i, &global_sum_massflow1, 1, myid);
    
}
}

if(! I_AM_NODE_ZERO_P)
{
    PRF_CRECV_REAL(node_zero, &global_sum_massflow1, 1, node_zero);
    
    #endif
    #endif

}

DEFINE_PROFILE(cyclon1,t,i)
{
    #if !RP_HOST

        face_t f;

        begin_f_loop(f,t)
        {
            F_PROFILE(f,t,i) = global_sum_massflow1;
        }
        end_f_loop(f,t)
        
    #endif

}
Bibliography


