VALIDATION AND UTILIZATION OF CFD FOR REDUCING CO EMISSIONS FROM AN FCC REGENERATOR

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INTRODUCTION

A North American refinery was seeking improvement to a full-burn FCC regenerator that had been experiencing high levels of carbon monoxide (CO) in the flue gas despite the presence of significant excess oxygen. The regenerator also experienced excessive refractory erosion in the upper freeboard near the cyclone inlets. A computational fluid dynamics (CFD) simulation was performed to calculate the three-dimensional, transient, coupled gas-particle hydrodynamic and thermal behavior of the regenerator simultaneously with heterogeneous coke-combustion and homogeneous gas-phase chemical kinetics. The model enabled informed discussions between the refinery and a technology supplier by identifying the root cause of the high CO emissions to be related to the spent catalyst distributor. The model was then used to verify that the suggested hardware changes would address the refinery's concerns without adversely affecting other aspects of regenerator reliability or performance.

DESCRIPTION OF THE WORK

Figure 1. Geometry

A three dimensional CFD model of the regenerator was constructed, as shown in Fig. 1. Major internal structures included three pairs of internal cyclones, spent catalyst distributor, two air rings and a portion of the regenerated catalyst standpipe. The computational model was constructed at full scale, with a regenerator height of approximately 70 ft (21.3 m).

Model initial and boundary conditions were taken from the operating conditions at the refinery. Moist air (5.5 mol% H_2O) entered at a rate of 2,000 mscfh (18.3 kg/s) at a temperature of 386°F (470 K) through hundreds of nozzles located on the air rings. Additional moist air was used to convey the spent catalyst into the regenerator at a rate of 1,050 mscfh (9.6 kg/s) with inlet temperature of 197°F (365 K). A pressure boundary condition was used to allow gases to and particles to leave the regenerator vessel at the cyclones, maintaining a freeboard pressure of 28 psig (294,325 Pa absolute).

Spent catalyst entered the model at a rate of 12.2 ton/min (184.4 kg/s) and a temperature of 980°F (800 K). Since the mixing of the spent catalyst exiting the stripper standpipe with the lift air was outside the scope if the computational model, it was assumed that the spent catalyst and conveyance air reached thermal equilibrium at 945°F (780 K) prior to entering the regenerator through the spent catalyst distributer. Catalyst entrained into the cyclone inlets was returned through the cyclone diplegs, and overall catalyst circulation was maintained by allowing solids to exit the vessel through the regenerated catalyst standpipe.

The model was initialized with 193,200 lb (87,600 kg) of catalyst, based on pressure drop data from unit operations. The particle size distribution (PSD) of the catalyst was determined by equilibrium catalyst sampling at the refinery and used in the computational model. The catalyst particles entering through the spent catalyst distributor contained 1.02 wt.% coke (H/C = 1.1), as determined by mass and energy balance data.

The chemical reactions and rates were taken from the open literature [Arbel et al., 1995], [Weisz and Goodwin, 1966], [Weisz, 1966]. Coke combustion included the carbon and hydrogen components reacting with oxygen to form CO, CO_2 and H_2O. The gas phase CO combustion included both homogeneous and catalyzed heterogeneous mechanisms.

The Barracuda Virtual Reactor® commercial CFD software package was chosen for the regenerator modeling due to several unique technical capabilities, all pertinent to the subject work, namely:

- The ability to model the particle size distribution of the catalyst;
- A discrete, multi-component formulation for the particles, including varying particle compositions and temperatures;
- A complete Lagrangian formulation of the solids, critical to the computation of wall-impact erosion;
- The capability to model any solids loading, from fully dilute up to close-packed, in the same simulation and without prior knowledge of what the loading is likely to be;
- Multi-phase thermal and chemistry model formulations; and
- The ability to model full-scale industrial systems with very large physical particle counts.

The CFD code is based on the CPFD® method [O'Rourke et al., 2009] which solves the transient fluid and particle mass, momentum and energy equations in three dimensions. The fluid is described by the Navier-Stokes equation with strong coupling to the discrete particles. The particle momentum has been adapted from the Multi-Phase Particle-In-Cell (MP-PIC) numerical approach [Andrews and O'Rourke, 1996], [Snider et al., 1998], [Snider, 2001]. This CFD code has been applied to a wide range of fluid-particle flows [Snider, 2007], [Parker, 2011], [Blaser and Corina, 2012], [Parker et. al, 2013] including FCC [Clark et al., 2012], [Blaser et al., 2013].

RESULTS & DISCUSSION

This work was undertaken in two stages. First the model was applied to the existing regenerator design in order to validate its applicability and to gain an understanding of the cause of the high CO emissions, thermal asymmetry, and high erosion that had been observed during operation. Once validated, the model informed decision-making regarding hardware changes and was used to verify that the suggested modifications would address the concerns without adversely affecting other aspects of regenerator performance or reliability.

Validation against Operational Data

A transient calculation simulated 100 seconds which required just under one week of real time on a GPU-enabled workstation computer. Time-averaged data, shown in Fig. 2, were analyzed to isolate longer-term trends from the significant instantaneous fluctuations that are present in a fluidized bed. The figure shows time-averaged data on centerline and radial cut planes with gas temperatures on the left, O_2 concentration in the center and CO concentration on the right.

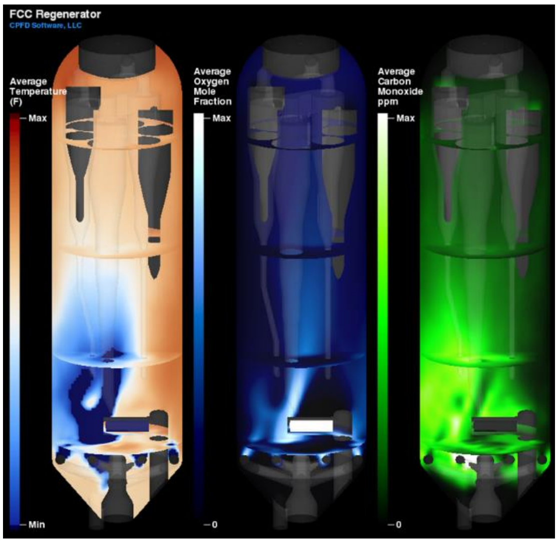

Figure 2. Time-averaged gas temperature and composition

Several trends are immediately apparent from Fig. 2. A distinct thermal asymmetry is observed with a cooler zone shown on the left near the outlet of the spent catalyst distributor. This region has a high concentration of oxygen, as shown in the center of the figure. This O_2-rich, cooler region is largely attributed to the air used to transport the spent catalyst into the regenerator, particularly since both the air and catalyst streams are cooler than the dense phase of the regenerator fluidized bed.

The CO concentrations are shown on the right of Fig. 2. The relative uniformity of CO below the spent catalyst distributor suggests that the O_2 being injected by the air ring nozzles is well-dispersed within the dense bed whereas the high concentration of oxygen extending from the spent catalyst distributor indicates that the O_2 entering from the spent catalyst distributor is generally bypassing the dense bed and is available for combustion in the freeboard. However, since this region is locally cooler, it is less conducive to CO oxidation than warmer regions of the freeboard, as can be observed by noting the correlation between the warmer temperatures and lower CO levels on the right of the regenerator as shown in Fig. 2.

An examination of the CO combustion rates reveals a strong temperature sensitivity near the regenerator operating conditions; a reduction of temperature from 1370°F (743°C) to 1320°F (716°C) reduces the CO combustion rates by 63% and 32% for the homogeneous and heterogeneous reactions, respectively. The effect of temperature is likely even more pronounced in the freeboard when the accelerating effect of the reaction exothermicity is considered as well.

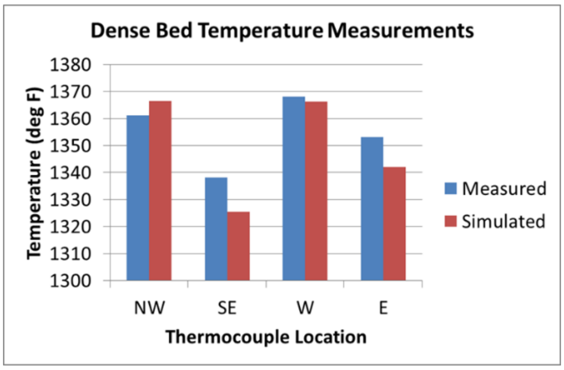

Figure 3. Dense bed temperatures

The simulated thermal profile in the dense bed agrees with thermocouple measurements taken at the refinery as shown by Fig. 3, both in magnitude and trend, validating the model.

Figure 4. Regions of high erosion

The computational model also predicted the high levels of refractory erosion near the cyclone inlets, as shown in red in Fig. 4. The model computed an erosion index as a function of particle mass, velocity and impact angle as described by Blaser et al. [2013]. The predicted areas are consistent with locations of severe erosion in the operating unit evidenced by high external skin temperatures and hot spots requiring active cooling during unit operation.

While geometry changes could be studied to reduce erosion, the erosion was deemed to be largely related to the high air flow necessitated by the poor mixing. If an improvement could be made to the thermal profile in the lower regenerator, less air flow would be required reducing both superficial velocity and subsequent catalyst entrainment into the cyclones. Since these effects have a compound, non-linear effect on erosion, design changes at the cyclone elevations were not considered further at the time.

Combining the self-consistent conclusions of the CFD results with the thermal validation data enabled further-informed discussions between the refinery and technology supplier. The model showed why the regenerator had both high CO levels and significant excess O_2 in the flue gas and also predicted the areas of high erosion seen at the refinery. The model results clearly demonstrated that the solution to the CO problem was not fundamentally to introduce more O_2 nor to add increased levels of a combustion promoter additive, but rather to improve the mixing of the cooler gas and particles entering through the spent catalyst distributor with the warmer dense bed.

Use of Model to Improve Performance

The model results pointed to the spent catalyst distributor performance as a primary cause of multiple issues. The technology supplier proposed a new spent catalyst distributor design which was evaluated using the CFD model prior to installation at the refinery.

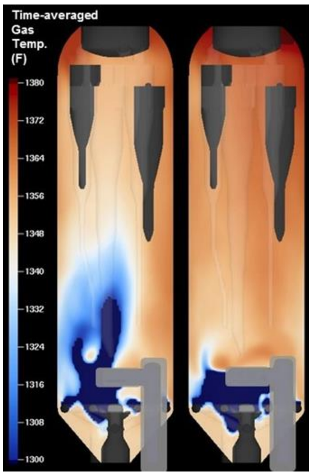

Figure 5. Effect of design changes on gas temperature

Figure 5 shows the effect of the spent catalyst distributor change on time-averaged gas temperatures as shown on a centerline slice through the model. The thermal asymmetry resulting from the use of the old spent catalyst distributor is visible on the left of the figure, while the right shows how the new design (details obscured) promotes significantly better thermal mixing.

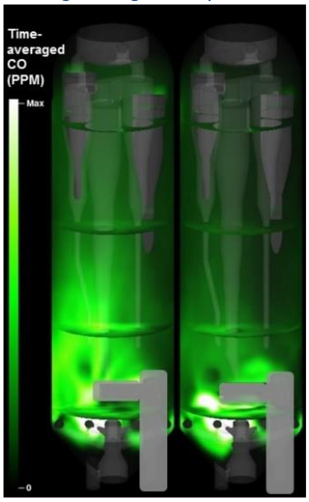

Figure 6. Effect of design changes on CO concentration

Figure 6 shows the resultant effect on time-averaged CO concentration in the regenerator. The higher average dense-phase temperatures enable more uniform CO combustion lower in the unit, reducing the CO entering the cyclones and subsequently reducing CO emissions.

Discussion

The CFD models utilized the same operating conditions allowing for a direct comparison of the thermal and gas composition profiles as influenced by the planned design changes. The analyses were completed within the timeframe allocated for selection of hardware, prior to the scheduled shutdown. While this represents a successful utilization of CFD modeling for turnaround planning, additional benefits of the modeling were not sought due to project timing constraints.

The next logical step in the optimization process would be to explore the effect of process conditions on performance and reliability. It is reasonable to expect that a more efficient spent catalyst distributor design would enable efficient regeneration with less excess oxygen. Alternately, the ratio of flow between inner and outer air rings could be altered. The effect of myriad process condition changes on regenerator performance and reliability is now enabled by a validated computational model. Such an approach represents a shift away from the use of computational models for turnaround planning toward that of continuous improvements. While hardware changes require FCC unit shutdown, operating conditions can be varied during operation.

CONCLUSIONS

This work included both the validation and subsequent utilization of CFD as part of a collaborative approach to reducing CO emissions for an FCC regenerator operated by a North American refinery. The baseline model predicted the presence of high CO levels and revealed the mixing of gas and catalyst from the spent catalyst distributor with the fluidized bed to be the root cause of thermal asymmetry leading to inadequate CO combustion. The baseline model was validated with thermocouple data and erosion observations at the refinery. The validated model informed discussions between the refinery and a technology supplier, and was used to verify that the suggested hardware changes would address the refinery's concerns without adversely affecting other aspects of regenerator reliability or performance. Modifications to the regenerator are scheduled for late 2014.

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