

Fine-tune operations through computational fluid dynamics

Advanced modeling methods assist engineers to troubleshoot existing processing equipment

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Engineers and managers involved in chemical and hydrocarbon processing industries are fully aware of the increased focus on equipment efficiency and plant productivity, as well as the need for improvement in these areas. Examples highlighting why performance and efficiency are more important include:

- Significant profit margin pressures exist on many downstream products. As the price of raw materials and fuel rises, consumers and distributors have been able to keep end-product prices low. Sustaining operational and utility costs at a minimum becomes critical.
- At the current market conditions, refineries and petrochemical plants cannot endure unplanned downtime and are striving to optimize production. Due to tight and well-planned operating schedules, any plant shutdown from fouling or equipment failure is enormously disruptive.
- Environmental regulations require plants to reduce pollutants. One example is the recent State Implementation Plan (SIP) to reduce NO_x emissions in the Houston/Galveston area in Texas.

As a result, many US Gulf Coast plants must retrofit processing equipment and upgrade operations to conform to these standards. Minimizing downtime, ensuring a smooth and efficient startup, and efficiently (quickly) reaching the unit's operating objectives collectively combine to mitigate revenue losses from changeovers.

Using innovative technologies, engineers can now effectively combine advanced computational tools and clever engineering to evaluate troubleshooting options and generate improved design concepts. These computational tools use computer simulation, combined with or in place of physical prototyping, to anticipate problems, evaluate retrofits and optimize design. Potential benefits are enhanced performance, minimized downtime for retrofitted equipment and more rapid design of new unit equipment with increased assurance of performance.

One such tool is computational fluid dynamics or CFD. The method involves solving the mathematical equations describing transport phenomena with a focus on fluid motion and heat transfer. Mass transfer, chemical reactions, and combustion and pollutant formation can be included via computational methods that are embedded within software products.

CFD is a well-established technology that historically was available for solving problems with simple geometries. It is now being used to solve problems including radiation, combustion and reaction, and heat transfer in very complex geometries, while

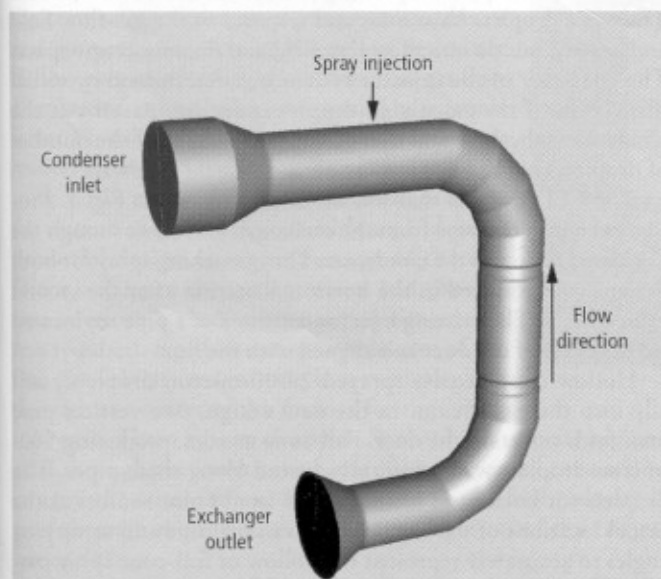


FIG. 1 CFD model domain of the flue-gas spray injectors.

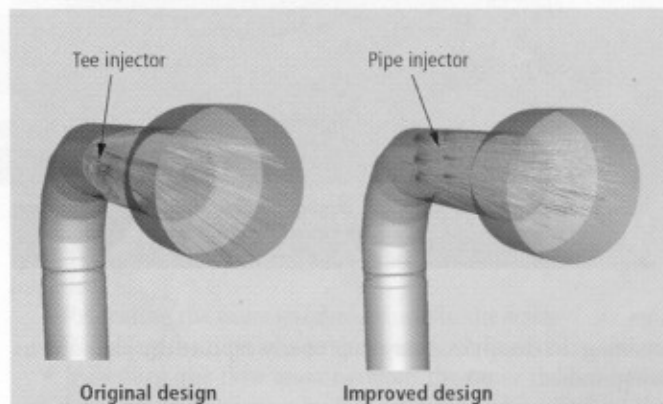


FIG. 2 CFD calculated tracks of the droplets in flow field.

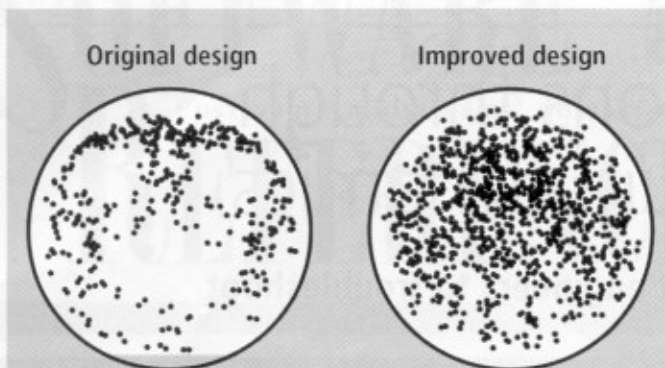


FIG. 3 Droplet locations at the condenser inlet plane.

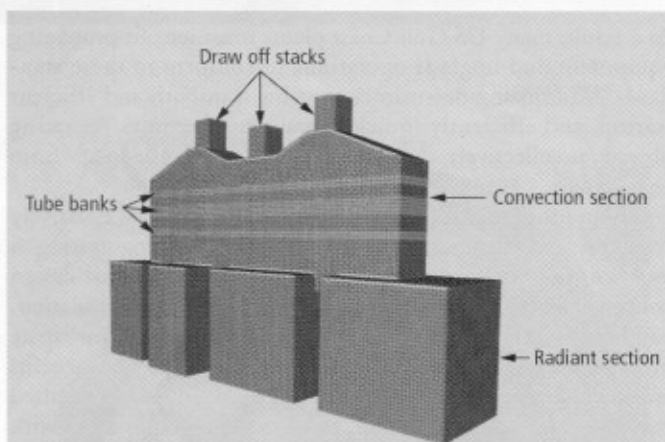


FIG. 4 CFD model for the reformer furnace.

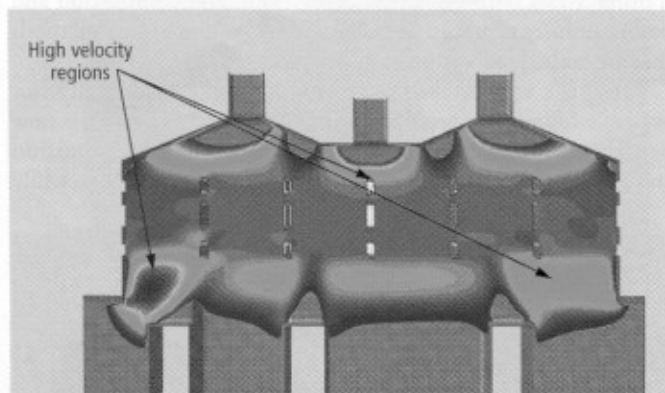


FIG. 5 Gas velocity profile at the furnace midplane.

retaining the detail necessary to properly capture the phenomena being studied.

Maximize design opportunities. The benefits that could be realized through CFD tools have been recognized for a long time. Historically, CFD studies were contracted only when design-

ers felt that it was the *only option*. While computing power limited the detail and scope of such projects, many empirical design relationships developed over the years provided information at same level of detail. This all changed with the exponential increase in computing power.

Extensive testing and model validation programs have been developed. To reap the full benefits of these applications, CFD engineers must not only know the software, but also fully understand the process technology being modeled. Interpreting CFD results requires that an engineer appreciate the fundamentals of chemical engineering design and can communicate the impact of the flow dynamics to the designers to find the appropriate design solutions.

CFD can be applied to a multiplicity of problems ranging from the simple to the very complex. In addition, CFD is being applied to design tasks that would normally be calculated using other methodologies. Yet through CFD studies, processing options can now be optimized and improved. Several examples of commercial applications of CFD will now be discussed.

Water spray quenching of a gas stream. In this example, CFD methods were used to determine the adequacy of water spray injectors to quench effluent from a waste-heat exchanger downstream of an ethylbenzene-to-styrene monomer reactor. The original unit was initially designed with empirical rules. The quenching is done in a line that connects the waste-heat exchanger to a downstream condenser. This condenser was fouling, and this was limiting unit availability. It was believed that the design of the quench spray system was a contributing factor to this fouling and caused a temperature maldistribution at the entrance to the condenser tubesheet.

In the study, the gas-flow field in the effluent line was first calculated without the injector. The spray patterns of the existing spray injector and a new design were evaluated by modeling the flow of an ensemble of droplets in the calculated gas-flow field. Since the mass rate of the quench water was less than 10% of the gas stream, a coupled droplet/vapor calculation was not needed. Thus, the droplets have mass and respond to the gas-flow field and gravity, but do not affect that field and do not occupy space. The adequacy of the injector system was determined by visual inspection of the calculated droplet trajectory pattern at the condenser tubesheet and by a quantitative count of the number of droplets that did not impact on the effluent line wall.

The CFD domain that was modeled is shown in Fig. 1. Process gas enters the pipe from the exchanger and flows through the U-shaped region to the condenser. The quenching spray for both designs is introduced in the horizontal section after the second 90° bend. The existing injector consisted of a pipe tee located at the center of the duct and aligned with the flow.

Hollow cone nozzles sprayed 2,000-micron droplets radially into the gas stream. In the new design, two vertical pipe manifolds traversed the duct. Full-cone nozzles, producing 500-micron droplets were uniformly spaced along these pipes. The droplets for both cases were released from point sources at the actual locations of the nozzle outlets in the pipe and at varying angles to accurately represent the hollow or full-cone spray pattern. The injectors were not modeled geometrically.

Fig. 2 shows the tracks of a large ensemble of droplets that were calculated by CFD for the existing nozzle and new improved design. The tracks clearly show that the new design, with its

Very Interesting

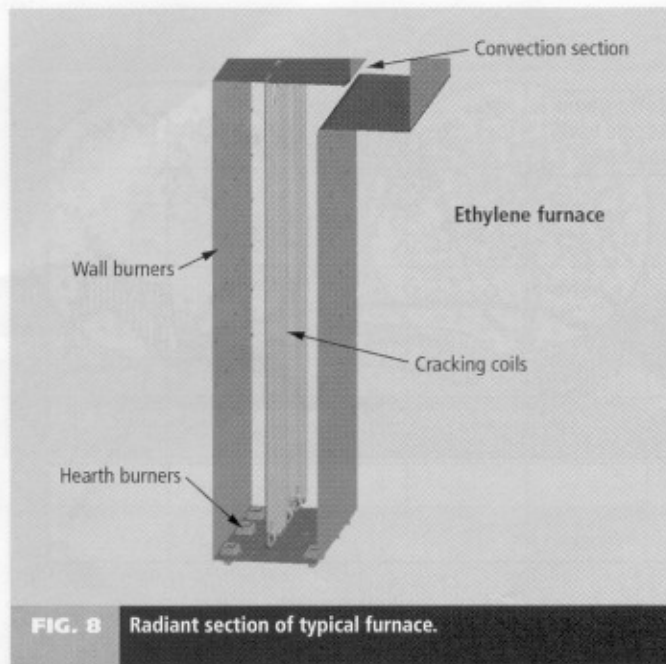


FIG. 8 Radiant section of typical furnace.

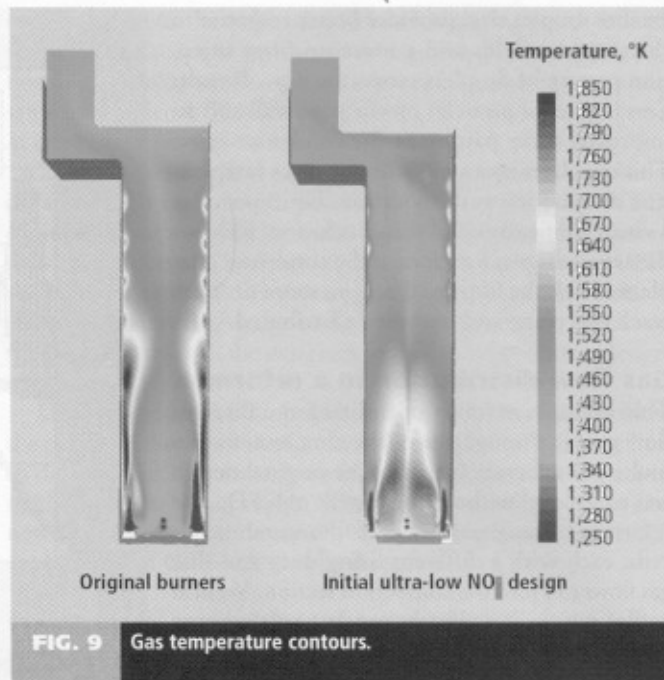


FIG. 9 Gas temperature contours.

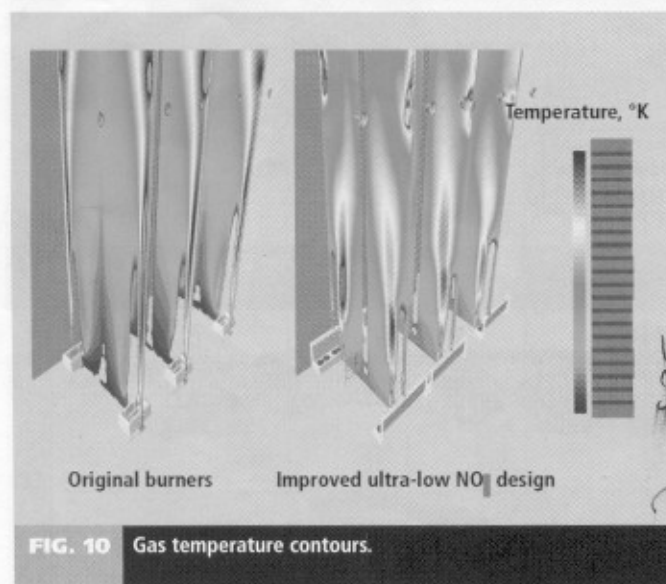


FIG. 10 Gas temperature contours.

Ultra-low NO_x burners for ethylene furnace. In this example, CFD methods are applied to improve the performance for a large ethylene furnace. In this furnace, light hydrocarbons are cracked in very-short-residence-time tubes that are suspended in a combustion chamber. The critical parameters of this furnace are:

- Transfer of the heat of cracking to the tube side hydrocarbons
- Control of the tube-metal temperatures for prolonged runlength
- Reducing pollutants emissions such as NO_x to meet regulatory statutes.

The radiant section of a typical furnace is shown in Fig. 8. Combustion heat is provided by burning fuel in both hearth burners (located on the floor of the furnace and firing vertically)

and in wall burners (that are positioned along the wall and fire radially along the wall).

With newly developed ultra-low NO_x burner (20 to 30 vppm), a portion of the fuel is premixed with all of the air in both the hearth and wall burners. The remaining fuel needed for the firing rate is introduced in a staged manner to control the temperature of the combustion gases; thus, minimizing NO_x production. This is achieved through staged ports located in front of the hearth tile at the furnace floor.

It was suspected that, when compared to the original conventional burners that generally produce straight vertical flames attached to the furnace wall, these lean premixed burners might produce shorter flames that could "roll over" at the bottom of the firebox and impinge on the tubes. This would obviously be detrimental to tube life and would also cause coking within the tubes and short runlength.

For the initial application of this new burner technology to a client's ethylene furnace, a CFD study was conducted to compare the expected performance of low- NO_x burners to the original burners. This simulation included these modeling features:

- A detailed geometric description of the furnace. This included locally refined meshes around the burner inlet ports as well as the process tubes. Considerable detail was required to achieve realistic and validated performance. A distinct model was developed for both the original burner and the new burner case.
- A combustion model on the firebox side to provide the heat generation.
- A model of the hydrocarbon cracking that occurs inside the tubes. Details of the model accurately reflect the heat absorption and thus provide realistic tube heat fluxes and coil metal temperatures.
- Turbulence and radiation models.

These CFD simulations contained between two and five million computational cells depending on the burner type and required up to a week's worth of CPU time on a high-speed computer cluster.

The initial simulations compared the new burners to the heater with the original burners. In the initial cases, the burners were simply located at the same position as the original burners. The results of this study indicated that, while the original burner design provided straight flames, the new low- NO_x configuration resulted in flames that impinged on the tube surfaces. This is clearly evident from the two temperature contour plot views (Fig. 9) comparing the two cases.

Based on these results, an optimization using CFD was done to develop design modifications that would allow the ultra-low- NO_x burner to perform acceptably in the heater. These modifications included re-designing the angle of the fuel that was being injected through the ports in front of the new burners and relocating the burners on the heater floor to provide lateral spacing into which the combusting gas could expand. These modifications reduced the tendency for the flames to "roll" into the tubes. Figure 10 compares the redesigned ultra-low-

NO_x burner to the original burner configurations. The modifications straightened the flames that, while still more diffuse than for the original burners, are more in line with those predicted for the original burners and are much improved from the original ultra-low- NO_x design.

This burner configuration, optimized by CFD, was installed in the client's furnace. Flame quality and runlength have been excellent, and low- NO_x emissions have been experienced. The startup was smooth and downtime was minimal.

Outlook. The applications of CFD described above are excellent examples of the value that can be realized in improving process operations and/or reducing cost. Properly validated CFD codes give insight that could only otherwise be obtained through high-cost experimentation. CFD also reduces the time required to answer questions that arise during plant design, troubleshooting, redesigning existing commercial equipment and scale-up of equipment for new processes. **HP**

ACKNOWLEDGMENT

The authors wish to acknowledge the cooperation of the John Zink Co., in the low- NO_x burner modification CFD studies.

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