CFD ANALYSIS OF BYPASS MIXING IN REACTION FURNACES

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This paper demonstrates the use of computational fluid dynamics (CFD) for analysing bypass gas mixing in reaction furnaces. Bypass flow injection method and location play a crucial role in the performance of these systems. When possible, a system should be designed for straight through reaction furnace operation rather than bypass.

1.0 INTRODUCTION

HEC Technologies manufactures a range of custom designed SRU equipment that includes: reaction furnaces, reheaters, reducing gas generators and tail gas incinerators. In the case of reaction furnace applications, equipment capacities have ranged from 4 to 1000 tonne/d and acid gas quality has varied from 8% H_2S to 80% H_2S by volume. Most units operate with air only but some are designed for any level of O_2 enrichment. For such a wide range of design capacities and feed conditions it is important to have access to robust tools that will help to optimize equipment designs. CFD has been found to be one of the most cost effective means for the simulation of performance of new or existing equipment.

1.1 Reaction Furnace with Bypass

In the production of sulphur, a reaction furnace is a chemical reactor; the feed of which is pre-processed in a flame to generate the heat and chemical reactants required for a reasonable product yield. When the flame temperature is too low for good flame stability or proper contaminant (NH_3, BTX hydrocarbons) destruction, one possible remedy involves bypassing a portion of the acid gas from the flame end of the reaction furnace (zone 1) to some point downstream of the acid gas flame (zone 2). This shifts the acid gas/air ratio closer to stoichiometric equivalence, yields a corresponding increase in flame temperature, and improves contaminant destruction and/or flame stability. The bypass gas represents approximately 20% of the total molar flow that leaves zone 2 of the reaction furnace.

The location and method of bypass injection into reaction furnace zone 2 can have a significant impact on plant performance. Inadequate mixing of bypass gas with zone 1 effluent can compromise sulphur conversion. In addition, bypassed acid gas usually contains hydrocarbon contaminants that can cause catalyst deactivation if they are not completely destroyed in the reaction furnace. For those reasons, it is important that bypass acid gas be properly mixed and given sufficient time to react in zone 2. One purpose of this paper is to demonstrate the use of CFD for analysing bypass mixing in reaction furnaces.

2.0 COMPUTATIONAL FLUID DYNAMICS

CFD can be described as finite element analysis applied to fluid flow. It involves finding a numerical solution to the Navier Stokes equations governing the conservation of energy, mass and momentum. When CFD is applied to a reaction furnace, the flow system is divided into a large number of volume elements called cells. The entire collection of cells in a system is called a mesh or grid. The accuracy of a CFD simulation depends on the relative coarseness of the mesh. A fine mesh will result in a more accurate solution than a coarse mesh. When the solution remains unchanged as the mesh is made finer, it is then considered to be grid independent. The iterative solution is considered converged when energy, mass and momentum are conserved at every cell and over the entire flow system. A typical engineering simulation will contain between 10^4 and 10^6 cells.

2.1 Turbulence Model

Turbulent flows are characterized by the eddies that form the fluctuating components of velocity and scalar concentrations. The presence of the eddy structures in a stream results in a bulk viscosity character that deviates from the laminar viscosity of the fluid. It is not computationally feasible to model the eddy structures within a flow field. As a result, the effect of eddy structures is incorporated as a turbulent or “eddy” viscosity in the mathematical model. The ideal turbulent viscosity model would dependent on the magnitude and direction of shear stresses as well as the turbulence intensity at any point in a system. There are a few different turbulence models available for use in CFD simulations. Sikorski et al. (2002) provided an example of the impact of turbulent viscosity model on a CFD simulation of a reaction furnace. Some models are much more demanding than others of computational resources. The averaging nature of any turbulence model is usually the largest single error factor in the CFD simulation of a flow field. The simulations performed for this paper were carried out using the hybrid SST model to ensure a reasonable flow field representation near solid boundaries as well as in the free stream.

2.2 Combustion Model

The most important chemical reactions in a reaction furnace are combustion (O2 consuming) and sulphur formation. Combustion releases the heat and chemical species that drive the sulphur forming reactions. The temperature and density changes that take place within a mixing, combusting flow field have a significant impact on the overall flow and mixing patterns. However, it is not necessary to resort to the use of rate dependent chemical reactions to obtain a reasonably accurate simulation of temperature, density and flow distribution. On that basis, the simulations for this paper were carried out using a simplified reaction scheme together with the mixed equals reacted (EDM = eddy dissipation) combustion model. The reaction scheme was developed to yield temperature and density predictions very close to what would be obtained from a chemical equilibrium model. This approach allowed a very reasonable solution convergence time without a significant loss of model accuracy.

For more detailed insight into CFD theory some of the books available on the subject include: Abbot and Basco (1994), Anderson (1995), Ferziger and Peric (1999), Wendt (1992) and Wilcox (1993).

2.3 Benefits of CFD

A reaction furnace can be described as a turbulent flow system that is undergoing simultaneous mixing and chemical reaction. Due to the high temperature and poisonous nature of the reaction furnace contents it is usually not feasible to conduct scale model testing of such systems. Water and air flow modelling are much more feasible than a test furnace; however, they have some drawbacks compared to CFD. The effects of temperature and density change associated with combustion may not be properly reflected in the flow and mixing patterns obtained from isothermal flow tests (Sikorski et al. 2002). The time and costs required for the construction and operation of water and air flow models are usually greater than what would be required to conduct a CFD simulation.

CFD is not intended as a means for making extremely accurate predictions of an absolute quantity (temperature, velocity, concentration) at a specific point in a system. It is best applied to analyse the effect of a change in a system variable on overall performance. System variables fall into two main categories: boundary conditions and geometry. Velocity characteristics, flow rates, chemical composition, temperature and pressure are typical boundary conditions that can be varied during an investigation. Geometric variations may include chamber length, diameter, transition angles, mixing obstacles (a choke ring, checker or baffle wall) as well as bypass injection method and location. Temperature, velocity and concentration profiles are typically the most useful information obtained from a CFD simulation of a reaction furnace. In a previous paper by Sikorski et al. (2002), it was discussed how, even in the absence of rate dependent chemical reactions, temperature, mixing and flow patterns can be used to diagnose a variety of reaction furnace problems, such as:

- hot spots and refractory damage
- cold spots and associated metal shell corrosion
- contaminant (NH_3, hydrocarbons) slippage
- poor sulphur conversion
- poor waste heat boiler efficiency
- waste heat boiler damage
- flame instability
- thermal damage of burner components

Ideally it would be very beneficial if CFD were able to predict species concentrations within the furnace and, most importantly in the effluent. The key species of concern include but are not limited to S2, H2, CS2, COS, NH3, and hydrocarbons. However, this goes beyond the scope of the current study. More details on the ongoing efforts at HEC Technologies to implement detailed chemical kinetics into the CFD code can be found in the work of Sikorski et al. (2002).

3.0 SIMULATION RESULTS

All of the CFD simulations here were based on the assumption of adiabatic (zero heat loss) operation of the reaction furnaces. Even though this would not be true in reality, the assumption has a negligible impact on the overall results and makes it easier to focus on evaluation of mixing quality. The simulations represent an SRU associated with a refinery that relies on the bypass of some amine acid gas to reaction furnace zone 2 to ensure adequate NH3 destruction. Cases 1 to 5 were based on a tangentially fired reaction furnace. The location, orientation and size of the bypass connection were varied to examine the impact on the mixing of the bypass stream with zone 2 effluent. Cases 6 and 7 were based on the same furnace except the tangential burner was replaced by a high intensity unit installed on the end of the furnace. The latter two cases were used to examine the effect of bypass versus no bypass, i.e. all of the acid gas going through the burner. All cases were based on the same total flow of air and acid gas.

The convergence criteria for all cases was 0.01% error for energy, mass and momentum balance at every cell and 0.1% balance error over the entire system. The temperature, concentration and velocity profiles shown below have the units of Kelvin, mass fraction and metres per second.

3.1 Case 1 - Single Bypass Inlet - Radial Injection

The computational grid and geometry for this case are shown in figure 1. The system volume was divided into about 10^6 cells. The reaction furnace is made up of two zones separated by a choke ring. The acid gas burner is oriented at a right angle to the furnace but offset from the centre line to impart a tangential flow path for the feed streams. Air and acid gas streams enter the furnace concentrically, the air surrounding the acid gas. The radial bypass connection is located just down stream of the choke ring, on the same side of the furnace as the burner. The furnace geometry is terminated at the plane of entry to the waste heat boiler.

Figure 2 shows a velocity vector and streamline plot for this system. The flow from the burner becomes attached to the furnace wall and continues through with a helical flow path. At the point where the bypass flow enters the furnace the rotating zone 1 effluent is partly disrupted by the shearing of the two streams.

Figure 3 shows a series of circular cross section profiles of the furnace temperature distribution. The profiles in zone 1 show the contrast in temperature between the un-reacted feed streams and the hot zones of reacted gas. When the bypass flow is injected into the furnace it penetrates through to the centre zone and creates a non-homogeneity that persists to the furnace outlet. Figure 4 shows an axial temperature profile of the system. It highlights the fact that most the volumes of zones 1 and 2 are in a highly stratified state. The O2 profile shown in figure 5 illustrates the fact that a significant portion of the zone 1 volume is required for complete O2 consumption by the acid gas flame.

3.2 Case 2 - Single Bypass Inlet - Opposite - Radial Injection

This case is identical to case 1 with the exception that the bypass was moved to the opposite side of the furnace. The temperature profiles of figures 6 and 7 show that there is a slight improvement in mixing relative to case 1.

3.3 Case 3 - Single Bypass Inlet - Tangential Injection - Co-Rotating

Case 3 is identical to case 1 with the exception that the bypass was oriented tangentially to cause the flow to co-rotate with the zone 1 effluent. The temperature profiles of figures 8 and 9 show that the bypass flow becomes attached to the furnace wall while the hot zone 1 effluent remains in the centre. The larger radial temperature difference at the furnace outlet compared to case 1 implies that a change to tangential injection would result in poorer bypass flow mixing.

3.4 Case 4 - Single Bypass Inlet - Tangential Injection - Counter-Rotating

This case is identical to case 3 with the exception that the tangential bypass flow counter-rotates relative to the zone 1 effluent. The temperature profiles of figures 10 and 11 show that the bypass flow penetrates to the centre zone while the hot zone 1 effluent tends to stay near the walls. While the simulation was being carried out it was found that there was a significant periodic oscillation that was taking place. This case was then solved on a time dependent basis. It was found that the counter rotating bypass jet behaved in a oscillatory manner. A pulse of gas would inject into the furnace followed by a momentary jet disruption by the opposing zone 1 flow. The overall result was that the zone 2 mixing was still somewhat compromised at the furnace outlet.

3.5 Case 5 - Four Bypass Inlets

The bypass geometry was changed from a single radial inlet to four small diameter, radial inlets evenly distributed around the furnace circumference. Each inlet has a total flow area equal to one quarter that of a single inlet. The temperature profiles of figures 12 and 13 show improved mixing compared to any of the four previous cases. This would be expected based on increasing the surface to volume ratio and evenly distributing the bypass around the furnace.

3.6 Case 6 - End Fired Furnace - Four Bypass Inlets

The case 5 side fired, tangential furnace geometry was changed to an end fired unit with a high intensity burner (figure 14). The temperature plots shown in figures 15 and 16 show that zone 1 mixing is faster than the side fired cases and allows more time for zone 1 destruction of NH_3. The bypass mixing quality in zone 2 suggests improved mixing relative to case 5. The O_2 profile of figure 17 shows that O_2 is fully consumed very early in zone 1.

3.7 Case 7 - End Fired Furnace - No Bypass

Case 7 is identical to case 6 with the exception that all of the acid gas was directed through the burner. The temperature plots of figures 18 and 19 show that system mixing is far better when all of the reaction furnace feed is directed through the burner. This case was presented to emphasize the fact that it is better for a reaction furnace to be operated on a straight through basis when it is feasible to achieve flame temperature enhancement by means such as O_2 enrichment or feed preheat.

4.0 DISCUSSION

A CFD simulation is only an approximation of the behaviour of a flow system. However, if done properly, it is usually a very good approximation. The issue that must always be considered when interpreting results is how accurate are the predictions compared with reality. The key performance factor evaluated in this study was zone 2 mixing quality and the effect of bypass injection geometry. By focusing on the effect of a system change on qualitative performance factor instead of a quantitative performance factor, the trends predicted by the CFD can be considered to be reasonable representations of reality.

When considering the cases evaluated in this study, the changes in mixing quality are in accord with what would be expected by the specific geometry changes. For example, CFD prediction of improved mixing when changing from a single inlet (case 1) to four small inlets (case 5) agrees with what would be seen in a real system.

It is also possible to assess CFD validity by comparing performance indicators of a real system to what might be inferred from a CFD simulation. Reaction furnaces, such as those studied here, with a single bypass inlet located close to the furnace outlet often experience catalyst problems and compromised sulphur conversion. Those problems are consistent with what would be expected from the poor bypass mixing combined with inadequate residence time downstream of a bypass inlet.

For more discussion on the issue of CFD validation in reaction furnace applications the reader is referred to the work of Sikorski et al.(2002).

5.0 CONCLUSIONS

1. For the furnace geometry investigated in this study utilizing a single radial bypass inlet, changing the bypass position from the burner side to the opposite results in a slight mixing improvement.
2. A single, radial bypass inlet yields better mixing than a tangentially oriented inlet regardless of whether the flow is co or counter rotating.
3. Four radial bypass inlets provide an improvement in mixing when compared to a single radial inlet.
4. It is better for a reaction furnace to be operated on a straight through basis when it is feasible to achieve flame temperature enhancement by means such as O2 enrichment or feed preheat.

6.0 REFERENCES

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Wilcox, D. C. (1993) Turbulence Modelling for CFD, DCW Industries

7.0 FIGURES

FIGURE 1. Computational Grid for Case 1, Tangential Furnace with Tangential Bypass

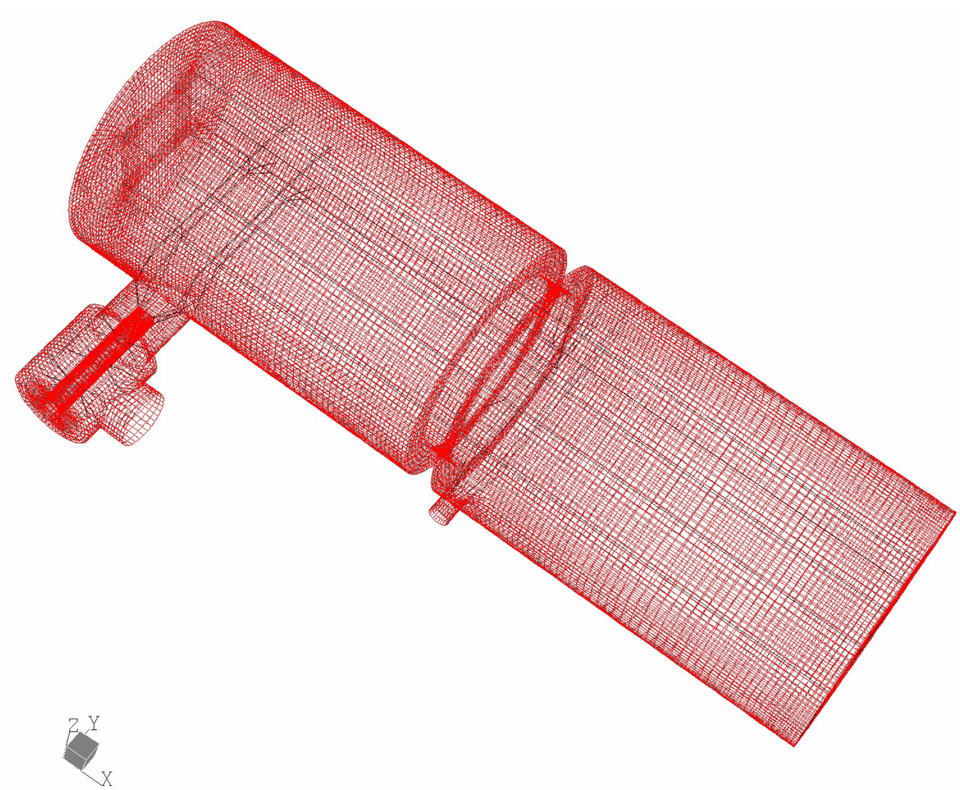

FIGURE 2. Velocity and Streamline Plot for Case 1, Tangential Furnace with Radial Bypass

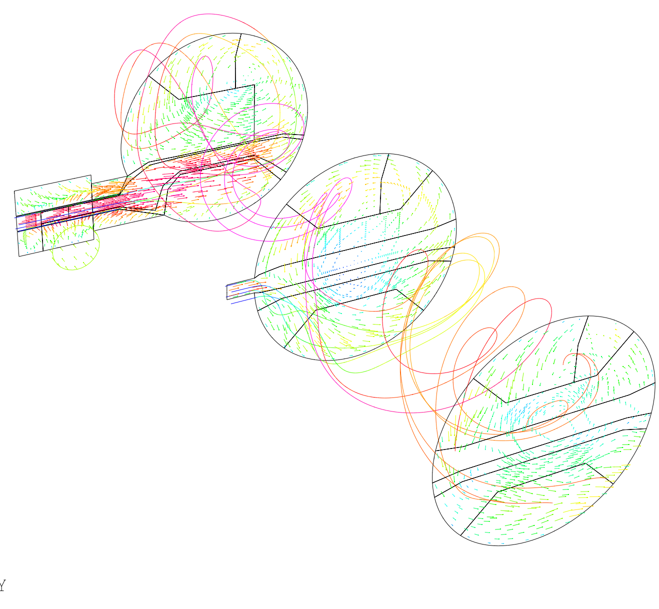

FIGURE 3. Temperature Distribution for Case 1, Tangential Furnace with Radial Bypass

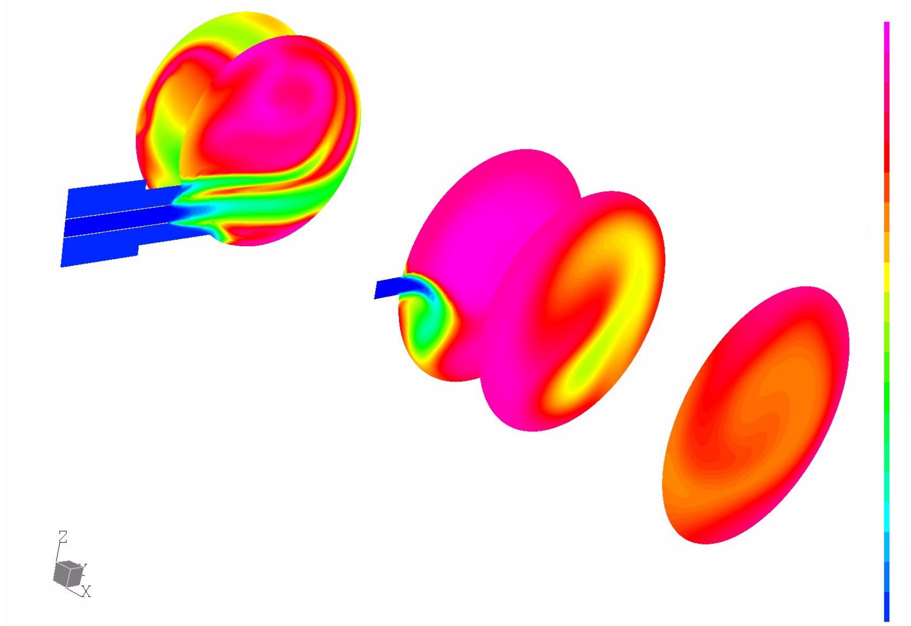

FIGURE 4. Axial Temperature Distribution for Case 1, Tangential Furnace with Radial Bypass

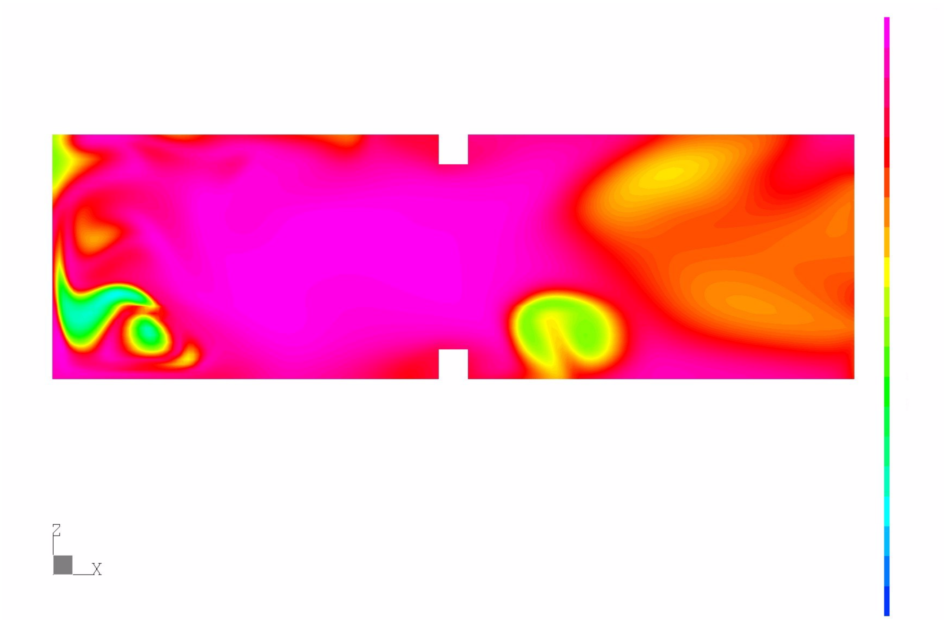

FIGURE 5. Axial O_2 Distribution for Case 1, Tangential Furnace with Radial Bypass

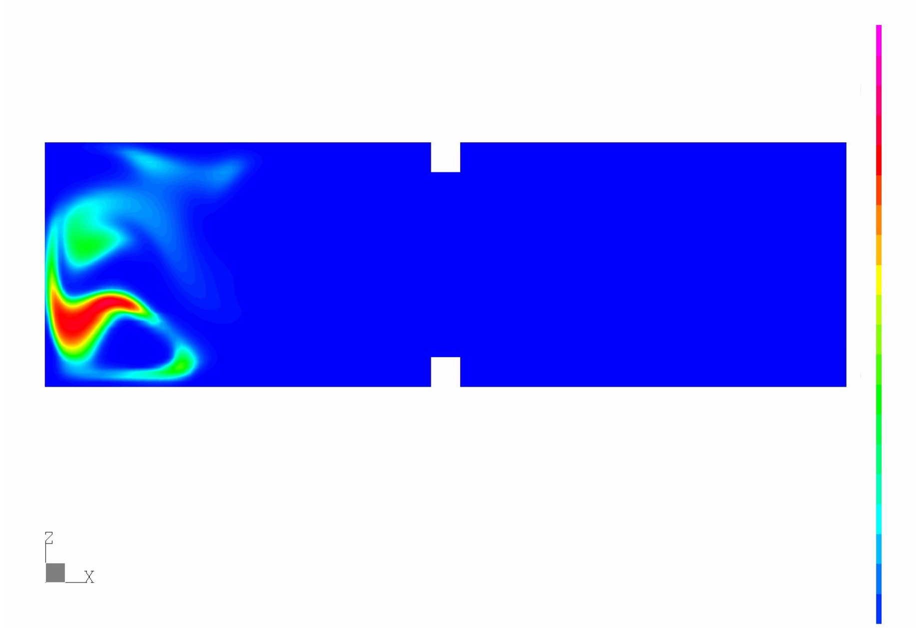

FIGURE 6. Temperature Distribution for Case 2, Tangential Furnace with Radial Injection Opposite Side

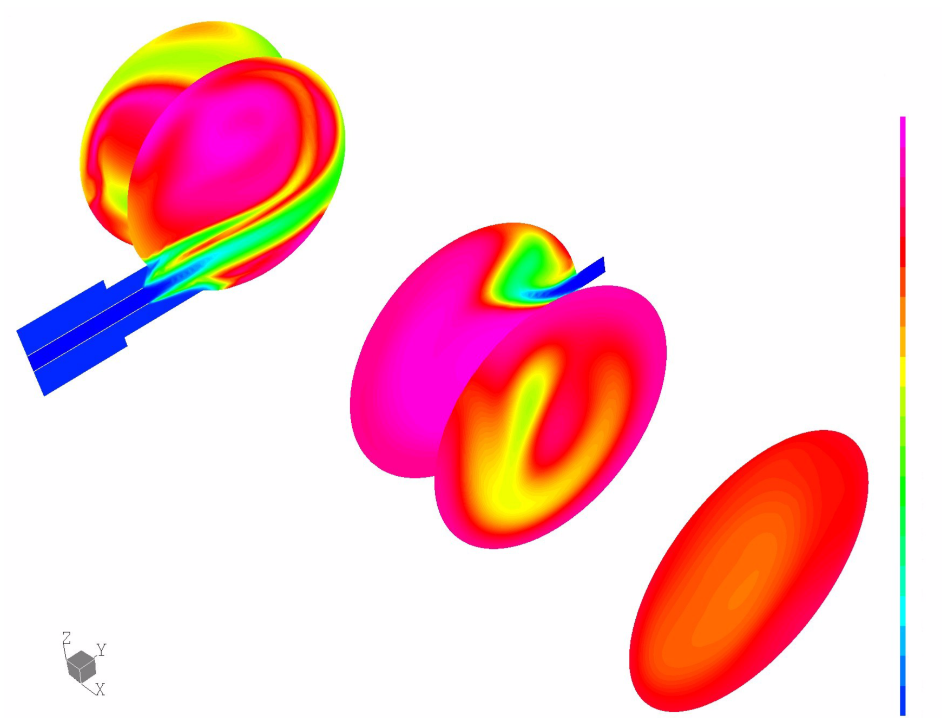

FIGURE 7. Axial Temperature Distribution for Case 2, Tangential Furnace with Radial Injection Opposite Side

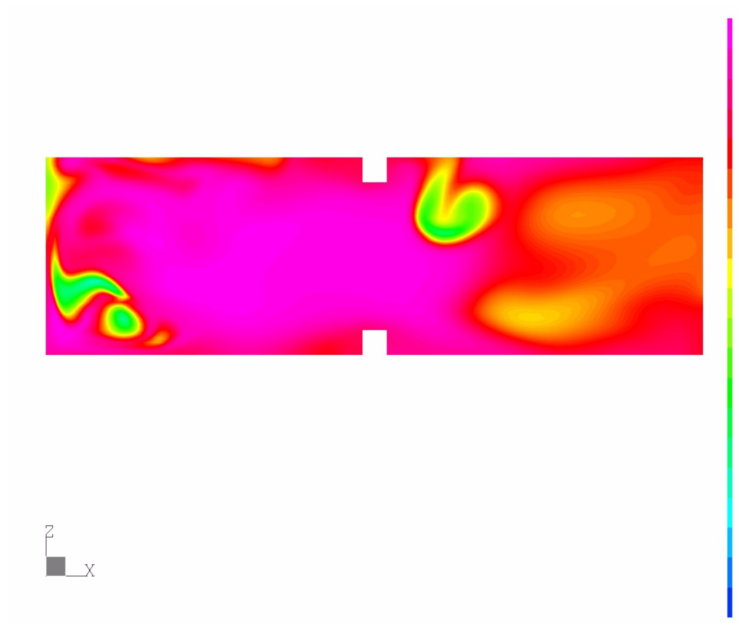

FIGURE 8. Temperature Distribution for Case 3, Tangential Injection - Co-Rotating

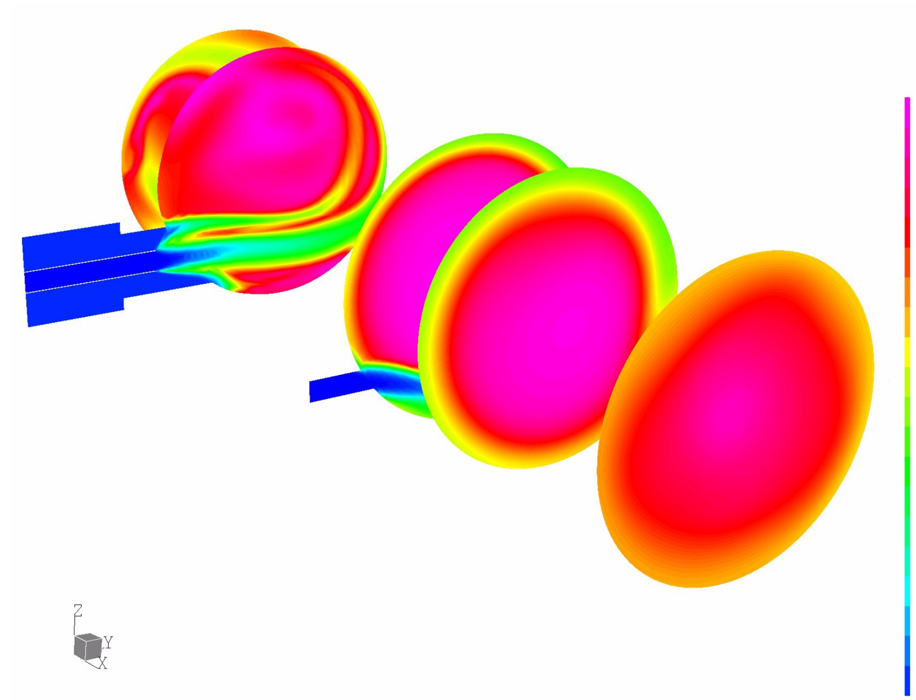

FIGURE 9. Axial Temperature Distribution for Case 3, Tangential Injection - Co-Rotating

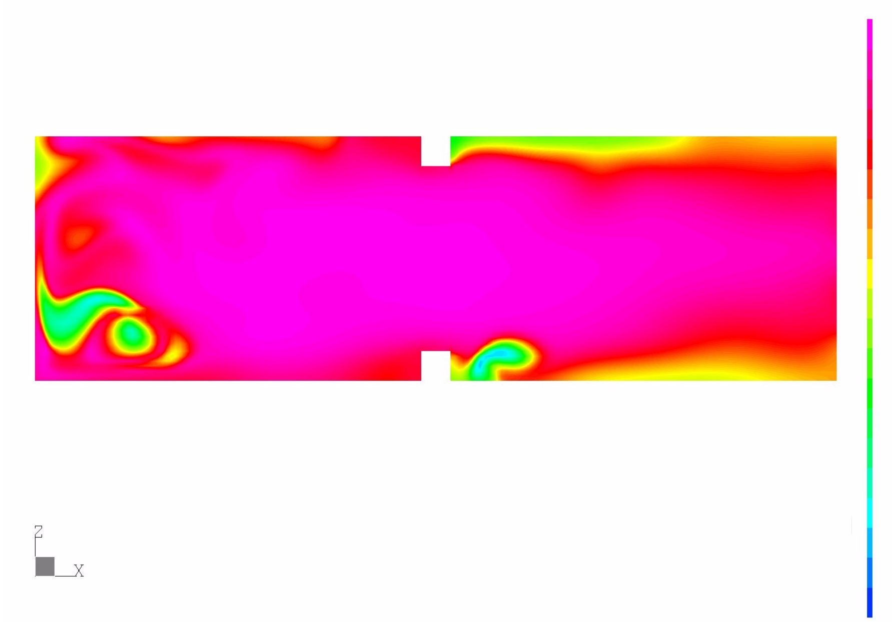

FIGURE 10. Temperature Distribution for Case 4, Tangential Injection - Counter-Rotating

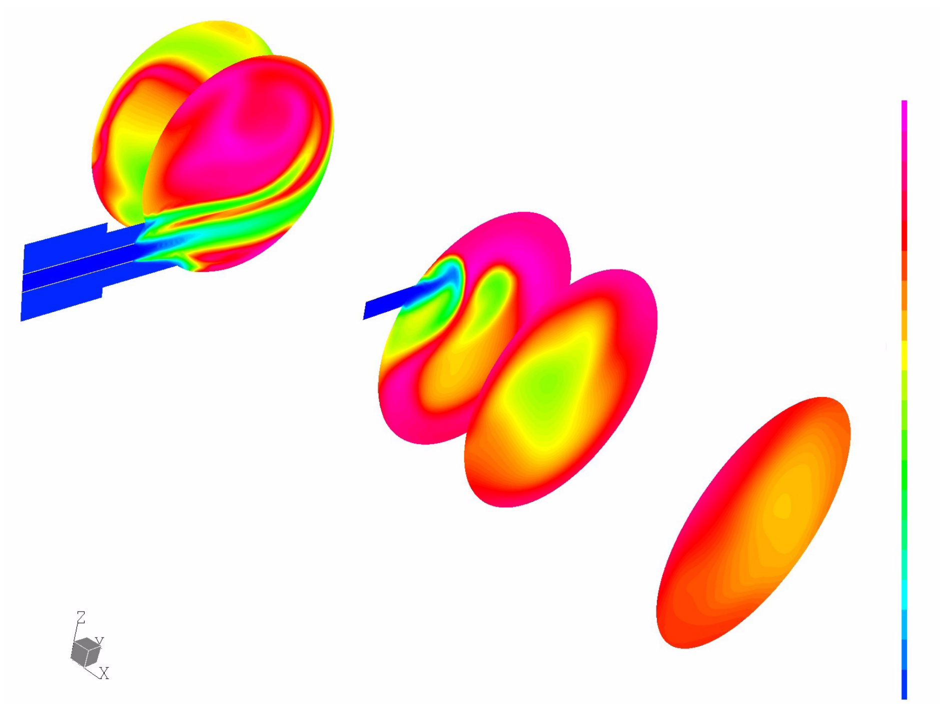

FIGURE 11. Axial Temperature Distribution for Case 4, Tangential Injection - Counter-Rotating

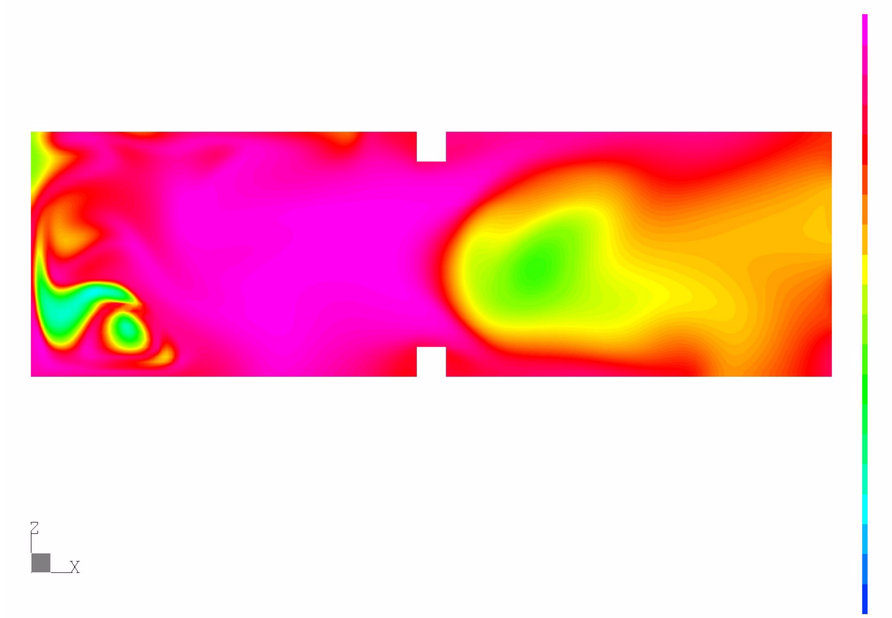

FIGURE 12. Temperature Distribution for Case 5, Four Radial Bypass Inlets

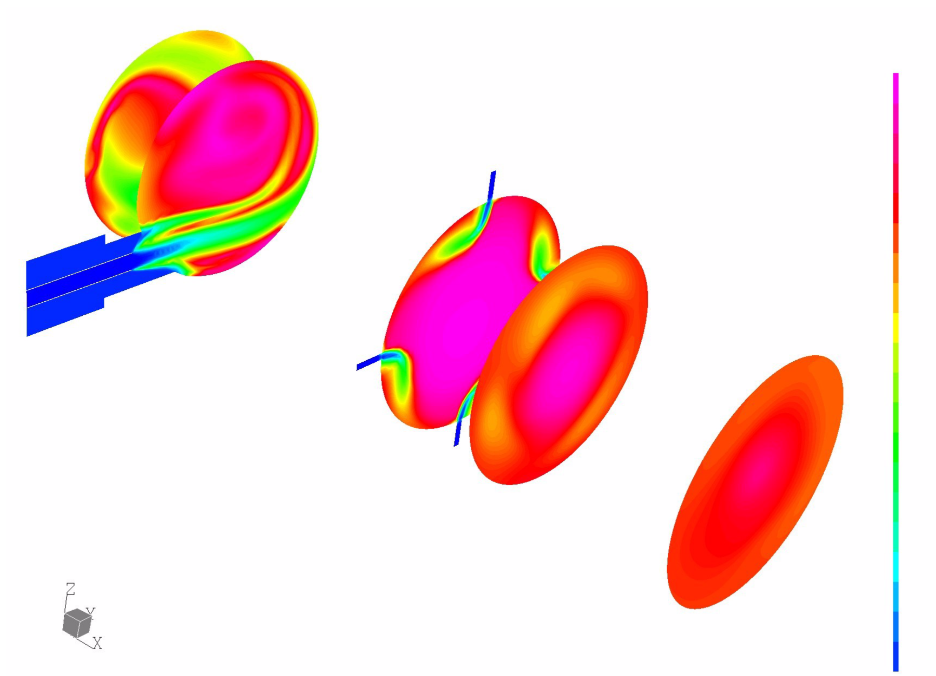

FIGURE 13. Axial Temperature Distribution for Case 5, Four Radial Bypass Inlets

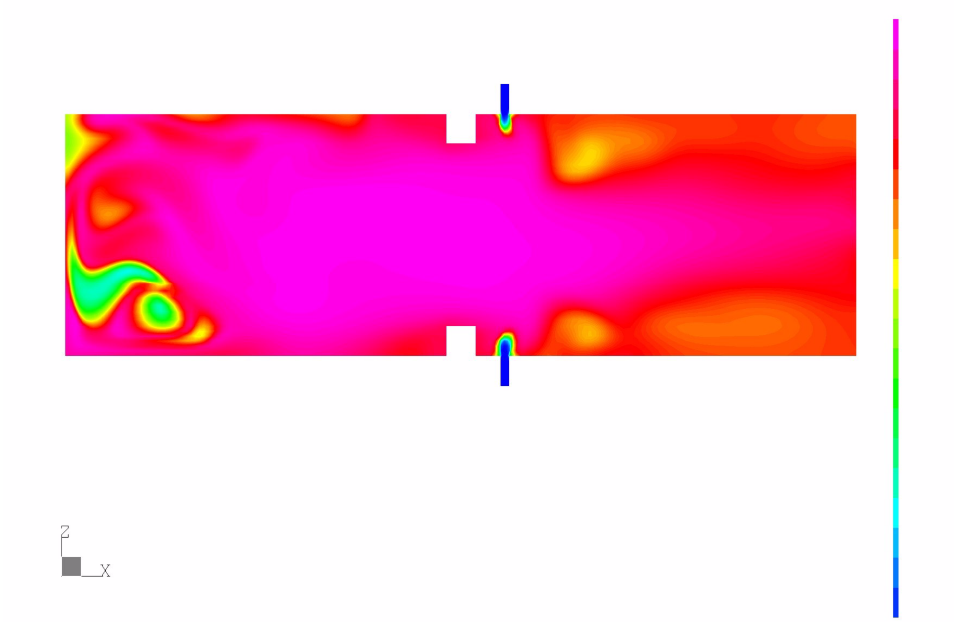

FIGURE 14. Computational Grid for Case 6, End Fired Furnace with Four Radial Bypass Inlets

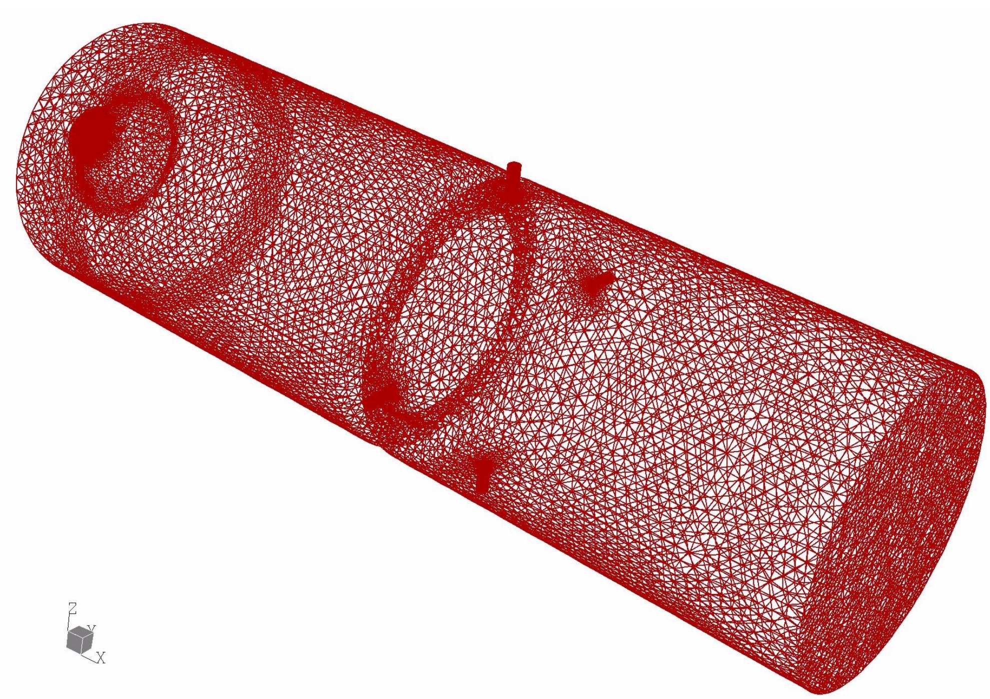

FIGURE 15. Temperature Distribution for Case 6, End Fired Furnace with Four Radial Bypass Inlets

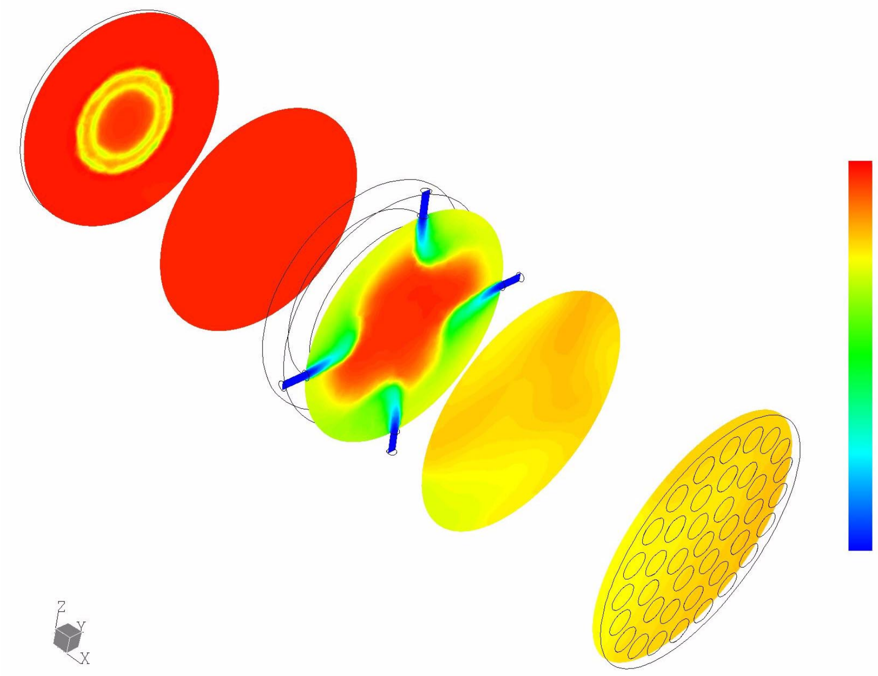

FIGURE 16. Axial Temperature Distribution for Case 6, End Fired Furnace with Four Radial Bypass Inlets

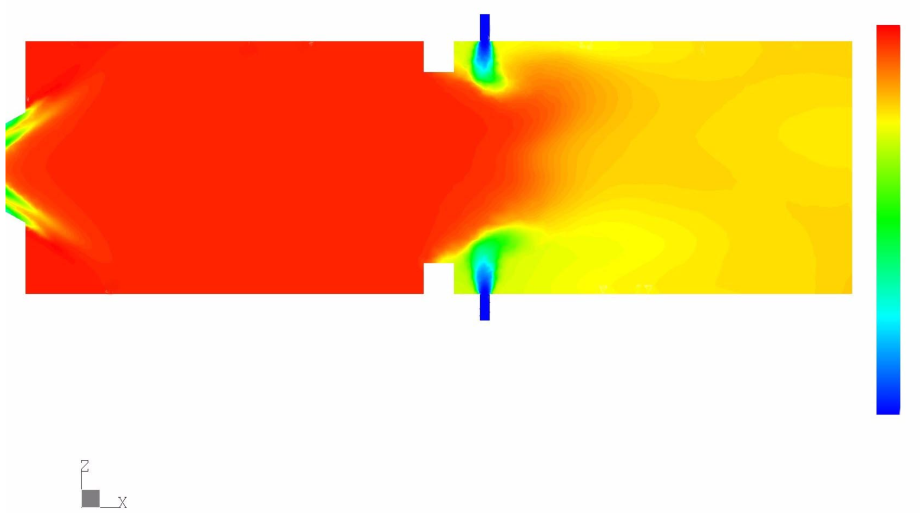

FIGURE 17. Axial O_2 Distribution for Case 6, End Fired Furnace with Four Radial Bypass Inlets

FIGURE 18. Temperature Distribution for Case 7, End Fired Furnace - No Bypass

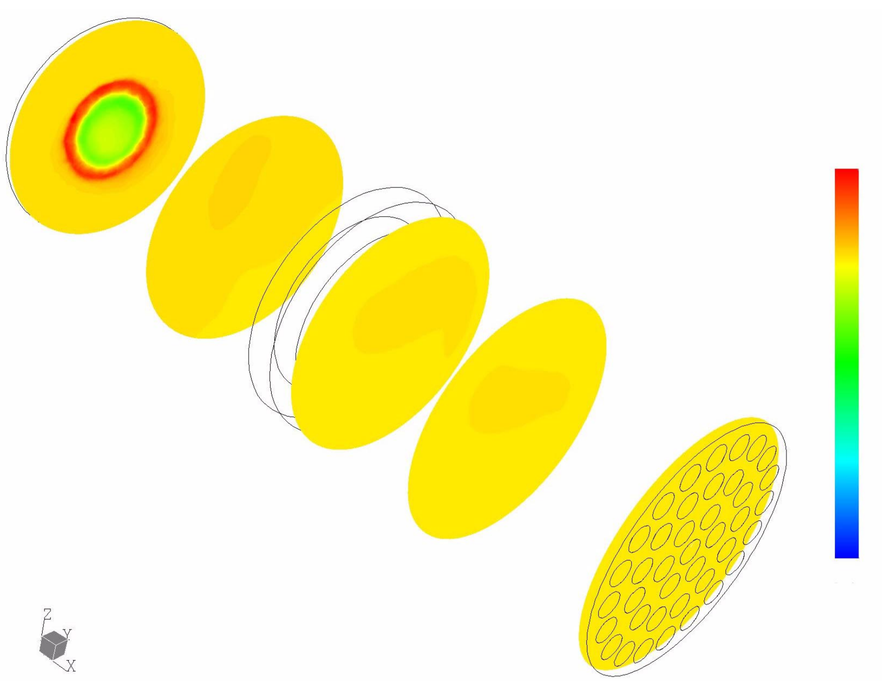

FIGURE 19. Axial Temperature Distribution for Case 7, End Fired Furnace - No Bypass