

# CFD Development for Fired Heater Applications

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AFRC 2022 Industrial Combustion Symposium

## 1. Introduction:

Industry values the ability to ‘virtually’ verify and optimize burner performance through CFD simulation and to evaluate the suitability of burner and furnace designs. Inaccurate results may lead us to falsely reject good burner designs or accept a poor design. Field problems can be far more expensive to fix in terms of reduced capacity, downtime, or field modifications compared to resolving issues in the CFD model and test furnace prior to fabrication.

We have extensive CFD modeling capabilities that we have developed in close coordination with our test facility and burner engineering staff. We also have unrivaled testing capabilities for single and multiple burner configurations that we have used to develop and validate our CFD simulation capabilities, including single flame and flame merging prediction. Our CFD engineers work closely with our process engineering team to optimize burner designs and tip drillings so that the burners we supply are optimized for performance in customer applications.

Our experience in modifying gas tip drillings and other burner design features can lead to a dramatic improvement in burner performance. We have the experience to know that a burner that looks excellent in a single burner test does not always perform well in a multi-burner situation where flame interactions and flue gas circulation patterns can result in lengthened or leaning flames. These situations can produce undesirable tubeskin temperatures, potentially leading to premature fouling and elevated NO<sub>x</sub> emissions. JZ has the expertise and experience, combined with our CFD and testing capabilities to anticipate and avoid these problems.

We have been developing optimization capabilities for the last several years and have applied this capability toward improving the predictive performance of our CFD simulations. In this effort we have deployed that capability to assess and improve our predictive models for a two-burner scenario with multiple burner spacings.

We have completed several efforts in the last few years to collect CFD validation data for single burners in our test facility. We have used these single-burner datasets to substantially improve the accuracy of our CFD models compared to test data. The combustion model parameters resulting from this work are referred to as the “B” parameters. The baseline parameters used before that work are referred to as the “A” parameters. However, an unforeseen consequence of using the “B” parameters is that our CFD predictions in multi-burner scenarios produce high levels of CO in burner action zones, contrary to our experience. The purpose of this study was to collect data that can help us generate more accurate CFD predictions in multiple-burner situations, without sacrificing our single-burner capability.

The result of this work is a set of eddy breakup parameters that we can use in simulations of customer furnaces that are optimized to accurately simulate the dual-burner testing we will do in this effort. We have also assessed the accuracy of our current model parameters for the dual-burner test data we generated.

## 2. Combustion Experiments:

Two Coolstar-15 burners were used to collect new data for this project. JZ Test Furnace 7 is large enough to install two free-standing burners in the floor. A floorplate design was devised that allowed us to easily vary the space between the burners between 30” and 45”. During testing we evaluated burner spacings of 30, 36, and 42 inches. Testing was performed for three fuel compositions: 100% Tulsa natural gas (TNG) and high and low hydrogen content refinery gas (RFG). Maximum and normal heat release rates were tested. Table 1 summarizes the test conditions:

Client Fuel Name		TEST FUEL COMPOSITION (VOL. %)							TEST FUEL PROPERTIES			
Test Fuel		TNG	Propane (C <sub>3</sub> H <sub>8</sub> )	Propylene (C <sub>3</sub> H <sub>6</sub> )	Butane (C <sub>4</sub> H <sub>10</sub> )	Nitrogen (N <sub>2</sub> )	Hydrogen (H <sub>2</sub> )	Carbon Dioxide (CO <sub>2</sub> )	LHV (Btu/lb)	Mol wt. (kg/kgmol)	Temp. (°F)	CP/CV
TNG fuel composition is 91.7% Methane, 6.2% Ethane, 0.3% Propane, 1.3% Nitrogen, 0.4% Carbon Dioxide.												
TNG	A	100							20933	16.69	Ambient	1.31
RFG 1	B	50	20				30		21472	17.77	Ambient	1.26
RFG 2	C	40	40				20		20710	24.72	Ambient	1.22
Test Point Number	Liberation (MMBtu/hr (LHV))	Fuel Type	Air Temp. (°F)	Percent O <sub>2</sub> (vol%, dry)	Burner dP (inH <sub>2</sub> O)	Comments						
<b>30 inches from BCL to BCL</b>												
1	8	A	Ambient	3.0	TBD	Maximum heat release: air register full open.						
2	5	A	Ambient	3.0	TBD	Normal heat release: design excess air by adjusting air register.						
3	8	B	Ambient	3.0	TBD	Maximum heat release: design excess air by adjusting air register.						
4	5	B	Ambient	3.0	TBD	Normal heat release: design excess air by adjusting air register.						
<b>36 inches from BCL to BCL</b>												
5	8	A	Ambient	3.0	TBD	Maximum heat release: air register full open.						
6	5	A	Ambient	3.0	TBD	Normal heat release: design excess air by adjusting air register.						
7	8	B	Ambient	3.0	TBD	Maximum heat release: design excess air by adjusting air register.						
8	5	B	Ambient	3.0	TBD	Normal heat release: design excess air by adjusting air register.						
9	8	C	Ambient	3.0	TBD	Maximum heat release: design excess air by adjusting air register.						
<b>42 inches from BCL to BCL</b>												
10	8	A	Ambient	3.0	TBD	Maximum heat release: air register full open.						
11	5	A	Ambient	3.0	TBD	Normal heat release: design excess air by adjusting air register.						
12	8	B	Ambient	3.0	TBD	Maximum heat release: design excess air by adjusting air register.						
13	5	B	Ambient	3.0	TBD	Normal heat release: design excess air by adjusting air register.						

**Table 1. Test conditions.**

All probing was done on the center plane between the two burners because test ports existed at those locations.

### 3. Optimization

Numerical optimization is the process of using computational algorithms to find the minimum or maximum of a nonlinear, multi-dimensional function. Numerous algorithms exist. The choice of an algorithm depends largely on two questions: 1. Can we calculate an analytical derivative of the function, or can we easily and accurately calculate the derivative numerically? 2. Is the calculation of the function to be minimized fast or slow? These questions are related because an expensive to evaluate function may prevent us from calculating numerical derivatives. For a function that we can evaluate quickly and expect to be continuous and smooth, methods that use gradients (the Jacobian matrix) may be good choice. For a function that can be evaluated quickly but is discontinuous a Monte Carlo method may be the best choice. For the problem considered here the function (RMS difference between CFD and measurements) is not known analytically. Each function evaluation requires converging a CFD case for a different set of parameters, so we would characterize the function evaluation as *slow*. For this situation the simplex algorithm<sup>1</sup> is a good choice and has proven to be robust and reliable. Figure 1 outlines the numerical optimization process.

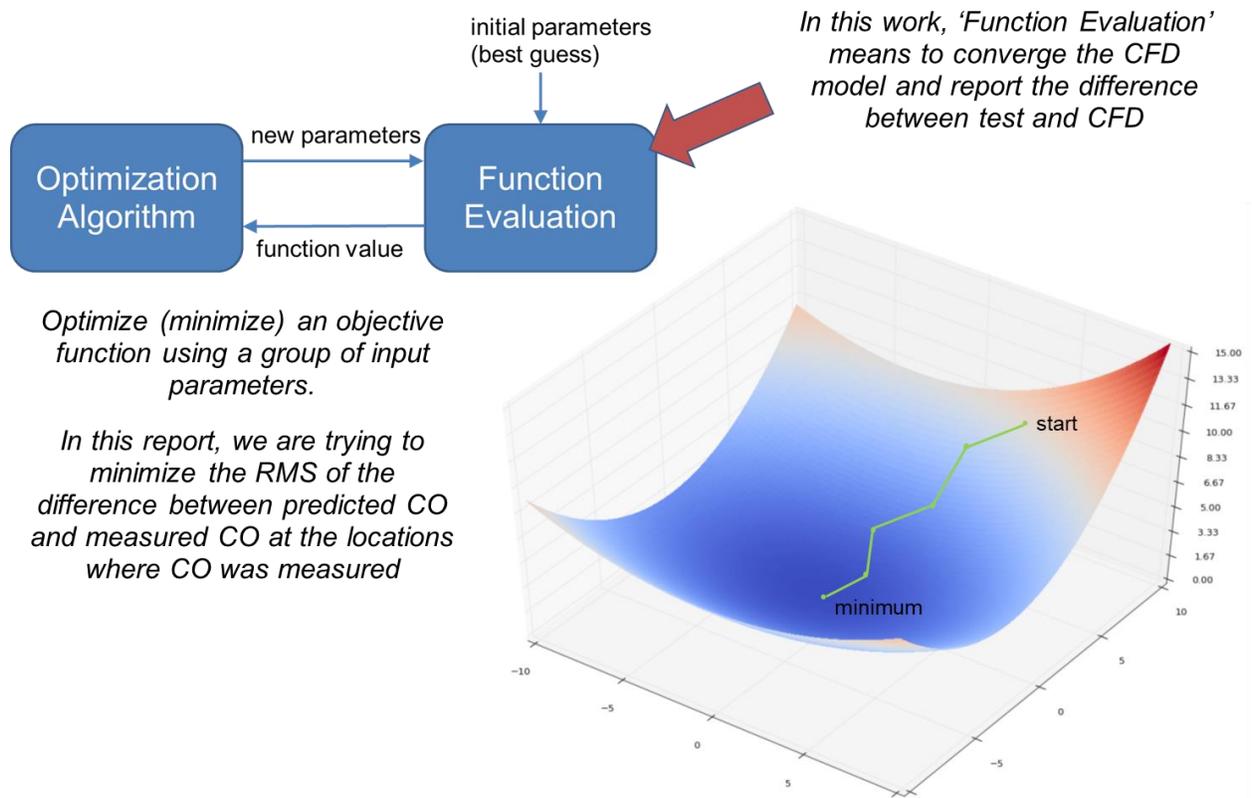
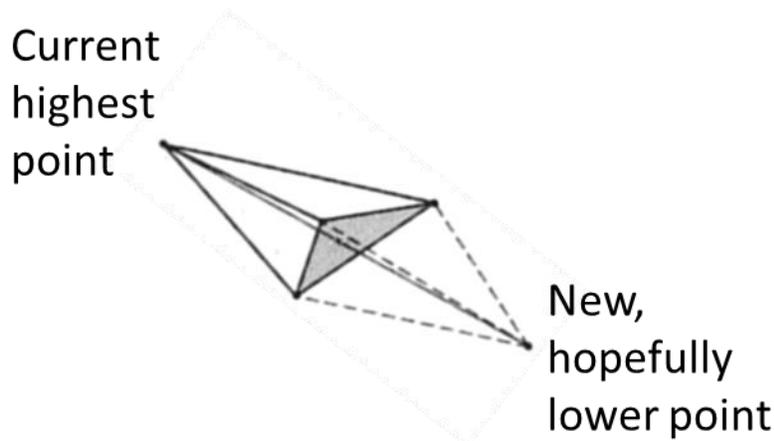


Figure 1. Optimization process overview.

The simplex algorithm can work in any number of dimensions (variables). A simplex in  $n$ -dimensional space is defined as geometric figure with  $n+1$  vertices; in two dimensions a simplex is a triangle, in three dimensions a simplex is a tetrahedron. In more dimensions visualization becomes extremely difficult but the process can be handled mathematically.

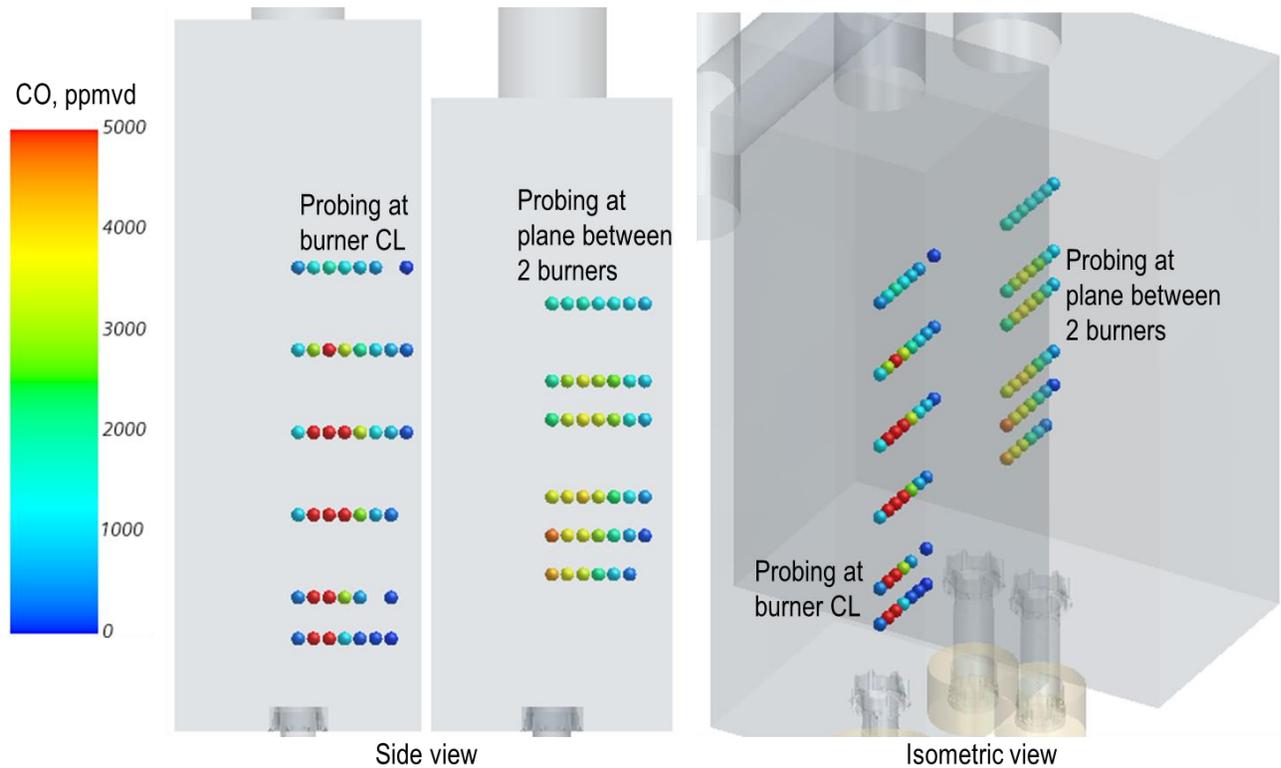
Most of the time the simplex algorithm chooses a new point by reflecting across face opposite the high point as illustrated in Figure 2. When needed the algorithm can also grow or shrink the step size for slowly or quickly changing functions or contract all dimensions of the simplex if the operating space becomes very tight, such as near a local optimum. Since the simplex algorithm is a downhill crawler, it cannot guarantee finding the global optimum, especially for a nonlinear multi-dimensional space. For this reason it is good practice to try multiple starting points.



**Figure 2. A typical simplex algorithm step visualized in three dimensions.**

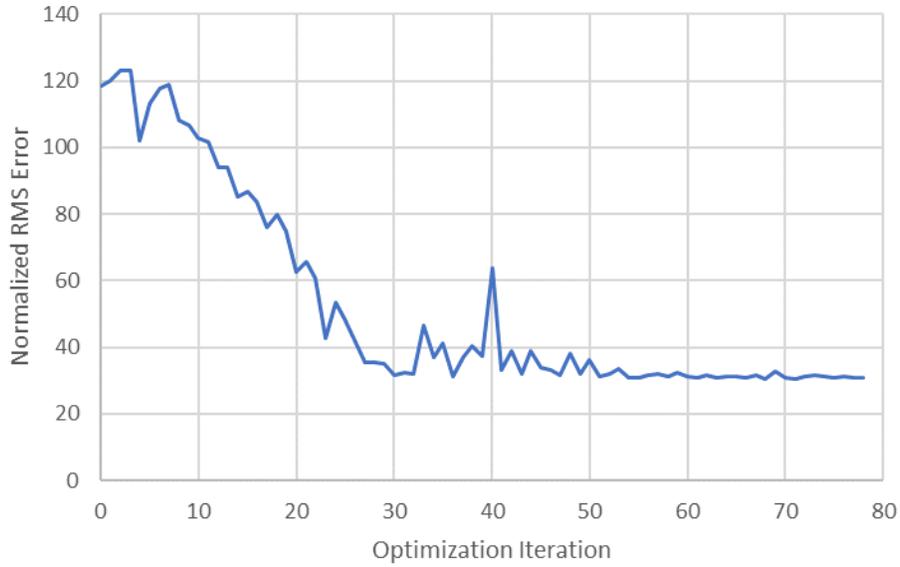
The algorithm needs an initial simplex to start but succeeding steps require only one function evaluation. The initial simplex is formed by choosing a baseline point and changing each variable by a selected delta. Variables are typically normalized to be of order one. If a variable might change over orders of magnitude, the logarithm of the variable is used for optimization.

The CFD parameter optimization setup included a single CoolStar burner in furnace 10 with accompanying in-flame CO probing data along with the dual-burner model of two CoolStars in Furnace 7 with a 30-inch centerline-centerline spacing. The smallest spacing was chosen because that configuration produced the greatest discrepancy between the measured and computed CO values using the “B” parameters. The two models were placed side-by-side in a single CFD simulation (Fig. 3) which used the same parameters for both furnace models.



**Figure 3. CFD optimization setup with a single CoolStar burner in furnace 10 and two CoolStar burners separated by 30" in furnace 7 with representative CO probing measurements.**

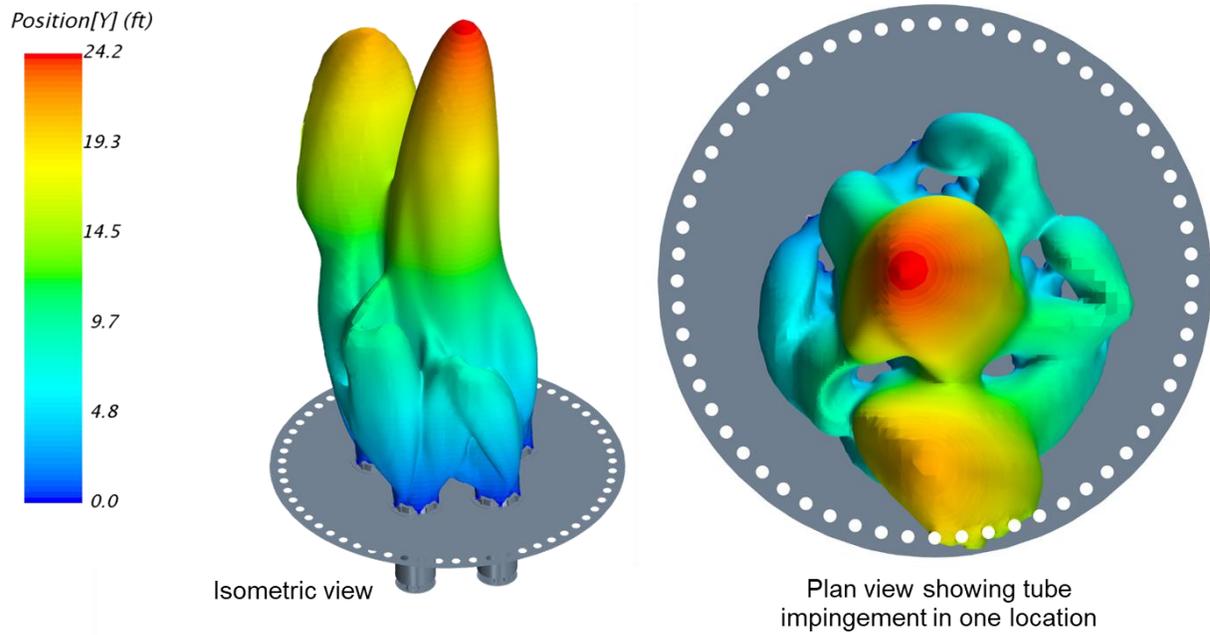
Four separate optimizations were performed with the same geometric setup: For cases with TNG and RFG fuels, the standard  $k-\epsilon$  model (SKE) and the realizable  $k-\epsilon$  model (RKE) were optimized. In most cases the objective function was adjusted to help achieve the desired outcome of modeling 2000 ppm CO iso-surface. In most cases more than one starting point was used to try to find a result closer to a global optimum rather than a local optimum. In most cases the starting point was the "B" parameters. Six or seven parameters were typically optimized in a single run. Figure 4 shows typical optimization performance, in this case reducing the normalized RMS error by nearly a factor of four.



**Figure 4. Simplex algorithm optimization performance.**

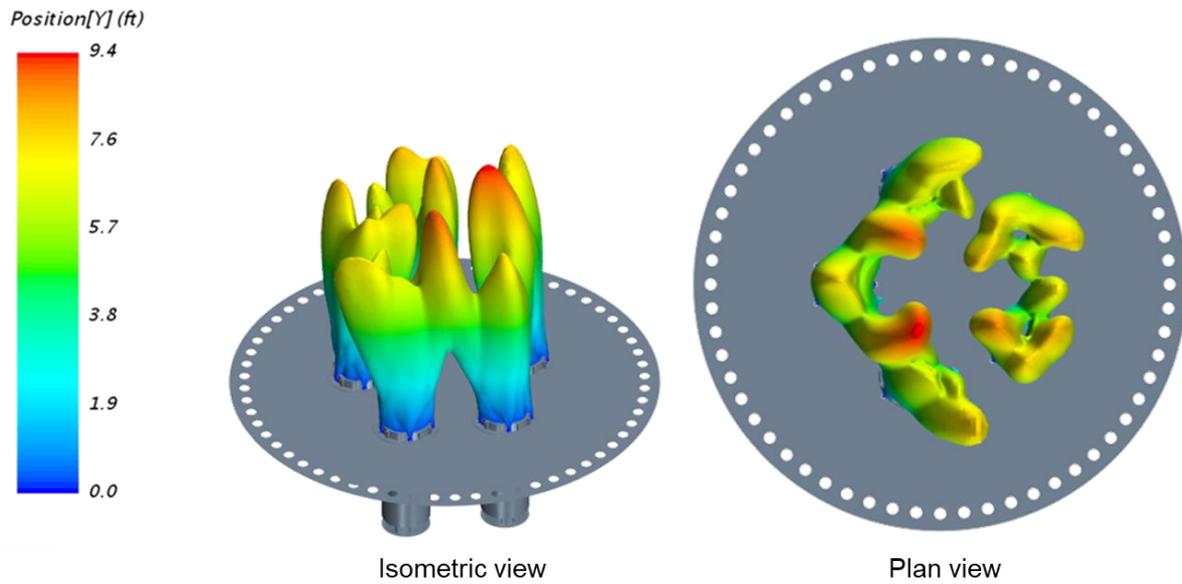
## 4. Application

An example of using optimized kinetic parameters to improve a customer furnace is a the radiant section of a heater containing five LN-SFR-17-LC ARIA burners. The customer observed flame overlap and tube impingement, which was also observed in the CFD results as shown in Figure 5.



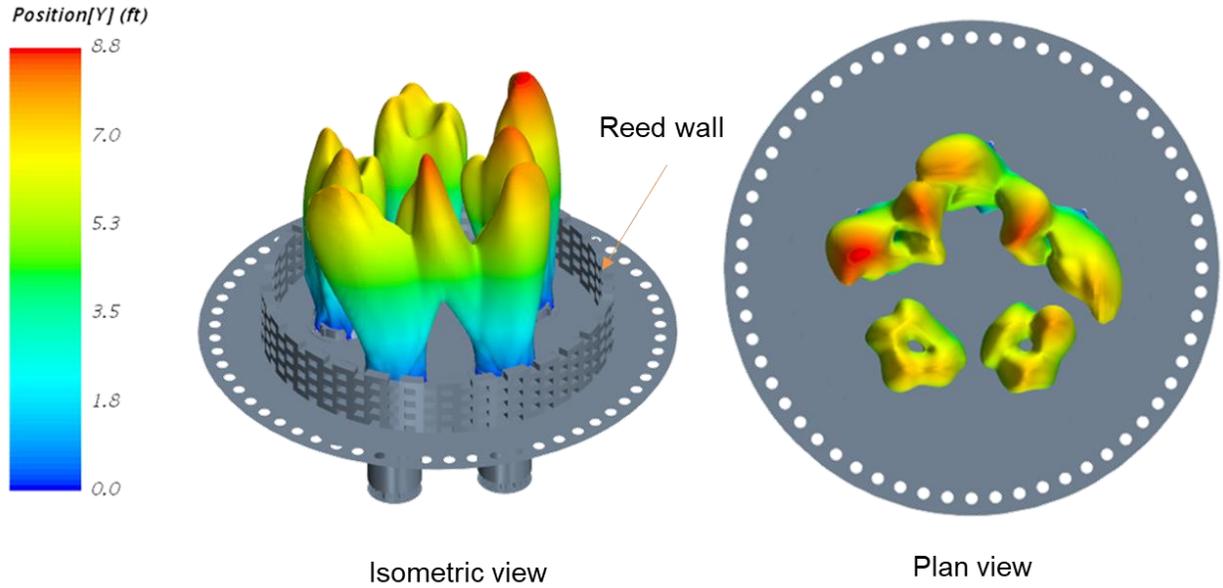
**Figure 5. Computed CO=2000 ppmvd iso-surfaces for a heater containing five LN-SFR-17-LC ARIA burners, original configuration.**

Based on previous test work, a gas tip revision was proposed to improve the flame shape. In the CFD simulation, the proposed revision made a significant reduction in flame interaction and eliminated flame impingement on the tubes, as shown in Fig. 6.



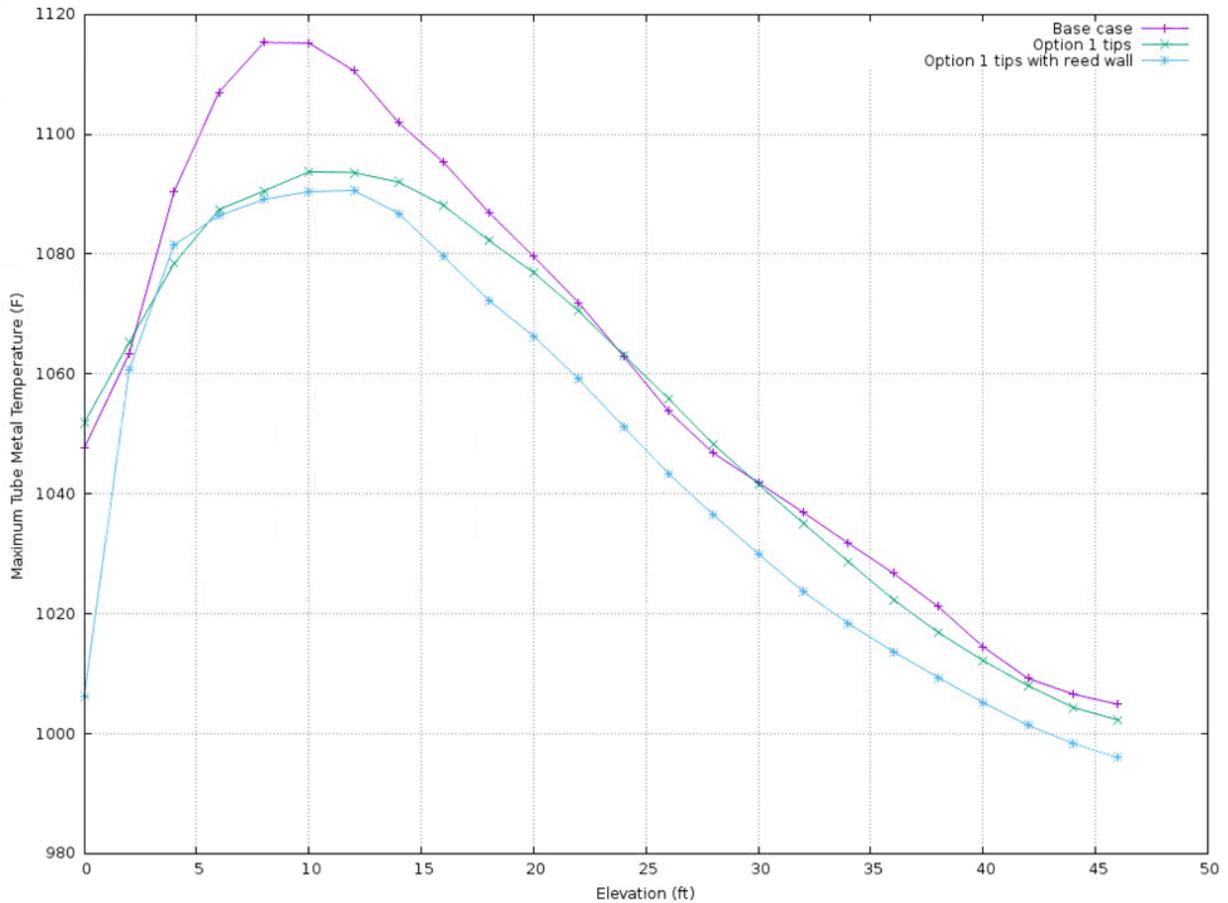
**Figure 6 Computed CO=2000 ppmvd iso-surfaces for a heater containing five LN-SFR-17-LC ARIA burners, revised tip drilling.**

In addition, a Reed wall with a checkered opening pattern was added. In previous work by John Zink adding a fairly tall reed wall has improved the symmetry of flue gas circulation in our CFD models. CFD results with the revised tip drillings and the Reed wall are shown in Fig. 7.



**Figure 7. Computed CO=2000 ppmvd iso-surfaces for a heater containing five LN-SFR-17-LC ARIA burners, revised tip drilling and Reed wall.**

The revised tip drillings and the Reed wall also improved the tube metal temperature (TMT) uniformity as shown in Fig. 8.



**Figure 8. Computed tube metal temperatures for the baseline case, the revised tip drillings and the revised tip drillings plus the Reed wall.**

The improved flame behavior and tube metal temperature uniformity were observed by the furnace operator in general agreement with the CFD predictions.

## 5. Conclusions

CFD results without comparison to measurements have limited usefulness. Our experience comparing CFD and measured data has shown that using the default parameters found in commercial CFD codes does not result in accurate results. Numerical parameter optimization, combined with in-furnace data for single and interacting burners is a powerful tool for improving the reliability of CFD. CFD parameters optimized against multi-burner are found to increase CFD reliability allowing CFD to be used to improve furnace performance.

## References:

Press, W.H., Teukolsky, S.A., Vetterling, W.T. and Flannery, B.T., *Numerical Recipes: The Art of Scientific Computing*, Cambridge University Press, 1986.