Combustion Modeling – What Should You Expect?

Two common types of combustion modeling are used when designing and troubleshooting furnaces: **chemical reaction modeling** and **fluid flow modeling**. Using computers, it is possible to combine these models to study furnace and burner operation. While the results become better each year, shortcomings prevent getting precise answers in most cases.

Chemical Reaction Modeling

Chemical reactions are modeled based on research in well mixed systems. If the mixture of reactants, the starting temperature and the starting pressure are known, reaction modeling can tell you what products will have been produced, how much heat has been liberated (or consumed), and the rest of the chemical and physical properties of the system. When burning methane in oxygen, the overall reaction can be written:

$$CH4 + 2O2 \rightarrow CO2 + 2H2O$$

This says that 100% of the methane and oxygen turn into carbon dioxide and water, but that is not what actually happens. There are several chemical reactions (paths) for this overall reaction, and unless the time allowed is infinite, there will always be traces of intermediate compounds remaining. For instance, in an efficient furnace there is always at least a trace of CO in the stack gas.

Fluid Flow Modeling

Fluid modeling is based on physical characteristics like momentum and evaporation and the transport properties of the fluids in a system. For instance, the path of a particle through an air duct can be predicted based on particle size, air temperature, duct size, etc. Likewise, the evaporation of a water droplet passing through a hot furnace can be described accurately using techniques presently available.

Chemistry and Flow Combined = CFD Model

Combining the two modeling approaches gives Computational Fluid Dynamic (CFD) modeling. Eventually, computing power and our understanding of chemical reactions will be sufficient to for us to draw a complete picture of what is happening (or will happen) in any furnace. Right now, though, the best CFD models give us only a "pretty good" picture of reality.

For most furnaces, a natural gas burner can be assumed to combine the gas stream with the air stream, ignite the mixture and completely react all constituents. We know that almost all of the methane will react completely with oxygen in the air, forming CO2 and H2O. We also know that a very small fraction of the mixture will end up as CO, NO, NO2, N2O and various other minor constituents. The exact amount of NOx and CO is important because air permits usually limit these compounds in stack gas, but we really can only estimate their amounts based on past experience – attempts to calculate exact values scientifically have not been very successful.

Attempts to model flames accurately have not been completely successful. Methane and oxygen don't react until they are mixed, so combustion reactions start where the fuel gas first contacts air – combustion radiates heat, affecting the surrounding hardware and affecting the flow pattern of nearby unburned gases. Reaction rates increase as temperatures rise. Reaction products change as the local chemistry changes. Unless your model can see all of this and accommodate the changes in volume, temperature, momentum, reactant concentration, etc., you won't be able to predict exactly what will happen. Usually, exact predictions aren't needed.

When to Use CFD Modeling

1. Is there enough time?

For an "average" incinerator allow around 3 weeks for setup and running the program till it converges on an answer. Shortcuts in setup can shorten the time, but the answers may be fuzzier than you would want.

2. What do you need to know?

Hand calculations are still usually the way to go – you get good answers as long as the designer (biological computer) is experienced. Going straight to CFD is more expensive and takes longer. On the other hand, unexplainable operating problems deserve special measures. CFD can provide that "Ah Ha!" moment when other approaches have failed.

3. Is the problem steady-state or transient?

CFD is good at solving steady-state problems. Examples are standing flow patterns – like a "core" of unburned waste that extends from the burner to the waste heat boiler. That type problem can be identified and solved using CFD modeling. Noise problems, resulting from rhythmic variations of the flame envelope are beyond most CFD efforts – unless you can get NASA to help.

4. CFD is only a tool – not a solution

A perfect CFD model only replicates the problem or design. It won't tell you what to do next. Combined with your own experience, it can certainly suggest changes to look at, though. The best approach is to model the system that has problems to duplicate what exists – that indicates the model is set up right. Then decide which parameters to change and model your best-guess changes. Repeat till the problem goes away (in the computer) and then call the welder.

5. Maybe a "sledgehammer" fix would solve the problem and avoid an expensive CFD project.

For instance, if you know you have a distribution problem (the flame favors one side of the furnace), shutting down long enough to install a brick choke ring might be the common sense thing to try. The amount of pressure drop the choke uses is easily calculable without CFD and you can visualize how the flame path would change. So, use the maximum amount of pressure drop available, and install the choke. If the easy-quick fix fails, and the next step will be expensive, start thinking about CFD.

Progress

Year by year, the tools available for CFD modeling become better – easier to use and more accurate. For now (2007), it can save you when the chips are down, but can't fully take the place of experience.

Acknowledgments

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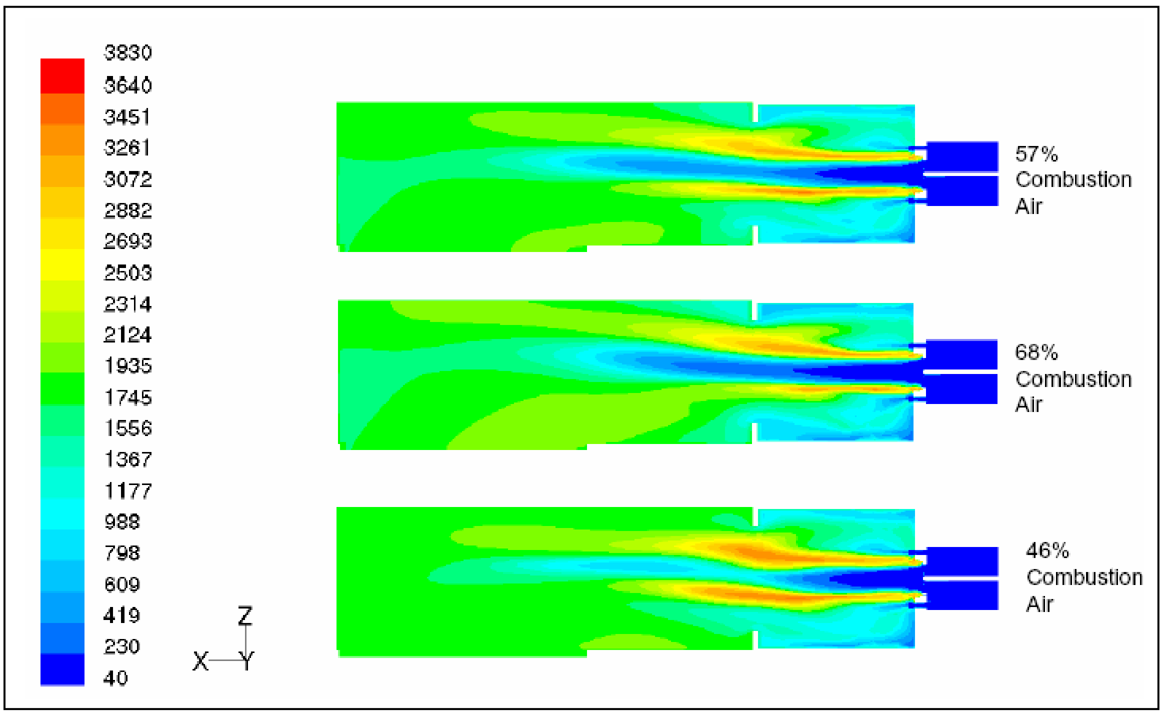
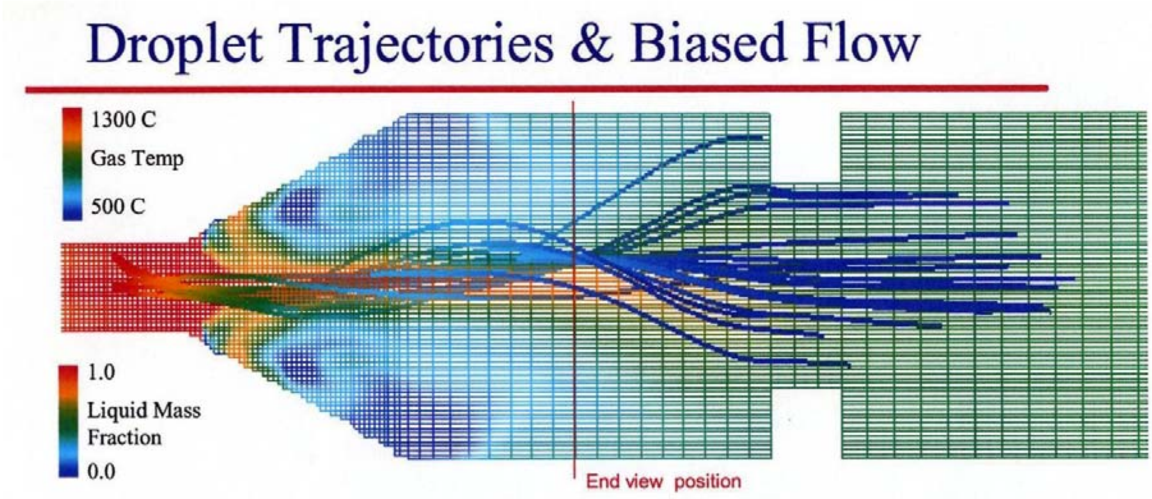
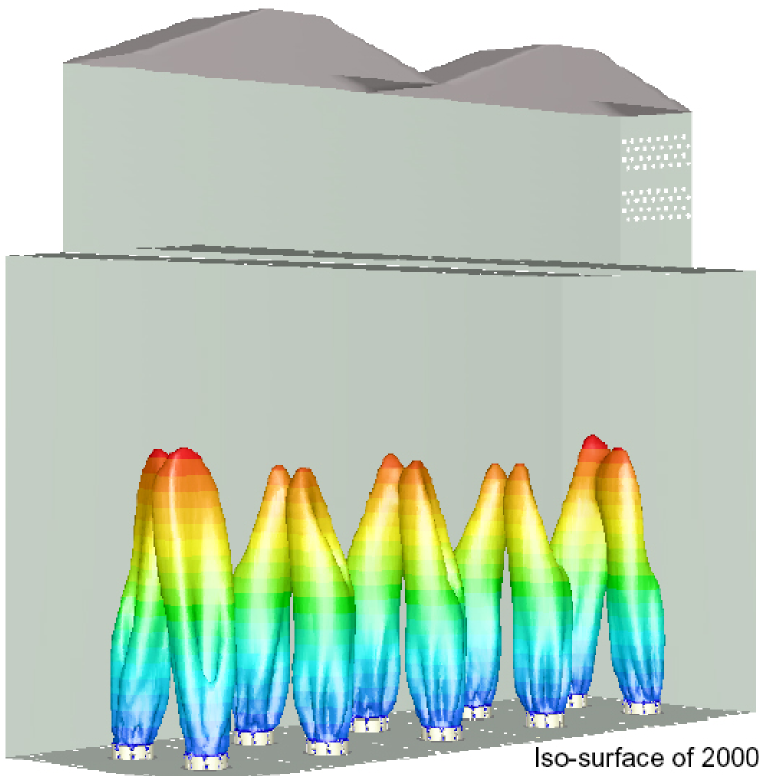
Examples of CFD Model results:



CFD Model of waste gas incinerator showing the effect of varying the amount of combustion air flowing to the burner – 46% air resulted in more even temperature distribution at the furnace exit. Note how the brick choke ring (white bars towards the burner end of the furnace) affects the temperature spread.



CFD model investigates the evaporation of waste liquid droplets in this waste gas incinerator. The white rectangles are a brick choke ring midway through the furnace. The fuel burner is at left. The exhaust exits to the right into a Watertube boiler, so complete droplet evaporation is needed to avoid tube fouling and emission problems. Note how the choke ring smoothes the flue gas temperature variations.



CFD can calculate hydrocarbon destruction – a visible flame contains more than 2000 ppm of carbon monoxide, providing a way to estimate the shape and size of burner flames.