
5 CFD in Burner Development

*Joseph D. Smith, Michael Lorra, Ph.D., Eric M. Hixson,
and Tom Eldredge, Ph.D.*

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5.1 INTRODUCTION

Computational fluid dynamics (CFD) has become an accepted tool to help in the design and operation of aerodynamic equipment. More recently, CFD has also found tremendous application in the analysis of combustion equipment, such as industrial burners. Widespread acceptance is limited due to the nonlinear relationship between reaction chemistry and turbulent fluid mechanics. Smith et al.¹ list several related issues that tend to limit the application of CFD to industrial problems, which include the following:

- *Limited understanding of the physics involved in reactive flow systems.* This includes uncertainty in fundamental chemical reaction kinetics for complex fuels, the chaotic nature of turbulent mixing, the heterogeneous chemistry related to solids (e.g., soot formation, catalysis, etc.), thermophoretic transport of solids to walls and the associated deposition mechanisms, and the radiative properties of complex multiphase systems.
- *The large disparity in both spatial and temporal time scales in typical reacting flow systems.* To capture the flow characteristics responsible for momentum transfer, one needs to resolve the flow to the smallest characteristic size (i.e., Kolmogorov scale). To capture the associated reaction kinetics, it is believed that one must further resolve the spatial features to the Batchelor scale. Pitts² points out that traditionally it was argued that one should resolve spatial features on the order of size of the Batchelor scale (product of Kolmogorov scale and inverse square root of Schmidt number), typically a few hundred micrometers for most laboratory flows. More recently, however, it has been suggested that the required spatial resolution may be 12 to 25 times larger than the Batchelor scale. Unfortunately, recent experiments, including scalar dissipation measurements along a line in an axisymmetric jet of propane into air at the National Institute of Standards and Technology, have shown that the larger estimates for the required spatial resolution will result in partial averaging of the scalar dissipation. Taken together, the studies suggest that to fully capture scalar dissipation fluctuations, the spatial resolution must be no larger than two to three times the Batchelor scale. The computational difficulty of coupling the many important aspects of chemistry and physics in a way that is efficient enough to be achievable for computations simulating practical furnaces, which have such a wide disparity of spatial and temporal scales.
- *Full-scale verification of actual CFD codes in real furnaces is difficult and costly.* In addition, local, detailed data for model validation is also expensive and tedious to obtain. This dearth of “realistic” data for evaluation of predictions brings with it uncertainty about both the numerical error in the predictions and the experimental error in the data.
- *Typical computational combustion tools have not been designed to optimize combustion equipment such as industrial burners.*

This leaves an engineer uncertain as to how to effectively use CFD predictions to address constrained design or operational problems. However, current trends in environmental and operational costs are making it increasingly necessary to explore operating conditions that are beyond the current empirical database of industrial burners. Recent work by Smith et al.³ and Henneke et al.⁴ have demonstrated the basic fact that CFD-based tools hold great promise for economically exploring new burner designs.

This chapter begins with a brief discussion of how these commercial codes are used to analyze a typical industrial burner. Attention focuses on producing an “appropriate” computational mesh. It also discusses different issues related to computational meshes. Next, it discusses in some detail the multi-physics involved in combustion modeling. In particular, it describes the necessary physical sub-models inherent in a typical CFD-based combustion simulation package. Finally, it provides three examples of how these types of tools have been used recently to address various issues related to industrial burners. In conclusion, the chapter summarizes key issues related to using CFD in industrial burner design, evaluation, and optimization. It also provides recommendations for future work needed to advance this science.

5.2 SOLVING BURNER PROBLEMS WITH CFD

Computational fluid dynamics (CFD) has been successfully used for many years in a number of industries, beginning with aerospace and expanding into aeronautics, automotive, electronics, and electric power generation. More recently, CFD has found application in the chemical process and the hydrocarbon process industries (HPI/CPI) where it has gained a foothold as a tested, validated, and

now regularly accepted, problem-solving tool. Engineers involved in designing and building advanced combustion equipment for the HPI and CPI industries routinely use CFD to advance new burner technology.

The science and technology of CFD has matured to the point where performance predictions are made with a degree of confidence from models covering a wide range of complex furnace, burner, and reactor geometries. CFD allows the engineer to explore operational parameters previously considered impossible or prohibitively expensive using normal testing procedures. Combustion-based CFD has become an extremely valuable tool in providing direction to the timely execution of industrial experiments, which further reduces the impact that retrofits and other equipment changes may have on an organization's bottom line.

Although a proven tool in modeling equipment behavior and performance, CFD is not without limitations. Most notable are the current limitations with respect to modeling turbulent reacting flow. Commercial CFD codes utilize a standard approach to simulate chemical kinetics, which approximate the consumption and production of chemical species. This causes the engineer to use simplifying assumptions about the chemistry considered in the simulation. While this simplified chemistry includes adequate information to predict flow patterns and local heat transfer, these models lack sufficient information to accurately predict NO_x and CO production. Alternatively, the NO_x chemistry is decoupled from the main calculation and obtained using post-processing techniques. However, for species more closely related to the base fuel, such as CO, a similar, abridged treatment is not currently available.

Recent efforts to include more complex chemical kinetics, such as those used by StarCDTM with the ChemkinTM* suite of programs, are helping push CFD technology closer to more fundamentally based mechanistic solutions. However, correctly coupling detailed kinetics with turbulent fluid mechanics is very difficult and, with the enhancement of mesh generation techniques, stands as one of the biggest areas for potential growth in the next five years.

Computer simulations are also only as good as the data with which they are validated. In many cases, sufficient data are not available to accurately calibrate a CFD model. Physical or scaled-flow modeling has traditionally been used to generate baseline data to help validate flow predictions. In addition, well-controlled, full-scale burner tests have been used to verify predictions of burner performance. CFD coupled with cold-flow physical modeling and hot-flow burner tests provides a powerful analytical tool to develop accurate, timely, and cost-effective burner designs.

5.2.1 KEY INGREDIENTS OF CFD

At its roots, CFD relies on three worlds (see [Figure 5.1](#)).⁵ First, CFD requires a comprehensive understanding of the physical phenomena involved in any process. Second, the physics of the phenomena must be translated into mathematical relationships. Third, due to the complexity of nonlinear mathematics (see [Table 5.1](#)), the governing equations must be solved using numerical algorithms. Effective use of CFD relies equally on each of these worlds. Error in any one translates into erroneous predictions, and failing to understand the limitations of each can lead to incorrect conclusions and potentially catastrophic results. For optimal use, the engineer must understand the physics, mathematics, and numerics to determine when simulation results represent reality.

When used appropriately, CFD helps reduce burner development cycle time, improves burner efficiency, and extends burner lifetime. This is due to reduced computer costs, increased computer power, and better and more detailed physics in commercially available CFD codes. CFD also helps reduce operating costs, improves product yield, and increases product quality through system optimization. In some instances, CFD helps the engineer evaluate various design options that otherwise

* Chemkin is a software tool for incorporating complex chemical kinetics into simulations of reacting flow. This commercial tool is supplied by Reaction Design, currently located in San Diego, CA.

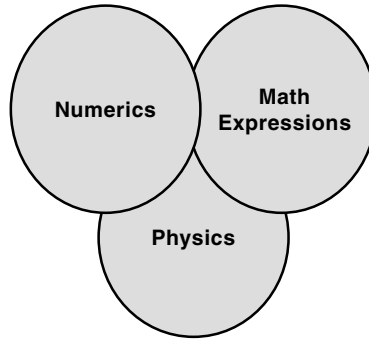


FIGURE 5.1 Three worlds of CFD.

TABLE 5.1
Cartesian Set of Differential Equations Solved in CFD

$$-\frac{\partial(\bar{\rho}\tilde{u}\phi)}{\partial x} + \frac{\partial(\bar{\rho}\tilde{v}\phi)}{\partial y} + \frac{\partial(\bar{\rho}\tilde{w}\phi)}{\partial z} - \frac{\partial}{\partial x}\left(\Gamma_\phi \frac{\partial(\phi)}{\partial x}\right) - \frac{\partial}{\partial y}\left(\Gamma_\phi \frac{\partial(\phi)}{\partial y}\right) - \frac{\partial}{\partial z}\left(\Gamma_\phi \frac{\partial(\phi)}{\partial z}\right) = S_\phi$$

Equation	ϕ	Γ_ϕ	S_ϕ
Continuity	1	0	0
X-momentum	$\tilde{u}$	μ_e	$-\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left(\mu_e \frac{\partial \tilde{u}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_e \frac{\partial \tilde{v}}{\partial x}\right) + \frac{\partial}{\partial z}\left(\mu_e \frac{\partial \tilde{w}}{\partial x}\right) + \bar{\rho}g_x - \frac{2}{3}\bar{\rho}\tilde{k}$
Y-momentum	$\tilde{v}$	μ_e	$-\frac{\partial p}{\partial y} + \frac{\partial}{\partial x}\left(\mu_e \frac{\partial \tilde{u}}{\partial y}\right) + \frac{\partial}{\partial y}\left(\mu_e \frac{\partial \tilde{v}}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu_e \frac{\partial \tilde{w}}{\partial y}\right) + \bar{\rho}g_y - \frac{2}{3}\bar{\rho}\tilde{k}$
Z-momentum	$\tilde{w}$	μ_e	$-\frac{\partial p}{\partial z} + \frac{\partial}{\partial x}\left(\mu_e \frac{\partial \tilde{u}}{\partial z}\right) + \frac{\partial}{\partial y}\left(\mu_e \frac{\partial \tilde{v}}{\partial z}\right) + \frac{\partial}{\partial z}\left(\mu_e \frac{\partial \tilde{w}}{\partial z}\right) + \bar{\rho}g_z - \frac{2}{3}\bar{\rho}\tilde{k}$
Mixture fraction	$\tilde{f}$	$\frac{\mu_e}{\sigma_f}$	0
Mixture fraction variance	$\tilde{g}$	$\frac{\mu_e}{\sigma_g}$	$-\frac{C_{g1}\mu_e}{\sigma_g} + \left[\left(\frac{\partial \tilde{f}}{\partial x}\right)^2 + \left(\frac{\partial \tilde{f}}{\partial y}\right)^2 + \left(\frac{\partial \tilde{f}}{\partial z}\right)^2\right] - C_{g2}\bar{\rho}\tilde{g}\frac{\tilde{\epsilon}}{k}$
Turbulent energy	$\tilde{k}$	$\frac{\mu_e}{\sigma_k}$	$G - \bar{\rho}\tilde{\epsilon}$
Dissipation rate	$\tilde{\epsilon}$	$\frac{\mu_e}{\sigma_\epsilon}$	$\left(\frac{\tilde{\epsilon}}{k}\right)(c_1G - c_2\bar{\rho}\tilde{\epsilon})$

where:

$$G = \mu_e \left\{ 2 \left[\left(\frac{\partial \tilde{u}}{\partial x} \right)^2 + \left(\frac{\partial \tilde{v}}{\partial y} \right)^2 + \left(\frac{\partial \tilde{w}}{\partial z} \right)^2 \right] + \left(\frac{\partial \tilde{u}}{\partial y} + \frac{\partial \tilde{v}}{\partial x} \right)^2 + \left(\frac{\partial \tilde{u}}{\partial z} + \frac{\partial \tilde{w}}{\partial x} \right)^2 + \left(\frac{\partial \tilde{v}}{\partial z} + \frac{\partial \tilde{w}}{\partial y} \right)^2 \right\}$$

would not be possible to evaluate experimentally because of safety constraints. Thus, CFD has also led to improvements in safe operations.

Because a model is only as good as the data it represents, CFD is best conducted hand-in-hand with experiments. CFD can help identify the key experiments needed instead of performing all tests required in a complete factorial design. This allows the researcher to spend more time on the tests

that will lead him or her closer to a determination or solution. In this way, CFD helps expand traditional methods instead of replacing them. While many plants have been designed and built using rules-of-thumb, empirical correlations, and spreadsheets, CFD bridges the gap between theory and practice by increasing the practical use of fundamentals in process design, operation, and optimization.

Today, engineers use commercially available, advanced CFD-based combustion packages, including Fluent and Star-CD. Other software tools such as Chemkin™ are used to simulate the chemical kinetics responsible for NO_x and CO emissions. The rapid expansion of computer power has led to more comprehensive CFD simulations that require large numbers of calculations. A typical burner simulation may require in excess of 10⁶ computational cells or nodes points. Based on current computer power, these simulations require between 24 and 72 hours each. As CPU power increases, more and more complex physics are added to the simulation, which improves an engineer's ability to solve "real" problems with CFD-based tools.

Today's challenge continues to be simulating fully three-dimensional, turbulent, reacting compressible flows inside very complex burner/furnace geometries. With recent advances in parallel computing, however, highly parallel workstation clusters are now used to solve problems with more than 10⁷ nodes with transient behavior.

5.2.2 MAIN GOAL OF CFD MODELING

The main goal for performing CFD related to industrial burners is to reduce the cost of developing new technology. When a new industrial burner is designed to meet certain performance standards, including heat release, reduced emissions levels, flame shape, and operational stability, an iterative testing process is common. Past experience shows that this process may require upward of 2 years and a minimum of \$1 million. Once the final prototype design is determined and installed in the field, the burner may undergo several subsequent modifications. A good example of this is the John Zink PSMR burner. Developed in the early 1990s as a low NO_x round-flame burner, it has become the industrial standard of today. However, the basic design has undergone several iterations to get to where it is today. During this development period, CFD has also become a common tool used to evaluate and optimize burner design.

Today, CFD is routinely used to investigate potential burner designs in conjunction with experimental testing. Using CFD to expand and understand test results, as well as using CFD to direct future testing to focus on key issues, is the most productive way of shortening the design cycle. Taken together, testing and CFD modeling have helped shorten the development cycle by an estimated 20%. In addition, CFD modeling has helped reduce warranty work once a new burner is installed in the field. This helps reduce expensive rework at the customer's facility, which helps maintain good will with customers.

5.2.3 CHOOSING THE DOMAIN

One of the key issues in developing a CFD model for an industrial burner is to select the appropriate domain for the analysis. A full-process furnace used in the hydrocarbon refining industry may include hundreds of burners of various designs and configurations (see [Figure 5.2](#), Reference 6). To reduce the computational demand for analyzing such a system in sufficient detail (see below), the recommended approach utilizes symmetry planes to reduce the overall computational domain. An example would be to use the natural symmetry in the furnace shown and only analyze half of the complete volume (see [Figure 5.3](#)⁶).

A simplified burner model can be used to reduce the overall complexity of the CFD model. Here, experience has shown that a model must resolve each fuel jet to capture the governing physics that result in flame shape and spread inside a furnace. Figure 5.4⁶ shows a typical burner model for

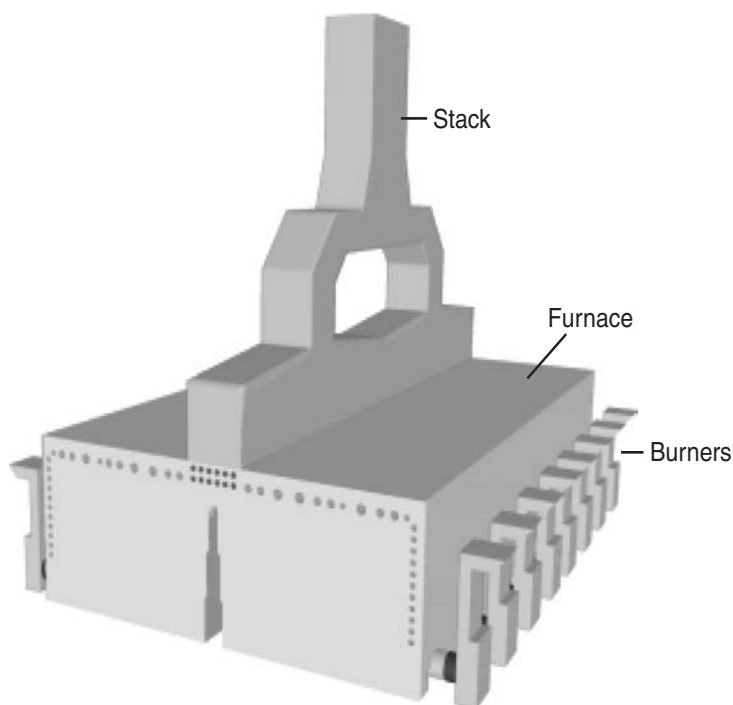


FIGURE 5.2 Outside view of a typical industrial furnace geometry with existing burners installed on furnace side with convection section and stack on top.

one of John Zink’s multi-fuel burners used in the furnace shown in Figures 5.3 and 5.4. Note that enough detail is included in each fuel tip to accurately approximate the respective flow dynamics around the refractory tile. In all cases, experience is required to understand what level of detail is required for a specific burner/furnace system. In some cases, one can avoid analyzing the full system geometry. On the other hand, one should include as much of the domain as is practically reasonable given available computer resources.

5.2.4 SELECTING BOUNDARY CONDITIONS

Before a CFD simulation is possible, the user must define the conditions around the entire boundary of the system. This means one must define what goes into and out of the system, as well as what conditions exist at the system walls. In general, these “boundary conditions” must provide adequate information to solve the governing second-order, elliptic partial differential equations describing the conservation of mass, momentum, and energy. This form of equation requires one boundary condition per order per equation. Thus, for the three momentum equations, one would need to specify two boundary conditions per equation. Typically, this would include inlet velocity and either the velocity at the wall or the centerline velocity (for axisymmetric geometries). The inlet velocity is a fixed or “Dirichlet”-type boundary condition. The wall condition would also be a fixed boundary condition while the centerline condition would be a flux or “Neumann”-type boundary condition. The same is true for the mass and energy equations. In general, the following boundary conditions are required to fully specify a system:

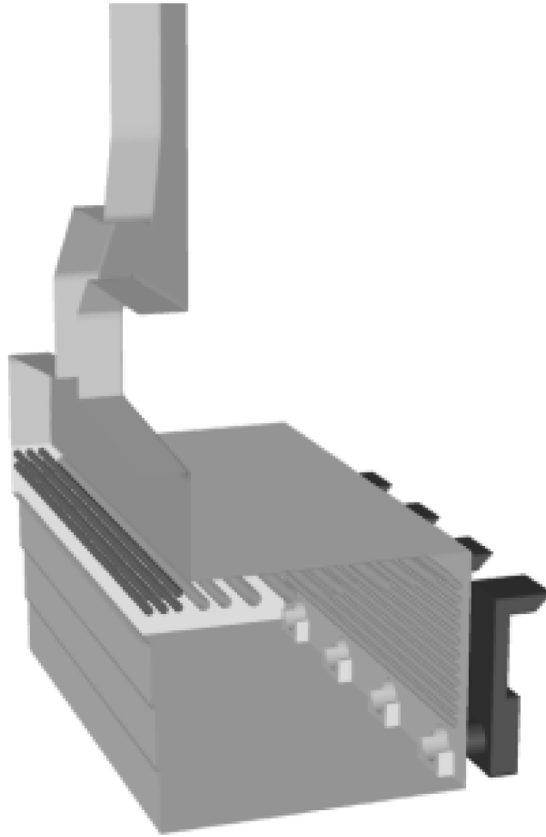


FIGURE 5.3 After applying natural symmetry planes, this view shows the actual section (1/4 entire furnace/ burner system) to be modeled.

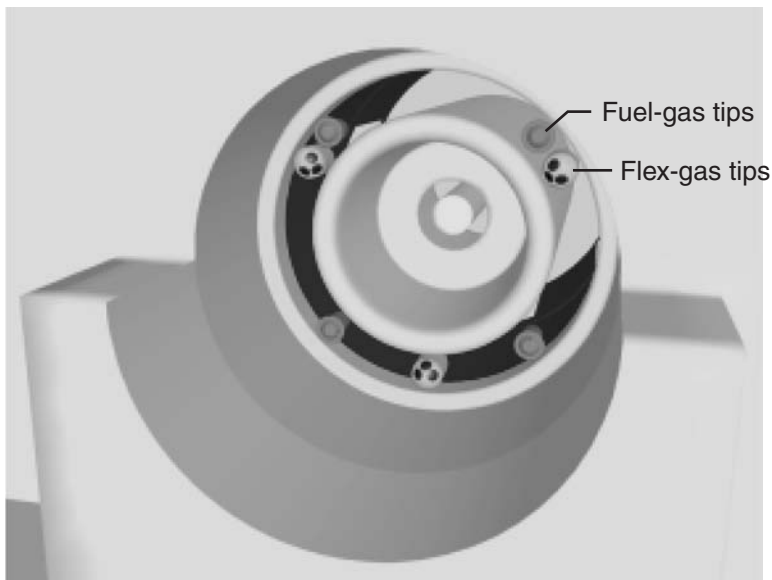


FIGURE 5.4 Detailed front view of one of John Zink's multi-fuel burners. Note the fuel-gas tips shown adjacent to the flex-gas tips. Note the local detail included in the fuel tips of this burner model.

1. All inlet streams must be characterized. Specific information should include mass flow rates, compositions, pressures, and temperatures. When a stream is composed of gas/liquid (as in atomization) or gas/solid (as in pulverized coal combustion), the relative percentage of each phase would also be required, as would information on droplet or particle size distribution.
2. Standard operating conditions for the reactor or furnace should be specified. This includes the system pressure, wall thermal properties such as thermal conductivity, construction materials (e.g., refractory, bare steel, water wall), refractory thickness, external wall temperatures, and internal wall radiative properties (e.g., surface emissivity and in some cases surface roughness).
3. Outlet conditions can also be set, including a flux condition for velocity (parallel exit flow, which means no velocity gradients at the exit). An exit pressure condition may be set as well.

5.2.5 NUMERICAL ANALYSIS AND COMPUTATIONAL MESHES

Closed-form mathematical relationships (either of a partial differential or integral form) that describe the general conservation equations are central to the simulation of engineering problems. These systems of nonlinear equations may have bifurcated solutions for a particular domain and set of boundary conditions. Simple analytical solutions to these theoretical relationships are most often intractable for anything other than very simple geometries and, therefore, offer very little practical value. To obtain a solution, the mathematical expressions must be reduced to simplified but analogous discrete algebraic equations that require solution at discrete points representing specific sub-volumes of the overall computational domain.⁷ This replacement of “continuum” equations with those utilizing discrete numbers is referred to as discretization. Hence, the simulation becomes possible with the associated computational load related to the number of discrete points where values of conserved scalars are calculated in the general domain. These discrete points are referred to as grid points and the collection of grid points represents a computational mesh. Once the calculation within the domain is broken down into these discrete points, the closed-form of the mathematical expressions can be expressed as a series of algebraic equations. This allows for numerical solution of the various flow-field variables at each of the grid points. For definition, if the partial differential equation form of the conservation relationships is used, the resulting methodology is known as a finite difference scheme. If the integral form of the equations is used, the resulting technique is known as the finite volume method. A third form of discretization, known as finite elements, also exists but is not part of this discussion.

The arrangement of the discrete points mentioned above is referred to as the computational mesh or grid and provides a segmented approximation of the system geometry to be analyzed or simulated by a CFD model. The density or number of grid points in any one portion of the computational domain should be sufficient to resolve the important geometric features, as well as capture the significant physics (e.g., boundary layer, shear layer, recirculation zone, reaction layer, etc.). The density of grid points typically varies from one region of the domain to another to help resolve these features. However, care must be taken to not take too large a jump in grid spacing from one section to another to maintain numerical stability. Typical expansion/contraction ratios for cells are in the range of 0.8 to 1.2. Too large a difference in neighboring grid spatial dimensions can lead to computational inaccuracy and numerical instability.

A couple of approaches are available to describe the geometry of a particular domain:⁸

1. Use regularly spaced or structured grid points with an orthogonal coordinate system.
2. Use an unstructured mesh with a boundary or body-fitted coordinate system.

Each approach handles the presence of curved surfaces differently. In the structured grid approach, the mesh is composed of hexahedral elements that simulate curved surfaces by allowing for a series of stair-steps to approximate the curve. Resolution of the curved surface depends on the

number of cells in this region. The three-dimensional elements retain their hexahedral shape but result in a curved, jagged surface. Increasing the refinement of the grid along these surfaces can reduce the impact this might have on the overall flow-field calculations; however, this will subsequently increase the computational load as cell refinements in one region of the grid are propagated into regions away from the curved surface. Another structured grid-based technique allows regularly shaped hexahedral cells to be “sliced” or “trimmed” at curved boundaries, resulting in element faces at the boundary that are irregularly shaped. Special algorithms then treat communication of flow-field information across these faces.

The use of body-fitted or unstructured grids allows for regularly shaped boundary surfaces to be more closely approximated by the grid elements that follow the curved surface using elliptic curvature. This approach reduces to a structured grid when all the domain elements are hexahedral and the edges of elements form continuous mesh lines. Unstructured grids allow the combined use of a wide variety of element shapes (e.g., tetrahedrons, pyramids, prisms, hexahedrons, and polyhedrons). This allows for the greatest amount of flexibility in approximating complex geometries.

Generally, it is acknowledged that greater grid densities (i.e., larger number of elements describing the domain) produce more accurate simulation results. However, in the particular case of unstructured grids, the quality of the mesh, which is directly related to the ability of a particular mesh to provide a reliable, robust solution, is also related to the shape of individual elements. Long, thin elements, as well as single faces with highly skewed angles or a high degree of curvature, can result in substantial errors in the calculation and cause the overall model to diverge in regions where these “bad” elements are used.

5.3 BUILDING BLOCKS OF CFD-BASED COMBUSTION MODELS

The mathematical simulation of turbulent combustion in industrial burners has been recognized as a difficult problem not only due to the numerical challenges associated with solving the differential equation set, but also the challenge of physically describing the important chemical and physical processes, such as chemistry–turbulence interactions, turbulent mixing, etc. Commercial CFD codes rely on available mathematical technology to combine knowledge of fluid mechanics with a reasonable approach to the reaction (combustion) processes. Care must be taken to maintain the scope of the simplifying approximations on an equivalent level.

CFD codes have been developed to address nonreacting flow systems, gaseous diffusion combustion, pulverized coal-fired systems, entrained flow gasification, droplet combustion, and slurry combustion or gasification. These codes typically utilize general coordinate systems to capture complex geometries common in industrial burner designs. Variation of properties can be included when deemed necessary. Symmetry planes can be used to simplify large-scale systems to reduce the computational demands required to simulate full furnaces. Models predict mean gas field properties for general three-dimensional, steady-state (and unsteady in special cases) turbulent flames (i.e., local velocity, temperature, density, and species composition). For special cases, multiphase combustion (e.g., gas/particle, gas/oil, etc.) is required. In these cases, particle/droplet properties are also computed, such as coal burnout, particle or droplet velocity, and temperature. [Figure 5.5](#) illustrates the various sub-models incorporated into a comprehensive CFD-based computer code used to simulate the relevant processes occurring inside industrial burners.

5.3.1 TURBULENT FLUID MECHANICS

5.3.1.1 Problem of Closure

The governing equations of fluid mechanics are derived from three physical laws: conservation of mass, conservation of momentum, and conservation of energy. If solving for additional species, such as required for a combustion model, conservation equations for the additional species are also required.

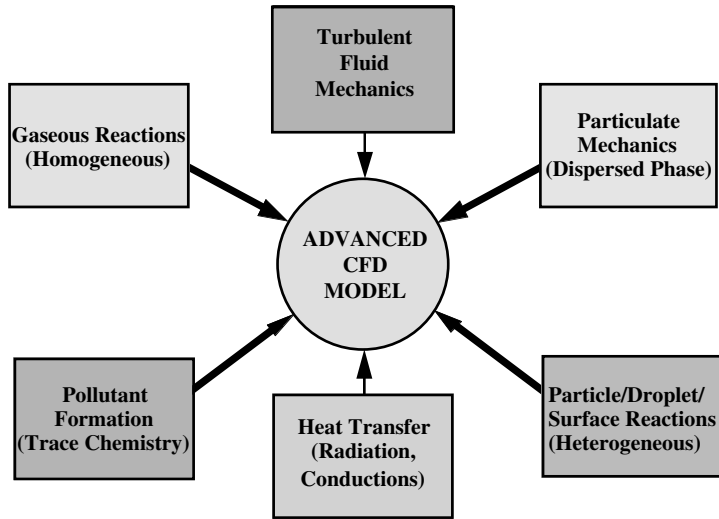


FIGURE 5.5 Typical sub-model components in comprehensive CFD code. Physical sub-models simulate specific physics involved in combustion processes that occur in industrial burners.

A conservation equation for each specie can be derived by performing a mass balance for that specie. Equations 5.1, 5.2a, 5.2b, and 5.3 show the continuity (conservation of mass), momentum equations, and species transport equations in Cartesian tensor form, respectively.

$$\frac{\partial(\rho u_i)}{\partial x_i} = 0 \quad (5.1)$$

$$\frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g \quad (5.2a)$$

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \frac{\partial u_k}{\partial x_k} \delta_{ij} \quad (5.2b)$$

$$\frac{\partial(\rho \Phi u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\Gamma_\Phi \frac{\partial \Phi}{\partial x_j} \right) + S_\Phi \quad (5.3)$$

where:

τ_{ij} = viscous stress tensor

δ_{ij} = Kronecker delta ($\delta_{ij} = 0$, when $i \neq j$)

μ = molecular viscosity of the fluid

λ = coefficient of bulk viscosity of the fluid

Φ = transported variable (chemical species, enthalpy, etc.)

Γ_Φ = molecular diffusion coefficient for Φ

S_Φ = source term for Φ

ρ = density of the fluid

P = static pressure

g = acceleration of gravity

White⁹ provides background information on the coefficient of bulk viscosity, and it remains a controversial quantity. Wilcox¹⁰ advises setting $\lambda = -\frac{2}{3}\mu$, which he says has been proven correct for monatomic gases, but White states that the kinetic theory actually assumes rather than proves this. Whatever the case, Wilcox states that the bulk viscosity of $\lambda = -\frac{2}{3}\mu$ is generally used in standard computational fluid dynamic (CFD) codes.

There are several characteristics that can be used to describe turbulence, as given by Tennekes and Lumley.¹¹ Turbulence flows are random and irregular, which makes deterministic methods very difficult. Turbulent diffusivity is almost always much larger than molecular diffusivity. This results in much higher rates of momentum, heat, and mass transfer for turbulent flows, as opposed to laminar flows. Turbulence is characterized by three-dimensional vorticity fluctuations. Turbulent vorticity fluctuations could not be maintained without vortex stretching, and vortex stretching does not occur in two-dimensional flows. Therefore, by nature, all turbulent flows are three-dimensional — turbulence is dissipative. Viscous shear stresses convert the turbulent kinetic energy of the fluid into internal energy. Therefore, turbulence needs a continuous supply of energy to replace the losses of viscous dissipation. Finally, turbulence occurs over a continuum and is governed by the continuum equations of fluid mechanics. The smallest turbulent scales are ordinarily much larger than molecular scales.

As mentioned, randomness and irregularity characterize turbulence. To characterize turbulence mathematically, quantities such as velocities, pressures, temperatures, etc. are expressed as having mean and fluctuating components. From a computational point of view, it is desirable to compute averaged quantities and, therefore, it is desirable to express the governing equations (Equations 5.1 through 5.3) in terms of average quantities. To do this, instantaneous values of quantities are put into the governing equations, and then the governing equations are averaged in some fashion. Because Equations 5.2 and 5.3 are nonlinear, averaging the equations results in unknown quantities ($\overline{u'_i u'_j}$ and $\overline{u'_i \Phi'}$). These unknown quantities must then be modeled. For most engineering applications, a semi-empirical turbulence model is used to compute the unknown quantities.

5.3.1.2 Favre and Reynolds Averaging

Turbulent transport occurs in the momentum, energy, and specie transport equations, and a turbulence closure model is required to correctly model the turbulent transport terms in each equation. At this point, the governing equations (Equations 5.1 through 5.3) plus any additional transport equations should be averaged in some fashion to determine the transport terms resulting from turbulence. It is assumed that the dependent variables in the governing equations are comprised of an average term plus a fluctuating term. There are two methods for averaging the equations: Reynolds averaging and Favre averaging. Wilcox² provides a good review of both methods. Favre averaging is applicable when compressibility is an important issue. Morkovin¹² hypothesized that the effects of density fluctuations on turbulence are insignificant, provided that the fluctuations are small relative to the mean density, $\frac{\rho'}{\bar{\rho}} \ll 1$. It is clear that for flows with combustion and/or significant heat transfer, the density fluctuations are not small relative to the mean density. Therefore, for modeling flows with combustion, Favre averaging is clearly preferable, as confirmed by Wilcox. Favre averaging of velocity is defined by Equation 5.4:

$$\tilde{u}_i = \frac{1}{\bar{\rho}} \lim_{T \rightarrow \infty} \int_{T-i}^{T+i} \rho u_i d\tau \quad (5.4)$$

Averaging of other transported variables, such as enthalpy or a chemical species, is done in a similar fashion to Equation 5.4. It should be noted for Favre averaging that the fluctuating velocities are denoted by double primes, $u_i = \tilde{u}_i + u''_i$; and, because products of velocity and density are

averaged, $\overline{u_i''} \neq 0$, but $\overline{\rho u_i''} = 0$. The Favre averaged mean continuity and momentum equations are given by Equations 5.5 and 5.6.

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial x_i} = 0 \quad (5.5)$$

$$\frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = -\frac{\partial\bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\bar{\tau}_{ij} - \overline{\rho u_j'' u_i''} \right) + \bar{\rho} g \quad (5.6)$$

The Favre-averaged Reynolds stress tensor is given by $\tau_{ij} = -\overline{\rho u_j'' u_i''}$.

5.3.1.3 Turbulence Models

There are generally four types of turbulence models commonly used in engineering practice:

1. Algebraic models
2. One-equation models
3. Two-equation models
4. Second-order closure models

Wilcox² and Rodi¹³ provide good reviews of various methods of turbulence modeling. Most of the models that fall into one of the first three categories have an underlying commonality; that is, the Boussinesq approximation. The Boussinesq approximation assumes that the Reynolds-stress tensor is proportional to the mean strain-rate tensor for every location in a turbulent flow. The constant of proportionality between the Reynolds-stress tensor and the mean strain-rate tensor is the eddy viscosity (μ_T).

5.3.1.3.1 Algebraic Models

Many algebraic models calculate an eddy viscosity from the Prandtl mixing-length hypothesis, given by Equation 5.7.

$$\mu_T = \rho(l_m^2) \left| \frac{\partial U}{\partial y} \right| \quad (5.7)$$

where:

l_m = mixing length
 U = mean velocity

Algebraic models are not very general because the mixing length depends on the flow scenario (i.e., jet, boundary layer, pipe flow, etc.). Therefore, an expression for the mixing length must be obtained for each type of flow when using an algebraic model.

5.3.1.3.2 One- and Two-Equation Models

One-equation and two-equation models attempt to overcome the difficulties with the Prandtl mixing-length hypothesis by solving transport equations for quantities that are related to the type of flow. In the above-mentioned algebraic model, there is a direct link between the fluctuating velocity scale and the mean velocity gradients, as shown by Equation 5.7. In one-equation and two-equation models, the link between the fluctuating velocity scale and the mean velocity gradients is found by solving one or more transport equations. Wilcox² describes two, more recent one-equation turbulence models that appear to show promise. The Baldwin-Barth¹⁴ model employs a transport equation for the turbulent Reynolds number and the Spalart-Allmaras¹⁵ model employs a transport equation for the eddy viscosity.

Prandtl chose the turbulent kinetic energy as the basis for a turbulent velocity scale shown in Equation 5.8. The eddy viscosity can be computed using the Kolmogorov-Prandtl expression given by Equation 5.9.

$$k = \frac{1}{2} \overline{u'_i u'_i} = \frac{1}{2} (\overline{u'^2} + \overline{v'^2} + \overline{w'^2}) \quad (5.8)$$

$$\mu_T = C_1 \rho \sqrt{kl} \quad (5.9)$$

where:

- k = turbulent kinetic energy
- l = turbulence length scale
- C_1 = constant of proportionality

Wilcox² provides a derivation of the Reynolds-stress equation, obtained by taking moments of the Navier-Stokes equation. The Reynolds-stress equation is a tensor equation and, by taking the trace of it, a transport equation is obtained for turbulence kinetic energy. This transport equation for the turbulence kinetic energy forms the basis for a number of one- and two-equation turbulence models. The turbulence kinetic energy transport equation has various terms that have been given physical interpretations. Included in the terms is a dissipation term (ϵ), which represents the rate at which turbulence kinetic energy is converted to thermal internal energy. From the turbulence kinetic energy equation, ϵ is the product of the viscosity and the square of the fluctuating vorticity. Therefore, based on dimensional arguments, the dissipation (ϵ) should be related to the turbulence kinetic energy and length scale as shown in Equation 5.10:

$$\epsilon = \frac{C_2 k^{3/2}}{l} \quad (5.10)$$

where C_2 = constant of proportionality.

5.3.1.3.3 k - ϵ Turbulence Model

Perhaps the most commonly used turbulence model for practical flow problems is the k - ϵ model. The earliest developments related to the k - ϵ model were by Chou,¹⁶ Davidov,¹⁷ and Harlow and Nakayama.¹⁸ The most well-known paper on the k - ϵ model is that of Jones and Launder,¹⁹ which according to Wilcox² has almost reached the status of the Boussinesq and Reynolds papers within the turbulence modeling community. The k - ϵ model is based on the turbulence kinetic energy transport equation discussed above, and a second transport equation for the dissipation rate. The equation for the dissipation rate (ϵ) is derived by taking a moment of the Navier-Stokes equation using the fluctuating vorticity. The resulting equation is a relatively complicated equation, which Wilcox² states needs “drastic surgery” to make it practical. The Standard k - ϵ model is shown below by Equations 5.11 through 5.13:

$$\rho U_j \frac{\partial k}{\partial x_j} = \tau_{ij} \frac{\partial U_i}{\partial x_j} - \rho \epsilon + \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_T}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right]; \quad \text{Turbulence Kinetic Energy} \quad (5.11)$$

$$\rho U_j \frac{\partial \epsilon}{\partial x_j} = C_{\epsilon 1} \frac{\epsilon}{k} \tau_{ij} \frac{\partial U_i}{\partial x_j} - C_{\epsilon 2} \rho \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_T}{\sigma_k} \right) \frac{\partial \epsilon}{\partial x_j} \right]; \quad \text{Dissipation Rate} \quad (5.12)$$

$$\mu_T = \frac{C_\mu \rho k^2}{\epsilon}; \quad \text{Eddy Viscosity} \quad (5.13)$$

The eddy viscosity relationship (Equation 5.13) follows from combining Equations 5.9 and 5.10. The empirical closure coefficients given by Wilcox² are shown below:

$$C_{\epsilon 1} = 1.44, \quad C_{\epsilon 2} = 1.92, \quad C_{\mu} = 0.09, \quad \sigma_k = 1.0, \quad \sigma_{\epsilon} = 1.3 \quad (5.14)$$

The optimal closure coefficients will vary somewhat, depending on the application and what investigators have found the coefficients should be to agree with experimental results. Therefore, the coefficients shown in Equation 5.14 are not universally optimal, and any CFD results obtained using the k - ϵ turbulence model should be closely scrutinized.

5.3.1.3.4 k - ϵ Turbulence Model Boundary Conditions

Establishing boundary conditions for the k - ϵ turbulence model results from an order of magnitude analysis of the boundary layer momentum equation in the log layer. The log layer is an overlap region between the viscous sublayer and the defect layer, where the law of the wall applies. An order of magnitude analysis of the boundary layer momentum equation suggests that convection, pressure gradient, and molecular diffusion terms can be neglected. Applying these simplifications to the transport equations for k and ϵ (Equations 5.13 and 5.14) results in relations for k and ϵ at the boundaries, which are referred to as wall functions. The standard wall functions are given by Equations 5.17 and 5.18:

$$k = \frac{u_{\tau}^2}{\sqrt{C_{\mu}}}: \quad \text{Standard Wall Functions for } k \quad (5.17)$$

$$\epsilon = \frac{k^{3/2} C_{\mu}^{3/4}}{\kappa y}: \quad \text{Standard Wall Functions for } \epsilon \quad (5.18)$$

where:

u_{τ} = friction velocity

$$u_{\tau} = \sqrt{\tau_w / \rho}$$

τ_w = wall shear stress

κ = Kármán constant ($\kappa \approx 0.4$)

y = distance measured normal from the wall

The wall functions (Equations 5.15 and 5.16) are applied to the node adjacent to the wall, which should lie within the log layer region. The law of the wall equation (Equation 5.19) is used to find the friction velocity (u_{τ}) at the node adjacent to the wall, and then the wall functions are used to specify k and ϵ :

$$U = u_{\tau} \left[\frac{1}{\kappa} \ln \left(\frac{u_{\tau} y}{\nu} \right) + B_1 \right] \quad (5.19)$$

where:

U = mean velocity

ν = kinematic viscosity

B_1 = constant

If the surface is smooth, Equation 5.19 should be used; however, if the surface is not smooth, an equation equivalent to Equation 5.19 is given by Equation 5.20, and was developed by Nikuradse.

Equations 5.19 and 5.20 are given in most engineering fluid mechanics texts, such as Roberson and Crowe.²⁰

$$U = u_{\tau} \left[\frac{1}{\kappa} \ln \left(\frac{y}{k_s} \right) + B_2 \right] \quad (5.20)$$

where:

k_s = surface roughness height

B_2 = constant

Wilcox² notes that numerical solutions are sensitive to the location of the node adjacent to the surface and recommends using near-wall grids. Another potential problem with using wall functions is that theoretically they do not apply for flows that separate from the wall. Finally, Wilcox points out that the standard k - ϵ model with standard wall functions does not perform well for boundary layers with adverse pressure gradients. Kim and Choudhury²¹ have proposed modifications to the standard k - ϵ wall functions to account for adverse pressure gradient.

5.3.1.4 Other Turbulence Modeling Approaches

The vorticity that characterizes turbulent flow has a large range of length and time scales that can exist in relatively close proximity to one another. When Reynolds-averaged Navier-Stokes (RANS) equations are utilized to simulate turbulent flow, all of the turbulent fluctuations are modeled using algebraic approximations rather than directly calculated, which results in a significant reduction in computational requirements. Various other approaches exist that are used to compute the turbulent relationships that exist in flowing systems. Two of the more popular methodologies are known as direct numerical simulation (DNS) and large-eddy simulation (LES).²²

DNS looks at solving the Navier-Stokes equations over the complete range of time and length scales present in a particular system. Perhaps the greatest issue with DNS is that the computational domain must be large enough to accommodate the largest length scales present, with a grid small enough to allow for resolution of the smallest scales where kinetic energy dissipation occurs. This criterion ensures that the number of grid points required to solve a problem of practical size will be quite large as compared to more conventional RANS-type calculations. By way of example, the number of grid points required in each direction of a three-dimensional calculation is proportional to $Re^{3/4}$, the Reynolds Number based upon the magnitude of the velocity fluctuations and the integral scale. Hence, for $Re = 10^6$ (which is not unusual for flows in typical engineering systems), the resulting grid requirement for a three-dimensional simulation would be on the order of 10^{15} . While the results of such calculations would contain very useful information, the current limits of available computer hardware make routine use of this approach to solve practical engineering problems prohibitive. In addition to the large grid requirements, the time scales required for this approach are constrained to very small time steps to capture the fluctuations at the very small end of the range, which further increases the computational load. Currently, DNS is used to solve small, low-Reynolds number flow circumstances based upon simple geometries.

Large-eddy simulation (LES) is positioned between DNS and the RANS approaches. This approach separates the range of length scales (eddies) into two groups. The first consists of relatively large eddies that can be numerically simulated and represent the majority of the turbulent energy. These are generally constrained more by boundary conditions and domain geometries. The second group is comprised of small eddies, which are more influenced by molecular viscous forces. The second group tends to be more isotropic and, therefore, it is easier to justify the use of numerical approximations to model them. Hence, the simulation rationale focuses on the direct resolution of the large eddies and filtering out eddies smaller than some lower limit or smaller than the local grid resolution and allowing them to be modeled. A significant issue related to the utilization of the LES

approach is the “communication” that must occur between the simulation of the two groups as large eddies degrade into smaller ones. The impact this has on grid requirements is that much coarser grids than are required by DNS can be used, although the grid requirements for LES are still much greater than for the Reynolds-/Favre-averaged approaches. Recent improvements in computer hardware performance have allowed this approach to be considered for engineering analysis.

5.3.2 HOMOGENEOUS CHEMISTRY

In general, the mathematical modeling of combustion processes includes the simulation of several physical and chemical processes in reacting flows. The modeling of any reacting or combustion process in a turbulent flow field can, at the very least, be called challenging. What can be observed as a flame is the result from interaction of convection and molecular diffusion with many chemical reactions and very small length and time scales. In general, a differentiation has to be made for types of flames as there are:

- Premixed flames
- Partially premixed flames
- Nonpremixed or diffusion flames

Depending on the Reynolds, Damkoehler, and Karlovitz numbers, a further separation has to be made in laminar, turbulent, wrinkled, corrugated flames, and homogeneous reaction zones.²³ Because almost every flow regime in a technical combustion application is highly turbulent, the laminar flame modeling will not be included in this discussion. Further information on laminar reaction systems can be found in Kee,^{24,25} Glarborg,²⁶ and Rogg.^{27–29}

The type of turbulent flame determines the combustion sub-model to be used. For premixed flames, the models available include:

- Progress variable C
- Transport equation for the flame front G
- Eddy breakup (EBU), eddy dissipation combustion model (EDX), and the eddy dissipation concept (EDC)
- Partially premixed presumed pdf model with equilibrium chemistry

For nonpremixed combustion, the models available include:

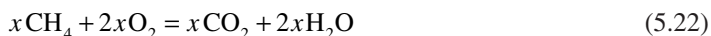
- Presumed pdf with equilibrium chemistry (adiabatic and nonadiabatic)
- Presumed pdf with finite rate chemistry (flamelet model)
- Eddy dissipation and eddy dissipation combustion model

The general form for a reaction with educts A and B and the products C and D can be written as:



where ν is the stoichiometric coefficient.

For example, in methane combustion, the global one-step formulation would be:



The reaction rate can formally be written as the product of the reaction rate coefficient and all participating species:

$$r_i = \left(\frac{dc_i}{dt} \right) = k c_1^{a_1} c_2^{a_2} c_3^{a_3} \dots c_N^{a_N} \quad (5.23)$$

with the reaction coefficient k , the reaction order a , and the species c_i , where the concentration of each species i is defined as:

$$c_i = \frac{\rho_i Y_i}{M}, \quad (5.24)$$

with M as the mean molar mass of the mixture. The rate coefficient k can be written in general form as:

$$k = AT^m e^{\left(-\frac{E_A}{RT}\right)}, \quad (5.25)$$

with R as the gas constant (8.3143 kJ/mole-K). The parameters here are the pre-exponential Arrhenius factor A , the temperature exponent m , and the activation energy E_A .

The final formulation for a concentration change of species i , over all elementary reactions k , can be formulated as:

$$\frac{\partial c_i}{\partial t} = \sum_{k=1}^M (v''_{i,k} - v'_{i,k}) (AT^a)_k \exp\left(-\frac{E_k}{RT}\right) \prod_{j=1}^N \left(\frac{\rho Y_j}{W_j}\right)^{v'_{j,k}} \quad (5.26)$$

or written as reaction rate:

$$\frac{\partial c_i}{\partial t} W_i = \dot{Y}_i = W_i \sum_{k=1}^K v_{ik} r_k \quad (5.27)$$

And, finally, the additional source term for the equation for energy conservation. The total released energy can be written as the sum of the product of reaction enthalpy H and the concentration change of species i :

$$q_r = \sum_{k=1}^K q_k = \sum_{k=1}^K -\left(\frac{\Delta H_k}{v_{i,k}}\right) \cdot \left(\frac{dc_i}{dt}\right)_k = -\sum_{i=1}^N h_i \omega_i \quad (5.28)$$

The equation governing species transport is:

$$\frac{\partial}{\partial t} \rho Y_i + \nabla \cdot (\rho \bar{u} Y_i) = \nabla \cdot (\rho D_i \nabla Y_i) + \dot{Y}_i, \quad (5.29)$$

where $\dot{Y}_i$ is the source term of the species i . The determination of that source term can be done according to aforementioned equations, or due to the complexity and number of involved species using approaches, which reduce the computational effort — as, for example, the EBU, EDX, and EDC models.

The eddy breakup model (EBU) was developed by Spalding³⁰ for the calculation of turbulent, premixed flame with irreversible one-step reaction. The assumption was that the rate of reaction is totally controlled by dissipation of eddies either containing unburned fuel or burned hot gases. The reaction rate of the unburned mixture $\dot{Y}_F$, as used in Equation 5.29, is determined by the decay rate of these eddies:

$$\dot{Y}_{F,\text{eddy}} = C(1-\tau)\rho \left| \frac{du}{dy} \right|, \quad (5.30)$$

following the mixing length hypothesis.

To estimate the actual rate of fuel consumption, we have to take into account the kinetically controlled reaction rate as defined by:

$$\dot{Y}_{F,\text{kin}} = AY_F Y_{\text{O}_2} \exp(-E_A/RT), \quad (5.31)$$

where A is the pre-exponential factor, E_A is the activation energy, and R is the universal gas constant. The actual rate of fuel consumption can be determined by:

$$\dot{Y}_{F,\text{actual}} = \frac{1}{\frac{1}{\tau \dot{Y}_{\text{kin}}} + \frac{1}{\dot{Y}_{\text{eddy}}}} \quad (5.32)$$

The major drawback of this approach is the assumption of homogeneous distribution and perfect mixing of fuel and oxidant. The formulation would only be valid for a turbulent, premixed flame with homogeneous distribution of fuel/air and flue gas pockets.

A development of the EBU model is the eddy dissipation combustion model (EDX) formulated by Magnussen.³¹ He takes into account the unmixedness of fuel and oxidizer and postulates that the rate of combustion will be determined by the turbulent intermixing of fuel and oxygen eddies on a molecular scale; or, in other words, by dissipation of these eddies. The reaction rate can be written in general form as:

$$\dot{Y}_i = C \bar{Y}_i \frac{\epsilon}{k}, \quad (5.33)$$

where C is a constant depending on the structure of the flame, and $\bar{Y}_i$ is the time-averaged concentration. This approach acknowledges the distribution and unmixedness of fuel oxidizer and hot products, and is therefore also valid for the calculation of nonpremixed flames. The actual reaction rate is determined by the minimum of the following criteria:

1. The reaction rate is determined by the concentration of fuel:

$$\dot{Y}_F = A \bar{Y}_F \frac{\epsilon}{k}, \quad (5.34)$$

where $A = 4.0$ and $\bar{Y}_F$ is the time-averaged fuel concentration.

2. The reaction rate is determined by the concentration of oxygen:

$$\dot{Y}_{\text{O}_2} = A \frac{\bar{Y}_{\text{O}_2}}{r_{\text{O}_2}} \frac{\epsilon}{k}, \quad (5.35)$$

with $\bar{Y}_{\text{O}_2}$ the local mean oxygen concentration and r_{O_2} the stoichiometric oxygen requirement.

3. The reaction rate is limited by the presence of hot products:

$$\dot{Y}_{\text{Pr}} = AB \frac{\bar{Y}_{\text{Pr}}}{1 + r_{\text{O}_2}} \frac{\epsilon}{k}, \quad (5.36)$$

with $A = 4.0$, $B = 0.5$, $\bar{Y}_{\text{Pr}}$ the local mean product concentration, and r_{O_2} the stoichiometric oxygen requirement.

The disadvantage of this approach is the fact that global reactions still have to be used. An extension of these models is the eddy dissipation concept (EDC).³² This model is still based on eddy dissipation along the turbulent energy cascade, but differentiates between areas of chemical reaction, the so-called fine structure region, and their surrounding nonreactive regions. These fine structures are situated at the end of the turbulent energy cascade. Their length scale is that of eddies in the Kolmogorov scale, where the species are mixed on a molecular level and react as the energy level meets their respective activation energy. The chemistry inside these fine structures can be treated as a perfectly stirred reactor.

This model takes into account that the dissipation is not homogeneously distributed in the computational domain, but takes place mainly in strained areas, the separating area from the reacting and nonreacting volumes. Magnussen proposes the following definition for the mass fraction contained in these fine structures:

$$\gamma = (u^*/u')^3, \quad (5.37)$$

where u^* is the characteristic velocity of the fine structure and u' is the turbulent velocity. Any mass transfer from surrounding nonreacting fluid into these fine structures follows the expression:

$$\dot{m} = 2 \frac{u^*}{L^*} \gamma^*, \quad (5.38)$$

where the characteristic velocity u^* and the characteristic length L^* can be expressed by:

$$u^* = 1.74(v\varepsilon)^{1/4} \quad (5.39)$$

and

$$L^* = 1.43v^{3/4}/\varepsilon^{1/4}, \quad (5.40)$$

where v is the kinematic viscosity and ε is the rate of dissipation of turbulent energy. Assuming isotropic turbulence, the mass fraction of the fine structure and the mass transfer between the fine structure and the surrounding can be written as:

$$\gamma^* = 9.7 \left(\frac{v\varepsilon}{k^2} \right)^{3/4} \quad (5.41)$$

and for the mass transfer:

$$\dot{m} = 23.6 \left(\frac{v\varepsilon}{k^2} \right)^{1/4} \frac{\varepsilon}{k} \quad (5.42)$$

If we assume that the reactions inside the fine structures are infinitely fast, the mass transfer between the surrounding fluid and the fine structure itself limits the reaction rate. Thus, the rate of reaction can be written as depending on the mass transfer:

$$\dot{Y}_F = 23.6 \left(\frac{v\varepsilon}{k^2} \right)^{1/4} \frac{\varepsilon}{k} \bar{Y}_{\min}, \quad (5.43)$$

where $Y_{\min}$ is the smallest concentration of Y_F or Y_{O_2} , limiting the reaction rate. It cannot be assumed that all fine structures are on the same temperature level, so the concentration of hot products must be taken into account. A correction factor:

$$\chi = \frac{\bar{Y}_{Pr}/(1+r_{O_2})}{\bar{Y}_{Pr}/(1+r_{O_2}) + Y_F} \quad (5.44)$$

is introduced and the final expression for the reaction rate becomes:

$$\dot{Y}_F = 23.6 \left(\frac{\nu \epsilon}{k^2} \right)^{1/4} \frac{\epsilon}{k} \chi \bar{Y}_{\min} \quad (5.45)$$

The main advantage of this approach is the possibility of including elementary reactions to describe the kinetics within the fine structures. Because any given set of reactions has only to be solved within these small regions, the computational time can be reduced significantly. Another method for the calculation of reacting flows is the mixture fraction approach.

5.3.2.1 Mixture Fraction Approach for Equilibrium or Nonequilibrium Chemistry

For nonpremixed or diffusion flames, one approach is using the presumed probability density function (ppdf) model, with or without equilibrium chemistry. Assuming that the chemistry is one-step, infinitely fast and irreversible (equilibrium chemistry), with equal diffusivities, this model can be interpreted as a zero-dimensional, perfectly stirred reactor with infinity residence time. The input for the PSR is given by the local value of the mixture fraction. Because the enthalpy is fixed by the mixture fraction, the temperature can be obtained using:

$$h_i = h_{f,i}^0 + \int_{T_0}^T c p_i(T) dT, \quad (5.46)$$

and

$$h = \sum Y_i h_i \quad (5.47)$$

with T_0 as reference temperature and $h_{f,i}^0$ the enthalpy of formation of species i . Values for $h_{f,i}^0$ can be found in Table 5.2. The results of these calculations can be stored in look-up tables and used afterward from the CFD code to determine the concentration distribution within the computational domain. This approach is often applied to turbulent flames using a presumed pdf for the mixture fraction. The schematics for an adiabatic calculation are shown in Figure 5.6.^{33,34}

The mixture fraction Z is defined as an element mass fraction of matter originating from the fuel stream. It is a so-called conserved scalar because elements are conserved during combustion and it is not directly influencing the underlying fluid mechanics. The element mass fraction of an element i in an N -species mixture is:

$$Z_i = \sum_{j=1}^N a_{ji} Y_j \frac{M_i^{\text{atom}}}{M_j}, \quad (5.48)$$

where a_{ji} is the number of atoms i in species j , M_j is the molecular weight of species j , and M_i^{atom} is the atomic mass of atom i . The mixture fraction Z is defined as linear combination of Z_i , where it is 0

TABLE 5.2
Standard State Values at $T = 298.15\text{K}$

Species	ΔH_f° (kJ/mol)	S° (J/K·mol)	ΔG_f° (kJ/mol)
Carbon			
C(s, graphite)	0	5.74	0
C(s, diamond)	1.895	2.377	2.9
C(g)	716.682	158.096	671.257
CH ₄ (g, methane)	-74.81	186.264	-50.72
C ₂ H ₂ (g, ethyne)	226.73	200.94	209.2
C ₂ H ₄ (g, ethene)	52.26	219.56	68.15
C ₂ H ₆ (g, ethane)	-84.68	229.6	-32.82
C ₃ H ₈ (g, propane)	-103.8	269.9	-23.49
C ₄ H ₁₀ (g, butane)	-888		
C ₆ H ₆ (l, benzene)	49.03	172.8	124.5
C ₆ H ₁₄ (l)	-198.782	296.018	-4.035
C ₈ H ₁₈ (l)	-249.952	361.205	6.707
CH ₃ OH(l, methanol)	-238.66	126.8	-166.27
CH ₃ OH(g, methanol)	-200.66	239.81	-161.96
C ₂ H ₅ OH(l, ethanol)	-277.69	160.7	-174.78
C ₂ H ₅ OH(g, ethanol)	-235.1	282.7	-168.49
CH ₃ COOH(l)	-276.981	160.666	-173.991
CO(NH ₂) ₂ (s, urea)	-333.5	104.6	-197.4
CO(g)	-110.525	197.674	-137.168
CO ₂ (g)	-393.509	213.74	-394.359
CS ₂ (g)	117.36	237.84	67.12
Hydrogen			
H ₂ (g)	0	130.684	0
H(g)	217.965	114.713	203.247
H ⁺ (g)	1536.202	—	—
H ₂ O(l)	-285.83	69.91	-237.129
H ₂ O(g)	-241.818	188.825	-228.572
H ₂ O ₂ (l)	-187.78	109.6	-120.35
Nitrogen			
N ₂ (g)	0	191.61	0
N(g)	472.704	153.298	455.563
NH ₃ (g)	-46.11	192.45	-16.45
N ₂ H ₄ (l)	50.63	121.21	149.34
NO(g)	90.25	210.76	86.55
NO ₂ (g)	33.18	240.06	51.31

(Continued)

TABLE 5.2
Standard State Values at $T = 298.15\text{K}$ (Continued)

Species	ΔH_f° (kJ/mol)	S° (J/K·mol)	ΔG_f° (kJ/mol)
Nitrogen			
$\text{N}_2\text{O}(\text{g})$	82.05	219.85	104.2
$\text{N}_2\text{O}_4(\text{g})$	9.16	304.29	97.89
$\text{HNO}_3(\text{l})$	-174.1	155.6	-80.71
$\text{HNO}_3(\text{g})$	-135.06	266.38	-74.72
$\text{HNO}_3(\text{aq})$	-207.36	146.4	-111.25
Oxygen			
$\text{O}_2(\text{g})$	0	205.138	0
$\text{O}(\text{g})$	249.17	161.055	231.731
$\text{O}_3(\text{g})$	142.7	238.93	163.2
Sulfur			
$\text{S}(\text{s, rhombic})$	0	31.8	0
$\text{S}(\text{g})$	278.805	167.821	238.25
$\text{S}_2\text{Cl}_2(\text{g})$	-18.4	331.5	-31.8
$\text{H}_2\text{S}(\text{g})$	-20.63	205.79	-33.56
$\text{SO}_2(\text{g})$	-296.83	248.22	-300.194
$\text{SO}_3(\text{g})$	-395.72	256.76	-371.06
$\text{H}_2\text{SO}_4(\text{l})$	-813.989	156.904	-690.003
$\text{H}_2\text{SO}_4(\text{aq})$	-909.27	20.1	-744.53

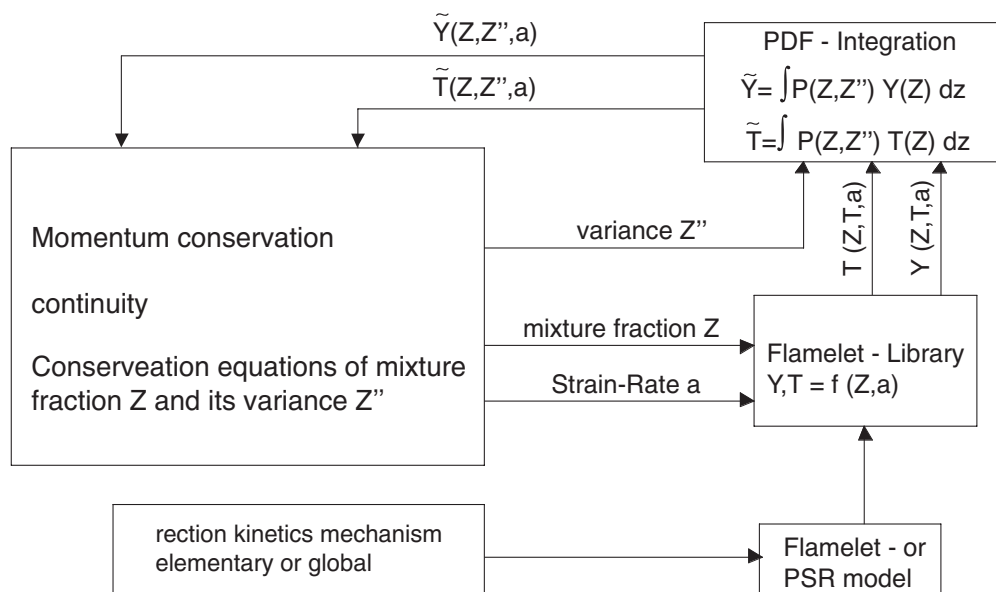


FIGURE 5.6 Application of a presumed pdf approach.

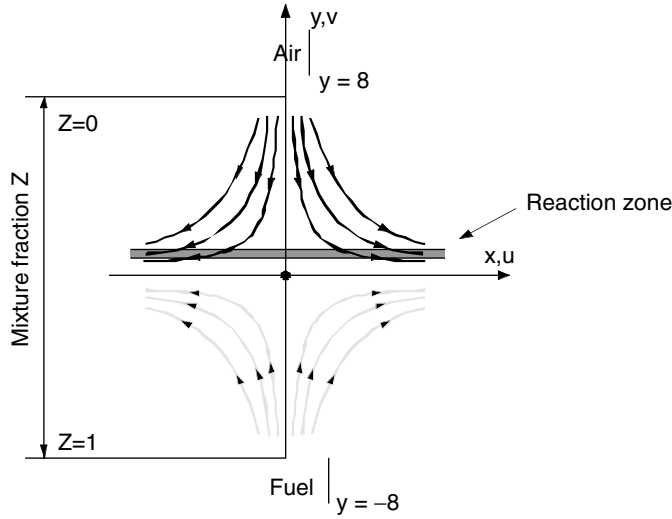


FIGURE 5.7 Illustration showing mixing process between fuel and oxidizer with resulting reaction zone.

in the oxidizer stream and 1 in the fuel stream (see Figure 5.7). In a two-feed system with a fuel stream mass flow $\dot{m}_1$ and an oxidizer stream mass flow $\dot{m}_2$, the mixture fraction represents the mass fraction of the fuel stream locally in the unburned mixture:

$$Z = \frac{\dot{m}_1}{\dot{m}_1 + \dot{m}_2} = \frac{Z_F}{Y_{F,1}} = 1 - \frac{Z_O}{Y_{O_2,2}} \quad (5.49)$$

with $Y_{F,1}$ the mass fraction of fuel in the fuel stream and $Y_{O_2,2}$ the mass fraction of oxygen in the oxidizer stream. Z_F and Z_O are the fuel element mass fraction coming from the fuel and from the oxidizer stream, respectively. The fuel element mass fraction Z_F is equivalent to the sum of fuel atoms. In the case of hydrocarbon combustion, it is equal to:

$$Z_F = Z_C + Z_H \quad (5.50)$$

The mixture fraction in the presence of combustion can be written as:

$$Z = \frac{vY_F - Y_{O_2} + Y_{O_2,2}}{vY_{F,1} - Y_{O_2,2}} \quad (5.51)$$

For the case of a stoichiometric mixture with $vY_F = Y_{O_2}$, the stoichiometric mixture fraction Z_{st} can be calculated from:

$$Z_{st} = \frac{Y_{O_2,2}}{vY_{F,1} - Y_{O_2,2}} = \left[1 + \frac{vY_{F,1}}{Y_{O_2,2}} \right]^{-1} \quad (5.52)$$

To include this approach in a CFD model, two additional equations must be solved. The first one is the conservation equation for the mixture fraction Z ; the second one is the conservation equation for the mixture fraction variance Z'' .

The transport equation for the mixture fraction Z as it is represented in a flow simulation

$$\frac{\partial(\rho u Z)}{\partial x} + \frac{\partial(\rho v Z)}{\partial y} + \frac{\partial(\rho w Z)}{\partial z} = \left(D_f + \frac{\mu_t}{Sc_f} \right) \left(\frac{\partial^2 Z}{\partial x^2} + \frac{\partial^2 Z}{\partial y^2} + \frac{\partial^2 Z}{\partial z^2} \right) \quad (5.53)$$

and the transport equation for the mixture fraction variance Z''

$$\begin{aligned} \frac{\partial(\rho u Z'')}{\partial x} + \frac{\partial(\rho v Z'')}{\partial y} + \frac{\partial(\rho w Z'')}{\partial z} - \left(D_g + \frac{\mu_t}{Sc_g} \right) \left(\frac{\partial^2 Z''}{\partial x^2} + \frac{\partial^2 Z''}{\partial y^2} + \frac{\partial^2 Z''}{\partial z^2} \right) \\ = 2 \frac{\mu_t}{Sc_g} \left(\frac{\partial Z}{\partial x} + \frac{\partial Z}{\partial y} + \frac{\partial Z}{\partial z} \right)^2 - 2\rho \frac{\epsilon}{k} g \end{aligned} \quad (5.54)$$

The pdf integration as shown in the preceding figure is commonly done using the β -pdf. The β -function is defined as:

$$\beta(\alpha, \chi) = \frac{\Gamma(\alpha)\Gamma(\chi)}{\Gamma(\alpha + \chi)}, \quad (5.55)$$

where;

$$\alpha = Z \left(\frac{Z(1-Z)}{Z''^2} - 1 \right) \quad (5.56)$$

and

$$\chi = (1-Z) \left(\frac{Z(1-Z)}{Z''^2} - 1 \right) \quad (5.57)$$

where:

$$\Gamma(\phi) = \int_0^\infty t^{\phi-1} e^{-t} dt \quad (5.58)$$

The shape of the β -function is shown in [Figure 5.8](#). This graph shows the distribution for a mixture fraction $Z = 0.6$ and several values for the mixture fraction variance Z'' .

The concentration and temperature distribution after integration over β -function can be determined from:

$$\tilde{Y}(Z, Z'') = \int Y(Z) P(Z, Z'') dz \quad (5.59)$$

and

$$\tilde{T}(Z, Z'') = \int T(Z) P(Z, Z'') dz \quad (5.60)$$

The result for Equation 5.60 is shown in [Figure 5.9](#). The graph shows the calculated temperatures of a methane/air flame for different variances Z'' .^{33,35}

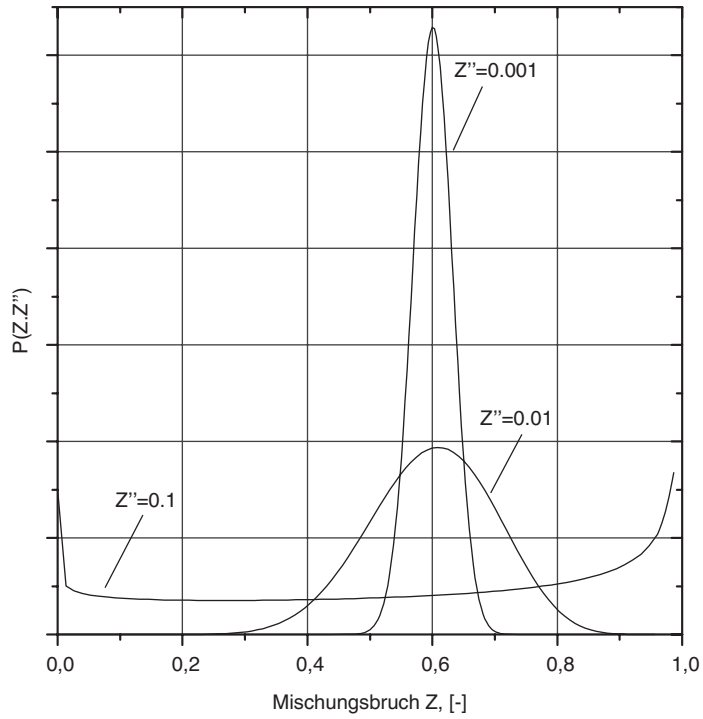


FIGURE 5.8 β -Function distribution for mixture fraction $Z = 0.6$ with several values for mixture fraction variance, Z'' .

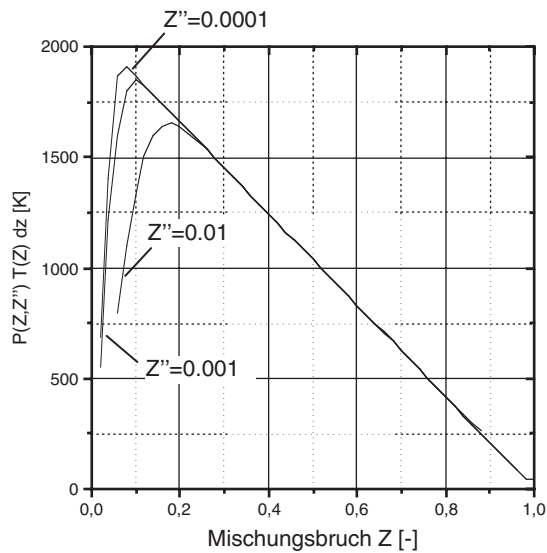


FIGURE 5.9 Temperature profile after integration over β -function for several values of mixture fraction variance Z'' .

5.3.3 WALL HEAT TRANSFER

Heat transfer between a burner flame and the furnace walls or tubes is a critical issue that must be resolved by a CFD simulation for the model to be useful for optimizing furnace efficiency. Thermal efficiency, defined as the total energy transferred to the furnace divided by the total available energy of the fuel, is largely dependent on radiative heat transfer within the industrial furnace and continues to be the focus of considerable research.

Radiative transfer theory deals with the propagation of intensity. Shuster³⁶ and Hamaker³⁷ were two of the first workers to describe the radiation process by writing equations for the rate of change of positive radiation fluxes in the positive and negative coordinate directions. Basic radiation transfer is governed by an integro-differential equation that accounts for the scattering and absorption of radiation by participating media:

$$(S \cdot \nabla)I_v = -(K_{a_v} + K_{s_v})I_v + K_{a_v}I_{b,v}(T) + \frac{K_{s_v}}{4\pi} \int_{\Omega'=4\pi} P_v(\vec{S} \rightarrow \vec{S}')I_v(S')d\Omega' \quad (5.61)$$

Figure 5.10 depicts the radiant energy balance in a specified direction. The term on the left-hand side of Equation 5.61 represents the net change in the intensity of radiation. The first term on right-hand side of the equation accounts for attenuation due to absorption and scattering while the second term on the right-hand side represents the addition due to emission. Finally, the integral term accounts for addition due to “in-scattering.” In-scattering is the radiation scattered by surrounding particles in the direction of travel of the radiation beam under consideration. This term, also known as the source term, is the most difficult to resolve given its integral nature of summing all incident radiation on a hemispherical section at a point. To simplify this equation, the source term is reduced to a differential form using various approaches.

5.3.3.1 Thermal Radiation Heat Transfer

Radiative heat transfer models for gas- or oil-fired^{38,39} and pulverized coal-fired furnaces⁴⁰ have been developed using the zoning method^{41,42} and the flux method.^{43–45} These approaches used simple empirical assumptions for flow characteristics, temperatures, heat release rates, and gas composition. However, they suffered from a lack of coupling between the individual directional fluxes. Other computational techniques developed to minimize this effect included the Monte Carlo method,⁴⁶ the diffusional method,⁴⁷ and, more recently, the discrete-ordinates method.⁴⁸

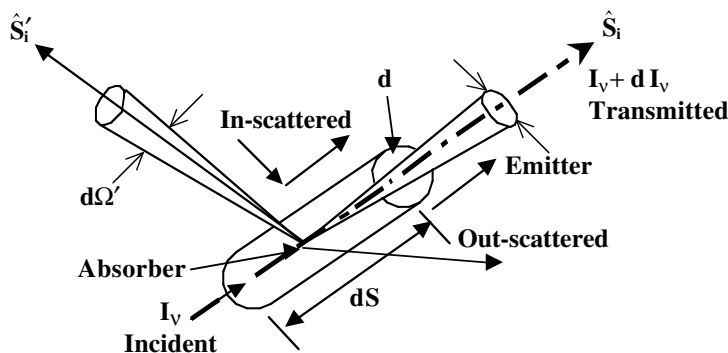


FIGURE 5.10 Radiant energy balance in a specified direction. (From Field, 1981.)

Zonal methods were first developed by Hottel and Cohen in 1958³¹ to simulate radiation exchange within a furnace chamber.³¹ Later, Hottel and Sarofim³⁷ refined the zone method to include non-ideality of the furnace and gases. This method is more rigorous on radiative transfer and combustion in industrial furnaces than the related flux methods.

Flux-based radiation models developed by Gosman and Lockwood³⁴ and by Varma³⁹ described geometrically simple systems that accounted for radiative transport via flux equations in two, four, or six flux directions. The derivation of the flux equations describing radiation transfer is relatively straightforward, and the computational demands for such an approach are far less than the comparative zonal approach. However, both the flux and zonal methods' inability to address coupling between directional fluxes makes them less popular today.

One method that captures the coupling between directional fluxes is the Monte Carlo method.³⁶ This method generates a "bundle" of intensities within a control volume and fires them in all directions and then traces the resulting rays throughout their lifetime as they undergo simulated absorption, emission, and scattering. This method provides a powerful and flexible solution to the nongray gas problem as well as the directional dependence of radiation. However, it suffers from poor economy in computer time. The discrete ordinates method attempts to address coupling between directional fluxes in a more efficient fashion.

Discrete ordinates (DO) solutions of the radiative transfer equation in multi-dimensional enclosures containing absorbing-emitting-scattering media have been developed for S_2 , S_4 , S_6 , and S_8 approximations (see Figure 5.11 for the S_2 and S_4 configurations). The S_4 approximation solves the radiative transport equation in 24 directions, the angular integral being discretized through the assumption of nonvariance of radiative intensities in prescribed solid angles surrounding representative directions. This discrete ordinates method has been tested in two-dimensional axisymmetric

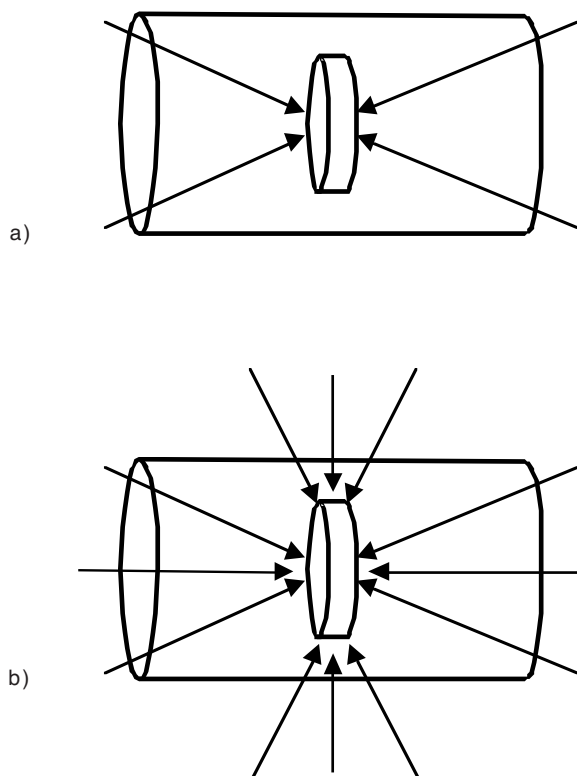


FIGURE 5.11 Directional intensities reaching a volume element: (a) S_2 and (b) S_4 .

geometries,⁴⁹ two-dimensional Cartesian geometries,⁵⁰ three-dimensional rectangular geometries,⁵¹ and three-dimensional geometries with generalized shapes.⁵² It has also been tested in nonscattering and scattering media. Comparison to exact solutions, the S_2 approximation is shown to have significant error while the S_4 approximation has been shown to be adequate. Today's CFD-based combustion models use this formulation of the DO method to approximate radiative transport in general furnaces and burners.

5.3.3.2 Properties of Radiating Gases

To carry out radiation calculations, information is needed on the absorption and scattering cross sections for particulates, as well as the scattering phase functions. These can be calculated using Mie theory⁵³ if the particle size, the wavelength of the radiation, and the complex refractive index of the particle are known.

Soot particles absorb but do not scatter radiation significantly due to their size. For this reason, soot radiation is typically ignored in most CFD codes.

Absorption coefficients for combustion gases are evaluated from gas emissivity data as:

$$k_{ag} = \left(\frac{1}{\ell} \right) [\ln(1 - \epsilon_g)] \quad (5.62)$$

where:

$$\epsilon_g = C_{\text{CO}_2} \epsilon_{\text{CO}_2} + C_{\text{H}_2\text{O}} \epsilon_{\text{H}_2\text{O}} - \Delta\epsilon \quad (5.63)$$

where ℓ is the mean beam length evaluated as:

$$\ell = 3.5(V_F/A_F) \quad (5.64)$$

and C_{CO_2} and $C_{\text{H}_2\text{O}}$ represent the pressure corrections to the gas emissivities, $\Delta\epsilon$ represents the spectral overlap correction, and V_F and A_F represent the averaged volume and cross-sectional area of the reactor. The gas emissivity data are taken from Hottel and Sarofim.⁴⁷

5.3.3.3 Radiative Boundary Conditions

In a well-controlled test furnace, the thermal boundary conditions along the wall, required by the radiation model, are well defined and can be supplied for the simulation. In most industrial furnaces, this is not the case. Instead, a wall heat transfer model is typically used that incorporates the local radiative fluxes (incident and emitted), local net convective heat flux, and a thermal resistance through the furnace wall (including any surface scaling or deposits). This model allows for specification of the boundary condition to be the local temperature outside the furnace wall. This requires specification of both a local temperature and the local thermal resistance of the wall.

Previous work has shown that the local radiation and temperature field is strongly dependent on this boundary condition. To improve accuracy, one can use measured external temperatures of the wall or ambient fluid or one can use the measured exit gas temperature to check this boundary condition. In the absence of local furnace data, a common assumption is that the wall resistance is uniform throughout the furnace. Although this is probably a weak assumption, the resistance is adjusted until the predicted and measured exit gas temperatures agree.

This definition of the boundary condition for the wall heat transfer also affects the reaction chemistry and the fluid dynamics. This assumption is believed to be the limiting assumption in the modeling of large industrial furnaces. Thus, more measurements and theoretical development

are needed to better resolve these boundary conditions for more thorough model definition and evaluation.

5.4 ILLUSTRATIVE EXAMPLES

5.4.1 FLAME SHAPE ANALYSIS CASE STUDY

CFD is commonly used to address customers' concerns directly related to thermal equipment performance in their individual applications. For example, our company used CFD to essentially duplicate conditions observed in an ethylene pyrolysis furnace, then devise a solution that was successfully implemented in the field.

Ethylene pyrolysis ("cracking") furnaces are found in many olefin plants and produce ethylene and propylene from feedstock containing ethane, propane, butane, and hydrocarbons through naphtha. The physical phenomena involved in this process include radiant heat transfer, gaseous combustion, convective heating of the process fluid in the process tubes, and convective cooling of the furnace effluent gases in the convection section of the furnace. In summary, the process entails rapidly heating the feedstock for a short time (less than 1 second is typical) to a temperature of about 1600°F (870°C). The feed gases are then quickly cooled and subjected to a number of separation processes. These phenomena are represented by the respective mathematical equations. The numerics required to solve these equations involve algorithms that solve large systems of nonlinear equations. As pointed out, successful application of CFD requires that all key physics are included in the simulation, that these physics are correctly captured in comprehensive mathematical expressions, and that the numerics accurately provide a reproducible solution to this nonlinear system of equations. If weakness exists in any of these three worlds, inaccurate CFD results are likely to occur.

Figure 5.12 is a photograph of burners operating in a cracking furnace. These burners are wall-fired and produce a flat flame. In this study, the installed flat flame burners produced a flame that "rolled off" the wall of the furnace and into the process tubes. Because flame impingement on the tubes can cause premature coking and tube failure, the furnace operators were forced to operate the furnace at only 50% capacity to avoid damaging the tubes.

In single burner tests at the lab, the flame shape observed in the furnace could not be reproduced, which required a CFD study of the burners in the actual furnace geometry.

Figure 5.13 illustrates three views of the CFD model of the burner. This model includes all the critical geometric features. The multiple jets created by the drillings in the primary and staged tips must be modeled in enough detail to simulate the individual jets. This requires significant experience with meshing tools as well as some knowledge of the fluid dynamic processes and resolution requirements. As observed in practical systems, the direction and size of these jets are critical to burner performance, and must be modeled in the CFD simulation to capture the correct flame shape and resultant heat flux profile.

Figure 5.14 shows a plan view of the furnace layout. The CFD model used to study the flame rollover problem assumed symmetry about certain planes to reduce the computational demands of the calculations, which allowed for rapidly generated solutions to the various burner changes. Figure 5.14 illustrates the symmetry planes used as dashed lines. This assumption allowed for study of flame interaction from adjacent burners while only including a "half-burner" in the model. This assumption greatly reduces the cell count to facilitate making several calculations to optimize the system.

5.4.1.1 Combustion Modeling and Boundary Conditions

The per-burner airflow is 5886 lbm/hr of ambient temperature air. The per-burner fuel flow is 325.3 lbm/hr. The fuel composition is given in Table 5.3. The lower heating value (LHV) of the fuel is 973 Btu/scf and its molecular weight is 18.5. The heat release per burner is 6.4 MMBtu/hr based on LHV.

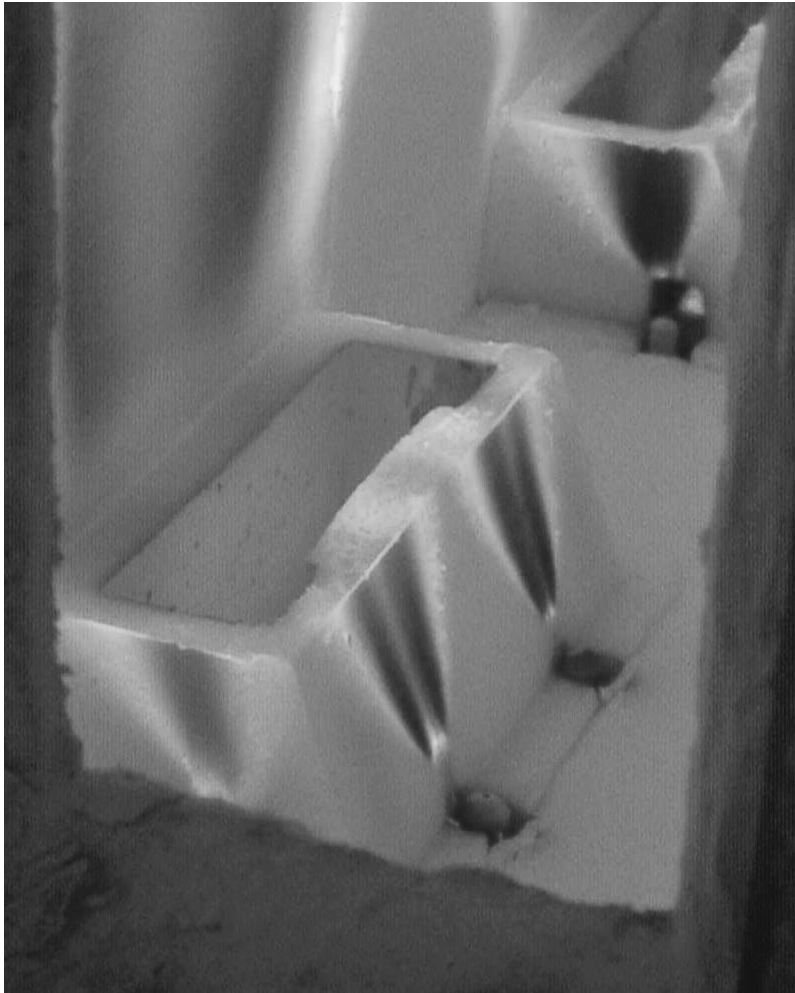


FIGURE 5.12 Closeup of burners firing in a cracking furnace.

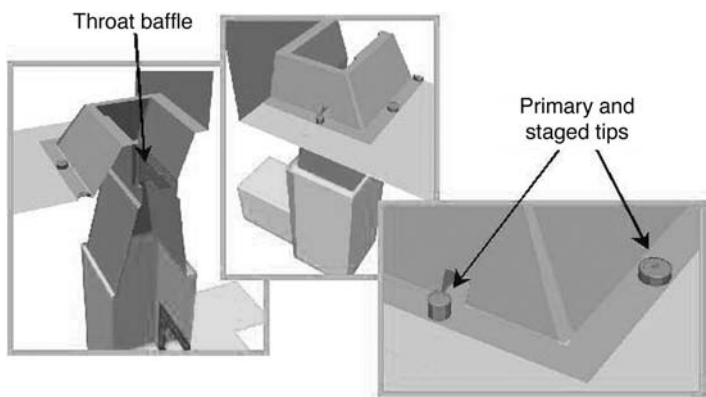


FIGURE 5.13 Closeup of CFD geometry for a flat-flame burner.

TABLE 5.3
Mole Fractions of Chemical Species
in Fuel and Combustion Air

Species	Fuel Fraction	Air Fraction
O ₂	0	0.206
N ₂	0.017	0.78
H ₂ O	0	0.014
CO ₂	0.0145	0.0003
CH ₄	0.861	0.0
C ₂ H ₆	0.0865	0.0
C ₃ H ₈	0.0166	0.0
C ₄ H ₁₀	0.0037	0.0

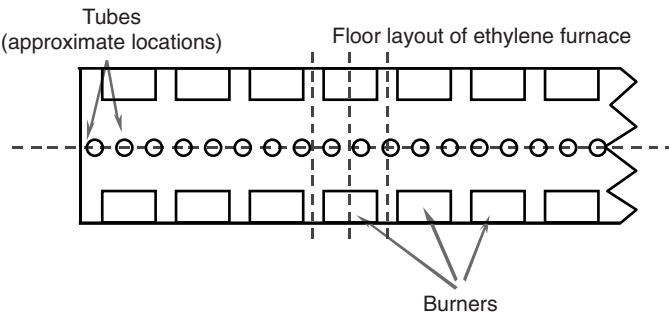


FIGURE 5.14 Plan view of furnace layout showing burner locations, tube locations, and symmetry planes used in CFD model (dashed lines).

Because these burners produce a nonpremixed flame, the presumed probability density function (PPDF) combustion model⁴ was used to simulate combustion. This model assumes that the combustion process is limited by fluid mixing rather than by chemical kinetics, a valid assumption for most hydrocarbon fuels in many combustion devices.

The CFD simulation used the realizable *k*- ϵ (RKE) turbulence model to simulate the effect of turbulence of the flow and mixing.^{54,55} Thermal radiation was simulated using the discrete ordinates model.⁵⁶ Thermal radiation is the most significant heat transfer mechanism in the radiant section of the furnace, and a significant fraction of the radiant flux to the tubes is directly from the gas, requiring a model capable of simulating optically thin gas radiation. The Weighted-Sum-of-Gray-Gases model⁵⁷ was used to compute the gas-phase absorption coefficients using an assumed surface emissivity of 0.85 on the tubes and 0.65 on refractory surfaces.

5.4.1.2 Predicted Flame Shapes and Modifications to Burner Geometry

Figure 5.15 shows the predicted flame shape (visualized by showing a constant mixture fraction isosurface) for the as-installed burners. The predicted flame shape is consistent with the observation that the flame rolls over into the tubes. The predicted flame shape also shows large “wings” of flame coming from the sides of the burner. These are consistent with the fuel placement in the burner, although the size of these wings is disconcerting. This burner was designed with an unusual constraint so that the burner could be easily operated when the furnace is in its “hot-standby” condition, which occurs regularly when the tubes undergo steam decoking.

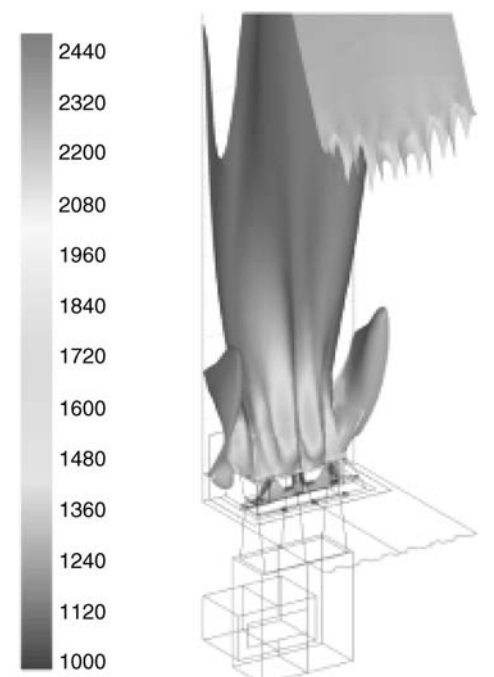


FIGURE 5.15 Flame shape ($\tilde{f} = 0.0575$ stoichiometric isosurface) predicted with initial burner geometry and tip drilling. The isosurface is colored by temperature ($^{\circ}\text{F}$).

After reviewing this predicted flame shape with burner engineers and furnace engineers, the conclusion was made that the combination of burner spacing in the furnace and the design constraint for hot-standby operation led to the flame rollover problem. This problem was not observed in single-burner tests or even in dual-burner tests, but the CFD model did reveal the problem. In a long row of burners as in the operating furnace, the combustion air will be “pinned” against the fired wall and unable to flow freely around the fuel. In a single- or dual-burner test, the air can flow around the flame and oxidize the fuel stream from both sides of the flame.

As a result of these discussions, seven additional CFD simulations were performed, each with a different fuel distribution around the tile. Figure 5.16 shows the flame selected as having the most optimal shape. This conclusion was reached by reviewing the predicted flame shapes for all seven tip-drilling changes with combustion engineers and furnace engineers.

Figure 5.17 shows the normalized heat flux profiles for the seven tip drillings considered. These are the heat fluxes to the process tube directly in front of the burner centerline.

Heat flux profiles are very important in ethylene pyrolysis furnaces because the tube metallurgy usually limits capacity. The furnaces are frequently operated with some portion of the tubes near the metallurgical temperature limit. For this reason, the more uniform the heat flux profile on the tubes, the higher the furnace capacity.

Upon completion of the CFD modeling study and test furnace evaluation of the selected tip drilling, new fuel tips were fabricated and delivered to the site. These tips were installed online. Upon installation, the flame impingement problem disappeared.

5.4.2 THERMAL OXIDIZER BURNER/REACTOR CASE STUDY

This case study considers the incineration of a dilute gas stream consisting of small amounts of sulfur-containing species (i.e., H_2S , COS , CS_2) and aromatic hydrocarbons. The thermal oxidizer had been operating for a period of time with a lower than desired destruction efficiency and this was developing into a regulatory compliance issue. It was suspected that mixing of the fuel, waste,

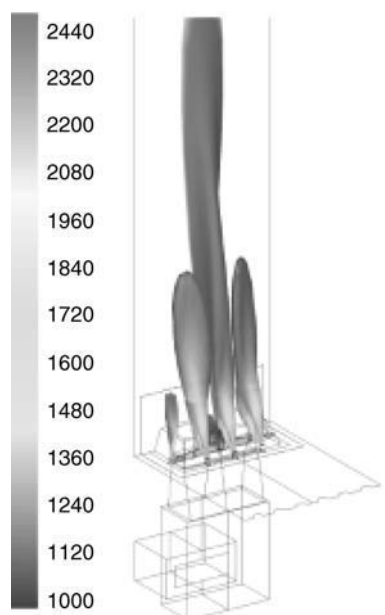


FIGURE 5.16 Flame shape ($\tilde{f} = 0.0575$ stoichiometric isosurface) predicted with optimized burner geometry and tip drilling. The isosurface is colored by temperature ($^{\circ}\text{F}$).

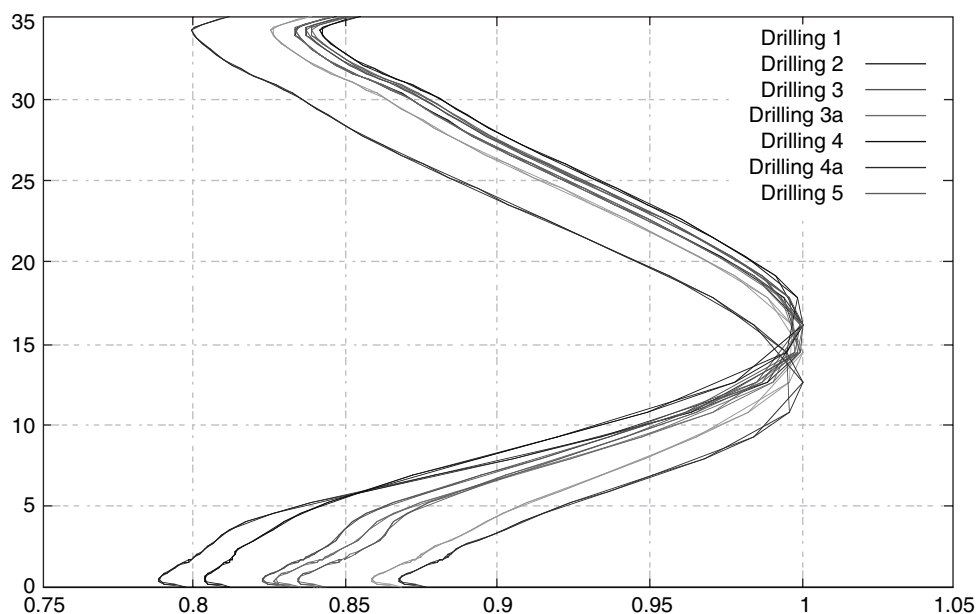


FIGURE 5.17 Normalized heat flux profiles for the various tip drillings studied.

and oxidant streams within the unit was less than optimal and a different style of burner was suggested to help improve this important parameter. Timing and the cost of renovation restricted the user to utilizing the existing reactor shell rather than make major modifications. The study was then designed to simulate the existing unit and then evaluate the effects related to the their replacement with the new, proposed burners.

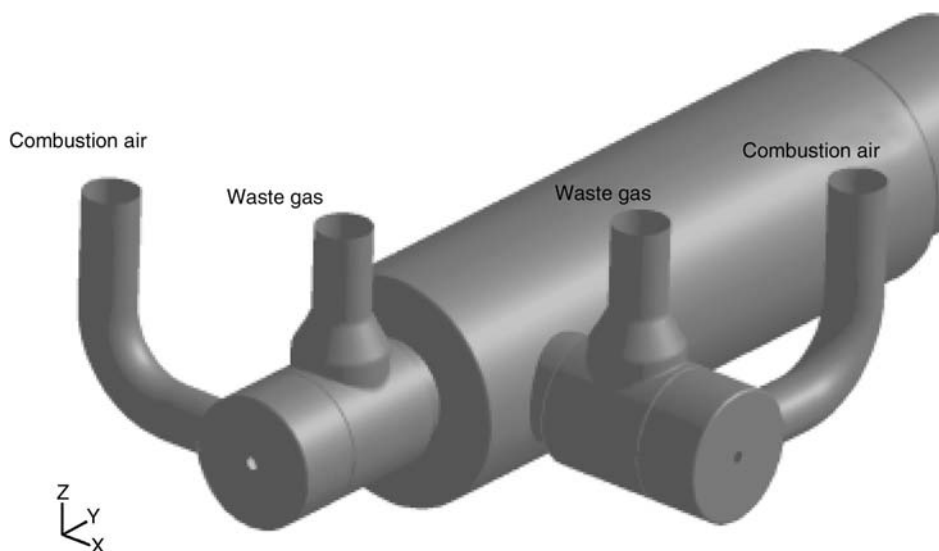


FIGURE 5.18 Overview of the modeled reactor.

The existing thermal oxidizer is a horizontal cylindrical furnace with two identical burners positioned at the head of the reactor perpendicular to one another on the reactor's horizontal mid-plane (see Figure 5.18). The original burners consisted of a single, center fuel gas riser, capped with a cone to help stabilize the flame. Air entered the burner by the gap around the center riser. Waste vent gas enters the burner assembly via a cylindrical gap concentric to the fuel gas riser's axis located outside of the burner tile. The fuel gas tip had drillings such that gas was allowed to enter in a conical pattern. The proposed burner modifications consisted of changing the fuel gas injection pattern by placing a number of individual tips around the interior burner periphery and providing drillings allowing for more tangential spin. Reducing the available concentric flow area slightly increased the pressure drop for the waste gas stream across the burner. A riser with a cone was added to allow for future fuel additions, but did not serve as an inlet to this particular burner simulation. The intent behind the new burner configuration was to increase local mixing sooner in the burner assembly, thereby helping to improve the potential for complete burnout of waste components. The two fuel gas tip arrangements are shown in Figure 5.19.

The fluid density was based on an ideal gas assumption, using a fixed value of system pressure. This approach is reasonable when large fractions of the pressure field fluctuations in the domain are expected to differ only slightly (<1%) from the user-input nominal system pressure. This approximation reduces the computational load per iteration. The RANS equations were used to account for momentum conservation and the "realizable k - ϵ " model was used to account for turbulent fluctuations. The combustion processes in these studies were modeled using the beta form of an assumed PDF (probability density function) of mixture fraction model. Heat loss from the reactor walls was assumed to be 1000 Btu/(hr-ft²).

The components that made up the fuel and waste gas streams are shown in Table 5.4. The air composition assumed to be at 94°F and 65% relative humidity.

Velocity profiles for the two different types of burners, shown along a plane perpendicular to the axis of the burner's centerline, are shown in Figure 5.20. The figures show the proximity of the plane to the burner's cone. The differences between the two are immediately obvious. The gas tip arrangement used in the older, existing burner was intended to provide a conical distribution of fuel gas with no swirl induced by the drilled pattern. The contours representing the calculation for the existing burner support this and show little to no rotation. The color map is shown to the left and

TABLE 5.4
Fuel and Waste Acid Gas Composition

Fuel Gas		Waste Acid Gas			
Specie	% Vol	Specie	% Vol	Specie	% Vol
CH ₄	82.5	CH ₄	0.16	H ₂ O	20.65
C ₂ H ₆	8.3	C ₆ H ₆	0.06	H ₂ S	0.5
C ₃ H ₈	3.9	CO	1.71	N ₂	41.61
N ₂	5.3	CO ₂	34.66	SO ₂	0.25
		H ₂	0.4		

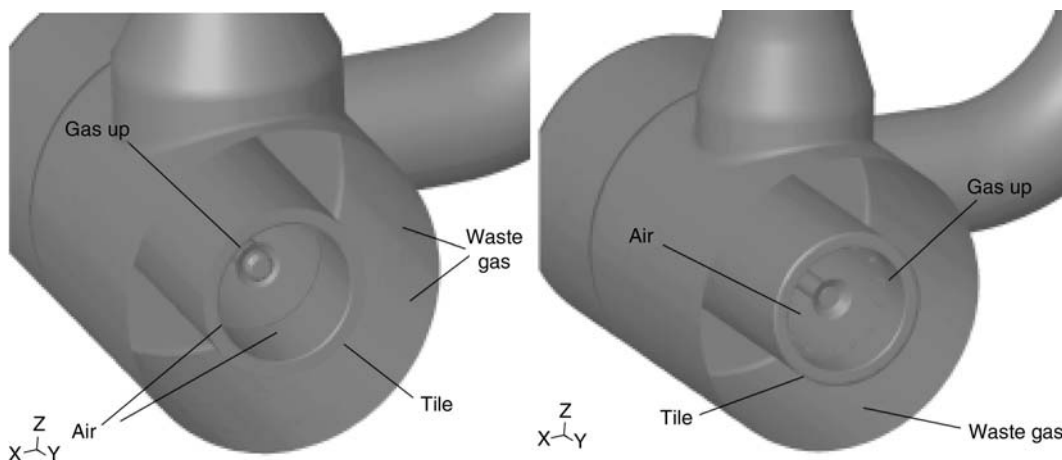


FIGURE 5.19 Existing and proposed burner modifications.

is in units of feet/second. The figure to the right shows the calculated result from the new burner configuration. The flow field now shows a swirling velocity pattern and seems to have a greater percentage of the flow area at a higher velocity.

Figure 5.21 shows the velocity profiles along the vertical mid-plane of the furnace, looking down from the top. The first profile (Figure 5.21a) shows the result from the existing burners. The velocity fields from the two burners combine and seem to form a “jet” that continues out toward the exit of the reactor. The implication is that the full reactor volume is not being utilized. The second profile (Figure 5.21b) shows the effect of the new burners. The overall magnitude of the combined jet is reduced; however, the slip that was occurring in the first case still seems to persist. This result prompted an additional study, with the addition of a choke ring to the reactor downstream of the burners. This addition could be made without major changes to the reactor as it currently existed.

As is shown, the addition of the choke ring significantly modified the flow fields in the reactor. Figure 5.22 shows the calculated temperature profiles from these three cases, and also the increase in field uniformity with the use of the new burners and more so with the choke ring.

The true impact this improvement in mixing has is best demonstrated by the contours shown in Figure 5.23. These represent H₂S mass fractions along the vertical mid-plane of the furnace, looking down from the top. The first, again, is from the simulation of the existing burner/reactor configuration. The second shows the impact of the new burners and indicates, for this particular metric, the addition of the new burners would make little improvement in the reactor’s effectiveness. There appears to be significant slip of the waste gas stream toward the exit. The case with the addition of the choke

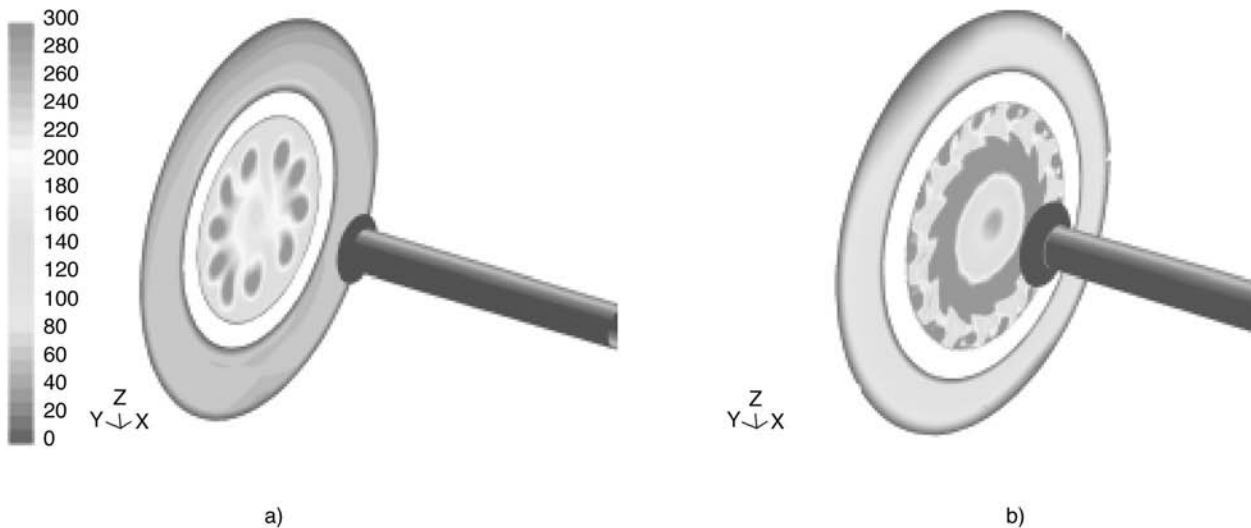


FIGURE 5.20 Velocity profiles near the burner face: (a) current burner and (b) modified burner design.

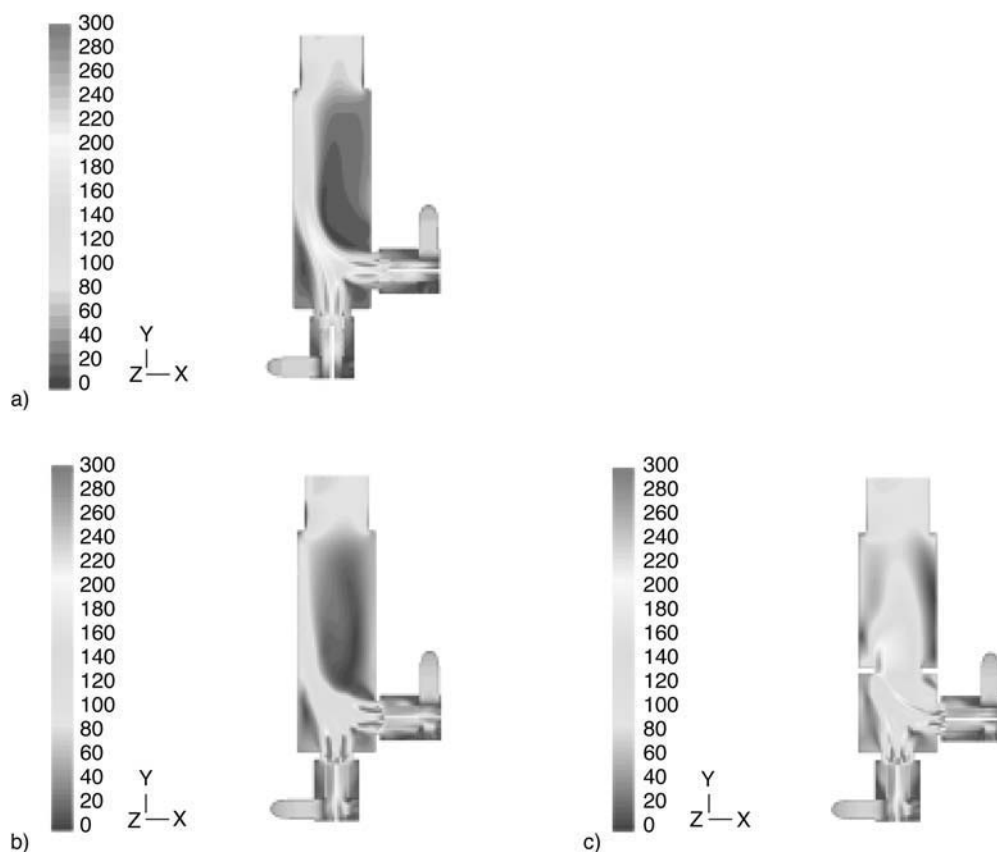


FIGURE 5.21 Velocity magnitude profiles along the reactor's vertical mid-plane (ft/sec): (a) existing burners, (b) new burners, no choke, and (c) new burners with choke.

ring shows the elimination of this slip, due to the increased utilization of the whole reactor volume. As can be seen, the improvement in mixing in the system utilizing the new burners and the choke seems to noticeably reduce the mass fraction of H_2S leaving the reactor. The improvement in mixing in the downstream section of the reactor also results in a more uniform temperature profile along the reactor walls, as shown in Figure 5.24. Figure 5.24a shows the expected temperature profiles from the existing burner configuration. The profiles seem to corroborate data taken during a site visit. Figure 5.24b and Figure 5.24c show that the temperature profiles along the reactor walls, with the addition of the new burners, becomes much more uniform, which should help improve the maintenance of the reactor as a whole.

The conclusion reached from this case study was that the addition of new burners in the existing reactor configuration should greatly improve the localized mixing, thereby helping with the incinerator's overall destruction efficiency. This was based on the calculated temperature and velocity fields from the CFD analysis. The addition of a choke seems to encourage better utilization of the reactor's available volume and subsequently improve the downstream uniformity of the resulting flow and temperature fields, as well as reduce the slip of waste gas from the side burner annulus. Temperature uniformity at the exit was considered important due to the presence of a waste heat boiler immediately downstream from the reactor exit. This improvement in mixing also appears to result in lower H_2S mass fractions leaving the oxidizer section. It was suggested that this addition should be considered an essential portion of the furnace upgrade.

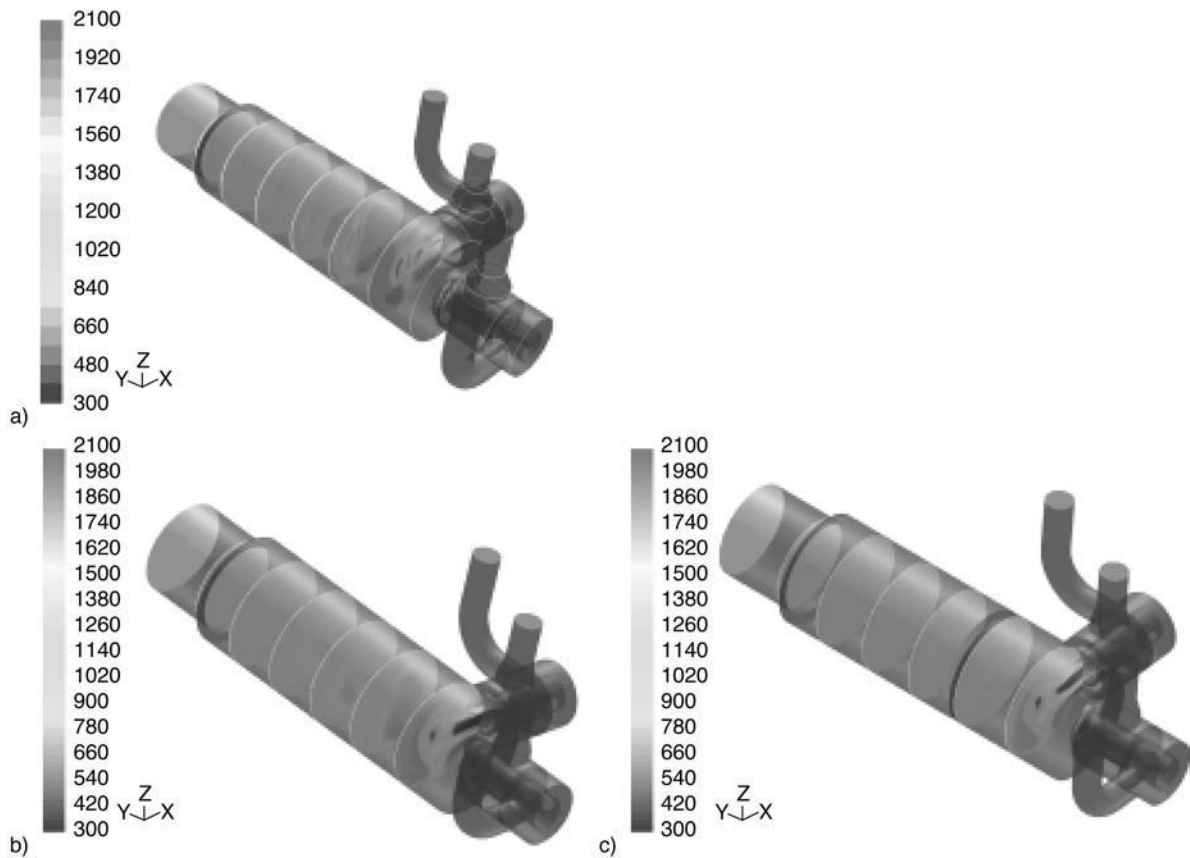


FIGURE 5.22 Temperature contour slices along the reactor axis (K): (a) existing burners, (b) modified burners without choke, (c) modified burners with choke.

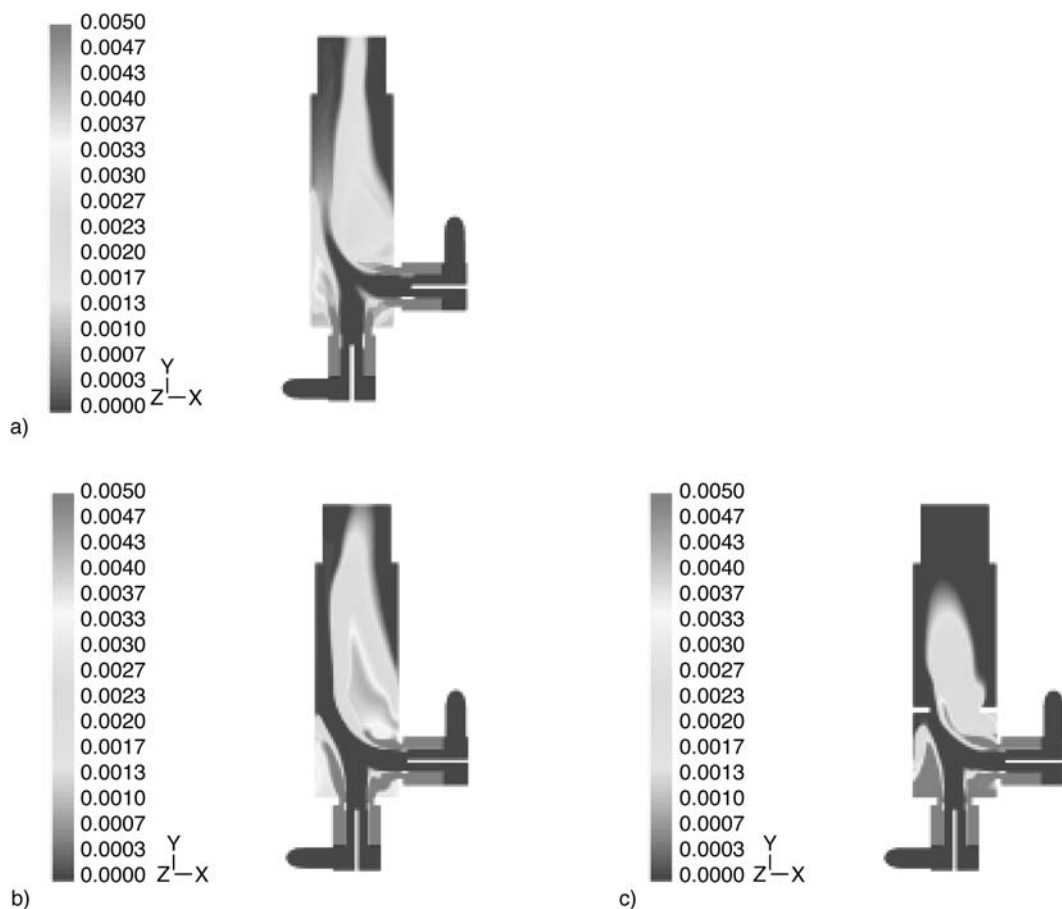


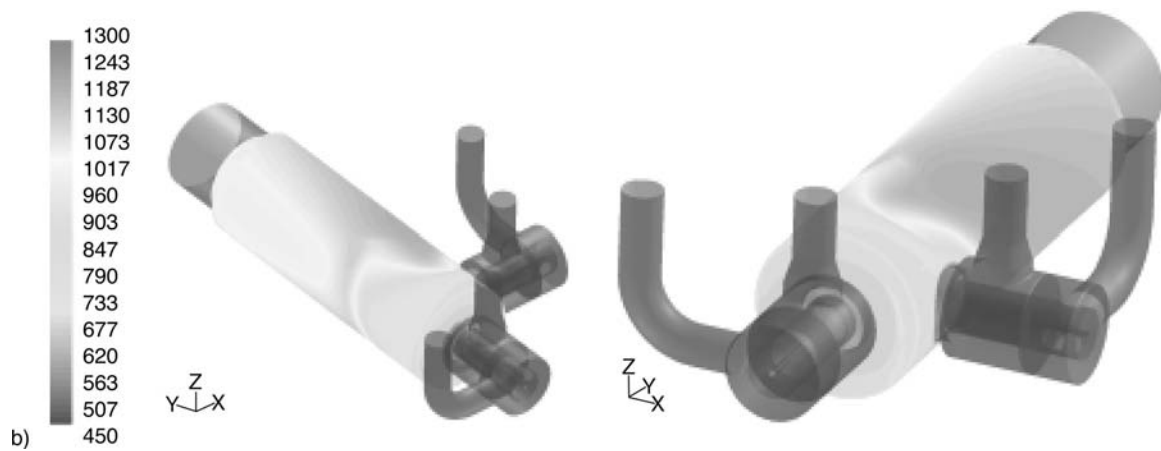
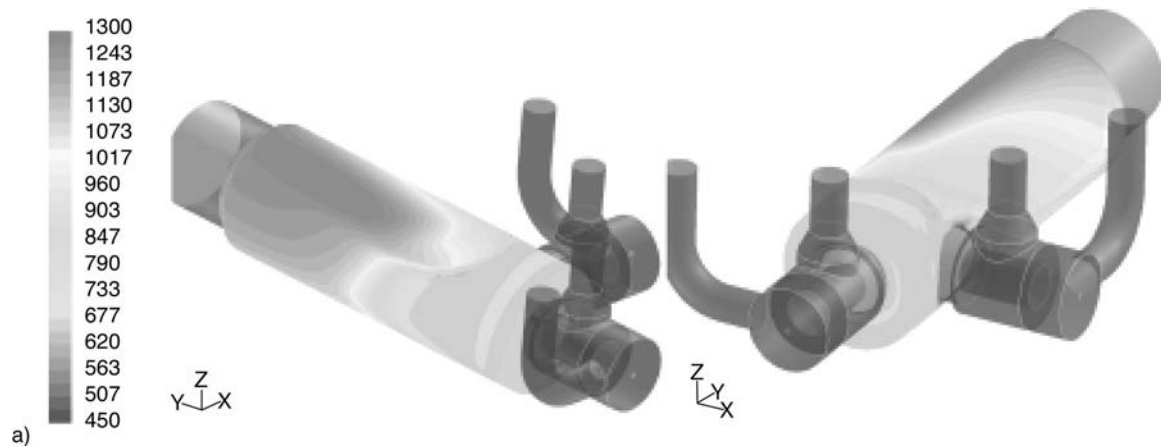
FIGURE 5.23 H_2S mass fraction profiles along the reactor's vertical mid-plane: (a) existing burners, (b) new burners, without choke, and (c) new burners with choke.

5.5 CONCLUSIONS AND SUMMARY

Time and experience in CFD-based combustion analysis have revealed their critical importance to the design and development of next-generation burners for the CPI/HPI. Recent advances in computer architecture, more comprehensive physics, and improved CFD solver algorithms have allowed engineers to address issues such as pollutant generation and equipment reliability. While tomorrow's supercomputers promise to open exciting new doors in the CFD field, today's challenge continues to be simulating fully three-dimensional turbulent reacting compressible flows inside very complex burner/furnace geometries.

Modeling continues to play a vital role in identifying complex problems. This approach provides a foundation to solve difficult problems, which in years past would have been intractable or exorbitantly expensive to address. In the examples presented in this chapter, the goals were to reduce fuel consumption without increasing combustion emissions or compromising burner turndown and carbon burnout at all loads. In each situation, operational improvements enabled the system to function at reduced excess air rates and higher efficiency, which translated into real savings.

Advanced modeling along with experimentation have also been used to address problems related to the thermal performance of ethylene pyrolysis furnaces. CFD has successfully identified and



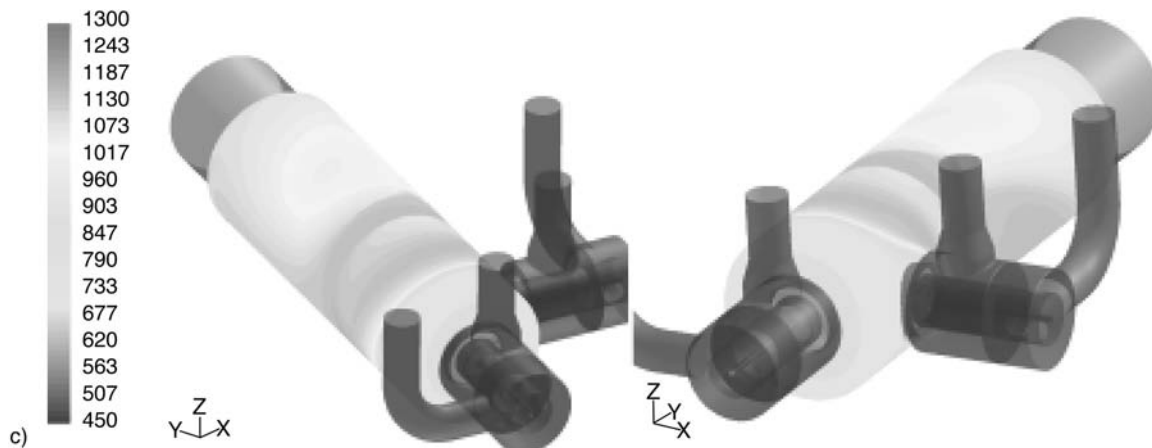


FIGURE 5.24 Temperature contour profiles along the reactor wall (K): (a) existing burners, (b) new burners, without choke, and (c) new burners with choke.

resolved the flame impingement/flame rollover problems in this specific furnace, which was implemented in the field quickly and cost-effectively. This same approach has been used on other similar furnaces with similar success. Solving these types of problems translates into significant cost savings in terms of higher online production rates for the operating unit.

Perhaps most importantly, advanced problem-solving techniques using CFD are making ultra-low emission burner design routine in today's ever-stringent economic and operating environment. This new tool has proven its ability to effectively help industry meet evermore stringent air quality regulations at acceptable costs.

REFERENCES

1. Smith, P. J., Heap, M. P., and Kertamus, N. J., Using Computational Combustion Simulations to Solve Industrial Problems, 92-JPGC-FACT-13, International Power Generation Conference, Atlanta, GA, October 18–22, 1992.
2. Pitts, W. M., Resolution Requirements for Scalar Dissipation Measurements in Turbulent Jets and Flames, 52nd Proceedings, American Physical Society/Division of Fluid Dynamics, November 21–23, 1999, New Orleans, LA, 1999, 37.
3. Smith, J. D. and Webster, T., Using CFD to Solve Challenges of Ultra-Low NO_x Burner Retrofit in Refinery Process Heaters, *Petroleum Technology Quarterly*, July 2002.
4. Henneke, M., Smith, J. D., Jayakaran, J. D., and Lorra, M., Computational Fluid Dynamics (CFD) Based Combustion Modeling, *The John Zink Combustion Handbook*, Baukal, C. E., Ed., CRC Press, Boca Raton, FL, 2001.
5. Engleman, M. S., Computational Fluid Dynamics in the 90's, Technology Trends in Automotive Engineering, Convex Computer Corporation, May 14–15, 1991.
6. Henneke, M., Lewellen, J., and Smith, J. D., Evaluating Burner Replacement Projects Using CFD, *Proceedings of the International Combustion Symposium: AFRC*, Ottawa, Canada, May 8–10, 2002.
7. Anderson, John D., Jr., *Computational Fluid Dynamics — The Basics with Applications*, McGraw-Hill, New York, p. 125, 1995.
8. Casey, M. and Wintergerste, T., Eds., *ERCOTAC Special Interest Group on "Quality and Trust in Industrial CFD" — Best Practice Guidelines*, European Research Community on Flow, Turbulence and Combustion, 2000, 14–15.
9. White, F. M., *Viscous Fluid Flow*, McGraw-Hill, New York, 1974.
10. Wilcox, D. C., *Turbulence Modeling for CFD*, DCW Industries, Inc., La Canada, CA, 1993.
11. Tennekes, H. and Lumley, J. L., *A First Course in Turbulence*, The MIT Press, Cambridge, MA, 1972.
12. Morkovin, M. V., Effects of Compressibility on Turbulent Flow, *The Mechanics of Turbulence*, Gordon and Breach, 1962.
13. Rodi, W., Turbulence Models and Their Application in Hydraulics — A State of the Art Review, *Association for Hydraulic Research*, 3rd ed., Delft, 1993.
14. Baldwin, B. S. and Barth, T. J., A One-Equation Turbulence Transport Model for High Reynolds Number Wall-Bounded Flows, NASA TM-102847, 1990.
15. Spalart, P. R. and Allmaras, S. R., A One-Equation Turbulence Model for Aerodynamic Flows, AIAA Paper 92-439, Reno, NV, 1992.
16. Chou, P. Y., On the Velocity Correlations and the Solution of the Equations of Turbulent Fluctuation, *Quart. Appl. Math.*, Vol. 3, 1945.
17. Davidov, B. I., On the Statistical Dynamics of an Incompressible Fluid, *Doklady AN. SSSR*, Vol. 136, 1961.
18. Harlow, F. H. and Nakayama, P. I., Transport of Turbulence Energy Decay Rate, Los Alamos National Laboratory, University of California Report LA-3854, 1968.
19. Jones, W. P. and Launder, B. E., The Prediction of Laminarization with a Two-Equation Model of Turbulence, *International Journal of Heat and Mass Transfer*, Vol. 15, 1972.
20. Roberson, J. A. and Crowe, C. T., *Engineering Fluid Mechanics*, Houghton Mifflin, Boston, MA, 1975.
21. Kim, S. E. and Choudhury, D., A Near Wall Treatment Using Wall Functions Sensitized to Pressure Gradient, ASME FED Vol. 217, Separated and Complex Flows, ASME, 1995.
22. Oran, E. S., Boris, J. P., *Numerical Simulation of Reactive Flow*, 2nd ed., Cambridge University Press, Cambridge, U.K., 2001.

23. Borghi, R., Turbulent Combustion Modelling, *Prog. Energy Combust. Sci.*, 14, 245–292, 1988.
24. Kee, R. J. et al., *Chemkin II: A FORTRAN Chemical Kinetics Package for the Analysis of Gas-phase Chemical Kinetics*, Sandia Report SAND 89-8009B-UC706, 1989, reprinted 1992.
25. Kee, R. J. et al., *SENKIN: A FORTRAN Program for Predicting Homogeneous Gas Phase Chemical Kinetics With Sensitivity Analysis*, Sandia Report SAND 87-8248UC401, reprinted 1991.
26. Glarborg, P. et al., *PSR: A FORTRAN Program for Modelling Well-Stirred Reactors*, Sandia Report SAND 86-8209UC4, reprinted 1992.
27. Rogg, B., *RUN-1DL: The Cambridge Universal Laminar Flamelet Computer Code*, in *Reduced Kinetic Mechanisms for Application in Combustion Systems*, Appendix C, Peters, N. and Rogg, B., Eds., Springer-Verlag, Berlin, 1993.
28. Rogg, B., *RUN-1DL: The Universal Laminar Flame and Flamelet Computer Code*, User Manual, 1994.
29. Rogg, B., *Numerical Modelling and Computation of Reactive Stagnation-Point-Flows*, in *Computers and Experiments in Fluid Flow*, Caromagno, G. M. and Brebbia, C. A., Eds., Springer Verlag, Berlin, 1989, 75–85.
30. Spalding, D. B., Mixing and Chemical Reaction in Steady Confined Turbulent Flames, *13th Symp. (Int.) on Combustion*, 1971, 649–657.
31. Magnussen, B. F. and Hjertager, B. H., On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion, *16th Symp. (Int.) on Combustion*, 1977, 719–727.
32. Magnussen, B. F., Hjertager, B. H., Olsen, J. G., and Bhaduri, D., Effects of Turbulent Structure and Local Concentrations on Soot Formation and Combustion in C_2H_2 Diffusion Flames, *17th Symp. (Int.) on Combustion*, 1978, 1383–1393.
33. Lorra, M., Investigation of NO_x Reduction in Turbulent Exhaust Gas Flows with Reburning Methods Using Experimental and Mathematical Modeling Regarding Detailed Reaction Mechanisms Using the Laminar Flamelet Theory, Ph.D. thesis, Ruhr-Universitaet Bochum, 1999 (in German).
34. Lorra, M. and Kremer, H., Mathematical Modelling and Experimental Evaluation of NO_x Reduction at Glass Melting Furnaces with Reburning, *Proc. 5th Int. Conf. of Combustion Technologies for a Clean Environment*, Lisbon, Portugal, 1999.
35. Lorra, M., Schnepfer, C., and Stephen, S., Investigation of a Duct Burner Design Using CFD Capabilities in Conjunction with Full-Scale Experiments, *Proc. 6th Eur. Conf. on Industrial Furnaces and Boilers*, Estoril, Portugal, 2002.
36. Shuster, A., *J. Astrophys.*, 21, 1, 1905.
37. Hamaker, H. C., *Phillips Research Reports*. Vol. 2, 55, 103, 112, 420, 1947.
38. Field, M. A., Gill, D. W., Morgan, B. B., and Hawksley, P. G. W., Combustion of Pulverized Coal, The British Coal Utilization Research Association, Leatherhead, Surrey, England (1967).
39. Bueters, K. A., Cogoli, J. G., and Habelt, W. E., Performance Prediction of Tangentially Fired Utility Furnaces by Computer Model, *15th Symposium (Int.) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1974, 1245.
40. Lowe, A., Wall, T. F., and Steward, I. McC., A Zoned Heat Transfer Model of a Large Tangentially Fired Pulverized Coal Boiler, *15th Symp. (Int.) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1974, 1261.
41. Hottel, H. C. and Cohen, E. S., Radiative Heat Exchange in a Gas-Fired Enclosure: Allowance for Non-Uniformity of Gas Temperature, *AIChE Journal*, 4, 3–14, 1958.
42. Johnson, T. R. and Beer, J. M., Radiative Heat Transfer in Furnaces: Further Development of the Zone Method of Analysis, *14th Symp. (Int.) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1972, 693.
43. Patankar, S. V. and Spalding, D. B., A Computer Model for Three-Dimensional Flow in Furnaces, *14th Symp. (Int.) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1972, 605.
44. Gosman, A. D. and Lockwood, F. C., Incorporation of a Flux Model for Radiation into a Finite-Difference Procedure for Surface Calculations, *14th Symp. (Int.) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1972, 661.
45. Varma, S. A., Radiative Heat Transfer in a Pulverized Coal Flame, in *Pulverized Coal Combustion and Gasification*, Smoot, L. D. and Pratt, D. T., Eds., Plenum Press, New York, 1979.
46. Steward, F. R. and Cannon, P., The Calculation of Radiative Heat Flux in a Cylindrical Furnace Using the Monte Carlo Method, *Int. J. Heat Mass Transfer*, 14, 245, 1971.
47. Hottel, H. C. and Sarofim, A. F., *Radiative Transfer*, McGraw-Hill, New York, 1967.
48. Fiveland, W. A., Discrete-Ordinates Solutions of the Radiative Transport Equation for Rectangular Enclosures, *ASME J. Heat Transfer*, 106, 699, 1984.

49. Jamaluddin A. S. and Smith, P. J., Radiative Transfer in Axisymmetric Cylindrical Enclosures Using the Discrete Ordinates Method, *Combustion Science and Technology*, 62(4–6), 173, 1988.
50. Jamaluddin A. S. and Smith, P. J., Predicting Radiative Transfer in Rectangular Enclosures Using the Discrete Ordinates Method, *Combustion Science and Technology*, 59, 321, 1988.
51. Jamaluddin, A. S. and Smith, P. J., Discrete-Ordinates Solution of Radiative Transfer Equation in Non-Axisymmetric Cylindrical Enclosures, *Journal of Thermophysics and Heat Transfer*, 6(2), 242, 1992.
52. Adams B. R. and Smith, P. J., Three-dimensional Discrete-Ordinates Modeling of Radiative Transfer in a Geometrically Complex Furnace, *Combustion Science and Technology*, 83, 1–15, 1992.
53. Mie, G., Optics of Turbid Media, *Ann. Phys.*, 25, 377–445, 1908.
54. Yakhot, V. and Orszag, S. A., Renormalization Group Analysis of Turbulence. I. Basic Theory, *J. Scientific Computing*, 1, 1–51, 1986.
55. Yakhot, V. Orszag, S. A., Thangam, S., Gataski, T. B., and Speziale, C. G., Development of Turbulence Models for Shear Flows by a Double Expansion Technique, *Phys. Fluids*, A4(7), 1510–1520, 1992.
56. Carlson, B. G. and Lathrop, K. D., Transport Theory — The Method of Discrete Ordinates, in *Computing Methods in Reactor Physics*, Greenspan, H., Kelber, C. N., and Okrent, D., Eds., Gordon Breach Science Publishers, New York, 1968.
57. Coppalle, A. and Vervisch, P., The Total Emissivities of High-Temperature Flames, *Combustion and Flame*, 49, 101–108, 1983.