Numerical simulations of turbulent non-premixed combustion in a regenerative furnace.

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UMI
NUMERICAL SIMULATIONS OF TURBULENT NON-PREMIIXED COMBUSTION IN A REGENERATIVE FURNACE

By Natalie Tyves

A Thesis
Submitted to the College of Graduate Studies and Research through the Department of Mechanical and Materials Engineering in Partial Fulfillment of the Requirements for the Degree of Master of Applied Science

Windsor, Ontario, Canada

1998

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Abstract

The research on gas-fired furnaces has been driven by the demand for fuel efficient processes and pollution reduction. In the past, this research has relied exclusively on empirical methods, which proved to be expensive and time consuming. With recent advances in numerical techniques and computer power, the dependence has now shifted to numerical simulations using computational fluid dynamics (CFD).

Computational fluid dynamics can be used as a useful design tool for studying new furnace configurations with different operating conditions. However, this potential cannot be realized until the numerical models that are used in the simulations are fully validated against experimental results. In the present work, the combustion process in an experimental regenerative, slab reheat furnace was simulated in order to validate several numerical models in the FLUENT code.

A total of 14 cases employing different numerical models were simulated with a uniform fuel distribution. Out of the 14 cases, only 11 obtained a converged solution. The results from these 11 cases were compared against experimental measurements in terms of the energy input and output rates and the temperature distribution in the center of the slab.

The three best cases in terms of both accuracy and computational effort were cases that employed the $k$-$\varepsilon$ turbulence model, the Delta PDF, and a constant absorption coefficient. These three cases were simulated again using a second set of operating conditions in order to evaluate their performance in the case of a non-uniform fuel distribution. The results of the simulations were validated against temperature measurements.
taken at several locations within the furnace. In all three cases, trends that were exhibited experimentally were accurately reproduced.

The work was successful in showing the potential of CFD in design. The cases clearly demonstrated the capability of predicting combustion in a regenerative, slab reheating furnace. Based on the results of the validations, it was concluded that the three cases that were simulated with the second set of operating conditions were also the best choices for use as design tools in studying new furnace geometries and operating conditions.
Acknowledgements

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Nomenclature

\( a \)  
absorption coefficient

\( a_0 \)  
pre-exponential rate constant

\( a_g, a_s \)  
absorption coefficients for gas and soot

\( a_{\varepsilon_i} \)  
emissivity weighting factors for the \( i \)th fictitious gray gas

\( A \)  
area

\( A \)  
constant in the RNG model

\( A \)  
Van Driest constant

\( A \)  
constant in the rate for soot combustion

\( A_\varepsilon, A_\mu \)  
constants in the two-layer zonal model

\( A_n' \)  
coefficients in the series for the radiation intensity

\( b_i, b_f \)  
constants in the generalized soot model

\( c_{\phi k} \)  
fitting coefficients in Modak’s model

\( c_\varepsilon \)  
constant in the two-layer zonal model

\( c_f, c_{ij} \)  
concentrations of fuel and oxidizer

\( c_\varepsilon \)  
soot concentration

\( C_{1\varepsilon}, C_{2\varepsilon}, C_\mu \)  
constants in the \( k-\varepsilon \) and RNG models

\( C_\gamma, C_\phi, C_\varepsilon, C_\epsilon \)  
constants in the RSM

\( C_d, C_\varepsilon \)  
constants in the mixture fraction variance equation

\( C_f \)  
constant in the nonequilibrium wall function
$D$ diameter

$E$ constant in the standard wall function

$f$ mixture fraction

$f$ linear branching coefficient

$f_{m,h}$ rich limit mixture fraction

$f'2$ mixture fraction variance

$F_1,F_2,F_3$ functions in Modak's model

$g$ linear termination coefficient

$g_0$ linear termination on soot particles

$g_i$ gravitational constant in the $i$ direction

$h$ enthalpy

$h_w$ enthalpy for a moving wall

$H$ enthalpy

$I$ radiation intensity

$I_0$ initial radiation intensity

$I_p$ blackbody intensity

$I^-$ intensity of the incoming ray

$k$ turbulent kinetic energy

$k_p$ turbulent kinetic energy at point $P$

$l_c,l_u$ length scales in the two-layer zonal modal

$L$ length
\[ L \] characteristic length

\[ L \] mean beam length

\[ m_r \] mass of a soot particle

\[ n \] local coordinate normal to the wall

\[ n \] nuclei concentration

\[ N_s \] number of soot particles per \( m^3 \)

\[ p \] pressure

\[ p \] sum of the partial pressures of all absorbing gases

\[ p_t \] total pressure

\[ p_c, p_w \] partial pressures of carbon dioxide and water vapor

\[ Pe \] Peclet number

\[ p_{\nu} \] production tensor

\[ Pr_m, Pr_t \] molecular and turbulent Prandtl numbers

\[ P_n^m \] Legendre polynomials

\[ q \] radiation flux

\[ q_{inc} \] incident radiation heat flux boundary condition

\[ q_n \] normal component of the radiation heat flux

\[ q_{rad} \] net radiation heat flux

\[ q_{rad}^- \] incident radiation heat flux

\[ \tilde{r} \] position vector

\[ r_f, r_s \] mass stoichiometries for the combustion of fuel and soot
\( \mathbf{r}_w \)  
position vector on the wall boundary

\( R_1, R_2 \)  
rates for soot combustion

\( R_n, R_i \)  
net rates for nuclei and soot generation

\( R_{n,e}, R_{S,e} \)  
rates for nuclei and soot combustion

\( R_{n,f}, R_{S,f} \)  
rates for nuclei and soot formation

\( \text{Re} \)  
Reynolds number

\( \text{Re}_\text{eff} \)  
effective Reynolds number

\( \text{Re}_t \)  
turbulent Reynolds number

\( R_i, R_{i-1} \)  
absolute sum of the residuals at the current previous iterations

\( R_0 \)  
initial residual on a grid level

\( s \)  
position

\( s \)  
path length

\( S \)  
mean rate-of-strain tensor modulus

\( S_g \)  
mean rate-of-strain tensor

\( S_h, S_u, S_\phi \)  
source terms in the energy, conduction, and scalar equations

\( t \)  
time

\( t' \)  
initial time

\( T \)  
total time

\( T \)  
temperature

\( T_i \)  
Chebyshev polynomials

\( T_g \)  
temperature of the gas
\( T_i \)  
incident radiation temperature from the source

\( T_w \)  
temperature of the wall

\( \nu \)  
kinematic viscosity

\( u \)  
velocity

\( u_i, u_j, u_k \)  
velocity components in the \( i, j, \) and \( k \) directions

\( u_{i,m} \)  
moving wall velocity component in the \( i \) direction

\( u_{i,\text{NB}} \)  
velocity component in the \( i \) direction at neighboring points

\( u_p \)  
velocity component in the \( i \) direction at point \( P \)

\( U \)  
mean velocity

\( U_i \)  
mean velocity in the \( i \) direction

\( U_p \)  
mean velocity at point \( P \)

\( U_z \)  
shear stress velocity

\( v_p \)  
velocity component in the \( j \) direction at point \( P \)

\( V \)  
mean velocity in the \( j \) direction

\( V \)  
volume

\( w_p \)  
velocity component in the \( k \) direction at point \( P \)

\( x_i, x_j, x_k \)  
Cartesian coordinates in the \( i, j, \) and \( k \) directions

\( y \)  
distance to the nearest wall

\( y \)  
thickness of viscous sublayer

\( y_e \)  
thickness of viscous sublayer

\( y_p \)  
distance from point \( P \) to the wall
\( y_f \)  
thickness of the thermal conduction layer

\( Z_k \)  
mass fraction of element k

\( Z_{k_f} \)  
mass fraction of element k at the fuel inlet

\( Z_{k_o} \)  
mass fraction of element k at the oxidizer inlet

**Greek Symbols**

\( \alpha \)  
inverse turbulent Prandtl number for energy

\( \alpha \)  
absorptivity

\( \alpha \)  
exponential in the Beta PDF

\( \alpha \)  
constant in the soot formation rate

\( \alpha \)  
termination criteria parameter

\( \alpha \)  
underrelaxation parameter

\( \alpha_0 \)  
constant in the RNG model

\( \alpha_s \)  
swirl constant

\( \alpha_k, \alpha_e \)  
inverse turbulent Prandtl numbers for the turbulent kinetic energy and its dissipation rate

\( \beta \)  
constant in the RNG model

\( \beta \)  
exponential in the Beta PDF

\( \beta \)  
constant in the soot formation rate

\( \beta \)  
residual reduction parameter

\( \delta \)  
Kronecker delta

\( \varepsilon \)  
turbulent kinetic energy dissipation rate
\( \varepsilon_c \)  
emissivity of carbon dioxide

\( \varepsilon_P \)  
turbulent kinetic energy dissipation rate at point \( P \)

\( \varepsilon_w \)  
wall emissivity

\( \varepsilon_w \)  
emissivity of water vapor

\( \Delta \varepsilon_{\infty} \)  
correction factor for gas emissivity

\( \phi \)  
dependent variable

\( \phi'_P, \phi_P_{\text{old}} \)  
the new and old values of the dependent variable at point \( P \)

\( \phi_i \)  
instantaneous dependent variable

\( \phi_0, \phi_L \)  
dependent variables at \( x = 0 \) and \( x = L \)

\( \Phi \)  
dependent variable

\( \Gamma \)  
diffusion coefficient

\( \eta \)  
Komolgorov scale

\( \eta_0 \)  
constant in the RNG model

\( \eta_0 \)  
kinetic rate for nuclei formation

\( \ell \)  
length scale

\( \kappa \)  
von Karman’s constant

\( \kappa_i \)  
absorption coefficient for the \( i \)th fictitious gray gas

\( \lambda \)  
Taylor scale

\( \Lambda \)  
integral scale

\( \mu_{\text{eff}}, \mu_{\text{mol}}, \mu_t \)  
effective, molecular, and turbulent dynamic viscosities

\( \nu \)  
kinematic viscosity
$\nu_{mol}$  
molecular kinematic viscosity

$\nu$  
velocity scale

$\theta_R$  
radiation temperature

$\rho$  
density

$\sigma$  
Stefan – Boltzmann constant

$\sigma_h, \sigma_k, \sigma_\phi$  
turbulent Prandtl numbers in the energy, conduction, and scalar equations

$\sigma_n, \sigma_s$  
turbulent Prandtl numbers in the nuclei and soot transport equations

$\sigma_k, \sigma_\varepsilon$  
turbulent Prandtl numbers in the turbulent kinetic rate and its dissipation rate equations

$\sigma_\lambda$  
scattering coefficient

$\tau$  
shear stress

$\tau_i$  
fraction of time $i$

$\tau_w$  
shear stress at the wall

$\omega$  
solid angle

$\Omega$  
characteristic swirl number

$\xi$  
local concentration of water vapor

Subscripts

$e, w$  
at the control volume faces to the east and west of point $P$

$E, W$  
at the control volume centers to the east and west of point $P$
Superscripts
-
\textsuperscript{time-averaged}
-
\textsuperscript{Favre-averaged}
-
\textsuperscript{fluctuating}
-
\textsuperscript{corrected}
-
\textsuperscript{dimensionless}
-
\textsuperscript{guessed}
1. Introduction

Economic competition in the steel industry has increased the demand for fuel-efficient uses in furnaces. In addition, due to stringent environmental laws the reduction of combustion generated pollutants has become equally important. Unfortunately, fuel efficiency and pollution control can be difficult to attain simultaneously. For example, preheating the incoming combustion air can increase fuel efficiency but the resulting elevated temperatures would promote NOx emissions. Low NOx burners that suppress fuel and air mixing in the initial stages of combustion have recently been developed to overcome this difficulty. Incorporation of these burners into a regenerative furnace results in lower peak temperatures and hence a decrease in the amount of NOx production. Despite these burners however, the demand for fuel efficiency and pollution reduction is still high and ways of keeping up with that demand are continuously being sought.

Although experimental techniques have been relied on almost exclusively for furnace research and development, they have been proven to be time-consuming and expensive. Fortunately, advances in numerical techniques and computing power have given birth to computational fluid dynamics, which have reduced the need for full-scale, prototype testing.

The computational fluid dynamics codes that are available today embody numerous models for simulating a variety of situations. The wide range of applicability of these models often makes it difficult to decide which ones would yield better results in a particular case. Through validation however, their range of applicability can be limited and an indispensable design tool for studying new furnace configurations with different operating conditions can be realized. The objective of this thesis therefore, is to validate the different models available
in FLUENT, a computational fluid dynamics code, against benchmark results in order to obtain the most viable design tool for simulating turbulent, non-premixed combustion in a regenerative furnace with a moving slab.
2. Literature Review

Computational fluid dynamics (CFD) has recently gained considerable popularity in the field of combustion. This is because researchers like Swithinbank et al. [1] are beginning to realize the value of using CFD as a design tool. To most, it is becoming apparent that when CFD is used instead of prototype testing, the expense and time are forgone with little if any compromise in predictive capability.

The majority of CFD research that has been done to date in the area of combustion has focused primarily on simple flames. Such focus has a great deal of merit since advanced combustion systems that are found in practical applications cannot be properly simulated without first understanding the underlying physical processes. In fact, the insight gained from modeling simple flames can almost always be used to model more complicated systems.

The most relevant research that has been done on simple flames is on turbulent, non-premixed types. Turbulent, non-premixed flames are often encountered in practical furnace applications and many different numerical models that simulate these particular flames have been investigated. The investigations have mostly been evaluations of existing flame models as in the case of Jones and Whitelaw [2] and Mechtoua and Viollet [3] and their study on turbulent, non-premixed methane jets. In some instances however, new numerical models that were proposed by the author(s) have been appraised. The work of Chen et al. [4] on a three-step reduction mechanism for predicting a CO/H$_2$/N$_2$ jet flame, and that of Cook [5] on an integral model for calculating the structure of turbulent, non-premixed jet flames in cross-flow are just two examples of such cases. Other researchers including Kent and Bilger [6],

3
Magnussen and Hjertager [7], Chen and Kollman [8], Smith et al. [9], Spalding [10], and Janicka and Kollmann [11] have also made similar contributions to the study of turbulent, non-premixed flames.

Significantly less research has been done on gas-fired furnaces. This is not surprising considering the complexity associated with such systems and the amount of computational effort required to model them. The reality is that advanced combustion systems demand exceptionally powerful processors for their simulation that most are unwilling to invest in because of their astronomical cost. Without them however, work is very time consuming and every effort is required to make the slightest bit of progress.

In lieu of the above, work has been published in order to drive the research on gas-fired furnaces. Such work has contributed little in the way of progress but has been a tremendous help to the research effort. Khalil [12] for example compared his numerical calculations of the flow characteristics in large furnaces with available experimental data solely for the purpose of illustrating the predictive capability of numerical models without any attempt at validation.

Validation however, is very important to research progress and the research on gas-fired furnaces has suffered because of it. Part of the reason there has been a lack of validation is due to computer requirements since in some cases, numerical accuracy has been sacrificed to overcome the inefficiencies of today’s systems. In such cases, numerical models simply cannot be validated with confidence against benchmark results. The other reason there has been such a lack of validation is because of the difficulty in obtaining adequate experimental measurements from full-scale furnaces. Not only are furnace measurements obtrusive, but they are also extremely expensive in a production setting.
To date, the number of publications validating numerical simulations of gas-fired furnaces is limited. Of particular significance is the work by Carvalho et al. [13] which shows comparisons of predicted and measured temperature profiles for different oxygen to fuel ratios in a ceramic glass kiln. Also of significance is the work by Zhang et al. [14-17], which because of the inadequacy of measurements from the full-scale, regenerative, slab reheat furnace shows comparisons of numerical data with measurements from a controllable, experimental furnace. The results of these works were very promising, however, only specific numerical models were validated. Further advances in research will require the validation of additional models. This is attempted in this work with the investigation of different models.
3. Furnace Description and Operating Conditions

Due to the unavailability of adequate combustion experiments in full-size, industrial furnaces, experimental data was collected from an experimental furnace that was developed by the NKK Corporation of Fukuyama, Japan. The experimental furnace is shown in Figure 3.1 and is used in the numerical simulation for validation against experimental results. The inner dimensions are 8x4x3 m³ and are on the same order of magnitude as in the full-size, industrial furnace. Steel slabs, four pairs of regenerative burners with full-size, industrial furnace burner capacity, and an auxiliary exhaust are all part of the experimental furnace configuration.

Figure 3.1 Experimental furnace configuration
The steel slabs are located on the inside bottom of the furnace and are 0.11 m thick, 3.5 m wide, and 0.5 m long. They are low-carbon steel (0.08% C) and when the furnace is in operation, they are fed into the centre of the furnace from left to right in the x-direction. They are also introduced into the furnace one after another, giving the appearance of one continuous slab.

The four pairs of regenerative burners are located 1.5 m from the furnace floor using the center of the burner as reference. In the x-direction, the spacing of the burners is as follows - 1.015 m between the wall and the first burner and the wall and the fourth burner, 1.97 m between the first and second and fourth and third burners, and 2.03 m between the second and third burners. The burners are paired up so that one burner from a pair is in a firing mode while the other, located on the opposite wall, is in an exhaust mode. When the furnace is in operation, adjacent burners on the same wall are alternated when fired. In this way, heat transfer to the slab occurs more uniformly. In the numerical simulation, burners 1 and 3 on the front wall and 2 and 4 on the back wall are in the firing mode. All other burners act as exhausts.

The burners themselves are regenerative burners, which means that they preheat the incoming air during the firing cycle using the heat from the flue gases that were expelled through the burner during the exhaust cycle. This is actually accomplished via a ceramic honeycomb regenerator in each burner that stores heat in its packing for approximately 20 s until the firing and exhaust cycles are reversed. In this way, fuel consumption is reduced because additional energy is no longer required to raise the temperature of the incoming air.

The burners are also low Ox burners. Their configuration allows the fuel and air to enter separately into the furnace and for the mixing to proceed gradually. Gradual mixing is
desirable since a more uniform temperature distribution can be attained and the high peak
flame temperatures responsible for promoting NOx can be avoided. The burner configuration
is depicted in Figure 3.2. Air is injected into the centre nozzle and the fuel is injected into
the top left and bottom right corner nozzles.

![Figure 3.2 Burner configuration](image)

Only about 80% of the flue gas volume exists through the exhaust burners. The
remainder 20% is discharged through a 0.16 m$^2$ auxiliary outlet on the left-hand side of the
furnace with the centre 2 m from the furnace floor and walls. The benefits of using this
auxiliary exhaust are twofold. First, smaller, less expensive blowers can be used and second,
the furnace pressure can be controlled more conventionally.
Also, although not shown in Figure 3.1, the outside bottom of the furnace is equipped with five cooling loops that extract heat from the slab. These cooling loops were incorporated into the experimental design in order to simulate heat losses from the bottom of the slab that occur in the full-size, industrial furnace.

There are two different sets of operating conditions. The operating conditions of the first set correspond to a uniform fuel load and are shown Table 3.1. The operating conditions of the second set correspond to a non-uniform fuel load and are shown in Table 3.2. In this table, Zone#1 and Zone#2 represent the left and right hand sides of the furnace. This zone division is clearly depicted in Figure 3.3. The two sets of operating conditions along with the properties of the slab, properties of the wall, etc. are used to specify boundary conditions in the numerical simulations.

<table>
<thead>
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<th>Parameter</th>
<th>Value</th>
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<tr>
<td>Air composition, vol.%</td>
<td>N₂, 79%; O₂ 21%</td>
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<tr>
<td>Air inlet temperature</td>
<td>1579 K</td>
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<tr>
<td>Air inlet velocity</td>
<td>83.7 m/s</td>
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<tr>
<td>Fuel composition, vol.%</td>
<td>CH₄ 10%; CO 23.7%; CO₂ 10.6%; H₂ 25.5%; H₂O 1.3%; N₂ 24.8%; C₂H₄ 1.2%</td>
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<tr>
<td>Fuel inlet temperature</td>
<td>293 K</td>
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<tr>
<td>Fuel inlet velocity</td>
<td>69.9 m/s</td>
</tr>
<tr>
<td>Slab inlet temperature</td>
<td>303 K</td>
</tr>
<tr>
<td>Slab inlet velocity</td>
<td>0.000833 m/s</td>
</tr>
<tr>
<td>Cooling water extraction rate</td>
<td>18.5 kW/m²</td>
</tr>
<tr>
<td>Surrounding temperature</td>
<td>300 K</td>
</tr>
</tbody>
</table>

Table 3.1 First set of operating conditions
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Zone #1</th>
<th>Zone #2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air composition, vol.%</td>
<td>N₂: 79%; O₂: 21%</td>
<td>N₂: 79%; O₂: 21%</td>
</tr>
<tr>
<td>Air inlet temperature</td>
<td>1455 K</td>
<td>1358 K</td>
</tr>
<tr>
<td>Air inlet velocity</td>
<td>69.5 m/s</td>
<td>41.0 m/s</td>
</tr>
<tr>
<td>Fuel composition, vol.%</td>
<td>CH₄: 10%; CO: 23.7%; CO₂</td>
<td>CH₄: 10%; CO: 23.7%; CO₂</td>
</tr>
<tr>
<td></td>
<td>10.6%; H₂: 25.5%; H₂O: 1.3%; N₂</td>
<td>10.6%; H₂: 25.5%; H₂O: 1.3%; N₂</td>
</tr>
<tr>
<td></td>
<td>24.8%; C₂H₄: 1.2%</td>
<td>24.8%; C₂H₄: 1.2%</td>
</tr>
<tr>
<td>Fuel inlet temperature</td>
<td>303 K</td>
<td>303 K</td>
</tr>
<tr>
<td>Fuel inlet velocity</td>
<td>70.8 m/s</td>
<td>44.6 m/s</td>
</tr>
<tr>
<td>Slab inlet temperature</td>
<td>296 K</td>
<td>296 K</td>
</tr>
<tr>
<td>Slab inlet velocity</td>
<td>0.000833 m/s</td>
<td>0.000833 m/s</td>
</tr>
<tr>
<td>Cooling water extraction rate</td>
<td>8.5 kW/m²</td>
<td>8.5 kW/m²</td>
</tr>
<tr>
<td>Surrounding temperature</td>
<td>300 K</td>
<td>300 K</td>
</tr>
</tbody>
</table>

Table 3.1 Second set of operating conditions

![Diagram](image)

Figure 3.3 Top view of the furnace showing the zone division
4. Conservation Equations

Determination of the velocity distribution and scalar distributions requires the solution of conservation equations. Normally, these conservation equations are time-dependent and the conserved fluid properties are functions of time. For turbulent flows, however, the time-averaged equations are usually used. This is because the wide range of length and time scales involved in turbulent flows make it difficult to solve for instantaneous values with the existing computer storage capacity. When time-averaged equations are solved, only mean values that are of interest in engineering applications are obtained.

The temporal variation of a fluid property, $\phi$, is depicted in Figure 4.1. As can be seen, for a particular time, $t$, the fluid property can be decomposed into its respective mean and fluctuating components \[20\]

$$\phi = \bar{\phi} + \phi'$$  \hspace{1cm} (4.1)$$

where

$$\bar{\phi} = \frac{1}{t} \int_{t}^{t} \phi dt$$

Substitution of this definition into the time-dependent conservation equations produces the more desirable time-averaged (Reynolds-averaged) equations.
Unfortunately, time averaging introduces density fluctuation terms into the conservation equations. These terms cannot be ignored. Since they constitute additional unknowns, they must be predetermined or modeled in terms of known quantities. However, a more favorable approach that has recently been adapted is Favre-averaging which is also referred to as mass-averaging or density-weighted averaging.

![Figure 4.1 Temporal variation of a scalar](image)

Favre-averaging involves making the following substitution into the time-dependent conservation equations [2]

\[ \rho \phi = \bar{\rho} \bar{\phi} + \rho' \phi' \] (4.2)

The resulting equations are still in terms of mean values but density fluctuation terms no longer appear. This is the main advantage of Favre-averaging over time averaging.
The Favre-averaged conservation equations governing steady state, turbulent combustion in a furnace are given by [20]

Continuity

\[
\frac{\partial}{\partial x_i} \left( \bar{\rho} \bar{u}_i \right) = 0
\]  \hspace{1cm} (4.3)

Momentum

\[
\frac{\partial}{\partial x_j} \left( \bar{\rho} \bar{u}_i \bar{u}_j + \bar{\rho} \bar{u}' \bar{u}'_j \right) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \bar{\mu}_{mol} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \bar{\mu}_{mol} \frac{\partial \bar{u}_i}{\partial x_i} \delta_{ij} \right] \]  \hspace{1cm} (4.4)

Energy

\[
\frac{\partial}{\partial x_i} \left( \bar{\rho} \bar{u} \bar{h} + \bar{\rho} \bar{u}' \bar{h}' \right) = \bar{S}_h
\]  \hspace{1cm} (4.5)

In furnaces with moving slabs, the above conservation equations must be coupled to an equation describing the heat transfer in the slab. This additional conduction equation is given below [20]

\[
\frac{\partial}{\partial x_i} \left( \bar{\rho}_w \bar{u}_i \bar{h}_w + \bar{\rho}_w \bar{u}'_i \bar{h}'_w \right) = 0
\]  \hspace{1cm} (4.6)

where the subscript \( w \) has been used to denote a wall representing the slab. In general, a conservation equation describing the transport of any scalar, \( \phi \), can be written as [12]
\[ \frac{\partial}{\partial x_i} \left( \overline{\rho u_i' \phi_i} + \overline{\rho u' \phi'} \right) = \overline{S_i} \quad (4.7) \]

In Equations 4.3 through 4.7, the tilde is used to denote Favre-averaged quantities while the overbar is used to denote time-averaged quantities.

The total number of governing equations from above is less than the number of unknown terms. Therefore additional information is required for closure. This additional information is obtained from models that approximate the unknowns in terms of known quantities. In the energy, conduction, and scalar equations, the terms \( \overline{\rho u' h'} \), \( \overline{\rho_u u_{,i} h_{,i}} \), and \( \overline{\rho u' \phi'} \), respectively, are modeled using the gradient transport analogy [2]:

\[
\begin{align*}
\overline{\rho u' h'} & = -\frac{\overline{\mu_t}}{\overline{\sigma_h}} \frac{\partial h}{\partial x_i} \\
\overline{\rho_u u_{,i} h_{,i}} & = -\frac{\overline{\mu_t}}{\overline{\sigma_{h, \omega}}} \frac{\partial h_{\omega}}{\partial x_i} \\
\overline{\rho u' \phi'} & = -\frac{\overline{\mu_t}}{\overline{\sigma_p}} \frac{\partial \phi}{\partial x_i}
\end{align*}
\quad (4.8)\]

where \( \overline{\sigma_h} \), \( \overline{\sigma_{h, \omega}} \), and \( \overline{\sigma_p} \) are the turbulent Prandtl numbers that have values of 0.7 [20].

The above models are the only ones used for approximating those three terms because of their wide acceptance. All other terms that are approximated have a number of different models for their prediction. The Reynolds stresses, \( \overline{\rho u' u'_i} \), in the momentum conservation
equation is one such term. Models relating to these stresses are categorized as turbulence models because they contain physical information about the statistical behavior of turbulent flows. The source term in the energy conservation equation is another term that can be approximated by different models. Models relating in particular to the determination of the radiation contribution to this source term are categorized as radiation models.

There are also four other categories of models that are not directly associated with the terms in the governing equations but that are required for the complete and accurate description of the problem. The first of these categories deals with the treatment of the near-wall region where large changes in the level of turbulence preclude the turbulence models from being used near the wall. Models falling under this category are collectively called near-wall treatment models. The models in the second category predict the variation of either the absorption coefficient or the absorptivity. They are therefore linked to the radiation models and are categorized as variable radiation parameter models. Soot models form the third category and they predict soot formation and the effect of soot on radiation transfer. The final category encompasses combustion models, which relate to species concentrations.

In chapters 5 through 10 these models will be described in detail. For sake of simplicity, the Favre-averaged notation will no longer be used but all relevant quantities will represent Favre averages.
5. Turbulence Models

FLUENT employs three turbulence models for the core flow. The first two, the $k-\varepsilon$ and the renormalization group $k-\varepsilon$ models, are very similar. Both of them are two-equation models that base the approximation of the Reynolds stresses on two turbulence quantities that can be obtained from the solution of their transport equations. The third turbulence model is the Reynolds stress model. It is much more rigorous in its evaluation than the other two, involving the solution of transport equations for each of the Reynolds stresses. The three models are discussed below.

5.1 The $k-\varepsilon$ Model

The $k-\varepsilon$ model is based on the eddy-viscosity concept. The concept relates the Reynolds stresses to the mean velocity gradients and is known as the Boussinesq hypothesis. When isotropy is assumed, the relationship reduces to the simple form shown below [20]

$$
\rho u_i' u_j' = \frac{2}{3} k \delta_{ij} - \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \frac{2}{3} \mu_t \frac{\partial u_i}{\partial x_j} \delta_{ij} \tag{5.1.1}
$$

The above expression is analogous to the shear stress-strain rate relation that arises in laminar flow. The turbulent viscosity in Equation 5.1.1 plays the same role as the molecular viscosity that appears in the shear stress-strain rate relation. Both are constants of proportionality,
however, in the above equation the viscosity is a function of the flow field instead of the fluid.

When Equation 5.1.1 is substituted into the momentum conservation equation, the form of the momentum equation stays the same. The change occurs in the molecular viscosity. It is replaced by the effective viscosity, which is defined as the following combination [20]

\[ \mu_{\text{eff}} = \mu_{\text{mol}} + \mu_t \]  \hspace{1cm} (5.1.2)

Since \( \mu_{\text{mol}} \) can be obtained from knowledge of the fluid properties, the task becomes determining \( \mu_t \).

Several expressions, ranging from simple algebraic forms to more complex partial differential equations have been proposed to represent the turbulent viscosity, \( \mu_t \). The one relevant to the \( k-\varepsilon \) turbulence model is based on the assumption that the local state of the fluid depends on two turbulence quantities that can be determined from the solution of their transport equations. These turbulence quantities arise from proper choice of scaling parameters that satisfy dimensional requirements. If the velocity scale [12]

\[ v = \sqrt{k} \]  \hspace{1cm} (5.1.3)

and the length scale [12]
\[ t = \frac{\sqrt{k^2}}{\varepsilon} \] \hspace{1cm} (5.1.4)

are chosen as the scaling parameters, then the expression for the turbulent viscosity used in the \( k - \varepsilon \) model becomes \([12]\)

\[ \mu_t = \rho C_\mu \frac{k^\frac{3}{2}}{\varepsilon} \] \hspace{1cm} (5.1.5)

where \( C_\mu \) is an empirically derived constant.

The two turbulence quantities in Equation 5.1.5 are the turbulent kinetic energy, \( k \), and its dissipation rate, \( \varepsilon \) \([20]\)

\[ k = \frac{1}{2} \langle u_i' u_i' \rangle \] \hspace{1cm} (5.1.6)

\[ \varepsilon = \frac{\mu}{\rho} \left( \frac{\partial u_i'}{\partial x_j} \frac{\partial u_i'}{\partial x_j} \right) \] \hspace{1cm} (5.1.7)

Although these two quantities are responsible for the name \( k - \varepsilon \) turbulence model, the model has been referred to more generally as the two-equation turbulence model since the solutions of two equations, \( k \) and \( \varepsilon \) transport, are required.

The turbulent kinetic energy and its dissipation rate transport equations are given
by [20]

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho u_i k) = \frac{\partial}{\partial x_i} \left( \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_i} \right) + \frac{\mu_t}{\partial x_i} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial u_j}{\partial x_i} - \rho \varepsilon \quad (5.1.8)
\]

\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho u_i \varepsilon) = \frac{\partial}{\partial x_i} \left( \frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_i} \right) + C_{1e} \frac{\varepsilon}{k} \left[ \mu_t \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial u_j}{\partial x_i} \right] - C_{2e} \rho \frac{\varepsilon^2}{k} \quad (5.1.9)
\]

where \( C_{1e} \) and \( C_{2e} \) are empirically derived constants and \( \sigma_k \) and \( \sigma_\varepsilon \) are respectively the turbulent kinetic energy and dissipation rate Prandtl numbers that govern diffusion. Values of the constants in Equations 5.1.5, 5.1.8, and 5.1.9 are given in Table 5.1.1 [20].

<table>
<thead>
<tr>
<th>( C_{1e} )</th>
<th>( C_{2e} )</th>
<th>( C_\mu )</th>
<th>( \sigma_k )</th>
<th>( \sigma_\varepsilon )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.44</td>
<td>1.92</td>
<td>0.09</td>
<td>1.0</td>
<td>1.3</td>
</tr>
</tbody>
</table>

*Table 5.1.1 The k-\( \varepsilon \) model constants*

The \( k-\varepsilon \) model has been successful in predicting the flow field for a wide variety of turbulent cases. However, the model is not without drawbacks. For one thing, it is not suitable for flows that are significantly affected by turbulence because of the assumption of isotropy. Also the model is semi-empirical in nature. This means that the constants appearing in its equations are limited to the range of parameters for which the experiments
were performed.

5.2 The ReNormalizion Group (RNG) $k - \varepsilon$ Model

The RNG $k - \varepsilon$ model is based on the same principle as the $k - \varepsilon$ model and the relationship between the Reynolds stresses and the mean velocity gradients is still the framework for this model. The main difference lies in the way the viscosity is determined. Instead of using a semi-empirical approach as in the $k - \varepsilon$ model, the viscosity is obtained using a Renormalization Group technique.

The Renormalization Group technique essentially describes a physical problem in terms of “coarse-grained” equations of motion. A good example of this technique is the application of Newton’s law to a collection of atoms instead of to individual atoms. The resulting equations of motion would then describe average behaviour on space and time scales that are much larger than the mean free path and the collision time of the individual atoms. In relation to turbulence, the RNG technique is used to incorporate small scale eddies in the equations of motion based on larger scale eddies.

Eddies range in size from the integral scale, $\Lambda$, which is the largest scale to the Komolgorov scale, $\eta$, or the smallest scale. The integral scale is on the same order of magnitude as the size of the volume containing the flow and has a high level of energy associated with it. The Komolgorov scale on the other hand, is of molecular size and has a low level of energy associated with it due to viscous dissipation. The eddies in between are
grouped together to form the Taylor scale, \( \lambda \). In the first step of the RNG method a band of smaller scales near \( \eta \) is removed and then represented in terms of the remaining larger scales. This process of removal results in a modified system of equations, with a different viscosity and force that requires substantially less computational effort. In the following steps, the above is repeated iteratively until the computational requirement for the solution of the system of equations becomes relatively reasonable.

As smaller scale eddies are eliminated, the effective viscosity of the system increases from its molecular value, \( \nu_{mol} \). Conversely, the effective Reynolds number decreases because of its inverse relationship with viscosity [20]

\[
\text{Re} = \frac{\mu L}{\nu} 
\]  

(5.2.1)

This variation of effective viscosity with Reynolds number is demonstrated in Figure 5.2.1 and is mathematically described by the following differential equation [20]

\[
\frac{d\mu}{dt} = \frac{A \epsilon t^3}{\mu(t)^3} 
\]  

(5.2.2)

where \( t \) is the length scale and \( A \), an analytically derived constant. Note that although the Reynolds number is not explicitly present in the equation, it is implicated through its dependence on the other variables. The exact derivation is beyond the scope of this paper and is left to the reader. Integration of the above expression results in an interpolation
formula for $\mu(t)$ between the molecular viscosity and the viscosity associated with the integral scale [20]

$$\mu(t) = \mu_{mol} \left[ 1 + \frac{3 A \varepsilon}{4 \mu_{mol}^3} \left( t^4 - \eta^4 \right) \right]$$  \hspace{1cm} (5.2.3)

![Graph showing modification of effective viscosity and Reynolds number by scale elimination procedure.](image)

*Figure 5.2.1 Modification of the effective viscosity and Reynolds number by the scale elimination procedure*

When Equation 5.2.3 is recast in terms of the turbulence quantities, it results in a differential relationship between the effective viscosity, $\mu_{\text{eff}} \left( \mu_{\text{eff}} = \mu_{mol} + \mu_{r} \right)$ and $k/\sqrt{\varepsilon}$. This is precisely the relationship that is used for calculating the viscosity in the momentum
conservation equation. It can be shown that for high Reynolds number flows associated with the integral scale, the form of the equation for turbulent viscosity is identical to Equation 5.1.5 that is used in the \( k - \varepsilon \) model. The value of the constant however is slightly different. \( C_\mu \) is 0.085 [20], which is very close to the empirically derived value of 0.09.

The transport equations for \( k \) and \( \varepsilon \) that the RNG \( k - \varepsilon \) model utilizes are given below [20]

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho u_i k) = \frac{\partial}{\partial x_i} \left( \alpha_{k} \mu_{eff} \frac{\partial k}{\partial x_i} \right) + \mu_{t} S^2 - g \frac{\alpha_{k}}{\rho} \frac{\partial \rho}{\partial x_i} - \rho \varepsilon \tag{5.2.4}
\]

\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho u_i \varepsilon) = \frac{\partial}{\partial x_i} \left( \alpha_{\varepsilon} \mu_{eff} \frac{\partial \varepsilon}{\partial x_i} \right) + C_{1\varepsilon} \frac{\varepsilon}{k} \mu_{t} S^2 - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} - R \tag{5.2.5}
\]

where \( C_{1\varepsilon} \) and \( C_{2\varepsilon} \) are now analytically derived constants having values of 1.42 and 1.68 respectively [20]. Also, \( C_\mu \) has a functional form that takes into account the effect of swirl on turbulence. Its value depends on the characteristic swirl number, \( \Omega \), the ratio \( k/\varepsilon \), and the swirl constant, \( \alpha_{s} \), which assumes different values that range from 0.05 for mildly swirling flows to higher values for more swirl dominated flows [20]
\[ C_\mu = f\left(\Omega, \frac{k}{\varepsilon}, \alpha_\varepsilon\right) \]  

(5.2.6)

\( \alpha_k \) and \( \alpha_\varepsilon \) in Equation 5.2.4 and 5.2.5 are respectively the inverses of the turbulent kinetic energy and turbulent kinetic energy dissipation rate Prandtl numbers. They are computed using the following formula [20]

\[
\frac{\mu_{mol}}{\mu_{eff}} = \frac{\alpha - 1.3929}{\alpha_a - 1.3929}^{0.6321} \frac{\alpha + 2.3929}{\alpha_a + 2.3929}^{0.3679}
\]

(5.2.7)

The constant \( \alpha_a \) has a value of unity [20]. The variation of the inverse Prandtl numbers with turbulence is similarly accounted for in the energy and the species conservation.

The \( R \) term in the transport equation for \( \varepsilon \) represents the effect of the mean rate of strain on the dissipation rate and is defined as [20]

\[
R = \frac{C_\mu \eta^3(1-\eta/\eta_a)}{1+\beta \eta^5} \frac{\rho \varepsilon^2}{k}
\]

(5.2.8)

where \( \eta = Sk/\varepsilon \), \( \eta_a \approx 4.38 \), and \( \beta = 0.012 \) [20]. When \( \eta < \eta_a \), i.e. mildly strained flows, \( R \) makes a positive contribution to the term representing the destruction of \( \varepsilon \) and the results are close to those of the standard \( k-\varepsilon \) model. When \( \eta > \eta_a \), \( R \) makes a negative contribution to the destruction of \( \varepsilon \). In these highly strained flow cases, the turbulent kinetic energy and hence the effective turbulent viscosity are reduced causing the results to deviate
from the standard $k - \varepsilon$ model. The $R$ term is a characteristic feature of the RNG model.

The RNG model is clearly an improvement over the standard $k - \varepsilon$ model. To summarize, the RNG model accounts for low Reynolds number effects and uses analytically derived constants. It also includes the effect of swirl on turbulence and provides an analytical formula for turbulent Prandtl numbers. However, even with all these improvements, the model still cannot be applied to situations where the flow is anisotropic.

5.3 The Reynolds Stress Model (RSM)

In this model, the Reynolds stresses are obtained from the solution of their transport equations [20]

$$\frac{\partial}{\partial t} (u'_i u'_j) + u_k \frac{\partial}{\partial x_k} (u'_i u'_j) = - \frac{\partial}{\partial x_k} \left[ \left( u'_i u'_j + \frac{P}{\rho} (\delta_{ij} u'_i u'_j + \delta_{ik} u'_k) - \nu \frac{\partial}{\partial x_k} (u'_i u'_j) \right) \right]$$

$$- \frac{\partial}{\partial x_k} \left[ \left( u'_i u'_j + \frac{P}{\rho} (\delta_{ij} u'_i u'_j + \delta_{ik} u'_k) - 2\nu \frac{\partial}{\partial x_k} (u'_i u'_j) \right) \right]$$

(5.3.1)

Term $A$ denotes the convective transport and term $B$ denotes the diffusive transport due to turbulence and viscosity. Term $C$ represents the production due to the interaction between the Reynolds stresses and the mean velocity gradient (the production tensor, $P_{ij}$) while term
$D$ denotes redistribution or pressure-strain. The last term on the right hand side of the equation, term $E$, represents the dissipation due to viscous action.

Several terms in Equation 5.3.1 constitute additional unknowns. In order to obtain closure of the equation set, these unknowns must be modeled within the RSM itself. The diffusive transport term is modeled using a scalar diffusion coefficient [20]

$$-rac{\partial}{\partial x_k} \left[ (u', u'_i, u'_k) + \frac{p}{\rho} (\delta_{ij} u'_i + \delta_{ik} u'_k) - \nu \frac{\partial}{\partial x_k} (u'_i u'_j) \right] = \frac{\partial}{\partial x_k} \left( C_i \frac{k u'_i u'_j}{\epsilon} \frac{\partial u'_j}{\partial x_i} \right)$$  \hspace{1cm} (5.3.2)

When isotropy is assumed, the above expression is simplified to the following form [20]

$$-rac{\partial}{\partial x_k} \left[ (u', u'_i, u'_k) + \frac{p}{\rho} (\delta_{ij} u'_i + \delta_{ik} u'_k) - \nu \frac{\partial}{\partial x_k} (u'_i u'_j) \right] = \frac{\partial}{\partial x_k} \left( \nu \frac{\partial u'_i}{\partial x_i} \right)$$  \hspace{1cm} (5.3.3)

The simplified form is used by FLUENT, however. Equation 5.3.2 may be activated to account for directional diffusivity. The ability to dispense with the assumption of isotropy makes the RSM model superior to the two turbulence models discussed previously in cases where the flow is highly turbulent.

Another term that is modeled is the redistribution or pressure-strain term. It is described in terms of $P_y$ and other known quantities [20]

$$\frac{p}{\rho} \left[ \frac{\partial u'_i}{\partial x_i} + \frac{\partial u'_j}{\partial x_i} \right] = -C_i \frac{\epsilon}{k} \left[ u'_i u'_j - \frac{2}{3} \delta_{ij} k \right] - C_2 \left[ P_y - \frac{2}{3} \delta_{ij} P - S_y \right]$$  \hspace{1cm} (5.3.4)
where

\[ P = \frac{1}{2} P_u \]  \hspace{1cm} (5.3.5)

and \( C_1 \) and \( C_2 \) are empirically derived constants.

The final term that is modeled is the dissipation term. The term is assumed to be isotropic with small scale turbulence at high Reynolds number. The resulting approximation is written in terms of the dissipation rate, \( \varepsilon \) [20]

\[ 2\nu \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_j}{\partial x_k} = \frac{2}{3} \delta_{ij} \varepsilon \]  \hspace{1cm} (5.3.6)

Equation 5.1.9 can be used for determining \( \varepsilon \) in the above expression when directional diffusivity is not being considered, otherwise, the following transport equation should be employed [20]

\[ \frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho u_i \varepsilon) = \frac{\partial}{\partial x_i} \left( C_e \frac{\rho k}{\varepsilon} u'_i u'_i \frac{\partial \varepsilon}{\partial x_i} \right) + \frac{1}{2} C_{1e} \rho P_u \frac{\varepsilon}{k} - C_{2e} \rho \frac{\varepsilon^2}{k} \]  \hspace{1cm} (5.3.7)

Four new constants appear in the RSM model. Their values are given in Table 5.3.1 [20].
\begin{table}[h]
\centering
\begin{tabular}{cccc}
\hline
$C_0$ & $C_1$ & $C_2$ & $C_e$ \\
\hline
0.22 & 1.8 & 0.6 & 0.18 \\
\hline
\end{tabular}
\caption{RSM constants}
\end{table}
6. Near-Wall Treatment Models

The turbulence models discussed in the previous chapter can only be applied with accuracy to core regions of the flow. In regions close to the boundaries such as walls, the models tend to breakdown mainly because there are significant changes in the level of turbulence. Closest to the wall turbulence is damped, while further away it is enhanced due to large gradients, accelerated transports, and turbulent kinetic energy production. For this reason, near-wall regions deserve special attention.

\[ U/U_c = 2.5 \ln(U_0 y/\nu) + 5.45 \]

*Figure 6.1 Near-wall region*

The near-wall region can be subdivided into three layers as shown in Figure 6.1. The first layer closest to the wall is called the viscous sublayer. In this layer, the flow is laminar-like with viscous effects dominating momentum, heat, and mass transfer. The layer farthest...
from the wall is called the fully turbulent layer. Here, turbulence is responsible for the transfer of momentum, heat, and mass and viscous effects are negligible. The middle layer, called the buffer layer, joins the other two with viscous effects and turbulence having equal importance.

One approach that is used to determine the values of variables in the near-wall region is the wall function approach. In this approach, the variables are obtained from semi-empirical formulas called wall functions that bridge the wall to the fully turbulent region. The effects that influence momentum, heat, and mass transfer are incorporated into these formulas so that they are properly accounted for in the viscous, buffer and fully turbulent layers.

The other approach that is used is called near-wall modeling. Near-wall modeling, with the area near the wall resolved, employs a one-equation turbulence model. Unlike the $k-\varepsilon$ or RNG two-equation turbulence models, the one-equation turbulence model only solves the transport equation for the turbulent kinetic energy, $k$. The dissipation rate, $\varepsilon$, is obtained from an algebraic equation. In addition, the definition of turbulent viscosity in the one-equation turbulence model varies from the one given in the two-equation models. The two approaches, wall functions and near-wall modeling are discussed in detail below.
6.1 Wall Function Models

6.1.1 Standard Wall Functions Model

Lauder and Spalding [18] had proposed the use of standard wall functions for various variables in the near-wall region. Instead of solving the relevant governing equations, the values of the variables are obtained from these functions. For mean velocity, the standard wall functions are dimensionless and are given below [20]

\[ U^* = y^* \quad y^* < 11.225 \]  \hspace{1cm} (6.1.1)

\[ U^* = \frac{1}{\kappa} \ln(Ey^*) \quad y^* > 11.225 \]  \hspace{1cm} (6.1.2)

where

\[ U^* = \frac{U_p C_{\mu}^{1/4} k_p^{1/2}}{\tau_w / \rho} \]  \hspace{1cm} (6.1.3)

\[ y^* = \frac{\rho C_{\mu}^{1/4} k_p^{1/2} y_p}{\mu} \]  \hspace{1cm} (6.1.4)

Von Karman's constant, \( \kappa \), and empirically derived constant, \( E \), in Equation 6.1.2 are equal to 0.42 and 9.81, respectively [20]. The non-dimensional thickness, \( y^* = 11.225 \), marks the end of the buffer layer and the beginning of the fully turbulent layer. Hence, two separate
formulas are used to delineate the regions where viscous effects prevail \( (y^* < 11.225) \) and where they become negligible \( (y^* > 11.225) \). A linear formula, Equation 6.1.1, is used in the viscous-affected region and a logarithmic formula, Equation 6.1.2, is used in the fully turbulent region. Given the physical properties of the fluid, \( y^* \) can be computed from Equation 6.1.4 and used to determine the applicable function for finding mean velocity.

Similar functions exist for temperature. This is not surprising since the Reynolds analogy between momentum and energy transfer has long been established. The standard wall functions for temperature are [20]

\[
T^* = Pr_{mol} y^* \quad \text{for} \quad y^* < y^*_T \tag{6.1.5}
\]

\[
T^* = Pr_t \left[ \frac{1}{\kappa} \ln \left( Ey^* \right) + P \right] \quad \text{for} \quad y^* > y^*_T \tag{6.1.6}
\]

where

\[
P = \frac{\pi/4}{\sin(\pi/4)} \left( \frac{A}{\kappa} \right)^{1/2} \left( \frac{Pr_{mol}}{Pr_t} - 1 \right)^{1/4} \left( \frac{Pr_t}{Pr_{mol}} \right)^{1/4} \tag{6.1.7}
\]

The constant \( E \) in this case is 9.793 while the Van Driest constant, \( A \), appearing in Equation 6.1.7 is 26 [20]. Again there are two formulas, one for the thermal conduction sublayer where conduction is important and one for the turbulent region where the effects of turbulence dominate conduction.
The appearance of the molecular Prandtl number, $Pr_{mol}$, in Equations 6.1.5 and 6.1.7 has certain significance. It establishes a relation between the thermal conduction sublayer thickness, $y^*_T$, and the viscous sublayer thickness, $y^*$. For high Prandtl number fluids such as oil, the thermal conduction layer is thinner in comparison to the viscous sublayer. For low Prandtl number fluids such as liquid metals, the inverse is true.

The dimensionless thermal conduction sublayer thickness, $y^*_T$, can be obtained by equating Equations 6.1.5 and 6.1.6. The molecular Prandtl number must be computed first from physical properties but once $y^*_T$ is known, a decision can be made as to which function to use in obtaining the temperature.

There is also an additional standard wall function proposed by Launder and Spalding for determining a turbulent quantity. The function is for the dissipation rate, $\varepsilon$, and is given below [20]

$$\varepsilon^*_T = \frac{C_\mu^{3/4} k^{3/2}}{\kappa y^*_T}$$

(6.1.8)

The above equation is based on the assumption that the production of $k$ and its dissipation rate are in equilibrium. Note that a similar function does not exist for the turbulent kinetic energy. In the near-wall region, the turbulent kinetic energy is obtained from its transport equation and the following imposed boundary condition [20]

$$\frac{\partial k}{\partial n} = 0$$

(6.1.9)
6.1.2 Nonequilibrium Wall Functions Model

The nonequilibrium wall function for mean velocity in the fully turbulent region is sensitized to pressure gradients. This is one of the reasons why this model is an improvement over the standard wall functions model. It is especially true in cases where severe pressure gradients are of concern. The nonequilibrium wall function for \( y^+ > 11.225 \) is given by [20]

\[
\frac{\bar{U} C_{\nu}^{1/4} k^{1/2}}{r_{\infty}, \rho} = \frac{1}{\kappa} \ln \left( E \frac{\rho C_{\nu}^{1/4} k^{1/2} y}{\mu} \right) \tag{6.1.10}
\]

where

\[
\bar{U} = U - \frac{1}{2} \left[ \frac{dp}{dx} \left( \frac{y_v}{\rho \kappa^* k^{1/2}} \ln \left( \frac{y}{y_v} \right) + \frac{y - y_v}{\rho \kappa^* k^{1/2}} + \frac{y_v^2}{\mu} \right) \right] \tag{6.1.11}
\]

and

\[
y_v = \frac{\mu y_v^*}{\rho C_{\nu}^{1/4} k^{1/2}} \tag{6.1.12}
\]

\[
y_v^* = 11.225 \tag{6.1.13}
\]
The nonequilibrium wall functions model also achieves increased improvement over the standard wall functions model in cases of highly nonequilibrium flows. These type of flows cause the proportions of the viscous sublayer and fully turbulent layer to vary along the wall boundary. Such variations render the local equilibrium hypothesis invalid. When the thickness of the viscous sublayer is relatively large, the turbulent kinetic energy dissipation rate will be greater than the turbulent kinetic energy production. Hence, there will be a negative contribution from the source term in the turbulent kinetic energy transport equation. When the thickness is relatively small, just the opposite will occur because the fully turbulent layer, which will exist in greater proportion, will augment the turbulence.

To account for the nonequilibrium effects, a two-layer concept is employed in the nonequilibrium wall functions model with two distinct functions for each of the viscous and fully turbulent layers. The resulting nonequilibrium wall functions for the turbulent quantities are given below [20]

\[
\begin{align*}
\tau &= \begin{cases} 
0, & y < y_v \\
\tau_w, & y > y_v 
\end{cases} \\
k &= \begin{cases} 
\left(\frac{y}{y_v}\right)^2 k_w, & y < y_v \\
k_w, & y > y_v
\end{cases} \\
\varepsilon &= \begin{cases} 
\frac{2\nu k}{y^2}, & y < y_v \\
\frac{k^{3/2}}{C_i y}, & y > y_v
\end{cases}
\end{align*}
\]  

(6.1.14)

where

\[
C_i = \kappa C_{\mu}^{3/4}
\]  

(6.1.15)
6.2 Two-Layer Zonal Model

Wall functions are applicable for high Reynolds number flows and ideal flow situations. For low Reynolds number flows and when the flow situations are less than the ideal, wall functions may not suffice and a more accurate two-layer zonal model may need to be employed. In the two-layer zonal model, the entire domain is divided into the viscous-affected region and the fully turbulent region. A turbulent Reynolds number, \( \text{Re}_t \), is used to distinguish between the two regions and is given by [20]

\[
\text{Re}_t = \frac{D \sqrt{k} y}{\mu} \tag{6.2.1}
\]

where \( y \) is the minimum distance between a point in the domain and the nearest wall [20]

\[
y = \min_{\tilde{r}_{\text{eff}}} \| \tilde{r} - \tilde{r}_w \| \tag{6.2.2}
\]

The above definition allows the demarcation of the two regions in complex geometries and in cases involving multiple walls. When \( \text{Re}_t > 200 \), the region is fully turbulent and when \( \text{Re}_t \leq 200 \), the region is viscous [20].

In the fully turbulent region, a two-equation turbulence model, either \( k-\varepsilon \) or RNG depending on which one is chosen, is employed. In the viscous-affected region, a one-equation model is used. This model solves the transport equation for the turbulent kinetic
energy. $k$ . and employs the following algebraic equation for the calculation of the turbulent kinetic energy dissipation rate, $\varepsilon$ [20]

$$\varepsilon = \frac{k^{3/2}}{\ell_c}$$  \hspace{1cm} (6.2.3)

where

$$\ell_c = c_f \sqrt{1 - \exp \left( - \frac{\text{Re}_e}{A_c} \right)}$$  \hspace{1cm} (6.2.4)

and

$$c_f = \kappa C_{\mu}^{-3/4}$$  \hspace{1cm} (6.2.5)

$$A_c = 2c_f$$  \hspace{1cm} (6.2.6)

The model also gives the following definition for the turbulent viscosity [20]

$$\mu_t = \rho C_{\mu} \sqrt{k \ell_c}$$  \hspace{1cm} (6.2.7)

where
\[ f_\mu = c_{i,y} \left[ 1 - \exp \left( -\frac{\text{Re}_y}{A_\mu} \right) \right] \] (6.3.8)

Note that this definition differs from the one given in the two-equation models. The constant \( A_\mu \), appearing in the above length scale formula is 70 [20].
7. Radiation Models

Radiation models approximate the radiation contribution to the source term in the energy conservation equation. All radiation models employ the radiative transfer equation (RTE) in one form or another. Assuming a gray gas, the radiative transfer equation for an absorbing, emitting, and scattering medium is given by [20]

\[
\frac{dl}{ds} = \frac{a\sigma T^4}{\pi} - (a + \sigma_s)l + \sigma_s \frac{4\pi}{4\pi} \int I(s, \omega) d\omega
\]  

(7.1)

where

\begin{itemize}
  \item \(a\) = absorption coefficient
  \item \(\sigma_s\) = scattering coefficient
  \item \(\sigma\) = Stefan-Boltzmann constant \((5.672 \times 10^{-8} W/m^2 K^4)\)
  \item \(I\) = radiation intensity
  \item \(T\) = temperature
  \item \(s\) = position
  \item \(\omega\) = solid angle
\end{itemize}

The above equation describes the change of radiation intensity in an infinitely small layer of thickness \(ds\). The first term on the right-hand side of Equation 7.1 represents the change in radiation intensity due to emission. The second term represents the change due to absorption and scattering loss while the last term represents that due to scattering gain. Refer to Figure 7.1 for illustration.
Figure 7.1 Radiation heat transfer

The two radiation models that are available within FLUENT are the discrete transfer radiation model (DTRM) and the P-1 radiation model. In the discrete transfer model, the radiation contribution to the source term is determined by solving the RTE for a series of rays. In the P-1 radiation model, the problem of finding the radiation contribution is reduced to solving an equation for the radiation temperature through various substitutions involving the RTE. Detailed descriptions of the two models are given below.
7.1 The Discrete Transfer Radiation Model (DTRM)

When scattering is relatively small in comparison to absorption and emission, the radiation transfer equation becomes [20]

\[
\frac{dI}{ds} = \frac{a \sigma T^4}{\pi} - aI
\]  \hspace{1cm} (7.1.1)

This is the equation used by the discrete transfer radiation model. It is integrated along a series of rays emanating from the faces of each discrete control volume. Integration leads to the change in radiation intensity along each ray and the sum of these changes constitutes the source term in the energy conservation equation.

If the absorption coefficient is constant, integration of Equation 7.1.1 gives [20]

\[
I(s) = \frac{\sigma T^4}{\pi} \left(1 - \exp[-as]\right) + I_o \exp[-as]
\]  \hspace{1cm} (7.1.2)

where \( I_o \) is the initial radiation intensity at the start of the ray. The difference between \( I(s) \) and \( I_o \) would then be the change in radiation intensity contributing to the source term in the energy conservation equation.

\( I_o \) is obtained from boundary conditions. Treatment of the walls, inlets, and outlets as diffuse emitters and reflectors allows \( I_o \) to be determined from knowledge of the net radiation heat flux [20].
\[ I' = \frac{q_{rad}'}{\pi} \quad (7.1.3) \]

The net radiation heat flux, \( q_{rad}' \), is the sum of the reflected portion of incident radiation and the emissive power [20]

\[ q_{rad}' = (1 - \varepsilon_w) q_{rad}^{-} + \varepsilon_w \sigma T^4 \quad (7.1.4) \]

The incident radiation heat flux, \( q_{rad}^- \), appearing in Equation 7.1.4 is defined as [20]

\[ q_{rad}^- = \int I^- d\Omega \quad (7.1.5) \]

where \( \Omega \) is the hemispherical solid angle and \( I^- \) is the intensity of the incoming ray.

The above discussion is valid only for gray gases. For increased accuracy, the DTRM may be utilized with an effective emissivity submodel, which takes into account the non-gray property of the radiating gas. This submodel dispenses with the use of an absorption coefficient in favor of averaged values of absorptivity, \( \alpha \), and emissivity, \( \varepsilon \). The resulting radiation transfer equation is [20]

\[ \frac{dI(0 \rightarrow s)}{ds} = -\frac{d\alpha(T_w, T_r, 0 \rightarrow s)}{ds} I_w - \int_0^{s'} \frac{d^2 \varepsilon}{dsds'} (T(s' \rightarrow s), s' \rightarrow s) I_b(s') ds' \]

\[ -\frac{d\varepsilon}{ds'} (T(s' \rightarrow s), s' \rightarrow s) I_{b,s'=s} \quad (7.1.6) \]
where

\[ I_n = \frac{\sigma T^4}{\pi} \]  

(7.1.7)

Note. the effective emissivity submodel does not alter the basic concept of the DTRM. Changes in radiation intensity, although computed from Equation 7.1.6, still make up the source term in the energy conservation equation.

### 7.2 The P-1 Radiation Model

The P-1 radiation model is actually the lowest order approximation of the more general P-N model. The P-N model was first suggested by Jeans [19] and is based on the expansion of the radiation intensity into an orthogonal series of spherical harmonics. The expansion is given by [12]

\[ I(\mathbf{s}, \omega) = \sum_{n=0}^{\infty} \sum_{m=0}^{n} A_n^m P_n^m \cos \phi \cos \phi + (P_n^m)^2 \sin \phi \cos \phi \]  

(7.2.1)

where \( A_n^m \) are coefficients to be determined by the solution and \( P_n^m \) are the Legendre polynomials. If the above equation were to be substituted into the RTE, an infinite set of
differential equations would have to be solved. For this reason, lower order approximations are used to reduce the equation set to a finite number.

In the P-1 model, \( n \) is set equal to 1 as suggested by the name of the model. This reduces the series in Equation 7.2.1 to the first four terms. Although retaining more terms would provide a more accurate approximation, the P-1 model gives good results in many circumstances without making the problem computationally intensive. When the truncated series of the P-1 model is substituted into the RTE, four differential equations are obtained which can then be solved for the four terms.

The need for a simultaneous solution of the equation set is eliminated through a simplification. If the following definition for the radiation temperature is introduced [20].

\[
\theta_k^* = \frac{I}{4\sigma} \tag{7.2.2}
\]

then an equation for the radiation flux can be obtained from three of the four differential equations in the set. This equation is given by [20]

\[
q = -\frac{4\sigma}{3(a + \sigma)} \nabla \theta_k^* \tag{7.2.3}
\]

The divergence of this radiation flux represents the radiation contribution to the source term in the energy conservation equation and is given below [20].
\[ \nabla q = -\nabla \frac{4\sigma}{3(a + \sigma)} \nabla \theta_R^4 \]  
(7.2.4)

A direct substitution of Equation 7.2.4 is possible provided the distribution of \( \theta_R \) is known.

The distribution of the radiation temperature may be obtained from the radiation heat flux and the other differential equation in the equation set that was not used in its determination. The resulting expression is given below [20]

\[ \frac{1}{3a} \nabla \frac{1}{a + \sigma} \nabla \theta_R^4 - \theta_R^4 + T^4 = 0 \]  
(7.2.5)

The boundary condition for Equation 7.2.5 is [20]

\[ q_n(0) = \frac{\sigma(T_w^4 - \theta_R^4)}{1 - \frac{1}{\varepsilon_w}} \]  
(7.2.6)

It was obtained by substituting Marshak's boundary condition for the incident heat flux \( q_{inc} \) on the boundary [20]

\[ q_{inc} = \varepsilon_w \sigma T_w^4 + (1 - \varepsilon_w) \sigma \theta_R^4(0) + \frac{\varepsilon_w - 1}{2} q_n(0) \]  
(7.2.7)

into the equation for the normal component of the radiation heat flux, \( q_n(0) \) [20]
\[ q_n(0) = \varepsilon \sigma T_w^4 - \alpha_{inc} \]  

(7.2.8)

Unlike the DTRM, the P-1 radiation model takes into account the effects of scattering. For this reason, the P-1 model may be preferred in cases where scattering cannot be neglected. Unfortunately, the P-1 model also has some limitations. For one, it may overpredict the radiation fluxes in problems with localized sources of heat. In addition, there is no option to take into account the non-gray property of gases as in the DTRM. Therefore, the effective emissivity model cannot be employed with the P-1 radiation model.
8. Variable Radiation Parameters Models

The absorption coefficient in the DTRM and the P-1 radiation model can be constant or it can be made to vary with composition. Two variable absorption coefficient models are available in FLUENT. Modak's model is based on Hottel charts that were developed from experiments. The expression for the absorption coefficient is obtained from a direct curve fit of these charts. The weighted-sum-of-gray-gases model (WSGGM) relates the absorption coefficient to the emissivity. In the limit of small pathlength, the gray gas approximation becomes valid and the general expression for the absorption coefficient reduces to a different form. Hence in the WSGGM, two functions for the absorption coefficient are employed.

In addition to the above models, there is a third variable radiation parameter model. This is the effective emissivity submodel mentioned earlier and it relates the absorptivity, \( \alpha \), to the emissivity, \( \varepsilon \). The expression for the emissivity is borrowed from the WSGGM. All three models are discussed next.

8.1 Modak's Model

In this model the emissivity for a gas, as determined from correlated data, is given by

\[ \varepsilon = \varepsilon_c + \varepsilon_{\omega} - \Delta \varepsilon_{\omega} \quad (8.1.1) \]
\( \varepsilon_c \) and \( \varepsilon_w \) are the emissivities for carbon dioxide and water vapor, respectively. They are functions of the gas temperature, \( T \), partial pressures, \( p_{c(w)} \), and mean beam length, \( L \), as shown below [20]

\[
\ln \varepsilon_{c(w)} = \sum_{i=0}^{3} T_i(x) \sum_{j=0}^{3} T_j(y) \sum_{k=0}^{3} c_{ik} T_k(z) \tag{8.1.2}
\]

where

\[
x = 1 + \frac{\ln p_{c(w)}}{3.45} \\
y = \frac{2.555 + \ln(p_{c(w)} L)}{4.345} \\
z = \frac{T - 1150}{850}
\]

\( T_i(x) \) are Chebyshev polynomials of order \( i \) and \( c_{ik} \) are fitting coefficients. The mean beam length, \( L \), may be interpreted as the radius of a hemispherical gas mass whose emissivity is equivalent to that for the geometry of interest. It has been determined for various shapes and representative values are listed in Table 8.1.1 [21].

The correction factor, \( \Delta \varepsilon_{c(w)} \), in Equation 8.1.1 accounts for the reduction in emission that is associated with the mutual absorption of radiation between carbon dioxide and water vapor when both of them are present in a mixture with other nonradiating gases. It is represented by the following expression [20]
\[ \Delta \varepsilon_{\omega} = \begin{cases} \frac{F_1(\xi)F_2(p_c, p_w, L)F_3(T)}{10.7 + 101\xi - \frac{\xi^{10.4}}{111.7}} & (p_c + p_w)L \geq 0.1 \\ 0 & (p_c + p_w)L < 0.1 \end{cases} \] \] (8.1.3)

where

\[ F_1(\xi) = \frac{\xi}{10.7 + 101\xi} - \frac{\xi^{10.4}}{111.7} \]

\[ F_2(p_c, p_w, L) = [\log(101.3(p_c + p_w)L)]^{2.76} \]

\[ F_3(T) = -1.0204\xi^2 + 2.2449\xi - 0.23469 \]

and

\[ \xi = \frac{p_w}{p_w + p_c} \]

\[ \zeta = 0.001T \]

The above expressions are direct curve fits of Hottel charts and hence only hold for the following experimental conditions [20]

\[ 300 \leq T \leq 2000 \text{ K} \]

\[ 0.0011 \leq p_{c(w)} \leq 1.0 \text{ atm} \] (8.1.4)

\[ 0.0011 \leq p_{c(w)}L \leq 5.989 \text{ atm} \cdot \text{m} \]
Table 8.1.1 Mean beam length for various geometries

<table>
<thead>
<tr>
<th>GEOMETRY</th>
<th>CHARACTERISTIC LENGTH</th>
<th>MEAN BEAM LENGTH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere (radiation to surface)</td>
<td>Diameter ($D$)</td>
<td>$0.65D$</td>
</tr>
<tr>
<td>Infinite circular cylinder (radiation to curved surface)</td>
<td>Diameter ($D$)</td>
<td>$0.95D$</td>
</tr>
<tr>
<td>Semiinfinite circular cylinder (radiation to base)</td>
<td>Diameter ($D$)</td>
<td>$0.65D$</td>
</tr>
<tr>
<td>Circular cylinder of equal height and diameter (radiation to entire surface)</td>
<td>Diameter ($D$)</td>
<td>$0.60D$</td>
</tr>
<tr>
<td>Infinite parallel planes (radiation to planes)</td>
<td>Spacing between planes ($L$)</td>
<td>$1.80L$</td>
</tr>
<tr>
<td>Cube (radiation to any surface)</td>
<td>Side ($L$)</td>
<td>$0.66L$</td>
</tr>
<tr>
<td>Arbitrary shape of volume $V$ (radiation to surface of area $A$)</td>
<td>Volume to area ratio ($V/A$)</td>
<td>$3.6V/A$</td>
</tr>
</tbody>
</table>

The absorptivity is related to the emissivity in Equation 8.1.1 through the relation [20]

\[
\alpha = \varepsilon \left( \frac{T}{T_i} \right)^{(0.6-0.25)}
\]  

(8.1.5)

where $T_i$ is the incident radiation temperature from the source. The absorption coefficient is in turn related to the absorptivity via [20]

\[
\alpha = 1 - \exp(-aL)
\]  

(8.1.6)
This is the Modak’s model expression for the variable absorption coefficient. Good results have been obtained with this model regardless of its empirical nature. Unfortunately, Modak’s model is only available for use with the DTRM and it cannot be employed with the effective emissivity submodel.

8.2 The Weighted-Sum-Of-Gray-Gases Model (WSGGM)

In this model, the general expression for the variable absorption coefficient, $a$, is given by [20]

$$a = \frac{-\ln(1 - \varepsilon)}{s} \quad (8.2.1)$$

Here, the emissivity, $\varepsilon$, is approximated using weighting factors [20]

$$\varepsilon = \sum_{i=0}^{I} \alpha_{\varepsilon,i}(T)[1 - \exp(-\kappa_i ps)] \quad (8.2.2)$$

where

- $\alpha_{\varepsilon,i}$ = emissivity weighting factors for the $i^{th}$ fictitious gray gas
- $\kappa_i$ = absorption coefficient for the $i^{th}$ fictitious gray gas
- $p$ = sum of the partial pressures of all absorbing gases
- $s$ = path length
The path length, $s$, can either be specified as a characteristic cell size or as a mean beam length. Using the characteristic cell size is more appropriate in cases where the primary interest is in the distribution of radiation around a source. The mean beam length would be a better choice if the objective is to determine radiation exchange between walls.

When $s \leq 10^{-4}$ m, the gray gas approximation becomes valid and Equation 8.2.1 reduces to [20]

$$a = \sum_{i=0}^{I} a_{e,i} \kappa_i p$$

Hence for $s > 10^{-4}$, FLUENT uses Equation 8.2.1 and for $s \leq 10^{-4}$, Equation 8.2.3 is employed. When $s \approx 10^{-4}$, the two equations are practically identical.

The above equations hold for a total pressure of 1 atm [20]. When the total pressure is not equal to 1 atm, $\kappa_i$ must be rescaled. For $0.9 \leq p \leq 1.1$, the approximations given by Equations 8.2.1 through 8.2.3 may still give reasonable results but for all other pressures $\kappa_i$ must be corrected according to [20]

$$\kappa_i \rightarrow \kappa_i p_i^m$$

where $m$ is a nondimensional value that depends on the total pressure, partial pressures of the absorbing gases, and temperature. The WSGGM has a wider range of applicability than
Modak’s model. In particular, it is not restricted to the range of temperatures for which Modak’s model is applicable and can be used successfully in cases where \( T > 2000 \) \( K \) [20].

### 8.3 The Effective Emissivity Submodel

As discussed previously in chapter 7, the radiation transfer equation used by the effective emissivity submodel is expressed in terms of emissivity and absorptivity. The expression for emissivity is borrowed from the WSGGM and is repeated here for convenience [20]

\[
\varepsilon = \sum_{l=0}^{l} a_{\varepsilon l} \left[T_{l}(1 - \exp(-\kappa_{l}ps))\right] \quad (8.3.1)
\]

Equation 8.3.1 is used to establish an expression for the absorptivity that is used in the effective emissivity model [20]

\[
\alpha(T_{\omega}, T_{\kappa}(0 \rightarrow s), 0 \rightarrow s) = \varepsilon(T_{\omega}, T_{\kappa}(0 \rightarrow s), 0 \rightarrow s) \sqrt{T_{\kappa}/T_{\omega}} \quad (8.3.2)
\]
9. Combustion Models

A reaction mechanism is used to obtain reaction rates that constitute the source terms in the species conservation equations and must therefore be specified whenever species conservation equations are solved. When a large number of species are involved, description of the combustion reaction mechanism becomes exceedingly complex. For the combustion system in this study, the fuel that is injected into the furnace is the by-product of the steel production process and is composed of a mixture of a large number of gases as shown in Table 9.1. Therefore, a reaction mechanism for this case would be difficult to determine.

<table>
<thead>
<tr>
<th></th>
<th>CH$_4$</th>
<th>CO</th>
<th>CO$_2$</th>
<th>H$_2$</th>
<th>H$_2$O</th>
<th>N$_2$</th>
<th>C$_2$H$_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.9</td>
<td>23.7</td>
<td>10.6</td>
<td>25.5</td>
<td>1.3</td>
<td>24.8</td>
<td>1.2</td>
<td></td>
</tr>
</tbody>
</table>

Table 9.1 Fuel composition (% volume)

To avoid specifying the reaction mechanism, it is possible to use a combustion model involving the solution of a conserved scalar from which individual species concentrations are derived. This combustion model is called the Mixture Fraction/Probability Density Function (PDF) formulation and the conserved scalar is the mixture fraction, $f$, defined as [20]
\[ f = \frac{Z_k - Z_{k(0)}}{Z_{kf} - Z_{kO}} \]  

(9.1)

where \( Z_i \) is the mass fraction of species \( k \) and subscripts \( F \) and \( O \) are respectively the fuel and oxidizer stream conditions at inlet. Since it is a conserved scalar, the value of the mixture fraction at a point in the domain can be computed from the solution of its transport equation. The transport equation is given by [20]

\[
\frac{\partial}{\partial x_i} \left( \rho u_i f \right) = \frac{\partial}{\partial x_i} \left( \mu_i \frac{\partial f}{\sigma_i \partial x_i} \right)
\]  

(9.2)

The above equation is Favre-averaged and is written assuming steady-state.

The functional relationship between the instantaneous values of species concentrations and the mixture fraction can be established from the description of the system chemistry. Two options are available for describing the system chemistry with the mixture fraction/PDF model. Both of them do not require knowledge of the reaction mechanism. The first option is the flame sheet approximation where it is assumed that the chemistry is infinitely fast. Hence, fuel and air never coexist. As soon as they mix, the reaction proceeds to the right and they become burned. Such a description of the system chemistry yields a straight-line relationship between the mixture fraction and species mass fractions.

Unfortunately, the flame sheet approximation requires the reaction stoichiometry. This limits its application to the prediction of single step reactions where intermediate species formation and dissociation effects are not considered. Often use of this
approximation in modeling combustion in furnaces with preheated air results in a serious over prediction of peak flame temperature. Luckily, the second option that is available for describing the system chemistry does not require the reaction stoichiometry and can therefore predict the formation of intermediate species and take into account dissociation effects. This option is referred to as the equilibrium assumption and it assumes that the chemistry is fast enough for chemical equilibrium to always exist at the molecular level. With this option, species concentrations or mass fractions are obtained from the mixture fraction by minimizing Gibbs free energy.

The equilibrium assumption can refer to either full or partial equilibrium. Full chemical equilibrium may not be representative of the real combustion process and although it is possible to carry out full equilibrium calculations, assumption of partial equilibrium gives better results in many cases. With this assumption full chemical equilibrium calculations are performed only where the mixture fraction is below a specified rich limit, \( f_{\text{rich}} \). Above this limit, the chemical composition is computed from knowledge of the conditions at the fuel stream inlet and the rich limit since it is assumed that unburned fuel coexists with the combustion products. The partial equilibrium approach is not only characteristic of actual combustion processes but is also less computationally intensive.

With the system chemistry defined, the relationship between the instantaneous values of species concentrations and the mixture fraction can generally be expressed as [20]

\[
\phi_i = \phi_i(f) \quad (9.3)
\]
where $\phi_i$ is the mass fraction or concentration of species $i$. For non-adiabatic systems, the species mass fractions also depend on the enthalpy since changes in enthalpy strongly affect chemical equilibrium calculations. Therefore, whenever heat losses come into play, the relationship between species concentration and mixture fraction generalizes to [20]

$$\phi_i = \phi_i(f, h)$$  \hspace{1cm} (9.4)

Equation 9.4 describes the instantaneous relationship between species concentrations and mixture fraction. In engineering applications however, it is the mean values (or Favre-averaged values) and not the instantaneous values that are of interest. When the mixture fraction/PDF formulation is used, the correlation between instantaneous and mean values is established via a probability density function (PDF). The probability density function is a weighting function and describes the fraction of time that a variable takes on a value in a certain range.

A graphical representation of the probability density function is shown in Figure 9.1. The fraction of time that the mixture fraction, $f$, spends in the range $\Delta f$ is equal to the banded area under the probability density function curve. Mathematically, the probability density function for the mixture fraction is defined as [12]

$$p(f)\Delta f = \lim_{T \to \infty} \frac{1}{T} \sum \tau_i$$ \hspace{1cm} (9.5)

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A joint probability density function extends the above description to two variables. For non-adiabatic systems, a joint PDF would be more appropriate since there is a species concentration dependence on two variables, mixture fraction and enthalpy. However, computation of a joint PDF is not practical. Therefore single variable PDFs are used with the assumption that changes in enthalpy do not significantly impact turbulent enthalpy fluctuations. Such an assumption has proven to be valid in a number of situations.

![Figure 9.1 Graphical representation of the probability density function, $p(f)$](image)

The shape of the probability density function depends on the nature of the fluctuations that are encountered as a result of turbulence. Normally, the shape is different for every situation but several shapes have been observed experimentally more
often than others. These common shapes have been expressed in terms of mathematical functions and are the only ones used in practice to obtain mean values from instantaneous values of species concentrations.

There are two mathematical functions for describing the shape of the PDF in FLUENT. The first function is the double delta function. It is the simplest of the two available functions and is therefore computationally less intensive. The double delta function is given by [20]

\[
p(f) = \begin{cases} 
0.5, & f = \tilde{f} - \sqrt{\tilde{f}''^2} \\
0.5, & f = \tilde{f} + \sqrt{\tilde{f}''^2} \\
0, & \text{elsewhere}
\end{cases} \tag{9.6}
\]

where \(\tilde{f}\) is the Favre-averaged mixture fraction and \(\tilde{f}''\) is the Favre-averaged mixture fraction variance. The shape of the double delta function is shown in Figure 9.2. It corresponds to a square wave temporal distribution of \(f\) and therefore may not be particularly accurate in certain situations. The alternate \(\beta\)-function might be more accurate. It is given by [20]

\[
p(f) = \frac{\int f^{\alpha-1}(1-f)^{\beta-1} \, df}{\int f^{\alpha-1}(1-f)^{\beta-1} \, df} \tag{9.7}
\]

where
\[ \alpha = \tilde{f} \left[ \frac{\tilde{f} (1 - \tilde{f})}{\tilde{f}^* - 1} \right] \]

and

\[ \beta = (1 - \tilde{f}) \left[ \frac{\tilde{f} (1 - \tilde{f})}{\tilde{f}^* - 1} \right] \]

One possible shape of the \( \beta \) function is shown in Figure 9.3 [20].

From Equations 9.6 and 9.7 it can be seen that the shape of the PDF functions depends solely on the Favre-averaged mixture fraction, \( \tilde{f} \), and its variance \( \tilde{f}^* \). As mentioned above, the mixture fraction is obtained from Equation 9.2. Like the mixture fraction, the mixture fraction variance is also obtained from its Favre-averaged transport equation [20]

\[
\frac{\partial}{\partial \tilde{x}_i} \left( \rho u_i \tilde{f}^* \right) = \frac{\partial}{\partial \tilde{x}_i} \left( \mu_i \frac{\partial \tilde{f}^*}{\partial \tilde{x}_i} \right) + C_x \mu_i \left( \frac{\partial \tilde{f}}{\partial \tilde{x}_i} \right) - C_d \rho \frac{\varepsilon}{k} \tilde{f}^* \tag{9.8}
\]

where \( \sigma_i = 0.7 \), \( C_x = 2.86 \), and \( C_d = 2.0 \) [20]. Hence, once the mixture fraction and its variance are known, the shape of the PDF can easily be ascertained. Favre-averaged values can then be computed from instantaneous values as follows [20]
Figure 9.2 Delta function

Figure 9.3 $\beta$-function for $\tilde{f} = 0.3$ and $f'^{1/2} = 0.005$
\[ \tilde{\phi}_i = \int_0^1 p(f) \phi_i(f, h) df \] (9.9)

The mixture fraction/PDF formulation seems to offer the only solution to systems with a large number of species where intermediate species formation and dissociation effects are important. There are unfortunately some restrictions that may render the model unsuitable. One major restriction is that the flow must be incompressible. Therefore, the model cannot be employed in systems where the pressure varies significantly and where compressibility effects have to be accounted. The other restriction is that the diffusion coefficients for all species and enthalpy must be equal. This implies a Lewis number of unity. For turbulent flow this is a good approximation but may not be applicable to every case.
10. Soot Models

Soot is a general term used to describe carbonaceous particulates that are generated during gas-phase combustion processes. In certain applications, soot is undesirable. For example in gas turbines, the erosive nature of soot drastically reduces the life of the turbine blades. Soot is also a major concern because it poses a serious health risk with its tendency to absorb carcinogenic materials. On the other hand, soot is highly beneficial in industrial furnace applications where radiation is the primary mode of heat transfer to the load. This is because in-flame soot exhibits nearly blackbody behavior that is responsible for increases in radiation heat losses from the flame. In industrial furnace applications therefore, the challenge is to promote soot production in such a way that would enhance radiative heat transfer to the load without increasing soot emissions that could pose potential health risks.

In nonpremixed or diffusion flames, soot is widely believed to be formed over a limited range of temperatures. The lower limit of 1300K [22] corresponds to the temperature below which soot combustion or burnout ceases. The upper limit of approximately 1600K [22] is the temperature at which soot emanates from a flame. The exact mechanism of soot formation within this temperature range however, has not yet been conclusively determined but different models describing the mechanism have been proposed. Application of these models results in the prediction of soot concentrations as well as the effect of soot on radiative heat transfer.

The two models within FLUENT for predicting soot concentration are empirically based. Both of them require information about the combustion system but only one is applicable for a wide range of hydrocarbons and does not require inputs that have to be
experimentally obtained specifically for the system being modeled. This model is the two-step Tesner model in which the formation of soot is assumed to occur in two stages. In the first stage, radical nuclei are generated from the gaseous fuel. In the second stage, soot is generated or formed from the nuclei. The model therefore predicts the concentration of the nuclei, \( n \), and through the dependency on these nuclei, the concentration of the soot, \( c_s \).

Both concentrations are obtained from the solution of their transport equations [20]

\[
\frac{\partial}{\partial x_i} \left( \rho u_i n \right) = \frac{\partial}{\partial x_i} \left( \frac{\mu_i}{\sigma_n} \frac{\partial n}{\partial x_i} \right) + \rho R_n \tag{10.1}
\]

\[
\frac{\partial}{\partial x_i} \left( \rho u_i c_s \right) = \frac{\partial}{\partial x_i} \left( \frac{\mu_i}{\sigma_s} \frac{\partial c_s}{\partial x_i} \right) + \rho R_s \tag{10.2}
\]

The terms \( R_n \) and \( R_s \) appearing in the above equations are respectively, the net rates of nuclei generation and soot generation. They are defined as the difference between the corresponding formation and combustion rates [20]

\[
R_n = R_{n,f} - R_{n,c} \tag{10.3}
\]

\[
R_s = R_{s,f} - R_{s,c} \tag{10.4}
\]

where the subscripts \( f \) and \( c \) have been used to denote formation and combustion.

The rate of nuclei formation depends on a spontaneous formation and branching process and is given by [20]
\[ R_{n,t} = \eta_{o} + (f - g)n - g_{o}nN_{s} \]  \hspace{1cm} (10.5)

where \( \eta_{o} \) is the kinetic rate

\[ \eta_{o} = a_{o}c_{f} \cdot \exp\left(-\frac{E}{RT}\right) \]  \hspace{1cm} (10.6)

and

\[ a_{o} = \text{pre-exponential rate constant} \left(1.16 \times 10^{31} \text{ particles/kg s} \right) \]
\[ E/R = \text{activation energy term} \left(9 \times 10^{7} \text{ K} \right) \]
\[ f = \text{linear branching coefficient} \]
\[ g = \text{linear termination coefficient} \left(f - g = 100/s \right) \]
\[ g_{o} = \text{linear termination on soot particles} \left(1 \times 10^{-15} \text{ m}^{3} / \text{ particles s} \right) \]
\[ N_{s} = \text{number of soot particles per m}^{3} \]

The default limiting nuclei formation rate is \(10^{-21}/\text{m}^{3} \cdot \text{s} \) [20] and when the kinetic rate is greater than this value, the term \((f - g)n\) in Equation 10.5 is ignored.

The rate of soot particle formation is a function of the radical nuclei concentration, \( n \), and is shown below [20]

\[ R_{\alpha\beta} = m_{p}(\alpha - \beta N_{S})n \]  \hspace{1cm} (10.7)

where
\( m_p \) = mass of a soot particle
\( \alpha = \) empirical constant \( (1 \times 10^5 / s) \)
\( \beta = \) empirical constant \( (8 \times 10^{-14} \text{ m}^3 \cdot s/\text{number}) \)

The rate of soot combustion is not defined by a single rate expression but is taken to be the minimum of two rate expressions [20]

\[
R_{S,\infty} = \min(R_1, R_2)
\] (10.8)

The first rate, \( R_1 \), is given below and is for regions where the local mean soot concentration is low in comparison to the concentration of the oxidizer [20]

\[
R_1 = Ac_s \frac{\varepsilon}{k}
\] (10.9)

The constant \( A \) appearing above is equal to 4 [20]. The second rate, \( R_2 \), is for regions where the oxidizer concentration is low. In these regions the competition for the oxidizer between the soot and the unburned fuel leads to the following alternative rate expression [20]

\[
R_2 = A \frac{c_{\Omega} \varepsilon}{r_s} \frac{c_s r_s}{k (c_s r_s + c_f r_f)}
\] (10.10)

where
\[ c_f = \text{concentration of oxidizer species} \]
\[ r_s = \text{mass stoichiometry for combustion of soot} \]
\[ c_f = \text{concentration of fuel} \]
\[ r_f = \text{mass stoichiometry for combustion of fuel} \]

The lowest rate from Equations 10.9 and 10.10 determines the rate of soot combustion.

The rate of nuclei combustion, \( R_{n,c} \), is assumed to be directly proportional to the rate of soot combustion as determined from Equation 10.8. This relationship between the rate of nuclei combustion and the rate of soot combustion is given by \([20]\)

\[ R_{n,c} = \frac{n}{c} R_{s,c} \tag{10.11} \]

Substitution of the rate expressions defined above into the transport equations of Equations 10.1 and 10.2 leads to the solution for soot concentration. The extent of the effect of soot on radiative heat transfer depends on soot concentration. However, an additional model has to be employed to estimate this effect.

The one model within FLUENT that can be used in conjunction with the Tesner model is the generalized soot model. The generalized soot model estimates the effect of soot on radiative heat transfer by incorporating the absorption coefficient for soot into the overall absorption coefficient in the radiative transfer equation. The overall absorption coefficient for a mixture of soot and a gas is then calculated as the sum of the absorption coefficient for a pure gas and pure soot \([20]\)
\[ a = a_e + a_i \]  \hspace{1cm} (10.12)

where \( a_e \) is obtained from either WSGGM or Modak's model and \( a_i \) is obtained from [20]

\[ a_e = b_i c_s [1 + b_f (T - 2000)] \]  \hspace{1cm} (10.13)

The constants \( b_i \) and \( b_f \) are equal to 1232.4 and \( 4.8 \times 10^{-4} \), respectively [20].
11. Numerical Solution Procedure

The numerical solution procedure is multi-faceted. A control-volume approach, employing a non-staggered computational grid, is used to transform the governing differential equations into computer solvable, algebraic equations. The resulting algebraic equations are expressed solely in terms of values at the grid cell centers by way of various interpolation schemes. Solutions are obtained with the Line Gauss-Seidel (LGS) solver and multigrid acceleration. In the case of pressure-linked equations, a sequential procedure of the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm is also employed. Details of the various facets of the numerical solution procedure along with a description of convergence can be found below.

11.1 Control-Volume Approach

Differential equations cannot be solved directly using today’s computers. Computers do not understand and cannot process these types of equations. Therefore, if differential equations are to be solved with computer codes, they have to be modified. FLUENT employs a control-volume approach for converting a governing differential equation into a computer solvable, algebraic equation set.

When the control-volume approach is employed, a computational grid has to be formed by dividing the physical domain into discrete control volumes. The size of the computational grid plays an important role in numerical accuracy since the exact solution of
a differential equation is approached with increasing grid size. In most cases, however, solving the governing equations on very fine grids is computationally too intensive. Thus, the size of the computational grid and therefore the numerical accuracy are limited by computer speed and storage capacity. The size of the grid in this work was based on a grid dependency test that was carried out by Zhang et al. [14] for the same experimental furnace. Refer to Appendix C for the grid distribution.

The exact manner in which a differential equation is converted into an algebraic set of equations involves integration over each of the discrete volumes in the computational grid. Integration can be demonstrated most easily for a one-dimensional equation of a scalar quantity, \( \phi \). From Chapter 4, the conservation equation describing the transport of this scalar in the x-direction is written as [12]

\[
\frac{\partial}{\partial x} \left( \rho u \phi \right) = \frac{\partial}{\partial x} \left( \frac{\mu_t}{\sigma_o} \frac{\partial \phi}{\partial x} \right) + S_{\phi} \tag{11.1.1}
\]

When the Divergence Theorem [20]

\[
\int_{V} \frac{\partial}{\partial x} (\rho u \phi) dV = \int_{A} \rho u \phi \cdot dA \tag{11.1.2}
\]

is employed, integration of Equation 11.1.1 over the one-dimensional control volume in Figure 11.1.1 yields [20]
\[(\rho u \phi A)_c - (\rho u \phi A)_w = \left( \frac{\mu_r}{\sigma_s} \right)_c \frac{\phi_E - \phi_P}{\Delta x_c} A - \left( \frac{\mu_r}{\sigma_s} \right)_w \frac{\phi_P - \phi_w}{\Delta x_w} A + S_v \Delta V \] (11.1.3)

The above algebraic expression is the integrated differential equation for that particular control volume. Similar integrations over all the control volumes lead to an algebraic equation set that has the potential of being solved for the discrete values of the unknowns at the control volume centers.

![Figure 11.1 One-dimensional control volume used in demonstrating volume integration](image)

11.2 Interpolation Schemes

The algebraic equations that are obtained from integration, Equation 11.1.1, are not yet in a form that can be solved directly. All of the algebraic equations have to first be expressed solely in terms of the unknowns at the control volume centers. This means that
interpolations schemes have to be applied in order that face values of the unknowns such as the ones appearing in Equation 11.1.3 (i.e. $\phi_e$ and $\phi_w$) are eliminated.

Different schemes are available within FLUENT for interpolating the face values of the unknowns. The scheme that is commonly used is the power law scheme. This scheme implements the following one-dimensional convection-diffusion equation [20]

$$\frac{\partial}{\partial x} (\rho u \phi) = \frac{\partial}{\partial x} \Gamma \frac{\partial \phi}{\partial x}$$

(11.2.1)

The exact solution of the above equation gives the interpolation formula that describes the manner in which the variable $\phi$ varies with $x$ [20]

$$\frac{\phi(x) - \phi_0}{\phi_i - \phi_0} = \frac{\exp \left( Pe \frac{x}{L} \right) - 1}{\exp( Pe ) - 1}$$

(11.2.2)

where $Pe$ is the Peclet number

$$Pe = \frac{\rho u L}{\Gamma}$$

(11.2.3)

Equation 11.2.1 is depicted in Figure 11.2.1.
11.3 Line Gauss-Seidel (LGS) Solver

The unknowns at the control volume centers are solved iteratively using the Line Gauss-Seidel (LGS) solver. This is a line-by-line solver that simultaneously solves the discretized algebraic equations for a single line of cells (control volumes). The process begins with the formulation of a tri-diagonal matrix from the coefficients of the corresponding discretized equations in the line. The matrix is then solved using Gaussian
elimination for the unknowns at the cell centers, giving a solution for a particular line in the domain. Once a solution is obtained for the first line, the LGS proceeds to the next line until the entire domain has been traversed. At that time, if the convergence criterion has not been met, the entire procedure used by the LGS is repeated using updated values from the previous iteration. Note that during the first iteration, unknown values that are required in order to solve the matrix are by default assumed to be zero except in the case of temperature which is assumed to be 273 K [20].

In FLUENT, the direction along which the discretized equations are grouped is not arbitrary and has to be specified. The direction along which the discretized equations are grouped is termed the sweep direction while the direction in which the LGS traverses the domain is called the marching direction. The sweeping direction is normally perpendicular to the flow direction and is often alternated such that boundary condition information is propagated to all parts of the domain.

For equations that have difficulty converging, it is also possible to specify that the equations be solved by marching across the domain a multiple number of times during a single iteration. This improves the accuracy during each iteration since updated values are propagated through the domain with each sweep.

11.4 Multigrid Acceleration

Generally, the LGS is a good solver for reducing local errors but is much less effective in reducing global errors. For this reason, multigrid acceleration of the line solver
is often used to speed up the convergence rate. The technique that is employed by multigrid acceleration involves solving discretized equations on a coarser grid level. The coarser grid level is constructed from the original computational grid by grouping together neighboring control volumes. The corresponding discretized equations that are to be solved on this coarser grid level are obtained by summing a group of discretized equations in various subregions of the original grid. Solution of the discretized equations via the alternating direction LGS yields a correction field, which is then transferred to the finer grid level in an effort to reduce the global error.

The criteria used for determining sufficient convergence of the correction equations is the termination criteria [20]

\[ R_i < \alpha R_o \]  

(11.4.1)

\( R_i \) is the absolute sum of the residuals at the current iteration and \( R_o \) is the residual that was originally obtained on that particular grid level. The termination criteria parameter, \( \alpha \), has a default value of 0.1 [20]. When the above condition is satisfied, the correction equations are considered to be sufficiently converged.

In cases where the coarse grid corrections are slow to converge, an even coarser grid may be used to compute the global corrections. The use of additional coarser grid levels creates a hierarchy of grid levels up to a maximum of eight levels. Coarser grids are visited when the residual reduction on the current level is too slow. The criteria for determining when the next grid level is visited is given by [20]
\( R_i > \beta R_{i-1} \)  \hspace{1cm} (11.4.2)

\( R_{i-1} \) is the absolute sum of the residuals at a previous iteration. The fraction, \( \beta \), is called the residual reduction parameter and has a default value of 0.7 [20].

11.5 The Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) Algorithm

Together with the continuity equation, the momentum equations in the three coordinate directions make up four equations that can be simultaneously solved for four unknowns, \( u_1, u_2, u_3 \) and \( p \). However, a simultaneous solution is computationally too intensive. For this reason, special algorithms are required to solve any pressure-linked equations in which pressure appears as an additional unknown. These algorithms employ a sequential solution procedure.

The default algorithm in FLUENT is the Semi-Implicit Method for Pressure-Linked Equations (SIMPLE). It begins with a guessed pressure field, \( p^* \). This guessed pressure field is substituted into the discretized momentum equation, which is shown below in shortened notation for the one-dimensional case [20]

\[
A_p u_p = \sum_{NB} A_{NB} u_{NB} + (p_w - p_c) A + S \quad (11.5.1)
\]
Coefficients $A_p$ and $A_{NB}$ represent the sum of the convective and diffusive contributions while subscript $NB$ represents the neighboring points $E$ and $W$. The resulting momentum equation is then solved iteratively using the LGS solver for the guessed velocity field, $u^*$.

Once the guessed velocity field is obtained, the actual pressure and velocity fields in the discretized momentum equations are replaced by the guessed fields and unknown field corrections [20]

\[ u = u^* + u' \]  \hspace{1cm} (11.5.2)

\[ p = p^* + p' \]  \hspace{1cm} (11.5.3)

The guessed fields are then eliminated from the resulting equation (i.e. by subtracting a momentum equation that is in terms of guessed values) yielding a momentum balance that is only in terms of the pressure and velocity field corrections, $p'$ and $u'$ [20]

\[ A_p u'_p = \sum_{NB} A_{NB} u'_{NB} + (p'_w - p'_e) A \]  \hspace{1cm} (11.5.4)

The term involving the summation in Equation 11.5.4 goes to zero at convergence. By dropping this term for convenience and rearranging, a useful relation between velocity and pressure corrections is obtained [20]

\[ u'_p = \frac{1}{A_p} (p'_w - p'_e) A \]  \hspace{1cm} (11.5.5)
This relation can be substituted into the continuity equation involving guessed and corrected velocities to yield an equation that can be solved for the pressure corrections [20]

\[
(\rho Au^*)_c - (\rho Au^*)_w + (\rho A)_c \frac{1}{(A_p)_c} (p'_r - p'_e) - (\rho A)_w \frac{1}{(A_p)_w} (p'_w - p'_r) = 0
\]  
\[\text{(11.5.6)}\]

With the pressure corrections known, the velocity corrections can in turn be obtained from Equation 11.5.5 and both corrections can then be used to update the actual velocity and pressure fields via Equations 11.5.2 and 11.5.3.

11.6 Judging Convergence and Speeding up the Convergence Rate

The residuals referred to in Equations 11.4.1 and 11.4.2 provide a measure of the state of imbalance of the discretized equations. Unless the solution is exact, the right-hand side of the discretized equations will not equal the left-hand side of the equations. As an example, the residual of Equation 11.5.1 summed over all the computational points is given by [20]

\[
R = \sum_{\text{nodes}} \left| \sum_{NB} A_{NB} u_{NB} + S_c - A_p u_p \right|
\]  
\[\text{(11.6.1)}\]

where the pressure term has been incorporated into \( S_c \).
Residuals that are reported in FLUENT are normalized by default. An example of a normalized residual is given below for a variable $\phi$ [20]

$$\bar{R} = \frac{\sum_{nodes\ P} \left| \sum_{NB} A_{NB} \phi_{NB} + S_c - A_P \phi_P \right|}{\sum_{nodes\ P} A_P \phi_P} \quad (11.6.2)$$

The normalized residuals for velocity and pressure are slightly different however. In the case of velocity, the denominator is given by [20]

$$\sum_{nodes\ P} \left| A_P \sqrt{u_P^2 + v_P^2 + w_P^2} \right| \quad (11.6.3)$$

and in the case of pressure, normalization is defined as [20]

$$\bar{R} = \frac{R_1}{R_2} \quad (11.6.4)$$

These normalized residuals are useful for monitoring the progress of a solution. Generally, for a solution to be considered converged, the normalized residuals for enthalpy and radiation have to be on the order of $10^{-6}$ and on the order of $10^{-3}$ for all other variables [20]. Hence, the speed at which normalized residuals approach these orders are an indication of the convergence rate of the solution. A steep reduction in the normalized residuals would indicate that the solution is converging quickly. On the other hand, if the normalized
residuals remain constant or are increasing, the solution is not advancing and steps have to be taken to speed up the convergence rate.

One way to speed up the convergence without altering the numerical procedure is by changing the underrelaxation parameters. Underrelaxation parameters are used to reduce the change in a variable during an iteration. Instead of being replaced by a new value computed at the current iteration, the old value is updated by adding to it a fraction of the change in the variable [20]

\[ \phi_p' = \phi_{p,old} + \alpha \Delta \phi_p \]  

(11.6.5)

where \( \alpha \) is the underrelaxation parameter. Generally, improvement in the convergence rate can be achieved by increasing the underrelaxation parameters when the normalized residuals are constant or decreasing. When the normalized residuals are increasing, more conservative values of the underrelaxation parameters should be used.
12. Results and Discussion

12.1 First Set of Operating Conditions

A total of 14 different cases were modeled using the first set of operating conditions. For a list of the cases, refer to Table 12.1.1. The first case consists of the $k-\varepsilon$ turbulence model, the standard wall function model, the P-1 radiation model with the weighted-sum-of-gray gases variable radiation parameters model and a path length that is based on the characteristic cell size, and the mixture fraction/probability density function combustion model that employs a Beta PDF. This is the control case from which the all other cases are derived. As can be seen, the models in each case are almost identical to Case 1 except for one model that separates it from the control.

12.1.1 Velocity and Temperature Distributions

The velocity and temperature distributions on the horizontal plane that cuts through the air injection ports and the temperature distribution for the slab were obtained for the first 11 cases and are shown in Appendix A. The distributions are similar from case to case and the corresponding contour maps that are shown for Case 3 in Figures 12.1.1, 12.1.2, and 12.1.3 are representative of the type of conditions that are obtained with the different cases.

Figure 12.1.1 shows the velocity distribution. From this figure, it can be seen that the jet streams from the burners maintain a direction that is almost straight toward the opposite
| Case 1 (Control) | $k-\varepsilon$ model, standard wall function model, P-1 model with WSGGM and a path length that is based on the characteristic cell size, mixture fraction/PDF model with a Beta PDF |
| Case 2 | **RNG model**, standard wall function model, P-1 model with WSGGM and a path length that is based on the characteristic cell size, mixture fraction/PDF model with a Beta PDF |
| Case 3 | **RSM**, standard wall function model, P-1 model with WSGGM and a path length that is based on the characteristic cell size, mixture fraction/PDF model with a Beta PDF |
| Case 4 | **RSM with directional diffusivity**, standard wall function model, P-1 model with WSGGM and a path length that is based on the characteristic cell size, mixture fraction/PDF model with a Beta PDF |
| Case 5 | $k-\varepsilon$ model, **nonequilibrium wall function model**, P-1 model with WSGGM and a path length that is based on the characteristic cell size, mixture fraction/PDF model with a Beta PDF |
| Case 6 | $k-\varepsilon$ model, standard wall function model, P-1 model with WSGGM and a path length that is based on the characteristic cell size, **mixture fraction/PDF model with a Delta PDF** |
| Case 7 | $k-\varepsilon$ model, standard wall function model, P-1 model with WSGGM and a path length that is based on the **mean beam length**, mixture fraction/PDF model with a Beta PDF |
| Case 8 | $k-\varepsilon$ model, standard wall function model, P-1 model with a constant absorption coefficient of 0.5, mixture fraction/PDF model with a Beta PDF |
| Case 9 | $k-\varepsilon$ model, standard wall function model, **DTRM with Modak's model**, mixture fraction/PDF model with a Beta PDF |
| Case 10 | $k-\varepsilon$ model, standard wall function model, P-1 model with a WSGGM and a path length that is based on the characteristic cell size, mixture fraction/PDF model with a Beta PDF, **Tesner model with C2H4 defined as the fuel** |
| Case 11 | $k-\varepsilon$ model, standard wall function model, P-1 model, P-1 model with a WSGGM and a path length that is based on the characteristic cell size, mixture fraction/PDF model with a Beta PDF, **Tesner model with CH4 defined as the fuel** |
| Case I | $k-\varepsilon$ model, **two-layer zonal model**, P-1 model with a WSGGM and a path length that is based on the characteristic cell size, mixture fraction/PDF model with a Beta PDF |
| Case II | $k-\varepsilon$ model, standard wall function model, **DTRM with WSGGM and a path length that is based on the characteristic cell size, mixture fraction/PDF model with a Beta PDF** |
| Case III | $k-\varepsilon$ model, standard wall function model, **DTRM with the effective emissivity submodel**, mixture fraction/PDF model with a Beta PDF |

*Table 12.1.1 List of cases*
end of the wall. Very little deviation occurs from a straight path since the air is injected into the burners at a high velocity and the distance between inlet and exhaust ports is relatively short. Distinct recirculation zones between the jet streams and the walls can also be seen from this figure. These recirculation zones are induced by the interaction between two opposing, high velocity jet streams and flow impingement on the walls.

![Figure 12.1.1 Case 3 velocity distribution on the horizontal plane that cuts through the air injection ports](Image)

The temperature distribution on the horizontal plane that cuts through the air injection ports is depicted in Figure 12.1.2. In this figure, the main reaction zones are represented by high levels of temperature. These temperatures generally tend to be higher downstream from the slab inlet and are a consequence of the heat that is transferred to the slab as it moves along the furnace floor. Maximum temperatures for the various cases range anywhere between 1758 K to 1832 K.
The last figure. Figure 12.1.3 shows the temperature distribution for the slab with a clearance of 0.25 m on either side (represented by additional horizontal lines on the top and bottom). As can be seen, the temperature of the slab increases from one end of the furnace to the other as it absorbs heat from the main combustion reaction. It can also be seen that the change in the temperature along the longitudinal direction gradually diminishes as the slab advances. This is indicated by the increase in the distance between the temperature contours. Depending on the case, the final temperature at which the slab exits the furnace ranges from 1585 K to 1621 K.
12.1.2 Validation

The energy flow rates and the centerline slab temperature distribution were validated against experimental data from the NKK Corporation [23] for which uncertainty information has not been provided. The results of the validation for the energy flow rates are summarized in Table 12.1.2 for cases 1 through 11. All of the values are in kilowatts except for the quantities in parentheses, which represent the percentage error between the predictions and the measurements, and the quantities in the square brackets, which represent percent difference between the energy input and predicted energy output rates.

The overall energy balances in the table appear to be quite good for all 11 cases. The differences between energy input and output rates are nearly equal and are all very close to
<table>
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<tr>
<th>Experimental Data</th>
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<td>Flue gas at burner exhausts</td>
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<td>8.75</td>
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<td>3279.66</td>
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</tr>
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<td>2137.58</td>
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<td>3694.65</td>
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<td>2137.58</td>
<td>3697.98</td>
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</tr>
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<td>Case 9</td>
<td>8.75</td>
<td>2137.58</td>
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<td>Case 10</td>
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<td>3698.91</td>
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<tr>
<td>Case 11</td>
<td>8.75</td>
<td>2137.58</td>
<td>3699.44</td>
<td>2306.66</td>
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Table 12.1.2 Energy flow rates for cases 1 through 11
0.9%. Cases 2, 6, and 8 appear to have the lowest percent differences at 0.89%, 0.88%, and 0.88%, respectively.

Unusually high percentage errors that fall in the range of 73.48% and 89.1% are also noticed for the auxiliary exhausts. These large errors can be attributed to the presence of temperature gradients in the vicinity of the outlet. When they are present, predicted results that report average values can deviate significantly from measurements taken at a single location. Increasing the number of measurements near the auxiliary exhaust should aid in establishing a better correlation between predicted and measured values.

Table 12.1.2 also shows that cases with different radiation models and models that have a direct impact on radiation heat transfer have the greatest slab heat transfer percentage errors. The results of these models are particularly sensitive since in all of the cases about 98% of the heat is transferred to the slab by radiation and the rest is transferred by convection. The largest percentage errors are exhibited by Cases 7 and 9, which underpredict the heat transfer rates by 3.5% and 4%, respectively. These percentages indicate that the cell based approach for defining the path length is more accurate than the mean beam length method of Cases 7 and 9.

Relatively high percentage errors for the slab are also seen in Cases 10 and 11. These cases were expected to predict the highest heat transfer rates because of the additional soot models. Instead, the soot models underpredicted the heat transfer to the slab by 1.44% for Case 10 and 1.38% for Case 11. These discrepancies can be attributed to a number of weaknesses in the soot models. Probably the greatest weakness in the Tesner soot model is its inability to base the calculations on a mixture of gases. It only allows one type of gas to be specified as the fuel, which lends itself to error when a mixture of gases is part of the
problem definition. The Tesner soot model is also semi-empirical in nature and unless experimental data is defined explicitly, the default soot modeling parameters are set for the combustion of acetylene. Although, these parameters are generally applicable for a wide range of hydrocarbons, they still introduce a certain level of uncertainty to the results. The generalized soot model that estimates the effect of soot on radiation is also a weak model. The model’s expression for the absorption coefficient of soot is based on the results of two other approximations. This reduces the accuracy with which it can predict results.

The results of the centerline slab temperature validation are presented in Figure 12.1.4. This figure shows good agreement between predicted and experimental results for all Cases except 7 and 9. In fact, the agreement is almost the same from case to case. At the slab inlet, the temperature is slightly overpredicted, and at the slab outlet, it is slightly underpredicted. The discrepancy at the slab inlet lies in the problem definition and in the fact that the slab speed is an average that is based on a 10 min interval. In reality, one slab (0.5 m long) is pushed into the furnace in 10s and 9 min and 50 s elapse before the next slab is introduced.

The large percentage errors that were noted in the slab heat transfer rates for Cases 7 and 9 are also evident in Figure 12.1.4. As can be seen, both of these cases exhibit strong deviation from experimental measurements. Cases 10 and 11 in the figure also appear to deviate slightly more than the other cases. This confirms the inadequacy with which the soot models simulate the effect on heat transfer.
Figure 12.1.4 Slab temperature distributions at $y = 2\ m$
12.1.3 Computational Effort

On average, a converged solution was obtained after four and a half days on a Silicon Graphics Indy (SGI) station using version 4.44 of Fluent. The SGI is a 133 MHz IP22 processor with 64 MB of main memory, a data cache size of 16 KB, and a secondary cache size of 512 KB. It is configured with IRIX 6.2 as a dataless client so that the operating system and applications are all loaded over the network. The size of the two local disks, the temp and swap file systems, are 1 GB and 512 MB, respectively.

In all of the cases, underrelaxation factors were changed to speed up the convergence. Some difficult cases however, required the use of conservative underrelaxation factors and initial guesses to further reduce the computational time.

Table 12.1.3 lists all of the cases, in order of increasing computational effort for each class of models. Since the number of iterations required to reach convergence is dependent on underrelaxation factors, the order was based on the complexity of the models. The type and number of equations in each model gives a good indication of the efficiency with which the model can predict the results in relation to the other models. For example, from the turbulence models, the \( k-\varepsilon \) model requires the least amount of computational effort. Since it has less terms and functions in the governing equations and a lesser degree of nonlinearity than either the RNG or RSM turbulence models, it is also the simplest model out of all the turbulence models. On the other hand, the RSM with directional diffusivity is the most complex model and requires the most amount of effort. It has six more transport equations than the \( k-\varepsilon \) and RNG models and the equations that are used to account for directional diffusivity are much more elaborate than the ones that do not take anisotropy into
consideration. In fact, due to the complexity that is associated with the RSM model, the solution that was obtained with the $k-\varepsilon$ model was used as a starting guess to initiate turbulent flow calculations for the RSM model. The same correlation between computational effort and level of complexity can be established for the remaining models in Table 12.1.3.

As can be seen from the table, the complexity of the models in some instances appear to be the same. This is true in the case of the soot models and the P-1 radiation models that use the WSGGM based on the mean beam length and the characteristic cell size. Unfortunately, without a quantitative comparison there is always some doubt as to whether these models have the exact same computational requirements.

Table 12.1.3 also shows that cases with roman numerals have the most computationally intensive models. In fact, a converged solution was not obtained in either Cases II or III. The amount of time (more than two weeks) that was estimated for a converged solution in these cases did not justify their use in furnace simulations. Case I on the other hand, did converge successfully. However, the results were completely unrealistic. In this case, the two-layer zonal model was rendered ineffective because the grid was too coarse in the near wall region. The only solution of increasing the grid size however, would have added to its computational effort. For this reason, no further attempts were made at simulating the case on a finer grid.

12.2 Second Set of Operating Conditions

From the first set of operating conditions, the three best cases in terms of both accuracy and computational effort are Case 1, Case 6, and Case 8. In all of these cases, good agreement was achieved between the predictions and the measurements. However, since
<table>
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<td></td>
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<td>DTRM with Modak’s model</td>
</tr>
<tr>
<td></td>
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<td>DTRM with the effective emissivity model</td>
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<tr>
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<td>1</td>
<td>Case 11</td>
<td>Tesner model with (CH_4) defined as the fuel</td>
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</tbody>
</table>

*Table 12.1.3 List of cases in order of increasing computational effort for each class of models*

the key in governing the selection. All three cases are therefore associated with models that require the least amount of computational effort from their class. These three cases, Case 1, 6, and 8, were modeled using the second set of operating conditions in order to study their performance when the fuel distribution is non-uniform. To reflect the fact that they were modeled with the second set of operating conditions, the cases were renamed to Case 12, 13, and 14, respectively.
12.2.1 Velocity and Temperature Distributions

The velocity and temperature distributions on the horizontal plane that cuts through the air injection ports and the temperature distribution for the slab are shown in Appendix B for the three cases with the second set of operating conditions. The velocity contour maps for the three cases appear to be very similar. As with the first set of operating conditions, the jet streams are aimed directly toward the opposite end of the wall. Recirculation zones are also noticed, however, this time they appear only in Zone#1. In Zone#2 the air is injected at a lower velocity and as seen in cases 13 and 14, this velocity is just low enough to preclude recirculation zones from forming. The velocity difference between the two zones is also evident from the flame size. The long flame in Zone#1 and the shorter flame in Zone#2, clearly indicate that the jet stream velocity in Zone#1 is higher.

The temperature distributions for the center of the furnace show high temperature levels in the main reaction zones. This was also evident in the cases with the first set of operating conditions. However, in Cases 13 and 14, the levels at the center of these zones differ from the ones seen in Case 12. In Case 12, the temperatures are highest in Zone#1 while in Cases 13 and 14 they are highest in Zone#2. This difference can be attributed to the competing effect that exists between Zone#1, which has the higher air and fuel input rates, and Zone#2, which has the higher slab temperature. It can also be noted that the temperature distribution in all three cases is more uniform then the temperature distributions that were obtained with the first set of operating conditions. This is a direct result of the non-uniform fuel input.
The slab temperature distributions for the three cases with the second set of operating conditions do not reveal anything new from the cases with the first set of operating conditions. From these distributions, it can still be seen that the slab temperature increases as it travels downstream from the slab inlet and that the temperature gradients in this same direction decrease gradually.

### 12.2.2 Validation

The temperatures predicted by the three cases were validated against experimental measurements on five horizontal planes at $z = 0.5, 1.0, 1.5, 2.0,$ and $2.5$ m. These measurements were also obtained from the NKK Corporation and the corresponding distributions for $x = 3, x = 5, y = 1.2,$ and $y = 2$ m are shown in Figures 12.2.1 through 12.2.4, respectively. As the figures show, the predicted temperature distributions are very similar from case to case. In addition, the agreement between the predictions and measurements is generally good for all three cases. Considering the uncertainty that is associated with the experimental data, the dependence of accuracy on the numerical solution, the assumptions that were made in the development of the various models, as well as the complexity that is involved in simulating the interaction between turbulence, combustion, and heat transfer, the predicted temperature distributions follow the trends of the experimental measurements quite well.

In Figures 12.2.3 and 12.2.4, the temperature distributions exhibit an increasing trend in the $x$-direction. This has been noted previously and is a result of heat from the slab being
Figure 12.2.1: Comparisons of flue gas temperatures at $x = 3\ m$ and a) $z = 0.5\ m$; b) $z = 1\ m$; c) $z = 1.5\ m$; d) $z = 2\ m$; e) $z = 2.5\ m$

Figure 12.2.2: Comparisons of flue gas temperatures at $x = 5\ m$ and a) $z = 0.5\ m$; b) $z = 1\ m$; c) $z = 1.5\ m$; d) $z = 2\ m$; e) $z = 2.5\ m$
Figure 12.2.3: Comparisons of flue gas temperatures at y = 1.2 m and a) z = 0.5 m; b) z = 1 m; c) z = 1.5 m; d) z = 2 m; e) z = 2.5 m

Figure 12.2.4: Comparisons of flue gas temperatures at y = 2 m and a) z = 0.5 m; z = 1 m; c) z = 1.5 m; d) z = 2 m; e) z = 2.5 m
transferred to the surrounding flue gases. The temperature of the flue gases increases due to an increase in the slab temperature as it advances in the x-direction.

The highest temperatures in Figures 12.2.3 and 12.2.4 are observed at z = 1.5 m, which corresponds to the horizontal plane that cuts through the air injection ports. On this plane, the peaks in the temperature distribution that represent the main reaction zones are higher than the peaks that are seen on the z = 1 m and z = 2 m planes. This is evident from a comparison between Figures 12.2.3 and 12.2.4 (b) through (d). The fact that peaks are not seen at z = 0.5 m and z = 2.5 m indicates that the high temperatures of the main reaction regions dissipate into the surroundings by the time these planes are reached.

In Figures 12.2.1 and 12.2.2, the temperature distributions exhibit a constant trend in the y-direction on all planes except z = 1.5 m. On the z = 1.5 m plane, the temperature distributions correspond to the temperature distributions of the main reaction zones. Figure 12.2.1 (c) depicts the temperature distribution of the second main reaction zone while Figure 12.2.2 (c) depicts the temperature distribution of the third main reaction zone. The two figures appear symmetrical because the second burner is fired from the back wall (y = 4 m) and the third burner is fired from the front wall (y = 0 m).

Both Figures 12.2.1 (c) and 12.2.2 (c) reveal that the maximum temperatures on the z = 1.5 m plane are reached approximately three quarters of the way downstream from the injection ports. In approximating this location, the high temperatures that are seen near the burner inlets at y = 4 m in Figure 12.2.1 (c) and at y = 0 m in Figure 12.2.2 (c) were not taken into consideration because they represent the incoming combustion air. The maximum temperatures that are referred to above only pertain to flue gases.
From Figures 12.2.1 through 12.2.4 it can be seen that at \( z = 1.5 \) m, the temperatures are overpredicted at a number of locations. This may be the result of buoyancy terms in the turbulence models, which have the effect of raising the flame temperature. Figures 12.2.3 (c) and 12.2.4 (d) also show that the temperature at \( x = 7 \) m, which corresponds to the temperature in the fourth main reaction zone, is overpredicted by a larger margin than any of the other temperatures on the same plane (\( z = 1.5 \) m). This larger discrepancy can be further attributed to the heat that is lost through the clearance around the slab at the downstream end of the furnace (slab outlet).

Figures 12.2.1 (d) and 12.2.4 (d) also show a very large discrepancy between the predicted and measured temperatures for the second main combustion zone. In Figure 12.2.1 (d), which shows the temperature profile for the second main combustion reaction, the experimental temperature at \( y = 2 \) m is significantly higher than the temperatures that were predicted with the different cases at that same location. This same discrepancy is evident at \( x = 3 \) m in Figure 12.2.4 (d). Since the temperature that was measured on this plane is about 40° higher than the temperature that was measured at the same location (\( x = 3 \) m, \( y = 2 \) m) on the \( z = 1.5 \) m plane, the discrepancy is probably partly a result of experimental error. As noted earlier, the temperatures of the main reaction zones are generally higher on the \( z = 1.5 \) m plane that cuts through the injection ports.
13. Conclusions and Recommendations

This work provided an evaluation of the numerical models within FLUENT in terms of their predictive capability in simulating combustion in a regenerative, slab reheat furnace. Based on this evaluation, a number of conclusions can be made. Firstly, the amount of time that is required to obtain a converged solution in cases with the two-layer zonal model, the DTRM with WSGGM based on the path length, and the DTRM with the effective emissivity model does not justify their use in furnace simulations. Computationally intensive and time-consuming models cannot be afforded due to the pressure that has been put on industry to reduce fuel consumption and pollution.

Secondly, radiation models that define the path length in terms of the characteristic cell size should take precedence over models that define it in terms of the mean beam length. Cases based on the mean beam length were less accurate and underpredicted the heat transfer to the slab by relatively larger percentages. Since the accuracy with which the heat transfer to the slab is predicted is absolutely critical in determining fuel efficiency and energy conservation, the cell-based approach is the better choice. The same argument can be used for cases that employ the soot models. However, it is important to note that soot models do play an important role in radiation heat transfer to the slab. The relatively large errors that were obtained when these soot models were introduced were attributed to a number of weaknesses in the models. Therefore other new and improved soot models should not be completely dismissed.

Lastly, it can be concluded that the three best cases in terms of accuracy and computational effort are also the best choices for use as design tools in simulating
combustion in a regenerative slab reheat furnace. These three cases, which employ the $k-\varepsilon$ turbulence model, the Delta PDF, and a constant absorption coefficient, showed very good agreement between the predictions and experimental measurements both when the fuel load was uniform and when it was non-uniform. Considering the difficulties that are associated with modeling such advanced combustion systems, the cases can be expected to reproduce the velocity and temperature fields with confidence in other situations as well.

Overall, the work was successful in showing the potential of CFD in design. One recommendation that can be made for the future is to improve the present soot models within FLUENT. Future work might also include attempts at validating cases that simultaneously incorporate the Delta PDF and a constant absorption coefficient and obtaining turbulence parameter measurements for validation of the turbulence models. A sensitivity analysis might also be conducted in order to investigate the effect of changes in the empirical parameters.
Bibliography


17. Hino, Y. Zhang, C., and Sugiyama, S. Comparison of Measurements and Predictions of Flame Structure and NOx Emission in a Gas-Fired Furnace


23. NKK Corporation, *Materials and Processing Research Center*, Fukuyama, Japan
APPENDIX A

Velocity and temperature distributions obtained with the first set of operating conditions
**CASE2**

Velocity Magnitude (M/S)

$L_{max} = 8.370E+01$  $L_{min} = 0.000E+00$

---

**Nov 19 1998**

Fluent 4.48

Fluent Inc.
CASE 6
Velocity Magnitude (M/S)
Lmax = 8.370E+01  Lmin = 0.000E+00
Fluent 4.48
Fluent Inc.
CASE 8
Velocity Magnitude (M/S)
Lmax = 8.370E+01  Lmin = 0.000E+00

Nov 19 1998
Fluent 4.48
Fluent Inc.
CASE 10
Velocity Magnitude (M/S)
Lmax = 8.370E+01  Lmin = 0.000E+00
CASE2

Temperature (K)

Lmax = 1.789E+03  Lmin = 1.379E+03

Nov 19 1998
Fluent 4.48
Fluent Inc.
CASE 5
Temperature (K)
Lmax = 1.778E+03  Lmin = 1.470E+03
CASE 7
Temperature (K)
Lmax = 1.830E+03  Lmin = 1.486E+03

Nov 19 1998
Fluent 4.48
Fluent Inc.
CASE 8
Temperature (K)
Lmax = 1.804E+03  Lmin = 1.449E+03

Nov 19 1998
Fluent 4.48
Fluent Inc.
CASE 9
Temperature (K)
Lmax = 1.832E+03  Lmin = 1.431E+03
CASE 3
Temperature (K) At Cell Centers
Lmax = 1.600E+03  Lmin = 3.720E+02
CASE 5
Temperature (K) At Cell Centers
Lmax = 1.595E+03  Lmin = 3.724E+02

Nov 19 1998
Fluent 4.48
Fluent Inc.
CASE 6
Temperature (K) At Cell Centers
Lmax = 1.585E+03   Lmin = 3.714E+02

Fluent 4.48
Fluent Inc.
CASE 9

Temperature (K) At Cell Centers

$L_{\text{max}} = 1.611E+03 \quad L_{\text{min}} = 3.533E+02$

Nov 19 1998
Fluent 4.48
Fluent Inc.
CASE 10
Temperature (K) At Cell Centers
Lmax = 1.591E+03  Lmin = 3.699E+02

Nov 19 1998
Fluent 4.48
Fluent Inc.
CASE 11
Temperature (K) At Cell Centers
Lmax = 1.592E+03  Lmin = 3.698E+02
APPENDIX B

Velocity and temperature distributions obtained with the second set of operating conditions
CASE 12
Temperature (K) At Cell Centers
Lmax = 1.436E+03  Lmin = 3.432E+02

Nov 19 1998
Fluent 4.48
Fluent Inc.
CASE 13
Temperature (K) At Cell Centers
Lmax = 1.441E+03  Lmin = 3.436E+02

Nov 19 1998
Fluent 4.48
Fluent Inc.
APPENDIX C

Computational grid and sample case file
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Centerra Resource Park
10 Cavendish Court
Lebanon, New Hampshire 03766 USA
(800) 445-4454

----------------------------------------
Number of Cells and Species Dynamically Allocated
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<td>N</td>
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<td>7</td>
<td>ACCELERATION</td>
<td>M/S2</td>
<td>1.000E+00</td>
</tr>
<tr>
<td>8</td>
<td>ENERGY</td>
<td>J</td>
<td>1.000E+00</td>
</tr>
<tr>
<td>9</td>
<td>POWER</td>
<td>W</td>
<td>1.000E+00</td>
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<td>10</td>
<td>MASS FLOW RATE</td>
<td>KG/S</td>
<td>1.000E+00</td>
</tr>
<tr>
<td>11</td>
<td>TEMPERATURE</td>
<td>K</td>
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<tr>
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<td>ENTHALPY</td>
<td>J/KG</td>
<td>1.000E+00</td>
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<td>DENSITY</td>
<td>KG/M3</td>
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<td>15</td>
<td>VISCOSITY</td>
<td>KG/M-S</td>
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<tr>
<td>16</td>
<td>K.E. OF TURBLNCE</td>
<td>M2/S2</td>
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<td>17</td>
<td>K.E. DISS. RATE</td>
<td>M2/S3</td>
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<tr>
<td>18</td>
<td>SPEC. HEAT CAP.</td>
<td>J/KG-K</td>
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<tr>
<td>19</td>
<td>THERMAL CONDUCT.</td>
<td>W/M-K</td>
<td>1.000E+00</td>
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DIFFUSIVITY M2/S 1.000E+00
ACTIVATION ENRGY J/KMOL 1.000E+00
ANGLE RAD 1.000E+00
HEAT FLUX W/M2 1.000E+00
PARTICLE DIAM. M 1.000E+00
MOMENTUM TR RATE KG-M/S2 1.000E+00
HEAT TRANSF COEF W/M2-K 1.000E+00
PERMEABILITY M2 1.000E+00
INTERNAL MISC. - 1.000E+00
VOLUME FLOWRATE M3/S 1.000E+00
AREA M2 1.000E+00
ARRHENIUS FACTOR CONSISTENT UNITS 1.000E+00
INERTIAL FACTOR /M 1.000E+00
VOL. HEAT RATE W/M3 1.000E+00
ABSORB./SCATTER. /M 1.000E+00
ANGULAR VELOCITY RAD/S 1.000E+00
MOL. SIZE PARM. A 1.000E+00
PRESSURE GRAD. PA/M 1.000E+00
VORTICITY /S 1.000E+00
MUSHY ZONE CON. KG/M3/S 1.000E+00
SURFACE TENSION N/M 1.000E+00
SURF. TEN. GRAD. N/M/K 1.000E+00
CONTACT RESIST. M2-K/W 1.000E+00
VOLUME M3 1.000E+00
NUCLEI CONC. 10^15/M3 1.000E+00

- GEOMETRY -

RECTANGULAR CARTESIAN COORDINATES

NI = 90   NJ = 26   NK = 32

--- GRID GENERATION INFORMATION ---

X-GRID SEGMENT INFORMATION

<table>
<thead>
<tr>
<th>SEGMENT</th>
<th>START-POINT</th>
<th>LENGTH</th>
<th># CELLS</th>
<th>WEIGHTING-FACTORS</th>
</tr>
</thead>
<tbody>
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<td></td>
<td></td>
<td></td>
<td></td>
<td>START-POINT</td>
</tr>
<tr>
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<td>6.1760E-01</td>
<td>5</td>
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<tr>
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<td>4</td>
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<td>1.3400E-01</td>
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<td>1.1752E+00</td>
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<td>14</td>
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<tr>
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<td>4.6176E+00</td>
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<td>1</td>
<td>0.0000</td>
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Y-GRID SEGMENT INFORMATION

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<th>LENGTH</th>
<th># CELLS</th>
<th>WEIGHTING-FACTORS</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0000E+00</td>
<td>5.0000E-01</td>
<td>4</td>
<td>START-POINT: 0.0000, END-POINT: 0.0000</td>
</tr>
<tr>
<td>2</td>
<td>5.0000E-01</td>
<td>1.3000E+00</td>
<td>7</td>
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</tr>
<tr>
<td>3</td>
<td>1.6000E+00</td>
<td>4.0000E-01</td>
<td>2</td>
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<tr>
<td>4</td>
<td>2.2000E+00</td>
<td>1.3000E+00</td>
<td>7</td>
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<td>5.0000E-01</td>
<td>4</td>
<td>START-POINT: 0.0000, END-POINT: 0.0000</td>
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Z-GRID SEGMENT INFORMATION

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<th>LENGTH</th>
<th># CELLS</th>
<th>WEIGHTING-FACTORS</th>
</tr>
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<tbody>
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<td>1</td>
<td>0.0000E+00</td>
<td>1.1000E+01</td>
<td>1</td>
<td>START-POINT: 0.0000, END-POINT: 0.0000</td>
</tr>
<tr>
<td>2</td>
<td>1.1000E+01</td>
<td>4.0000E-02</td>
<td>1</td>
<td>START-POINT: 0.0000, END-POINT: 0.0000</td>
</tr>
<tr>
<td>3</td>
<td>1.5000E+01</td>
<td>6.0000E+00</td>
<td>1</td>
<td>START-POINT: 0.0000, END-POINT: 0.0000</td>
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<tr>
<td>4</td>
<td>2.1000E+01</td>
<td>1.0266E+00</td>
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<td>2.4800E+02</td>
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<tr>
<td>6</td>
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<td>1.7160E+01</td>
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<td>1.5670E+00</td>
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<td>5.0000E+00</td>
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- AXIS BOUNDARY IS NOT ACTIVE -

- CHEMICAL SPECIES DEFINITIONS -

TOTAL NUMBER OF CHEMICAL SPECIES = 15

<table>
<thead>
<tr>
<th>SPECIES NUMBER</th>
<th>SPECIES NAME</th>
<th>SPECIES TYPE</th>
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<tbody>
<tr>
<td>1</td>
<td>CH</td>
<td>GAS PHASE</td>
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<tr>
<td>2</td>
<td>CH2</td>
<td>GAS PHASE</td>
</tr>
</tbody>
</table>
3 CH3 GAS PHASE
4 CH4 GAS PHASE
5 CO GAS PHASE
6 CO2 GAS PHASE
7 H GAS PHASE
8 H2 GAS PHASE
9 H2O GAS PHASE
10 N2 GAS PHASE
11 O GAS PHASE
12 O2 GAS PHASE
13 OH GAS PHASE
14 C2H4 GAS PHASE
15 N GAS PHASE

SCALAR NUMBER SCALAR NAME
--------- --------
1 F-MEAN
2 F-VAR

- MULTI-GRID PARAMETERS -
U-VELOCITY IS SOLVED BY MULTI-GRID METHOD.
TERMINATION CRITERION: 0.1000000
RESIDUAL REDUCTION RATE: 0.7000000
MAX. LEVEL OF BLOCK CORRECTIONS IN I-DIR.: 0
MAX. LEVEL OF BLOCK CORRECTIONS IN J-DIR.: 0
MAX. LEVEL OF BLOCK CORRECTIONS IN K-DIR.: 0

V-VELOCITY IS SOLVED BY MULTI-GRID METHOD.
TERMINATION CRITERION: 0.1000000
RESIDUAL REDUCTION RATE: 0.7000000
MAX. LEVEL OF BLOCK CORRECTIONS IN I-DIR.: 0
MAX. LEVEL OF BLOCK CORRECTIONS IN J-DIR.: 0
MAX. LEVEL OF BLOCK CORRECTIONS IN K-DIR.: 0

W-VELOCITY IS SOLVED BY MULTI-GRID METHOD.
TERMINATION CRITERION: 0.1000000
RESIDUAL REDUCTION RATE: 0.7000000
MAX. LEVEL OF BLOCK CORRECTIONS IN I-DIR.: 0
MAX. LEVEL OF BLOCK CORRECTIONS IN J-DIR.: 0
MAX. LEVEL OF BLOCK CORRECTIONS IN K-DIR.: 0

PRESSURE IS SOLVED BY MULTI-GRID METHOD.
TERMINATION CRITERION: 0.1000000
RESIDUAL REDUCTION RATE: 0.7000000
MAX. LEVEL OF BLOCK CORRECTIONS IN I-DIR.: 0
MAX. LEVEL OF BLOCK CORRECTIONS IN J-DIR.: 0
MAX. LEVEL OF BLOCK CORRECTIONS IN K-DIR.: 0

ENTHALPY IS SOLVED BY MULTI-GRID METHOD.
TERMINATION CRITERION: 0.1000000
RESIDUAL REDUCTION RATE: 0.7000000
MAX. LEVEL OF BLOCK CORRECTIONS IN I-DIR.: 0
MAX. LEVEL OF BLOCK CORRECTIONS IN J-DIR.: 0
MAX. LEVEL OF BLOCK CORRECTIONS IN K-DIR.:  0

P-1 RADIATION       IS SOLVED BY MULTI-GRID METHOD.
TERMINATION CRITERION:  0.1000000
RESIDUAL REDUCTION RATE:  0.7000000
MAX. LEVEL OF BLOCK CORRECTIONS IN I-DIR.:  0
MAX. LEVEL OF BLOCK CORRECTIONS IN J-DIR.:  0
MAX. LEVEL OF BLOCK CORRECTIONS IN K-DIR.:  0

F-MEAN       IS SOLVED BY MULTI-GRID METHOD.
TERMINATION CRITERION:  0.1000000
RESIDUAL REDUCTION RATE:  0.7000000
MAX. LEVEL OF BLOCK CORRECTIONS IN I-DIR.:  0
MAX. LEVEL OF BLOCK CORRECTIONS IN J-DIR.:  0
MAX. LEVEL OF BLOCK CORRECTIONS IN K-DIR.:  0

F-VAR       IS SOLVED BY MULTI-GRID METHOD.
TERMINATION CRITERION:  0.1000000
RESIDUAL REDUCTION RATE:  0.7000000
MAX. LEVEL OF BLOCK CORRECTIONS IN I-DIR.:  0
MAX. LEVEL OF BLOCK CORRECTIONS IN J-DIR.:  0
MAX. LEVEL OF BLOCK CORRECTIONS IN K-DIR.:  0

MAXIMUM NO. OF FINE GRID ITERATIONS:  30
MAXIMUM NO. OF ITERATIONS PER LEVEL:  500
COARSE GRID SPACING IN I-DIRECTION:  2
COARSE GRID SPACING IN J-DIRECTION:  2
COARSE GRID SPACING IN K-DIRECTION:  2
MONITOR MG SOLVER: NO
MAX.-MG-LEVEL:     4

- VELOCITY/PRESSURE BOUNDARY CONDITIONS -

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<thead>
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<th>ZONE</th>
<th>U-VEL.</th>
<th>V-VEL.</th>
<th>W-VEL.</th>
<th>NORMAL</th>
<th>PRESSURE</th>
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<td>N/A</td>
<td>N/A</td>
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<tr>
<td>W2</td>
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<td>N/A</td>
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<tr>
<td>W3</td>
<td>8.33E-04</td>
<td>0.00E+00</td>
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<td>N/A</td>
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<tr>
<td>I1</td>
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<td>8.37E+01</td>
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<td>N/A</td>
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<tr>
<td>I2</td>
<td>0.00E+00</td>
<td>6.96E+01</td>
<td>0.00E+00</td>
<td>N/A</td>
<td>N/A</td>
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<tr>
<td>I3</td>
<td>0.00E+00</td>
<td>-8.37E+01</td>
<td>0.00E+00</td>
<td>N/A</td>
<td>N/A</td>
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<td>I4</td>
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<td>0.00E+00</td>
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<td>N/A</td>
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<td>I0</td>
<td>FIXED PRESSURE</td>
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<td>FIXED PRESSURE</td>
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<td>IW</td>
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<td>0.00E+00</td>
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- TURBULENCE BOUNDARY CONDITIONS -

- TWO EQUATION MODEL -

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<th>CHAR.-LENGTH</th>
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<td>SET</td>
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<td>SET</td>
<td>SET</td>
</tr>
<tr>
<td>W3</td>
<td>SET</td>
<td>SET</td>
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<tr>
<td>I1</td>
<td>1.000E+01</td>
<td>1.510E-01</td>
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<tr>
<td>ZONE</td>
<td>F-MEAN</td>
<td>F-VAR</td>
</tr>
<tr>
<td>------</td>
<td>--------</td>
<td>---------</td>
</tr>
<tr>
<td>W1</td>
<td>LINK CUT</td>
<td>LINK CUT</td>
</tr>
<tr>
<td>W2</td>
<td>LINK CUT</td>
<td>LINK CUT</td>
</tr>
<tr>
<td>W3</td>
<td>LINK CUT</td>
<td>LINK CUT</td>
</tr>
<tr>
<td>I1</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>I2</td>
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<td>0.00E+00</td>
</tr>
<tr>
<td>IW</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
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</table>

- SCALAR BOUNDARY CONDITIONS -

- TEMPERATURE BOUNDARY CONDITIONS -

<table>
<thead>
<tr>
<th>ZONE</th>
<th>TEMPERATURE</th>
</tr>
</thead>
<tbody>
<tr>
<td>W1</td>
<td>EXT. H-T</td>
</tr>
<tr>
<td>W2</td>
<td>HEAT FLUX</td>
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<td>W3</td>
<td>COND. WALL</td>
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<td>3.0300E+02</td>
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- SPECIAL TEMPERATURE BOUNDARIES -

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<tr>
<th>ZONE</th>
<th>HEAT FLUX BOUNDARY</th>
<th>HEAT FLUX VALUE</th>
<th>EXT. H-T BOUNDARY</th>
<th>EXTERNAL HEAT TRANSFER COEFF.</th>
<th>EXT. TEMP.</th>
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<tbody>
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<td>W1</td>
<td>N</td>
<td>N/A</td>
<td>Y</td>
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<td>3.0000E+02</td>
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<tr>
<td>W2</td>
<td>Y</td>
<td>-1.85000E+04</td>
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<td>N/A</td>
<td>N/A</td>
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<table>
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<th>ZONE</th>
<th>EXT. RAD BOUNDARY</th>
<th>T-INFINITY</th>
<th>EXT. EMISS.</th>
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<tbody>
<tr>
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<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>W2</td>
<td>N</td>
<td>N/A</td>
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CONDUCTING WALL ZONE PROPERTIES:

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<th>ZONE</th>
<th>THERMAL CONDUCTIVITY</th>
<th>SPECIFIC HEAT</th>
<th>DENSITY</th>
<th>VOLUMETRIC HEAT RATE</th>
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<td>7.6000E+03</td>
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<tr>
<td>0.0000E+00</td>
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</tbody>
</table>

- BODY FORCE -

IMPROVED TREATMENT OF BODY FORCE IN DISCRETE EQNS. - YES
INCLUDE BODY FORCE TERMS IN VELOCITY INTERPOLATION - YES

GRAVITATIONAL ACCELERATIONS:

\[ \begin{align*}
  x &= 0.000E+00 \\
  y &= 0.000E+00 \\
  z &= -9.800E+00
\end{align*} \]

REFERENCE DENSITY LOCATION:

\[ \begin{align*}
  i &= 2 \\
  j &= 2 \\
  k &= 3
\end{align*} \]

- TURBULENCE MODEL CONSTANTS -

\[ \begin{align*}
  C1 &= 1.4E+00 \\
  C2 &= 1.9E+00 \\
  CMU &= 9.0E-02
\end{align*} \]

- WALL FUNCTION TURBULENCE MODEL CONSTANTS -

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<tr>
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<th>CAPPA</th>
<th>ELOG</th>
</tr>
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<tbody>
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<td>W1</td>
<td>4.187E-01</td>
<td>9.793E+00</td>
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<tr>
<td>W2</td>
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<td>9.793E+00</td>
</tr>
<tr>
<td>W3</td>
<td>4.187E-01</td>
<td>9.793E+00</td>
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- ZONAL EMISSIVITIES (RADIATION MODEL) -

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<td>W3</td>
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<td>I4</td>
<td>1.0000E+00</td>
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<tr>
<td>IO</td>
<td>1.0000E+00</td>
</tr>
<tr>
<td>IS</td>
<td>1.0000E+00</td>
</tr>
<tr>
<td>IW</td>
<td>1.0000E+00</td>
</tr>
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</table>
- P-1 RADIATION MODEL CONSTANTS -

CARBON DIOXIDE SPECIES = CO2
WATER VAPOR SPECIES = H2O
WEIGHTED SUM OF GRAY GASES MODEL
CELL-BASED APPROACH
SCATTERING COEFFICIENT = 1.000E-08

- USER DEFINED PROPERTIES -

FLUID VISCOSITY - NO
FLUID DENSITY - NO
FLUID SPECIFIC HEAT - NO
FLUID THERMAL CONDUCTIVITY - NO
TURBULENT VISCOSITY - NO

- USER DEFINED SOURCE TERMS -

X-MOMENTUM EQUATION - NO
Y-MOMENTUM EQUATION - NO
Z-MOMENTUM EQUATION - NO
PRESSURE CORRECTION EQUATION - NO
TURBULENT K.E. EQUATION - NO
TURB. K.E. DISSIPATION EQUATION - NO
ENTHALPY EQUATION - NO
SPECIES EQUATIONS - NO

- USER STARTUP SUBROUTINE IS NOT ACTIVE -

- USER DEFINED REAL VARIABLES -

USPAR1 = 0.00000E+00
USPAR3 = 0.00000E+00
USPAR5 = 0.00000E+00
USPAR7 = 0.00000E+00
USPAR9 = 0.00000E+00
USPA11 = 0.00000E+00
USPA13 = 0.00000E+00
USPA15 = 0.00000E+00
USPA17 = 0.00000E+00
USPA19 = 0.00000E+00
USPAR2 = 0.00000E+00
USPAR4 = 0.00000E+00
USPAR6 = 0.00000E+00
USPAR8 = 0.00000E+00
USPA10 = 0.00000E+00
USPA12 = 0.00000E+00
USPA14 = 0.00000E+00
USPA16 = 0.00000E+00
USPA18 = 0.00000E+00
USPA20 = 0.00000E+00

- USER DEFINED INTEGER VARIABLES -

IUFGL1 = 0
IUFGL2 = 0
IUFGL3 = 0
IUFGL4 = 0
IUFGL5 = 0
IUFGL6 = 0
IUFLG7 = 0  IUFLG8 = 0
IUFLG9 = 0  IUFL10 = 0
IUFL11 = 0  IUFL12 = 0
IUFL13 = 0  IUFL14 = 0
IUFL15 = 0  IUFL16 = 0
IUFL17 = 0  IUFL18 = 0
IUFL19 = 0  IUFL20 = 0

- DENSITY IS CALCULATED FROM THE PDF LOOKUP TABLE
- THE OPERATING PRESSURE = 1.0100E+05

- SPECIES MOLECULAR WEIGHTS -

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<td>CH</td>
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<tr>
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<td>1.4027E+01</td>
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<tr>
<td>CH3</td>
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<td>1.6043E+01</td>
</tr>
<tr>
<td>CO</td>
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</tr>
<tr>
<td>CO2</td>
<td>4.4010E+01</td>
</tr>
<tr>
<td>H</td>
<td>1.0080E+00</td>
</tr>
<tr>
<td>H2</td>
<td>2.0159E+00</td>
</tr>
<tr>
<td>H2O</td>
<td>1.9015E+01</td>
</tr>
<tr>
<td>N2</td>
<td>2.8013E+01</td>
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<tr>
<td>O</td>
<td>1.5999E+01</td>
</tr>
<tr>
<td>O2</td>
<td>3.1999E+01</td>
</tr>
<tr>
<td>OH</td>
<td>1.7007E+01</td>
</tr>
<tr>
<td>C2H4</td>
<td>2.8054E+01</td>
</tr>
<tr>
<td>N</td>
<td>1.4007E+01</td>
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</table>

- MIXTURE VISCOSITY DEFINITION -

- VISCOSITY DEFINITION
VISCOSITY = 1.720E-05

- SPECIFIC HEAT DEFINITION -
SPECIFIC HEAT IS DEFINED FROM THE PROPERTIES DATABASE

- MIXTURE THERMAL CONDUCTIVITY DEFINITION -

- THERMAL CONDUCTIVITY DEFINITION
\[ K = 2.410E-02 \]

- BINARY DIFFUSION COEFFICIENT DEFINITION -
BINARY DIFFUSION COEFFICIENT FOR CH IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR CH2 IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR CH3 IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR CH4 IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR CO IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR CO2 IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR H IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR H2 IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR H2O IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR N2 IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR O IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR O2 IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR OH IN THE MIXTURE:
DIJ = 2.880E-05

BINARY DIFFUSION COEFFICIENT FOR C2H4 IN THE MIXTURE:
DIJ = 2.880E-05

OPERATING PRESSURE FOR NON-IDEAL GAS: 1.0100E+05

- PDF MODEL FOR DIFFUSION FLAMES -
ADIABATIC CASE - NO
SECONDARY INLET STREAM ALLOWED - NO
LOOKUP TABLE FILE -

/home/cae/tvyes1/furnadi.pdf
NUMBER OF ITERATIONS PER PDF TABLE LOOKUP - 5

- SOLUTION CONTROL PARAMETERS -

SOLVER MARCHING DIRECTION - J-DIRECTION
SOLVER SWEEP DIRECTION - I-DIRECTION
ALTERNATE SWEEP DIRECTION - YES
SOLUTION METHOD - SIMPLE
ALLOW PATCHING OF BOUNDARY VALUES - NO
CONVERGENCE/DIVERGENCE CHECK ON - YES
MINIMUM RESIDUAL SUM - 1.000E-03
MINIMUM ENTHALPY RESIDUAL - 1.000E-06
NORMALIZE RESIDUALS - YES
CONTINUITY CHECK - YES

- INTERPOLATION SCHEME ON CELL FACES -

FOR DENSITY - UPWIND
FOR PRESSURE - MOMENTUM WEIGHTED
FOR VELOCITY - LINEAR

TEMPERATURE CHANGE LIMITER - 1.000E-00
REYNOLDS STRESS TURBULENCE MODEL - NO
RNG TURBULENCE MODEL - NO
INCLUDE BUOYNACY TERMS IN TURB. MODEL - NO
MONITOR SOLVER - NO
FIX VARIABLE OPTION ENABLED - NO
SET PRESSURE REFERENCE LOCATION - NO
VISCOS DISSIPATION - NO
INCLUDE SPECIES DIFF. EFFECTS IN ENTH. - NO

DIFFERENCING SCHEME - POWER LAW

FIXED PRESSURE BOUNDARIES ARE ACTIVE

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<tr>
<th>VARIABLE</th>
<th>UNDERRELAX 1</th>
<th>UNDERRELAX 2</th>
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162
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</tbody>
</table>
Vita Auctoris

Natalie Tyves was born in 1973 in Moscow, Russia. She received most of her childhood education in Canada after her family moved there in 1981. She attended Belle River District High School and graduated from there in 1992. In the fall of the same year, she enrolled in the mechanical engineering co-op program at the University of Windsor and obtained her Bachelor of Applied Science Degree in 1996. She continued with her formal education in mechanical engineering at the Master's level and is currently candidate for the Master's degree at the University of Windsor.