

# On the Modeling of Industrial Furnaces and Combustion Chambers

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## Abstract

The recent advances in numerical methods and the vast development of computers had directed the designers to better development and modifications to airflow pattern and heat transfer in furnaces. Extensive efforts are exerted to adequately predict the heat transfer characteristics in the combustor zones and to reduce the emitted pollution and noise abatement to ultimately produce quite and energy efficient combustor systems. The present paper introduces a newly developed Computational Fluid Dynamics (CFD) program (3DTCFD) to predict the airflow characteristics in the furnaces. The present paper fosters mathematical modeling techniques to primarily predict what happens in three dimensional combustion chambers simulating boiler and industrial furnaces in terms of heat transfer characteristics and interactions. The present work also demonstrates the effect of chamber design and operational parameters on performance under various operating parameters. The governing equations of mass, momentum and energy are commonly expressed in a preset form with source terms to represent pressure gradients, turbulence and heat transfer. Fluid flow and heat transfer characteristics in combustors play an important role in the efficiency, thermal balance and performance. The present paper discusses the various modeling assumptions in furnaces. The present paper discusses the various combustion modeling assumptions in the furnaces. The numerical grid comprises; typically, 200000-grid node covering the combustion chamber volume in the X, R or Y and Z coordinates directions. The numerical residual in the governing equations typically less than 0.001 %. Examples of large industrial furnace are shown in the present paper are in good agreement with available measurements in the open literature. The present modeling capabilities are shown to adequately predict the local flow pattern and turbulence kinetic energy levels in complex furnaces.

**Keywords:** *CFD, Combustion Modelling, Furnaces*

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## Introduction

Combustion chamber designers always endeavor to achieve the optimum operating conditions that give maximum combustion efficiency together with minimum pollutant formation rate [1]. This can be attained if details of the combustion process are well known. Since the Sixties, after the advance of computers, numerical procedures became one of the most convenient tools, which aid the design procedure at sufficient accuracy and proper cost. The mathematical and numerical simulation of the combustion processes involve some of the following physicochemical phenomena: aerodynamic flow pattern, heat and mass transfer, turbulence, two-phase flow, chemical kinetics, and radiation. The exact treatment of any of these individual processes is very complex and requires excessively large computing facilities.

To aid the designer and to ease his mission, mathematical models that simplify the exact treatment of these processes are proposed, and embodied in the numerical procedure to yield the conservation equations solvable [2]. Furnace design would be greatly facilitated by the use of the mathematical and numerical procedures. These procedures can simulate different operating conditions for various designs to obtain the optimum design conditions. Different combinations of inlet velocities, combustor geometry, jet temperatures and equivalence ratios may produce very different flame and flow patterns, which in turn, may lead to undesired thermo-acoustically induced combustion instabilities [3]. Numerical simulation of reacting flows – developing spatially and temporally – is ideally designed to properly address most of the designer requirements. In the earlier investigations, the calculations of furnace flow properties

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were carried out using steady and two-dimensional procedures [4, 5]. These calculations were verified against some reliable experimental data and indicated good agreements with the some discrepancies in recirculation zone vicinity. In the recent investigations, the numerical calculations were carried out using the three-dimensional models, [6] and using the time-dependent models [3]. The main purpose of the present paper is to investigate the time dependent nature of reacting flows in a furnace after ignition and commencement of reaction, documenting the flame progress to enhance the future modeling developments, and marking up several observations to enhance the physical modeling of the reacting flows and flame propagation.

**Calculation Procedure**

The present research is carried out using a numerical method by solving the elliptic form of the governing differential equations in three-dimensional cylindrical configurations under transient conditions. Various assumptions are necessarily added to yield the differential equations solvable. The turbulence characteristics are modeled using the two-equation k- turbulence model. The values of the kinetic energy and dissipation rate are corrected near the wall using the wall functions, [7]. Solution technique utilized two combustion models, when attempting to simulate the turbulent combustion process, flow and combustion chemistry simplifications are carried,[8-17] .More details concerning the solution technique, its procedure, and its validation procedure can be found in previous publications and description of the 3DTCOMB , [18,19].

**Mathematical Modeling Equations and Combustion Models**

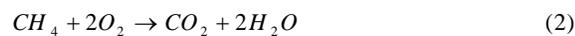
The governing equations of mass, three momentum, energy and species concentrations were all expressed in the finite difference counterpart of the time dependent version as indicated here after.

$$\frac{\partial}{\partial t} \dots \Phi + \frac{\partial}{\partial x} \dots U \Phi + \frac{1}{r} \frac{\partial}{\partial r} \dots r V \Phi + \frac{1}{r} \frac{\partial}{\partial \theta} \dots W \Phi =$$

$$\frac{\partial}{\partial x} \left( \Gamma \frac{\partial \Phi}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \Gamma \frac{\partial \Phi}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \Gamma \frac{\partial \Phi}{\partial \theta} \right) + S_{\Phi} \dots (1)$$

Where  $\Phi$  represents the various variables as in Table 1, the values of  $\Gamma$  and also the source/sink terms  $S_{\Phi}$  are given in the table 1.

Model 1: this model assumes a physically controlled, one step reaction, as shown in Equation 2, with supposing the fuel and oxidant cannot exist at the same place at any time and the reaction is infinitely fast and equilibrium is attained. The only species equation to be solved is that for the mixture fraction  $f$ , and this equation has no source as represented above .The prevailing chemical reaction is simplified as one-step as follows:



In regions of flame where oxidant and products exist  $0 < f < f_{st}$  Where  $f$  is Mixture fraction

$$m_{fu} = 0 \quad (3)$$

$$m_{ox} = (1 - f / f_{st})$$

In regions of flame where fuel and products exist ;  $1 >$

$$f > f_{st}$$

$$m_{fu} = (f - f_{st}) / (1 - f_{st}) \quad (4)$$

$$m_{ox} = 0$$

$$\text{And } m_{pr} = 1 - m_{ox} - m_{fu} \quad (5)$$

Model 2: In contrast to first model, a finite reaction rate is introduced in this model. In particular, both  $m_{fu}$  and  $m_{ox}$  can coexist at the same location at the same time. In solving the PDE for  $m_{fu}$ , its source term ( $R_{fu}$ ) (rate of the fuel consumption) is represented by an Arrhenius type source term or by an eddy-break-up term. The smaller of these two expressions at a given point in the flow field dominates the reaction and is used; the eddy dissipation rate  $\epsilon$  often slowing chemical reaction.

$$R_{fu} = A \rho^2 m_{fu} m_{ox} \exp(-E/RT) \quad (6)$$

or

$$R_{fu} = 0.55 g^2 (\rho \epsilon / k) \quad (7)$$

Where  $A = 10^{10} \text{ m}^3/\text{kg s}$ ,  $E/R = 1.84 \times 10^4 \text{ K}$

$K$  kinetic energy of turbulence &  $\epsilon$  is its dissipation rate .

In terms of the number of differential equations considered, model 2 requires the solution of the  $f$ ,  $g$ ,  $m_{fu}$  equations. Further modifications were added in several researches, but these modifications were not fully justified [6].

**Time Dependent Flame Behavior**

The time dependent flame propagation and behavior, obtained with the present numerical model, is described here. The present work is devoted to the flow configuration of furnace described in the Table 2, [16] .For a one step fast chemical reaction progress (Model 1), no special treatment was followed to start the flame simulation. In model 2 (finite reaction rate) the initiation of ignition simulation is needed. Simulation starts by diffusion of the fuel and combustion air to be mixed; this needs a catalyst. This catalyst is simply a spark as was assumed earlier. 18 With the Arrhenius reaction model in mind, it can be deduced that the flame would not start without high temperature mixture. So, at the present work, a simulated spark at the burner downstream is carried out. The temperature is artificially raised in this region to high temperature (about 1600 oK) at small time intervals (from start 0 second to 0.3 second) as indicated in Figures 1 and 2.

**Results and Discussions**

The predicted mixture fraction and fuel mass fraction distributions are presented here together with corresponding temperature patterns. The obtained results of model 1 are found to be beyond the known measured results. The model 1 is so simple and depends on simplified assumptions, that the chemical reaction is influenced by the reactants concentration decay. The fast chemical reaction may represent the real process in the well-mixed fuel and oxidant mixture. The fast chemical reaction, also, need a very fast flame propagation with

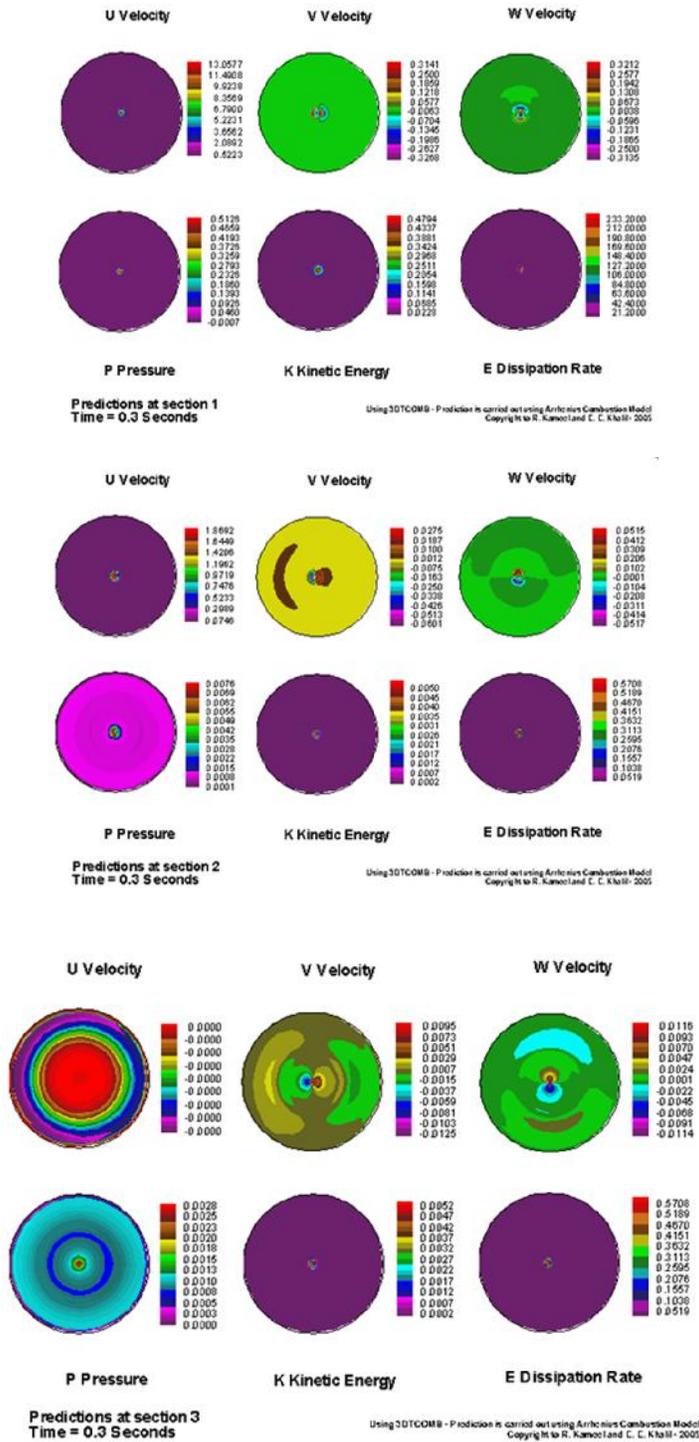


Figure 1: Predicted Flow Characteristics across the Furnace at End of Ignition

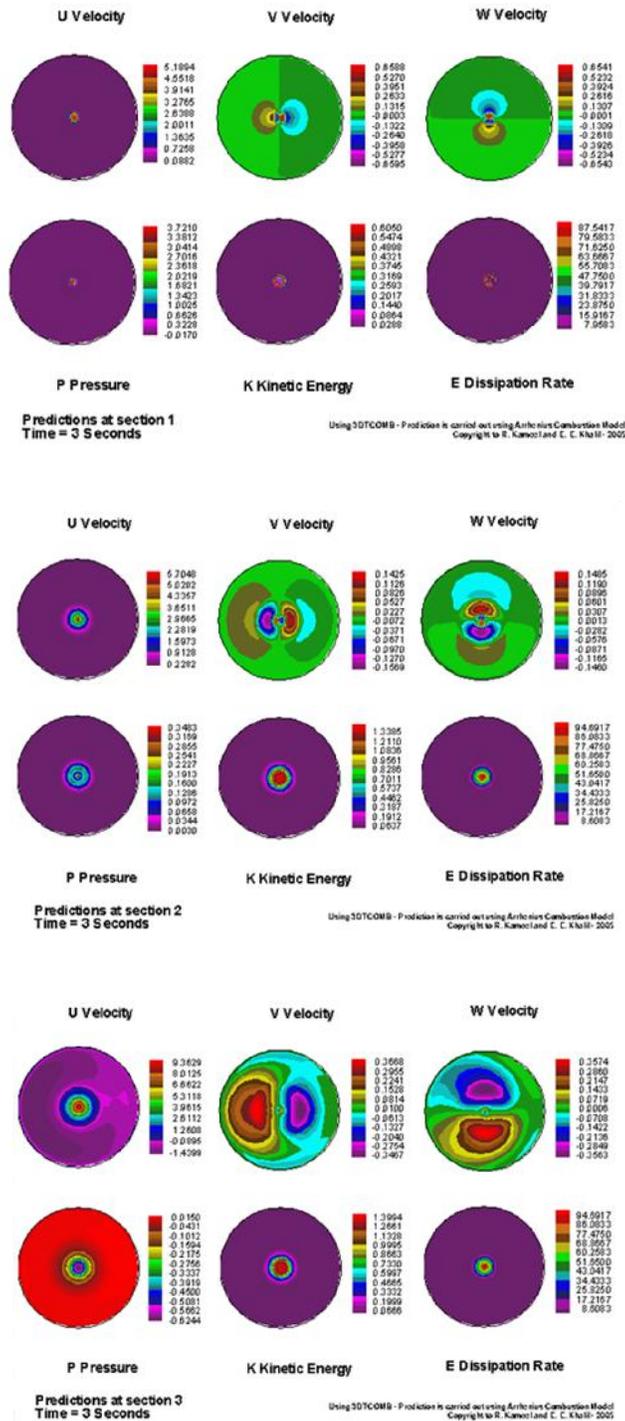


Figure 2: Predicted Flow Characteristics across the Furnace after 3 Seconds from Ignition

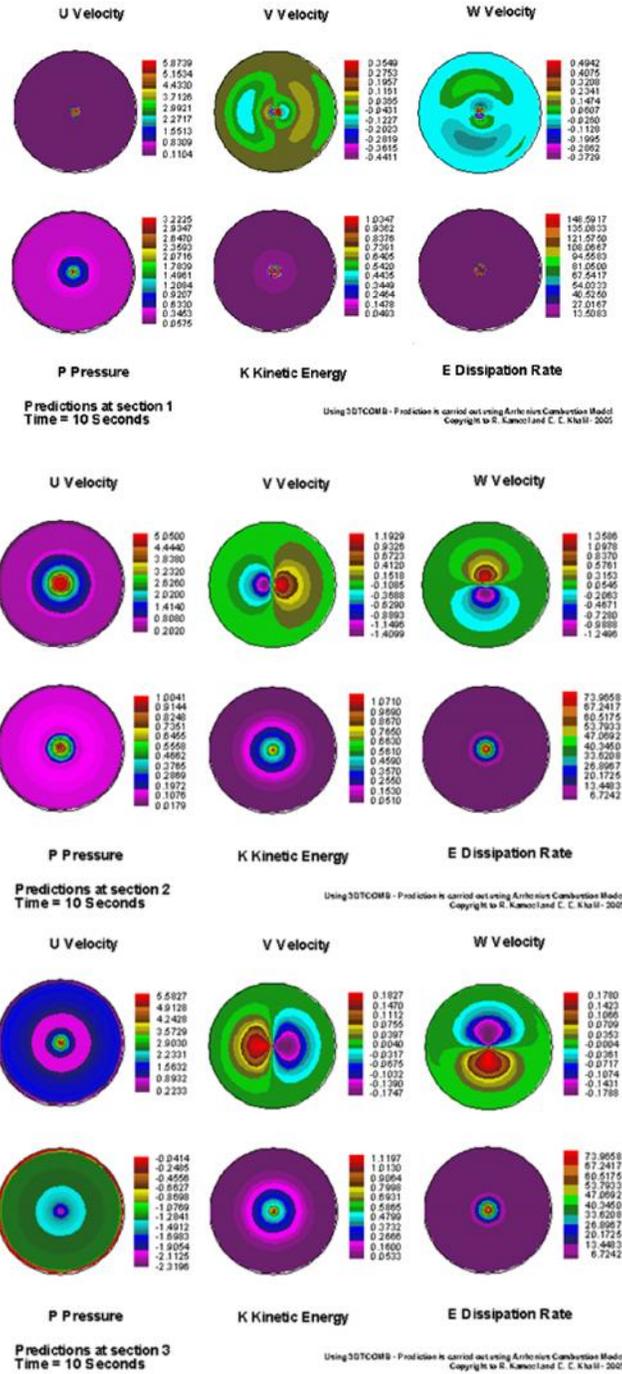


Figure 3: Predicted Flow Characteristics across the Furnace after 10 Seconds from Ignition

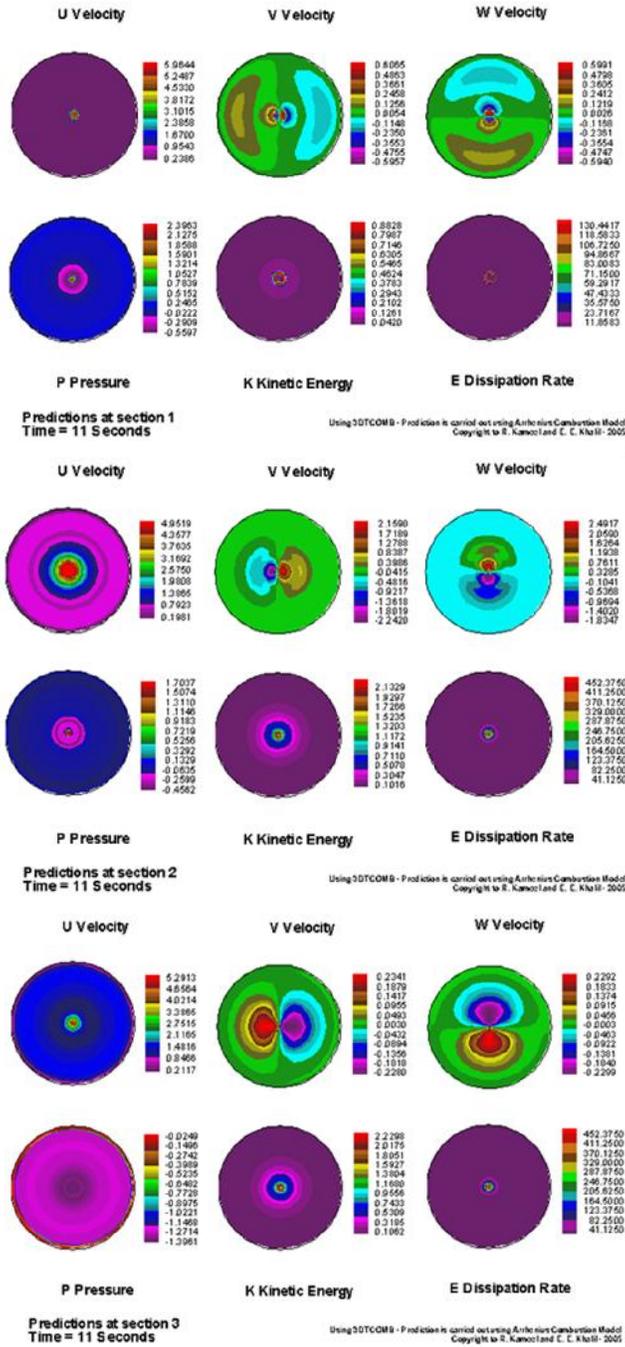


Figure 4: Predicted Flow Characteristics across the Furnace after 11 Seconds from Ignition

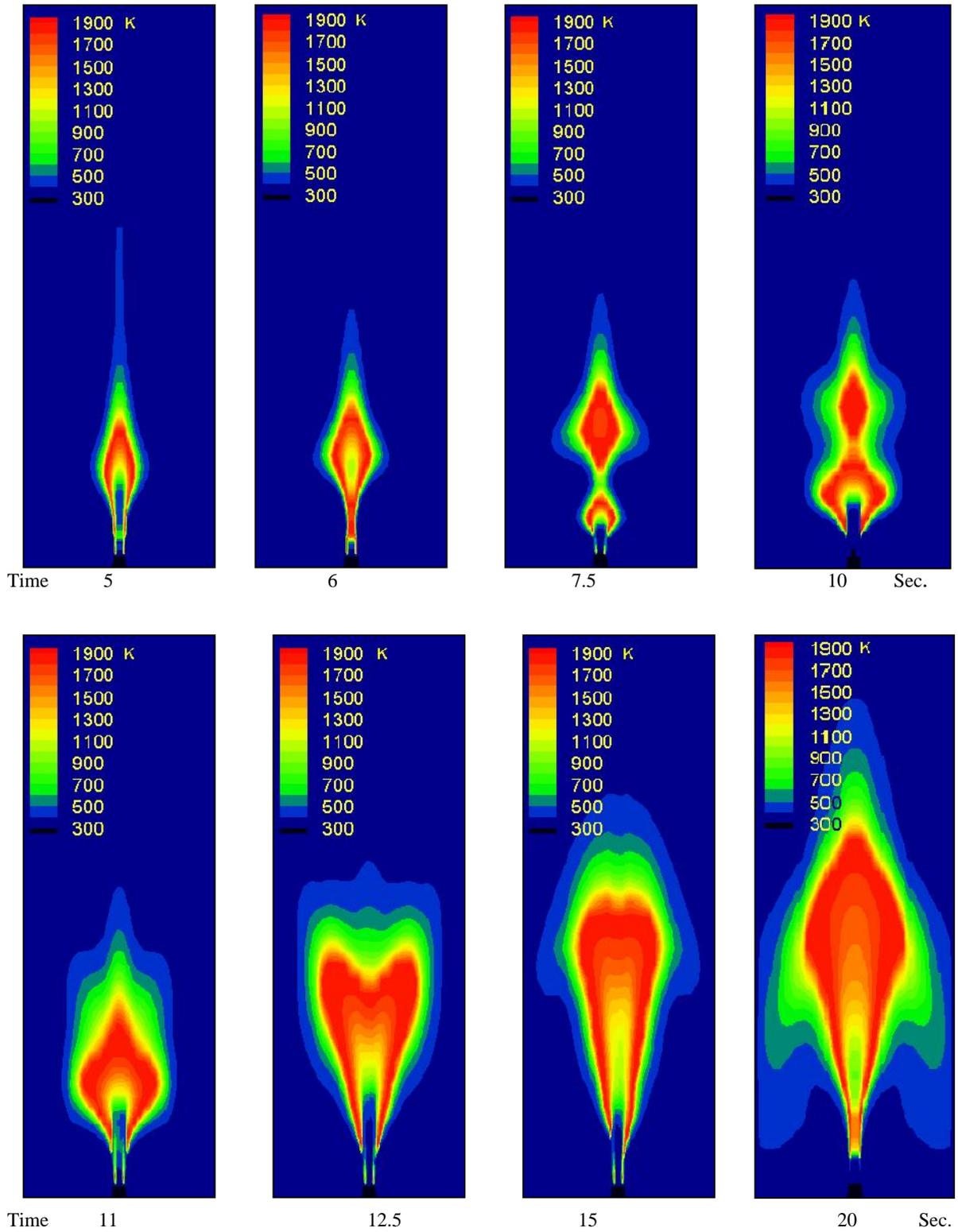


Figure 5: Predicted Temperature Contours in a Confined Flame up to 20 Seconds from Ignition

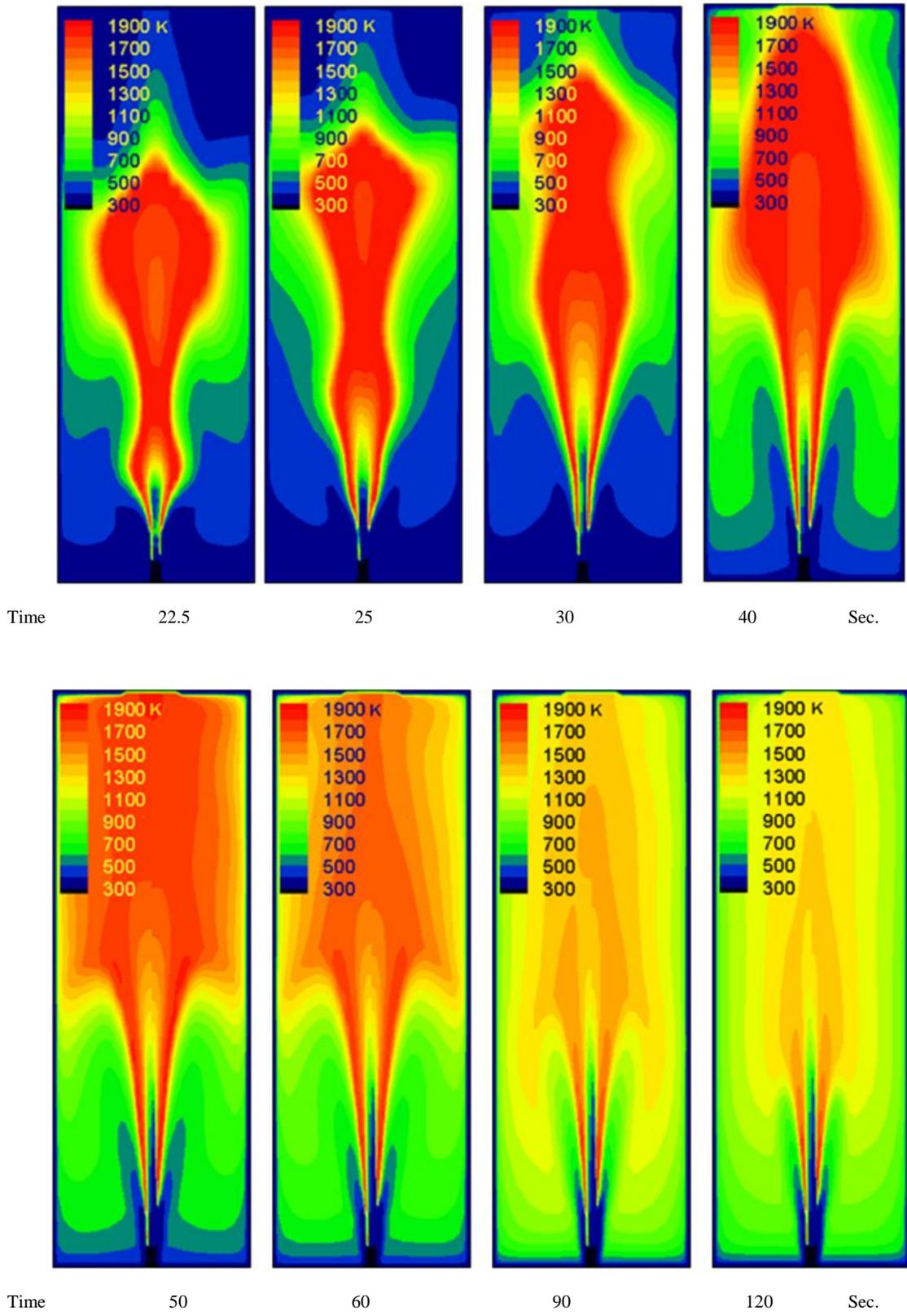


Figure 6: Predicted Temperature Contours in a Confined Flame Up To 120 Seconds from Ignition

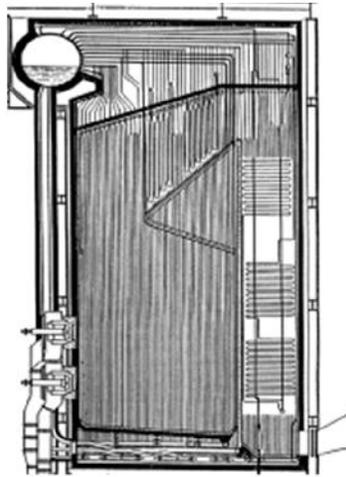


Figure 7: An Example of Steam Boiler Configuration

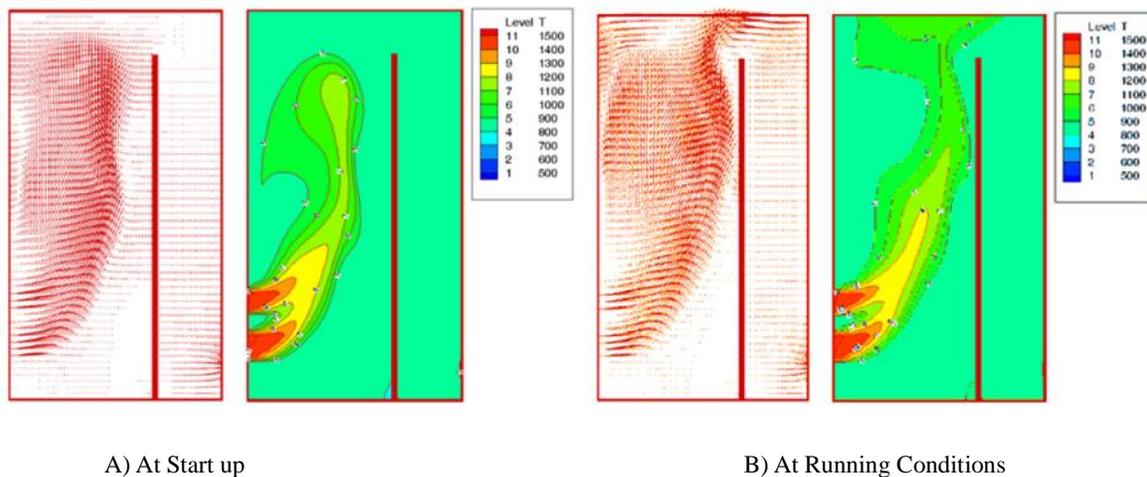


Figure 8: Predicted Time Averaged Velocity Vectors and Temperature Contours in Boiler Furnace

unconfined diffusion. Model 1 successfully predicts the flame nature qualitatively; the longitudinal and lateral wavy nature of the flame was so clear in the transient simulation using the first model. The prediction procedure using this model doesn't require large computing time, but it can not be adequately used as a simple design tool.

In the present non-swirl combusting flow, the Arrhenius model yields very good representative model. Such model is so sensitive to the boundary conditions especially near or at the flame regions. In high temperature regions, the switching between the Arrhenius model and the eddy-break-up model was frequently observed, which consequently influences the transient prediction and the steady state results. When Model 2 is incorporated, the results were recorded for 120 seconds. The steady state results were attained at about 110 seconds approximately after ignitions. It is observed that the flame had expanded longitudinally and laterally after 11 seconds of the

ignition, as shown in figures 3 and 4, [18, 19]. The flame reaches the end of chamber after nearly 41 seconds from ignition. This observed phenomenon would influence the outflow condition at the exit of the furnace. High disturbances in the flow and the turbulence were increasingly observed. The flame impinging on rear wall and back flow to the half of the furnace length was observed after 3-4 seconds from impingement at furnace end wall. At this instance, the hot gases were reverted backward toward the burner and expanded laterally toward the furnace side walls. The temperature temporal distribution in the furnace is represented in Figures 5 and 6. The propagation scenario of the flame can be directly extracted from that Figure.

The time dependent flame propagation is described and explained in the present work through a "squashing and stretching" process. The most important events are displayed here in the Figures 5 and 6. The flame envelope can be

identified based on the based on the flame temperature definition. An example of the application in power plant boilers is shown in Figure 7 that depicts an 85 ton/hr Steam generator whose furnace was modeled utilizing the same computer package used in this paper to predict local velocity and thermal patterns in furnaces under turbulent reacting conditions with Cartesian grid selection. Figure 8 shows the predicted time averaged velocity vectors and temperature contours at start up and normal operation.

**Concluding Remarks**

This paper introduces a well developed Computational Fluid Dynamics (CFD) program (3DTCOMB) to predict the airflow and flame characteristics in the furnaces, based on two combustion models. It was found that the Arrhenius rate-based model represented the furnace flow better than the fast reaction model. In the non-swirl confined flame simulation, the exit flow conditions should be considered with great care. The temporal nature of the flame propagation is described and explained in the present work. It is observed that the numerical results based on the Model 1 have insufficient agreement with

the previous experimental and numerical results. However, this first model successfully predicted a qualitative preliminary indication to the flame performance. The simulation process based on the first model was quicker than the simulation process based on the model 2. The propagation scenario of the flame can be extracted from these Figures. The transient nature of the flame propagation is described and explained in the present work through a “squashing and stretching” process. The flame envelope can be identified based on the flame temperature definition.

The agreement between the numerical results based on the Arrhenius reaction rate model and the experimental results was shown, [18, 19 & 20] to be qualitative; and further refinements and developments are needed. The time dependent flame behavior would aid the future development of the combustion models on a large-scale furnace. Attention and emphasis should be directed to the micro-scale modeling. The present program (3DTCOMB) will be subjected to further development in future to extend its capabilities to more adequately describe the combustion-time processes and turbulence-chemistry interactions. The final goal is to support the engineers and designers of the furnaces and combustors.

**Table 1: Generalized Partial Differential Equations**

Conservation of	W	X	S <sub>W</sub>
Mass	<i>I</i>	<i>0</i>	<i>0</i>
Axial momentum	<i>U</i>	$\sim_{eff}$	$-\partial P/\partial x + S_U$
Radial momentum	<i>V</i>	$\sim_{eff}$	$-\partial P/\partial r + S_V$
Tangential momentum	<i>W</i>	$\sim_{eff}$	$-(1/r)(\partial P/\partial \theta) - g_{gr} \dots (1-S_U t) + S_W$
Stagnation enthalpy	<i>h</i>	$\sim_{eff}/\dagger_h$	<i>0</i>
Mixture fraction	<i>f</i>	$\sim_{eff}/\dagger_f$	<i>0</i>
Concentration fluctuation	<i>g</i>	$\sim_{eff}/\dagger_g$	$C_{g1}G_{g1} - C_{g2} \dots g \nu/k$
Mass fraction of fuel	<i>m<sub>fu</sub></i>	$\sim_{eff}/\dagger_{fu}$	<i>R<sub>fu</sub></i>
Kinetic energy	<i>k</i>	$\sim_{eff}/\dagger_k$	<i>G - ... v</i>
Dissipation rate	<i>v</i>	$\sim_{eff}/\dagger_v$	$C_1 v G/k - C_2 \dots v^2/k$

$$\sim_{eff} = \sim_{lam} + \sim_t \quad \sim_t = \dots C_- k^2 / \nu$$

$$G = \sim_t [2\{(\partial U/\partial x)^2 + (\partial V/\partial r)^2 + (\partial W/r\partial \theta + V/r)^2\} + (\partial U/\partial r + \partial V/\partial x)^2 + (\partial V/r\partial \theta + \partial W/\partial r - W/r)^2 + (\partial U/\partial \theta + \partial W/\partial x)^2]$$

$$S_U = \partial/\partial x (\sim_{eff} \partial U/\partial x) + (1/r) \partial/\partial r (r \sim_{eff} \partial V/\partial x) + (1/r) \partial/\partial \theta (\sim_{eff} \partial W/\partial x)$$

$$S_V = \partial/\partial x (\sim_{eff} \partial U/\partial r) + (1/r) (r \sim_{eff} \partial V/\partial r) + (1/r) \partial/\partial \theta (\sim_{eff} r \partial(W/r)/\partial r) - 2(\sim_{eff}/r) (\partial W/r\partial \theta + V/r) + \dots W^2/r$$

$$S_W = \partial/\partial x (\sim_{eff} \partial U/r\partial \theta) + (1/r) \partial/\partial r (r \sim_{eff} ((1/r) \partial V/\partial \theta - W/r)) + (\sim_{eff}/r) (r \partial(W/r)/\partial r + (1/r) \partial V/\partial \theta) + (1/r) \partial/\partial \theta (\sim_{eff} (\partial W/r\partial \theta + 2V/r)) - \dots VW/r$$

$$C_{g1} = \sim_{eff} ((\partial m_{fu}/\partial x)^2 + (\partial m_{fu}/\partial r)^2 + (\partial m_{fu}/\partial \theta r\partial \theta)^2)$$


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$$C_1 = 1.44, C_2 = 1.92, C_- = 0.09, C_{g1} = 2.8, C_{g2} = 2.0, C_R = 1.0$$

$$\dagger_h = 0.9, \dagger_{fu} = 0.9, \dagger_f = 0.9, \dagger_g = 0.9, \dagger_k = 0.9, \dagger_v = 1.225$$

**Table 2: Dimensions of Furnace of reference [16]**

Furnace diameter	<i>D<sub>f</sub></i>	300 mm
Furnace length	<i>L<sub>f</sub></i>	900 mm
Fuel inlet diameter	<i>D<sub>1</sub></i>	12 mm
Inlet diameter of the air annulus	<i>D<sub>2</sub></i>	27 mm
Outlet diameter of the air annulus	<i>D<sub>3</sub></i>	55 mm
Diameter of exit	<i>D<sub>out</sub></i>	90 mm
Section 1	<i>L<sub>1</sub></i>	22 mm
Section 2	<i>L<sub>2</sub></i>	134 mm
Section 3	<i>L<sub>3</sub></i>	450 mm

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