



MATHEMATICAL MODELING OF SWIRLING TURBULENT NATURAL GAS COMBUSTION IN AXISYMMETRIC COMBUSTORS

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Abstract: A mathematical model is developed to numerically simulate the burning of natural gas in an axisymmetric combustor under turbulent swirling flow conditions. The gas phase is modeled in terms of Eulerian continuum conservation equations of mass, momentum, energy and species concentrations, for Favre-averaged quantities. The highly-coupled, non-linear set of elliptical partial differential equations that describe the system are solved by an iterative line-by-line technique after transferring it to a system of finite difference equations. The gas turbulence is described by the standard k- ϵ two-equation model. The model assumes equilibrium gas-phase chemistry and turbulence-chemistry coupling is modeled using the probability density function and mixture fraction concept. The model involves a staggered grid system for axial and radial velocities, and a relaxation technique for efficient numerical solution of the governing equations. The developed model is used to simulate the combustion processes in an axisymmetric, laboratory-scale combustor. In the model calculations of the significant features of the flow field are illustrated with velocity and temperature fields and gaseous species concentrations. One set of validation data are used for comparison and the computed results agree fairly well with the available experimental data.

Key words: Mathematical Modeling, Natural Gas, Swirl, Turbulent combustion,

DOĞAL GAZIN EKSENEL SİMETRİK FIRINLARDA TURBULANSLI YANMASININ MATEMATİKSEL MODELLENMESİ

Özet: Doğal gazın türbülanslı yanmasını simüle eden bir matematiksel model oluşturulmuştur. Bu modelde, kütle, momentum, basınç ve entalpi için gaz fazı hareket denklemleri, bir dizi eliptik kısmi türevsel denklemlerle tanımlanır. Bu denklemler, sonlu fark denklemler sistemine aktarıldıktan sonra iterasyon tekniğiyle çözümlenirler. Türbülans, standart doğrusal bir k- ϵ modeli olarak düşünülmüştür. Gaz fazı reaksiyonları, bölgesel anlık dengelerin var olduğu kabul edilerek modellenmiştir. Belirtilen model eksenel simetrik pilot ölçekli fırındaki yanma olayının modellenmesi için kullanılmıştır. Bu hesaplamalarda, akış alanının önemli özellikleri, hız alanı, sıcaklık alanı, ve gaz bileşenleri konsantrasyonu ile gösterilmiştir. Literatürden alınan bir set karşılaştırma verisi yazılan programın doğrulanması için kullanıldı ve hesaplanan sonuçların mevcut deneysel veriye oldukça yakın olduğu görüldü.

Anatar Kelimeler: Matematiksel Modelleme, Doğal gaz, Türbülans Yanma,

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NOMENCLATURE

Roman Symbols

C_μ	A constant in the k- ϵ turbulence model
f	Mixture fraction
g_f	Variance of the mixture fraction f
k	Mean turbulent kinetic energy
r	Radius
S	Gas source term
SN	Swirl Number
t	Time
u	Velocity along x-direction
$\mathbf{V}$	The velocity vector
v	Velocity along y-direction
$\mathbf{v}$	Velocity vector
w	Velocity along z-direction
x, y, z	Cartesian coordinates

Greek Symbols

Γ	General turbulent exchange coefficient
ϕ	General variables, Equivalence ratio
ϵ	Dissipation rate of turbulence energy
κ	Mean turbulent kinetic energy
μ	Dynamic Viscosity
ν	Kinematic Viscosity
ρ	Density
σ	Schmidt or Prandtl number.

Subscripts

f	Mixture fraction, formation.
g	Gas, mean square fluctuations (variance) of f
$g1, g2$	Empirical constants in the equations of g
m	Mean
x	Axial
t	Turbulent
ϕ	General dependent variable

INTRODUCTION

Turbulent swirling flows are often used in combustion systems in order to meet many of the performance requirements. Experimental studies show that swirl can prevent flow separation and enhance flame stability by producing higher rates of entrainment of the combustion air and fast flow mixing. In reacting flows the degree of swirl in the flow field strongly affects the flame size, shape, stability and combustion intensity. In axisymmetric geometries swirl creates flow recirculation zones that constitute a well-mixed region containing hot combustion gases and provide heat and active chemical species to the incoming fuel and air streams. The optimization of the combustion

process depends on accurate information describing these recirculation zones.

The degree of swirl is characterized by the swirl number SN, which is a dimensionless number representing the axial flux of swirl momentum divided by the axial flux of axial momentum times equivalent nozzle diameter (Sloan et. al. 1986).

$$SN = \frac{G_\phi}{R_o G_x} = \frac{\int_{R_i}^{R_o} \rho u w r^2 dr}{R_o \int_{R_i}^{R_o} (\rho u^2 + p) r dr} \quad (1)$$

Where

G_x = Axial flux of axial momentum (units of force)

G_ϕ = Axial flux of angular momentum (units of torque)

R_o = Equivalent nozzle or orifice radius

Traditionally, designers have mostly relied upon experiments in seeking an optimum combustor design procedures and parameters. One obvious difficulty with this approach is that, in general, changing the experiment or any of the parameters, such as geometry, inlet conditions, etc., may change the obtained conclusion. This approach is now being supplemented with computational modeling techniques, which provide the designer with the predictive capabilities and the freedom to change and alter the parameters in order to optimize the combustion process.

THE MATHEMATICAL MODELS

A complete mathematical model for prediction of the turbulent natural gas diffusion flames consists of the following parts:

The Flow Field Model

The gas phase equations that are modeled in this study can be classified as Eulerian, steady state, second-order, non-linear, elliptical partial differential equations and they are described by Navier-Stokes equations, coupled with appropriate equations for density and viscosity. For closure of the turbulence equations, the standard κ, ϵ turbulence model is used.

The gas phase governing equations may take the following general form (provided that ϕ , Γ_ϕ , and S_ϕ are chosen appropriately):

$$\nabla \cdot (\rho_g \mathbf{V} \phi) - \nabla \cdot (\Gamma_\phi \nabla \phi) = S_\phi \quad (2)$$

The first term in the left-hand side of Eq. (2) is the convection term describing the transport of ϕ by means of the mass flow. The second term is the diffusion term, which neither creates nor destroys ϕ , but rather just redistributes it about the flow domain due to gradient-driven diffusion. In the right-hand side, S_ϕ is the source term in the gas phase that describes the production and destruction of ϕ .

In terms of cylindrical coordinates appropriate to 2-dimensional, axisymmetric flow in the cylindrical geometry Eq. (2) may be written as:

$$\frac{\partial}{\partial x}(\rho u \phi) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v \phi) = \frac{\partial}{\partial x} \left(\Gamma_\phi \frac{\partial \phi}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \Gamma_\phi \frac{\partial \phi}{\partial r} \right) + S_\phi \quad (3)$$

Where u and v are the axial (x) and radial (r) gas phase velocity components.

When ϕ equals one, Eq. (3) will represent the mass conservation equation, otherwise it represents one of the following dependent variables: u (axial velocity), v (radial velocity), w (tangential velocity), κ (turbulence kinetic energy), ϵ (turbulence kinetic energy rate of dissipation), h (enthalpy), f (mixture fraction), g (variance of the mixture fraction).

For example, if ϕ represents the axial velocity u , Γ_ϕ will be equal to the effective viscosity μ_e , and the source term S_ϕ will be equivalent to:

$$S_\phi = -\frac{\partial p}{\partial r} + \frac{\partial}{\partial x} \left(\mu_e \frac{\partial u}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu_e \frac{\partial v}{\partial r} \right) \quad (4)$$

The explicit equations for all of the dependent variables can be written in a similar way and can be found elsewhere (Judeh, 2001).

The Turbulence Model

The turbulence model accounts for the transport within the turbulent flow field. The turbulence model adopted in this paper is the standard $k-\epsilon$ model (Launder and Spalding, 1972). Besides the equations for the mean velocity, the turbulent kinetic energy (κ) and the dissipation of turbulent kinetic energy (ϵ) transport equations are solved, along with an expression for the eddy viscosity (Khalil et. als. 1975). This model relates the eddy viscosity ν_t to κ and ϵ via the following Kolmogorov-Prandtl equation:

$$\nu_t = C_\mu k^2 / \epsilon \quad (5)$$

The Combustion Model

The combustion model is the model that simulates the production/consumption of species and energy. In the present study transport equations for the major gaseous species mass fractions are not solved. Instead, a simpler model based on experimentally obtained state relationships measured in laminar diffusion flames is employed (Gore and Faeth, 1988). These state relationships involve a presumed functional dependence of the major gas species mass fractions, Y_i , on an appropriately defined gas-phase mixture fraction, f (fraction of mass in the gas phase that originated in the fuel stream) (Bilger, 1977). Thus this turbulent combustion model assumes that the chemistry in a turbulent flame occurs in a manner similar to that of a laminar flamelet at that location in the mixture. A drawback of this model is that minor gas species are not predicted with this approach. Another drawback is that finite-rate chemistry effects such as ignition and flame extinction events cannot be captured.

The application of this combustion model requires the solution of two differential equations for the time-mean mixture fraction f and for g_f , the variance of f . These two equations for f and g_f in cylindrical coordinates are shown below in Eqs. (6) and (7).

$$\begin{aligned} \rho u \left(\frac{\partial f}{\partial x} \right) + \rho v \left(\frac{\partial f}{\partial r} \right) \\ = \frac{\partial}{\partial x} \left((r \Gamma / \sigma_f) \frac{\partial f}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left((r \Gamma / \sigma_f) \frac{\partial f}{\partial r} \right) \end{aligned} \quad (6)$$

$$\begin{aligned} \rho u \left(\frac{\partial g_f}{\partial x} \right) + \rho v \left(\frac{\partial g_f}{\partial r} \right) = \frac{\partial}{\partial x} \left((\Gamma / \sigma_g) \frac{\partial g_f}{\partial x} \right) \\ + \frac{1}{r} \frac{\partial}{\partial r} \left((r \Gamma / \sigma_g) \frac{\partial g_f}{\partial r} \right) + C_{g1} \Gamma \left[\left(\frac{\partial f}{\partial r} \right)^2 + \left(\frac{\partial f}{\partial x} \right)^2 \right] \\ - C_{g2} \rho \epsilon (g_f / k) \end{aligned} \quad (7)$$

Beside these two equations, a certain shape of the probability distribution function should be assumed. The assumed probability density function (PDF), will describe the statistical distribution of the mixture fraction (f), at any local point in space due to the fluctuations of f in time.

To describe the statistics of the mixing process mathematically, one needs the time-mean mixture fraction, the variance about the mean and the shape of the (PDF). In most of the applications, the shape of the (PDF) is assumed and the other two variables are calculated. In the literature several shapes of (PDF) are assumed, for example: Clipped Gaussian, Top-hat, β - functions and multiple δ -functions. In the current study the Clipped Gaussian pdf is used (Kuo, 1986). In this function, the local $f(t)$ varies randomly between two limits f_{min} and f_{max} , lying in the closed interval (0,1).

NUMERICAL SOLUTION PROCEDURE

The non-linear partial differential equations governing the gas phase flow field were presented in the previous sections. Since these equations are too complicated to be solved analytically, a numerical solution is required. In this study, the widely used finite difference technique is employed to transform these equations into numerically solvable ones. This technique is based upon the TEACH technique developed Gosman and Pun (1974), which is an iterative, steady state, finite-difference approach to solve the gas equations in the primitive variables (u, v, p) using a staggered-mesh system (Lilley and Rhode, 1982). In such a grid system the variables u and v are evaluated at the boundary of the cell while p and ρ being evaluated at the cell center.

According to this method, first the solution domain is divided into a finite number of discrete volumes and the numerical values of the dependent variables are determined at the center of these cells. The finite difference equations FDEs are derived by integrating the partial differential equations over the given control volume. The solution of the resulting system of FDEs must be performed in an iterative manner because of the high degree of non-linearity and interconnection of equations involved. A line-by-line technique; a tri-diagonal algorithm (TDMA) is used to solve these finite difference equations along a line using appropriate boundary conditions. The tri-diagonal algorithm is solved iteratively for a specific variable until convergence is achieved.

The primitive variable formulation does have a difficulty in dealing with the pressure gradient terms that appear in the momentum equations. To overcome this difficulty the SIMPLER approach developed by Patankar (1980), has been used. For the boundary conditions, uniform distribution condition, no-slip condition, fully developed flow condition and axi-symmetrical condition are taken at the inlet, wall, exit and axis, respectively.

Simulations have been done for the combustor shown in Figure 1 where reactants enter in separate

streams, a primary inlet tube for the injection of the natural gas and a secondary inlet tube for the injection of the swirling secondary air stream with a swirl number of 1.50. A two-dimensional grid of 94x88 was used for the predictions. Under-relaxation technique was employed for better numerical stability. The under-relaxation factors for the two gas velocity components; u and v are 0.6, for k and ϵ of the standard $k - \epsilon$ turbulence model, are 0.8, 0.6 and 0.5 under-relaxes gas density and turbulent viscosity, respectively.

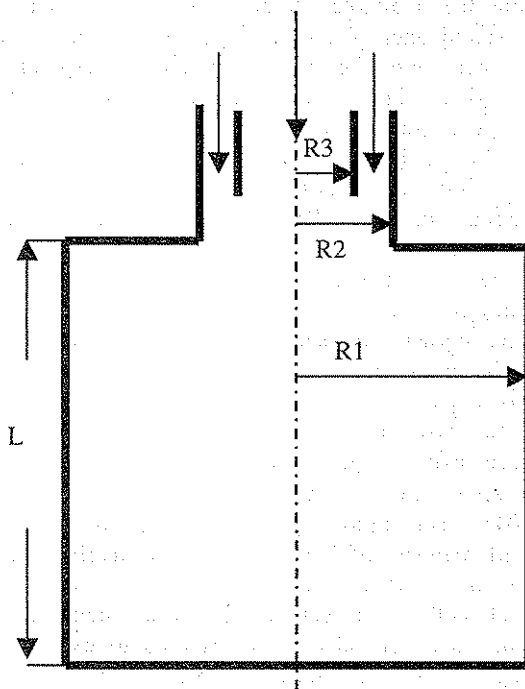


Figure 1. Schematic drawing of the confined jet sudden expansion combustor geometry used in current numerical simulation. (For dimensions see Table I below)

Table 1. Input data for the natural gas combustion case.

R1 = Primary tube diameter (cm)	1.28
R2 = Secondary tube diameter (cm)	9.34
R3 = Combustor diameter (cm)	80
L = Combustor length (cm)	250
Primary gas flow rate (g/s)	2.656
Secondary gas flow rate (g/s)	45.0
Primary swirl number	0.0
Secondary swirl number	1.5
Primary air inlet temperature (K)	298.0
Primary air turbulence intensity (%)	10.0
Secondary air inlet temperature (K)	298.0
Secondary air turbulence intensity (%)	10.0
Reactor pressure (Pa)	86 000

RESULTS AND DISCUSSION

In this paper, calculations have been made to demonstrate the ability of the above described mathematical models and to predict the capabilities of the code developed to simulate the flow field in axisymmetric sudden expansion combustor. In order to evaluate the quality of the predictions obtained using the code under consideration, one set of experimental natural gas combustion data reported by Eaton et. al. (1999) have been selected from the available literature because it contains measured data of several experimental parameters together with the results of the corresponding numerical simulations obtained by some other different researchers.

One of the important features of the incoming flow into a combustor is the creation of the recirculation zones. The resulting flow field domain possesses a central recirculation zone in the middle of the region around the centerline of the reactor, in addition to a corner recirculation zone near the upper corner provoked by the sudden enlargement of the cross sectional area of the combustor. The two zones can be identified clearly in Figures 2 and 3 that show the contour lines of the predicted gas mean axial velocity field calculated using two different values of the C_μ coefficient of 0.09 and 0.045. Each figure is also drawn for two different swirl numbers of 1.0 and 1.5, respectively. These two figures show that with an increase in the swirl level, both of the central and corner recirculation zone have generally been observed to expand in length toward the combustor upstream.

Comparison of the experimental and predicted centerline gas mean axial velocity is given in Figure 4. Predicted velocity is calculated using the standard k- ϵ turbulence model with C_μ value of 0.09. From this figure, it is apparent that the prediction is rather poor in the vicinity of the recirculation zone, but it does approach to be adequate near the wall and in the downstream region. Indeed, over the outer three-fourths of the chamber radius, the standard k- ϵ model matches the data well. Calculated values of centerline mean axial velocity indicates that the largest discrepancy occurs in the initial flow region where the flame front develops and this discrepancy almost disappear in the down stream region near the reactor exit where the effect of the recirculation zone disappear

The source of the discrepancy in Figure 4 seems to lie predominantly in the disability of the standard k- ϵ model to accurately predict the recirculation zone. In order to enhance the model ability to

predict the flow correctly inside the recirculation zone, the C_μ coefficient can be modified to simulate well the turbulent eddy viscosity. The modified C_μ coefficient is limited numerically between the value of 0.025 and its standard value of 0.09. As the value of C_μ decreases, this corresponds to a decrease in the eddy viscosity and leads to increasing contribution of laminar effects.

Figure 5 shows the centerline axial velocity predictions using three different values of C_μ : 0.09, 0.045, and 0.03 together with the experimental profile. The comparison shows that the modified C_μ coefficient helps somewhat to predict more correctly both the size and strength of the recirculation zone near the chamber axis, relative to the standard k- ϵ model. Prediction obtained using C_μ value of 0.045 was found to match almost exactly the experimental data.

Figure 6 shows the comparison between predicted and measured centerline mean gas temperature profiles for stoichiometric air-fuel mixture. For engineering purposes, it can be seen that the two sets of data are in good agreement. The reaction zone was clearly identified and the maximum flame temperature was well predicted.

The maximum temperature generally appears to lie immediately within the central recirculation zone that was identified earlier in Figure 2. High entrainment rates and rapid mixing between the fuel and air in diffusion flame systems characterize this zone. Hence, the recirculation zone is regarded as a well-mixed region with higher combustion rate that stabilizes the flame by continuous mixing of hot active species and fresh reactants.

In Figure 7, the predicted centerline gas temperature profiles are plotted for three different combustion air temperatures of 300, 350 and 400 K. As the inlet air temperature becomes higher, the maximum flame temperature has been identified to increase. This is not a desired increase since the high flame temperature increases formation of the soot precursor and increases formation of the other pollutants such as NO and CO.

Figures 8, 9 and 10 give the comparisons between predicted and measured radial profiles for gas mean axial velocity, tangential velocity and temperature at three different axial locations of 26, 86 and 126 cm. from the burner outlet. Examining these figures indicates that a reasonable agreement between model predictions and experimental measurements in both magnitude and shape exists in the downstream flow region far from the recirculation zone that develops near the inlet and around the centerline of the combustor, where deviations are serious. As the flow moves down the

reactor the profiles tend to become flat and constant along the combustor diameter.

Differences between measurements and the predictions of the current work and both PCGC-3 (Hill et. al. 1993) and FLUENT (Eaton et. al., 1999) codes shown in the last three figures demonstrate the complex nature of turbulent swirling flow combustion calculations. Possible reasons for observed differences could be attributed to:

1. Inadequacy of the two-equation turbulence model, which assumes that the turbulence is isotropic, which is not the case in a highly swirling flow.
2. Simplicity of the combustion model that does not account for the reaction kinetics and chemistry-turbulence interactions.
3. Lack of adequate information of the boundary conditions and suitable velocity, turbulent kinetic energy and its dissipation rate inlet profiles.
4. Alteration of the flow caused by the measuring probe intrusion while the measurements were taken.

A major motivation of many combustion calculations is the predictions of the various species concentrations especially the pollutant such as CO and NO_x . Accurate predictions of these variables are highly dependent on the sensitivity of the flow field solution.

Figure 11 represents calculated concentrations of fuel and major gas species CO_2 , CO and O_2 for three different equivalence ratios corresponding to lean, stoichiometric and rich air/fuel mixtures at the combustor centerline. The axial distribution of fuel concentration decreases more rapidly with the higher air/fuel ratio since more oxygen will be available to burn the fuel as soon as they mix. As a result, the flame sheet thickness will decrease by increasing air/fuel ratio.

The combustion model used for the present calculations postulates a physically controlled, infinitely fast one-step reaction, limited only by the extent of mixing process between fuel and oxygen. The recirculation region developed near the combustor entrance is playing an important role to enhance the mixing of fuel and oxygen resulting in a highly reactive zone i.e. the flame front where almost no oxygen can appear separately. In fuel-rich mixture case of Figure 11, not enough oxygen is available for complete combustion and the carbon in the fuel is oxidized initially to CO rather than CO_2 . The opposite of this trend is observed for lean-fuel mixture case where the carbon fuel is converted to CO_2 rather than CO. At the combustor downstream, locations far behind the initial mixing region for the case of lean fuel-air mixture case, the available oxygen will be consumed to convert CO to CO_2 resulting in almost negligible oxygen, larger CO_2 and less CO concentrations.

Figure 12 and Figure 13 illustrate the variations of mean gas temperature profiles measured along the combustor centerline for different rich and lean fuel-air mixtures. For fuel-lean mixtures as ϕ increases towards unity, the flame temperature and the gas temperature at combustor exit both increase until they reach their maximum at $\phi = 1.0$. On the other hand for fuel-rich mixtures as ϕ becomes larger than unity ($1.2 \geq \phi \geq 1.0$) the flame temperature obtained will be slightly larger than that obtained at stoichiometric conditions. In this case also, the gas exit temperature will have its largest value at ϕ equal unity.

The variation of the gas temperature at the combustor exit as a function of the equivalence ratio is shown in Figure 14. It is clear from this figure that the exit gas temperature has its maximum value at ϕ equal unity and for less or large values of ϕ , this temperature will decrease.

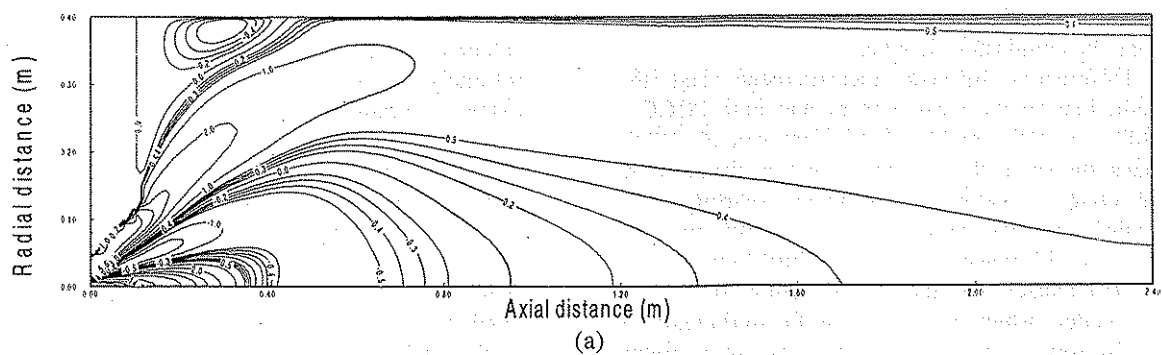
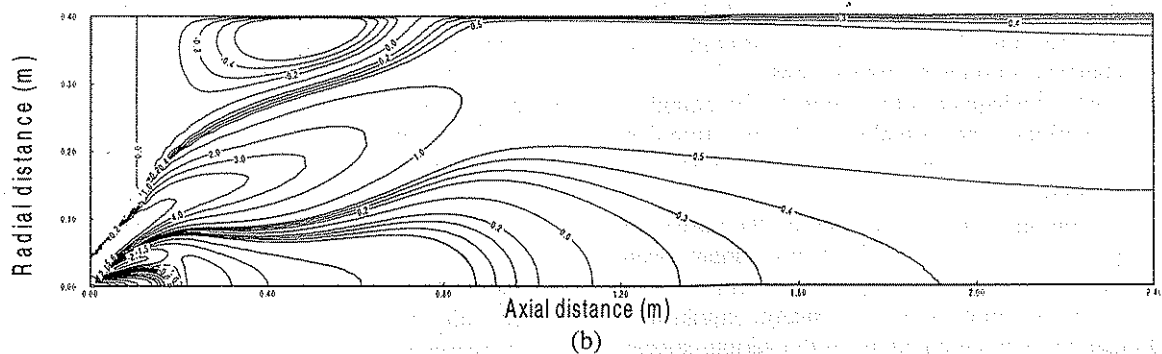


Figure 2. Contour lines of the gas mean axial velocity for natural gas combustion case for $C_\mu = 0.045$ and grid size=94x88: (a) Swirl number = 1.0, (b) Swirl number = 1.5.

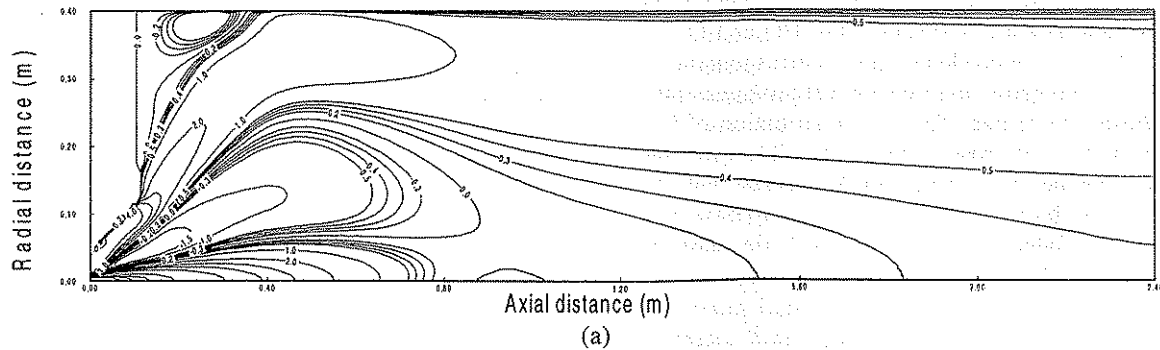
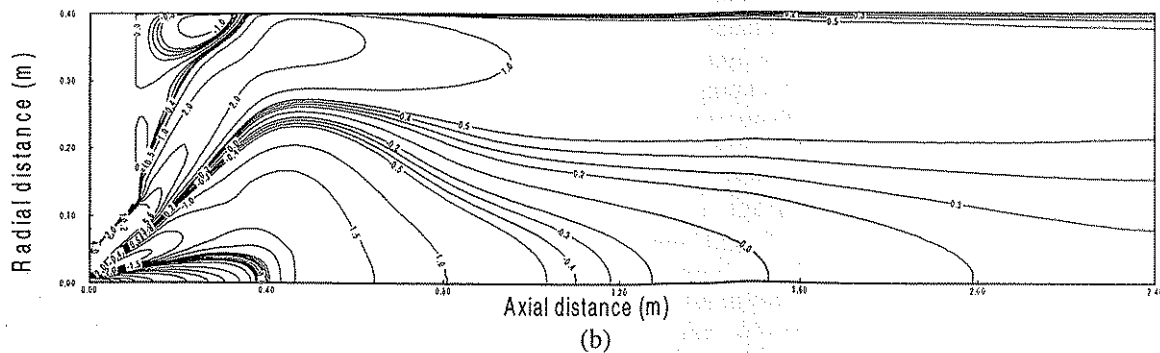


Figure 3. Contour lines of the gas mean axial velocity for natural gas combustion case for $C_\mu = 0.09$ and grid size=94x88: (a) Swirl number = 1.0, (b) Swirl number = 1.5.

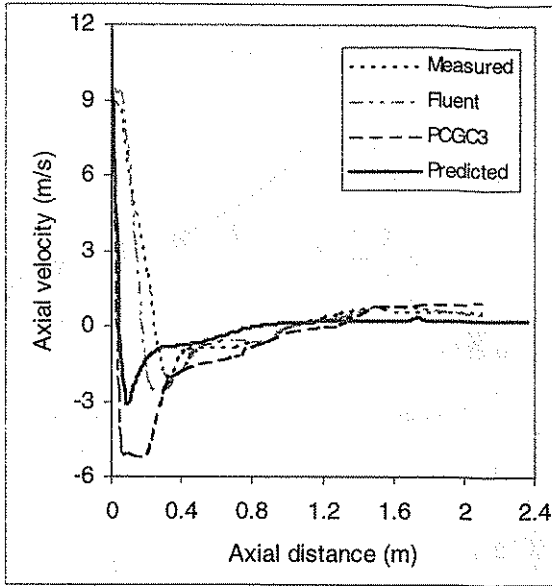


Figure 4. Predicted and experimentally measured gas axial velocity distributions along the combustor centerline during natural gas combustion. Swirl number =1.5, $C_{\mu} = 0.09$, equivalence ratio =1.0, grid size = 94x88 (Data from Eaton et. al. 1999).

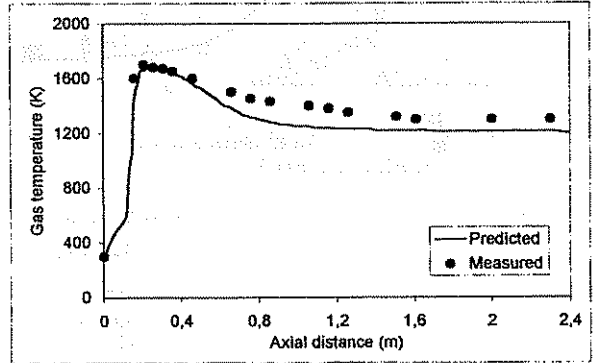


Figure 6. Predicted and experimentally measured gas mean temperature distributions along the combustor centerline during natural gas combustion. Swirl number =1.5, equivalence ratio =1.0, grid size = 94x88 (Data from Tree et. al. 1998).

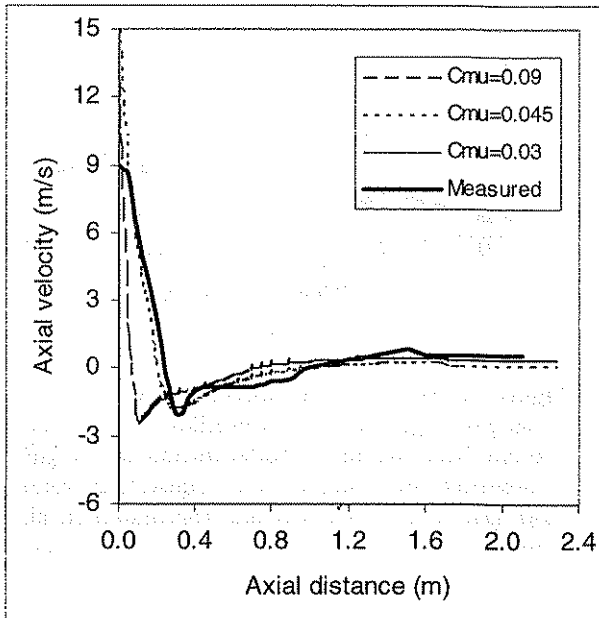


Figure 5. Predicted and experimentally measured centerline axial velocity distribution along the centerline during natural gas combustion. Predictions done for three different C_{μ} coefficients of 0.09, 0.045, and 0.03, swirl number =1.5, equivalence ratio =1.0, grid size=94x88. (Measured data from Eaton et. al. 1999).

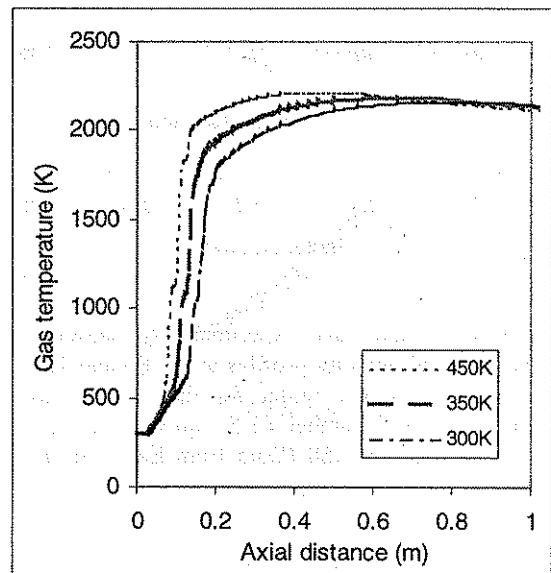


Figure 7. Predicted gas mean temperature distributions along the combustor centerline during natural gas combustion under three different combustion entrance air temperatures of 300, 350 and 400 K. Swirl number =1.5, equivalence ratio =1.0, grid size = 94x88.

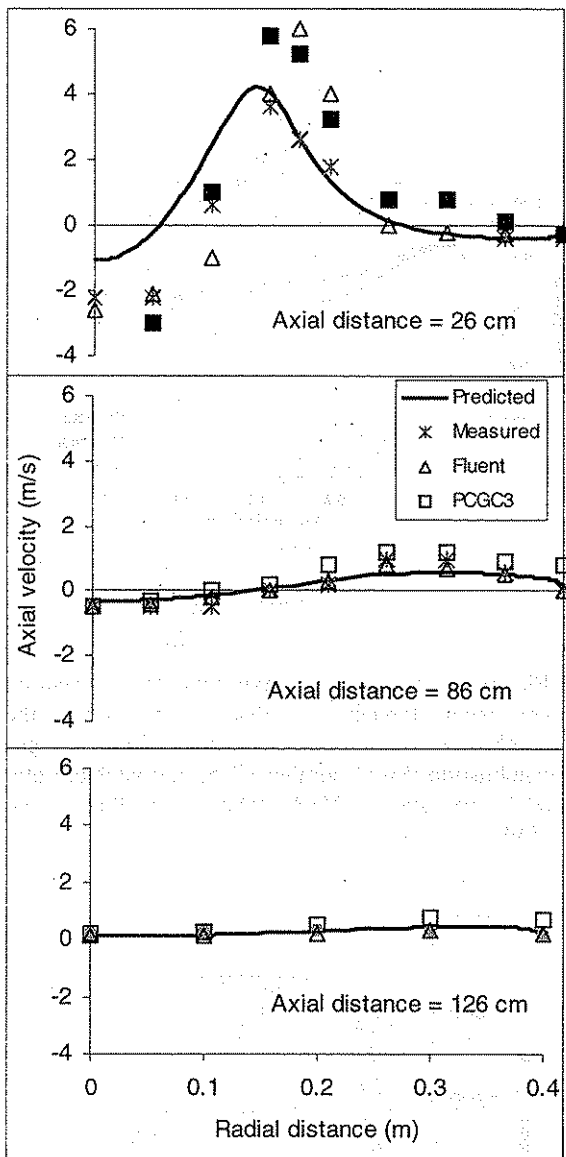


Figure 8. Predicted and experimentally measured radial gas axial velocity profiles at 26, 86 and 126 cm. from the burner outlet for the natural gas combustion. Swirl number =1.5, equivalence ratio =1.0, grid size = 94x88 (Data from Eaton et. al. 1999).

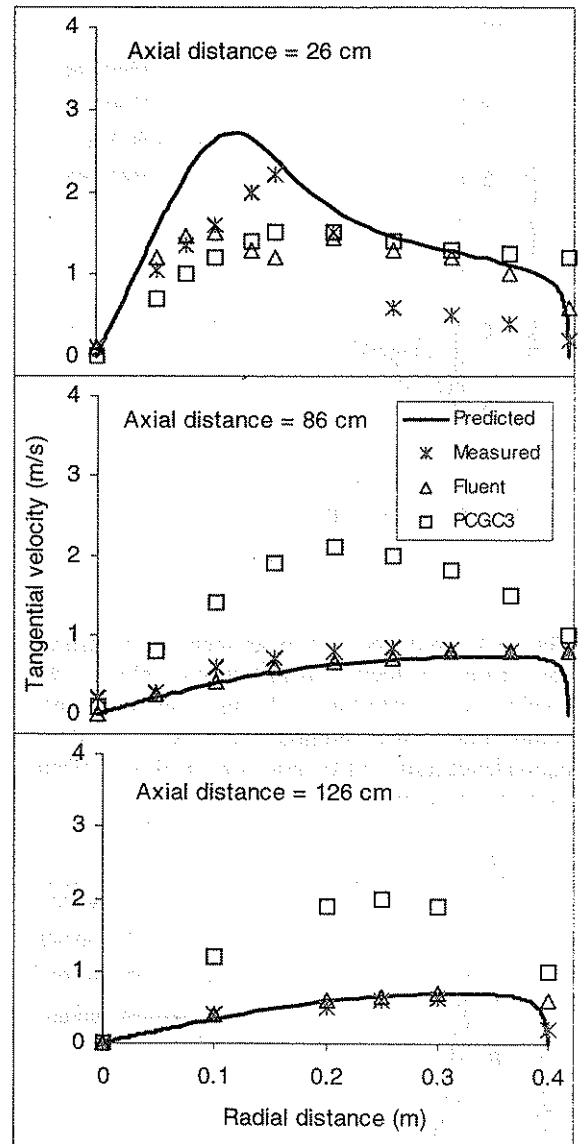


Figure 9. Predicted and experimentally measured radial gas tangential velocity profiles at 26, 86 and 126 cm. from the burner outlet for the natural gas combustion. Swirl number =1.5, equivalence ratio =1.0, grid size = 94x88 (Data from Eaton et. al. 1999).

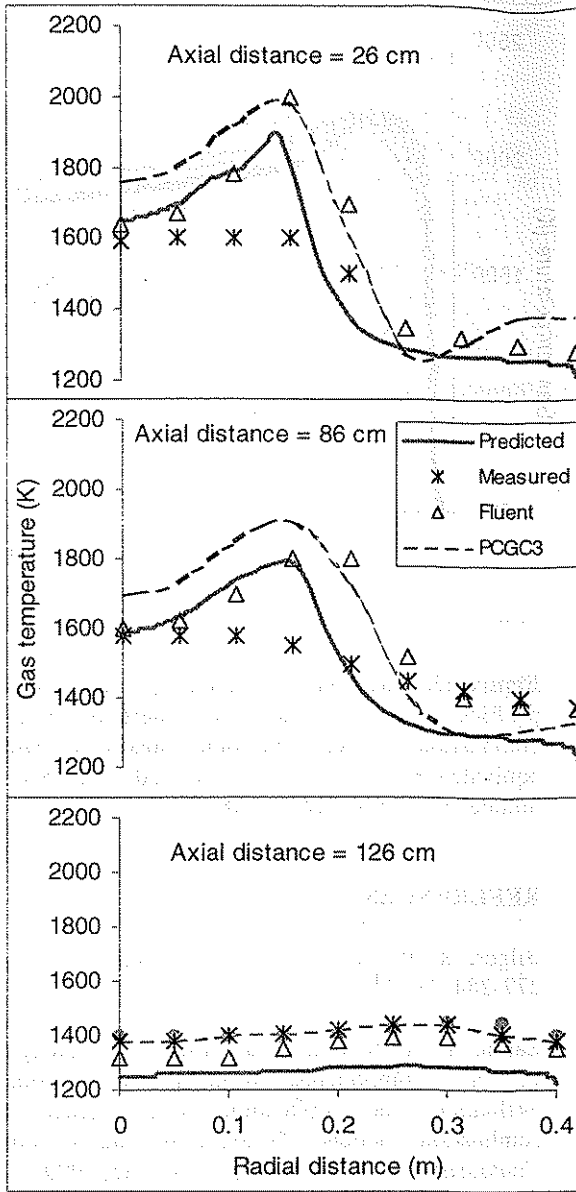
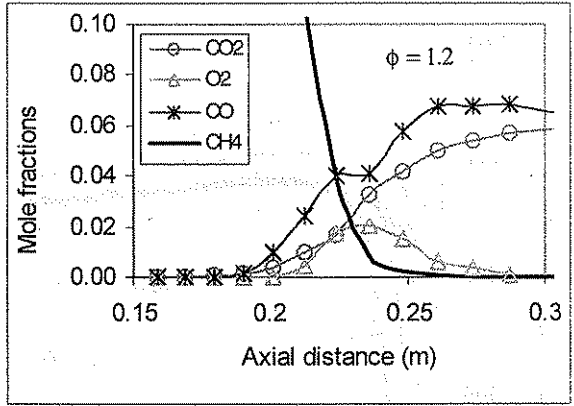
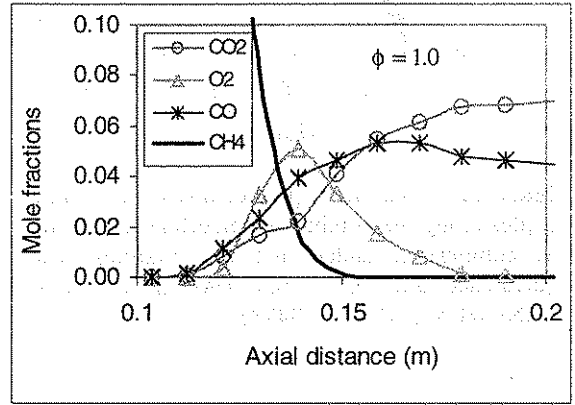


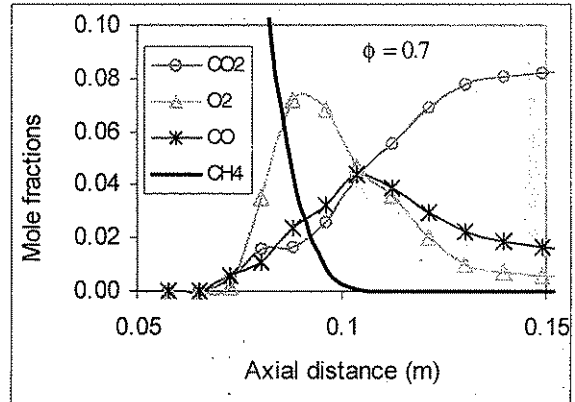
Figure 10. Predicted and experimentally measured radial gas temperature profiles at 26, 86 and 126 cm. from the burner outlet during natural gas combustion case. Swirl number =1.5, equivalence ratio =1.0, grid size = 94x88. (Data from Eaton et. al. 1999).



(a)



(b)



(c)

Figure 11. Variations of predicted fuel and gas species mole fractions along the combustor centerline during natural gas combustion under three different equivalence ratios: (a) $\phi = 0.7$, (b) $\phi = 1.0$ and (c) $\phi = 1.2$. Swirl number =1.5, grid size = 94x88.

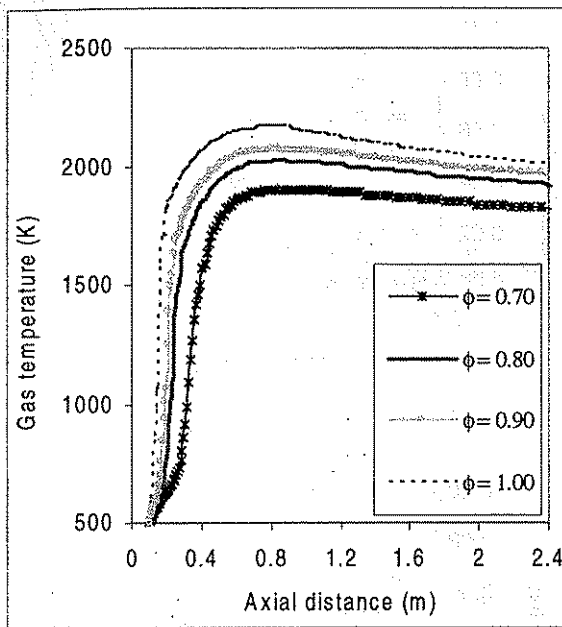


Figure 12. Variations of predicted gas temperature profiles along the combustor centerline for natural gas combustion under fuel-lean mixtures with equivalence ratios of 0.7, 0.8, 0.90, and 1.0. Swirl number = 1.5, grid size = 94x88.

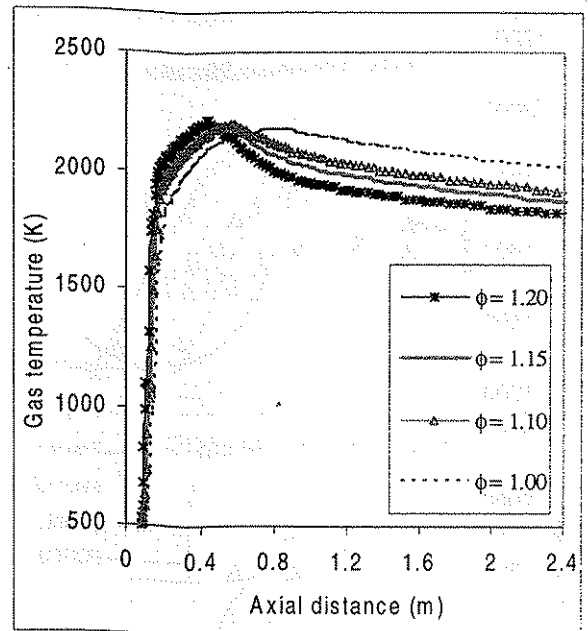


Figure 13. Variations of predicted gas temperature profiles along the combustor centerline for gas combustion under fuel-rich mixtures with equivalence ratios of 1.0, 1.10 and 1.20. Swirl number = 1.5, grid size = 94x88.

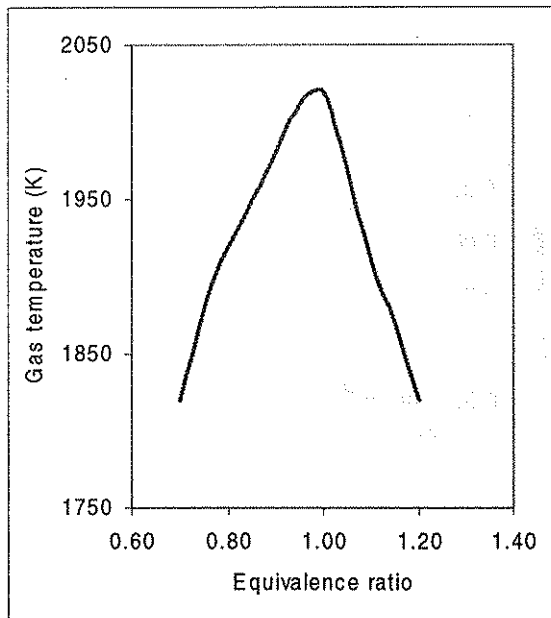


Figure 14. Variation of the predicted gas temperature profile with equivalence ratio along the combustor exit plane during natural gas combustion. Swirl number = 1.5, grid size = 94x88.

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