Numerical study of effect of oxygen fraction on local entropy generation in a methane–air burner

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Abstract. This study considers numerical simulation of the combustion of methane with air, including oxygen and nitrogen, in a burner and the numerical solution of local entropy generation rate due to high temperature and velocity gradients in the combustion chamber. The effects of equivalence ratio (ϕ) and oxygen percentage (γ) on combustion and entropy generation rates are investigated for different ϕ (from 0.5 to 1.0) and γ values (from 10 to 30%). Combustion is simulated for the fuel mass flow rate resulting in the same heat transfer rate ($\dot{Q}$) to the combustion chamber in each case. Numerical calculation of combustion is performed individually for all cases with the use of the Fluent CFD code. Furthermore, a computer program has been developed to calculate the volumetric entropy generation rate and the other thermodynamic parameters numerically by using the results of the calculations performed with the FLUENT code. The predictions show that the increase of ϕ (or the decrease of λ) significantly reduces the reaction rate levels. Average temperature in the combustion chamber increases by about 70 and 35% with increase of γ (from 10 to 30%) and ϕ (from 0.5 to 1.0) respectively. With increase of γ from 10 to 30%, volumetric local entropy generation rate decreases by about 9 and 4% for $\phi = 0.5$ and 1.0 respectively, while total entropy generation rate decreases exponentially and the merit numbers increase. The ratio of the rates useful energy transfer to irreversibility therefore improves as the oxygen percentage increases.

Keywords. Air–fuel combustion; local entropy generation; exergy; computational fluid dynamics.

1. Introduction

During combustion fossil and renewable fuels are converted into a different fuel and/or heat and/or electricity. Combustion of fuel involves converting the chemical energy contained in the fuel into chemical energy contained in the gaseous products and sensible energy of the produced gas. Burners are used widely in a variety of industrial combustion systems, where there is need to ensure efficient combustion conditions which is associated with good

fluid mixing and long reaction times. In many combustion devices, both air and fuel are in the gaseous phase and coaxial geometry is commonly used to merge the two streams. The principal objectives of research work in the area of combustion are to improve the combustion process in order to achieve higher combustion efficiency with a uniform exit temperature and allowable linear wall temperature distribution and to reduce combustion-generated polluting gases. However, the chemical and physical processes involved in combusting flows and their interactions are extremely complex and are often not well understood.

Combustion phenomena are a complex mixture of fluid dynamics and chemistry. Therefore, CFD (computational fluid dynamics) can serve as a powerful tool, and can be used to perform low-cost parametric studies involving critical burner design parameters. The CFD-codes solve the governing mass, momentum and energy equations in order to calculate the velocity, pressure and temperature fields. The main advantage of this computational approach is in its potential for reducing the extent and number of experiments required to describe such types of flow. In the near future, it may well be that computer simulation of combustion system will become a standard design tool.

On the other hand, the thermodynamic performance of a device or process can be assessed through the measure of the irreversibility generated. According to the first law of thermodynamics, energy can never be lost. Therefore it is justifiable to state that energy conversion processes do not have energy losses, except for losses from the process system into the environment. However, the second law of thermodynamics should also be considered for evaluating the sources of irreversibility in flow and thermal systems. Conserving useful energy depends on designing efficient thermodynamic heat-transfer processes. Energy conversion processes are accompanied by an irreversible increase in entropy, which leads to a decrease in exergy (available energy). Thus, even though energy is conserved, the quality of energy decreases because energy is converted into a different form of energy, from which less work can be obtained. Reduced entropy generation results in more efficient designs of energy systems. Therefore, in recent years, entropy minimization has become a topic of great interest in the thermo-fluid area. Bejan (1996a) focused on the different reasons behind entropy generation in applied thermal engineering where the generation of entropy destroys the available work (exergy) of a system. Therefore, it makes good engineering sense to focus on the irreversibility of heat transfer and fluid flow processes, and to try to understand the function of associated entropy generation mechanisms. Bejan (1996b) also conducted an extensive review on entropy generation minimization. The review traced the development and adoption of the method in several sectors of mainstream thermal engineering and science. Furthermore, many researchers have studied the entropy generation in various flow cases. Second-law analysis of heat transfer in swirling flow through a cylindrical duct was investigated by Mukherjee *et al* (1987), who calculated the rate of entropy generation. They also defined a merit function and discussed the influence of swirling on this function. Mahmud & Fraser (2003) also investigated the second-law analysis in fundamental convective heat transfer problems and the thermodynamic analysis of flow and heat transfer inside channel with two parallel plates (Mahmud & Fraser 2002). Sahin (1998, 1999, 2000, 2002), Yilbas *et al* (1999), Shuja *et al* (2001a), Demirel & Kahraman (1999) and Abbassi *et al* (2003) performed many studies on second law analysis and the entropy generation due to the heat transfer and fluid friction in duct flows under various conditions. Shuja and coworkers analysed entropy generation in swirling jet impingement on an adiabatic wall (Shuja & Yilbas 2001b; 2003) and an impinging jet (Shuja *et al* 2001b) for various flow conditions.

The present study considers the combustion of methane with air and the local entropy generation rate due to the high temperature and velocity gradients in combustion chamber

of burner. In order to investigate the effect of oxygen percentage on the combustion and entropy generation rate, the combustion of methane with air is examined at various oxygen percentages in the air by using Fluent CFD code (Fluent Inc. 2003).

2. Mathematical model

2.1 Burner geometry

The main aim of this study is to estimate numerically the rate of local entropy generation in the combustion chamber of a burner. For this purpose, the combustion of methane (CH_4) with air in a burner was considered. The two-dimensional axisymmetric model and geometric configuration of the burner are shown in figure 1. As apparent from this figure, the methane and air inlets are coaxial and merge downstream. It is assumed that the burner wall is under ambient conditions and that the walls neighbouring the air and fuel inlets are isolated.

In order to estimate the effects of oxygen percentage in the air and equivalence ratio, defined in section 2-2, on below combustion and entropy generation rates, different (consecutive) oxygen percentages and equivalence ratios were studied. In this study, combustion is simulated for the fuel mass flow rate resulting in the same heat transfer rate ($\dot{Q}$) to the combustion chamber in the each case. Simulations performed with equal heat transfer rate approximation would facilitate comparison of the local entropy generation in the combustion chamber due to other geometries. Numerical calculation of the combustion was performed using the Fluent CFD code.

2.2 Mathematical model

The model used for the numerical calculations include:

- for turbulent flow, the RNG (renormalization group theory) $k-\varepsilon$ model (Yakhot & Orszag 1986)
- for chemical species transport and reacting flow, the eddy-dissipation model with the diffusion energy source option

The assumptions made are as follows.

- the Flow is steady, two-dimensional axisymmetric, turbulent and compressible
- the Fuel–air mixture is assumed to behave as an ideal gas
- No-slip condition is assumed at the burner walls

Figure 1. Coordinate system and two-dimensional axisymmetric model of the burner (dimensions are not to scale).

2.2a Governing conservation equations: Governing mass, momentum and energy conservation equations for steady-state gas flow are given in tensor notation as follows.

Mass conservation equation (species transport equations) –

$$\frac{\partial}{\partial x_i} (\rho u_i m_{i'}) = - \frac{\partial}{\partial x_i} J_{i',i} + R_{i'} \quad (1a)$$

$J_{i',i}$ (mass diffusion) is written for turbulent flows as follows:

$$J_{i',i} = - \left(\rho D_{i',m} + \frac{\mu_t}{Sc_t} \right) \frac{\partial m_{i'}}{\partial x_i}, \quad (1b)$$

where $D_{i',m}$ is the diffusion coefficient for species i' in the mixture and

$$D_{i',m} = (1 - X_{i'}) / \sum_{j', j' \neq i'} X_{j'} / D_{i'j'}, \quad (1c)$$

$D_{i'j'}$ is the binary mass diffusion coefficient for species i' in species j' .

An equation of this form is solved for $N-1$ species where N is the total number of fluid phase chemical species present in the system.

The momentum conservation equation –

$$\frac{\partial}{\partial x_j} (\rho u_i u_j) = - \frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}, \quad (2a)$$

and

$$\tau_{ij} = \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \frac{2}{3} \mu \frac{\partial u_l}{\partial x_l} \delta_{ij}. \quad (2b)$$

The energy conservation equation –

$$\frac{\partial}{\partial x_i} [u_i (\rho E + P)] = \frac{\partial}{\partial x_i} \left(\lambda_{eff} \frac{\partial T}{\partial x_i} - \sum_{j'} h_{j'} J_{j'} + u_j (\tau_{ij})_{eff} \right) + S_h \quad (3a)$$

where $J_{j'}$ is the diffusion flux of species j' , S_h includes heat of chemical reaction and any other volumetric heat sources,

$$E = h - \frac{P}{\rho} + \frac{u_i^2}{2}, \quad (3b)$$

where h is defined for ideal gases as:

$$h = \sum_{j'} m_{j'} h_{j'}, \quad (3c)$$

where

$$h_{j'} = \int_{T_{ref}}^T C_{p,j'} dT. \quad (3d)$$

λ_{eff} is the effective conductivity and for the RNG k - ε model,

$$\lambda_{\text{eff}} = \alpha \cdot C_p \cdot \mu_{\text{eff}}, \quad (3e)$$

where α , the inverse effective Prandtl number, is computed using the following formula derived analytically by the RNG theory:

$$\left| \frac{\alpha - 1.3929}{\alpha_0 - 1.3929} \right|^{0.6321} \cdot \left| \frac{\alpha + 2.3929}{\alpha_0 + 2.3929} \right|^{0.3679} = \frac{\mu}{\mu_{\text{eff}}} \quad (3f)$$

where

$$\alpha_0 = \lambda / \mu C_p. \quad (3g)$$

Two additional equations for the RNG k - ε turbulence model – The turbulence kinetic energy, k , and the dissipation rate, ε , are determined using the following transport equations, respectively:

$$\frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_i} \left(\alpha_k \mu_{\text{eff}} \frac{\partial k}{\partial x_i} \right) + G_k - \rho \varepsilon, \quad (4a)$$

$$\frac{\partial}{\partial x_i}(\rho u_i \varepsilon) = \frac{\partial}{\partial x_i} \left(\alpha_\varepsilon \mu_{\text{eff}} \frac{\partial \varepsilon}{\partial x_i} \right) + \frac{\varepsilon}{k} (C_{1\varepsilon} G_k - C_{2\varepsilon} \rho \varepsilon) - \chi \quad (4b)$$

where α_k and α_ε the inverse effective Prandtl numbers for k and ε , respectively, are calculated from (3f) by using $\alpha_0 = 1$,

$$\mu_{\text{eff}} = \mu + \mu_t, \mu_t = \rho C_\mu (k^2 / \varepsilon), \quad (4c,d)$$

C_μ , C_1 and $C_{2\varepsilon}$ are the model constants,

$$G_k = \mu_t S^2, \quad (4e)$$

and

$$\chi = C_\mu \rho \frac{\eta^3 (1 - (\eta / \eta_0)) \varepsilon^2}{1 + \beta \eta^3} \frac{1}{k}. \quad (4f)$$

S the modulus of the mean rate-of-strain tensor is defined as

$$S = (2S_{ij}S_{ij})^{1/2}. \quad (4g)$$

S_{ij} (the mean strain rate) is given by:

$$S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad (4h)$$

$$\eta = S \cdot (k / \varepsilon), \quad (4i)$$

$\eta_0 = 4.38$, and $\beta = 0.012$.

Thermal properties of the mixture – Fluid density is calculated using the ideal-gas law. Density, viscosity, specific heat and thermal conductivity of the mixture are calculated from the relevant properties of the species in the mixture according to the ideal-gas-mixing-law as follows:

$$\rho = (P_{op} + P) / \Re T \sum_{i^1} (m_{i^1} / M_{i^1}), \quad (5a)$$

$$C_p = \sum_{i^1} m_{i^1} C_{p,i^1}, \quad (5b)$$

$$\lambda = \sum_{i^1} \left[X_{i^1} \lambda_{i^1} / \left(\sum_{j^1} X_{j^1} \varphi_{i^1,j^1} \right) \right], \quad (5c)$$

$$\mu = \sum_{i^1} \left[X_{i^1} \mu_{i^1} / \left(\sum_{j^1} X_{j^1} \varphi_{i^1,j^1} \right) \right], \quad (5d)$$

and

$$\varphi_{i^1,j^1} = \frac{\left[1 + (\mu_{i^1} / \mu_{j^1})^{1/2} (M_{j^1} / M_{i^1})^{1/4} \right]^2}{\left[8 (1 + M_{i^1} / M_{j^1}) \right]^{1/2}}. \quad (5e)$$

Boundary conditions –

$$\text{At the fuel inlet } (x = 0 \text{ and } 0 < r < r_f), u_x = U_f, u_r = 0, \text{ and } T = T_{in} \quad (6a-d)$$

$$\text{At the air inlet } (x = 0 \text{ and } r_i < r < r_o), u_x = U_{air}, u_r = 0, T = T_{in}, \quad (6e-g)$$

$$\text{At the isolated walls } (x = 0, r_f < r < r_i \text{ and } r_o < r < R), \partial T / \partial x = 0 \quad (6h)$$

$$\text{At the burner wall } (r = R, \text{ and } 0 < x \leq L),$$

$$u_r = 0, \quad (6i)$$

natural convection is assumed, i.e.

$$q''_w(x) = -h_{amb} [T(x, R) - T_{amb}], \quad (6j)$$

and the no-slip condition is assumed, i.e.

$$u_x = 0. \quad (6k)$$

Since the profiles of velocity and temperature are both symmetric with respect to the axis of the burner, the relevant boundary conditions at the symmetry axis ($r = 0$) are

$$\partial \psi / \partial r = 0 \quad (6l)$$

where ψ is any arbitrary variable.

$$\text{At the outlet, } \partial \psi / \partial x = 0, \text{ All velocities are zero except the axial velocity.} \quad (6m)$$

2.2b Combustion of fuel with air: The simplest description of combustion is that it is a process that converts the *reactants* available at the beginning of combustion into *products* at the end of the process. The most common combustion processes encountered in engineering are those which convert a hydrocarbon fuel (which might range from pure hydrogen to almost pure carbon (C), e.g. coal) into carbon dioxide (CO₂) and water (H₂O). They are usually exothermic (i.e. they release the chemical (or bond) energy contained in the fuels as thermal energy).

Reaction mechanism – In this study, the combustion of methane with oxygen is modelled with a two-step reaction mechanism ($N_R = 2$ and species number, $N = 5$) where production and combustion of carbon monoxide (CO) is taken into account. In the first stage, methane is oxidized into carbon monoxide and water vapour and in the second, carbon monoxide oxidizes into carbon dioxide. The reaction mechanism takes place according to the constraints of chemistry, and is defined by:

A lean mixture occurs when the quantity of air available for combustion is greater than the chemically correct quantity for complete oxidation of the fuel; this means that there is excess air available. The equation for combustion of a lean mixture of methane–air is

divided by the actual air/fuel ratio, AFR_{act} , i.e.:

$$\phi = \frac{AFR_{\text{sto}}}{AFR_{\text{act}}} \quad (8a)$$

where

$$AFR_{\text{sto}} = 2 \left(M_{\text{O}_2} + (100 - \gamma)/\gamma M_{\text{N}_2}/M_f \right), \quad (8b)$$

and

$$AFR_{\text{act}} = \dot{m}_{\text{air}}/\dot{m}_f. \quad (8c)$$

The combustion reactions, (7a,b), give reaction enthalpy and the value of this enthalpy is the negative of the lower calorific value (LCV) of methane because it is based on gaseous water in the products. However, its value is taken to be a positive value for the flowing fluid because it is transferred into the flowing fluid inside the burner chamber during the combustion process. Therefore, the reaction energy released in the chemical reaction is added to the S_h term in (3a) as the positive volumetric energy source.

The lower heating value, LHV, and LCV of the fuel can be calculated as

$$\text{LHV} = \sum H_P - \sum H_R \quad \text{and} \quad \text{LCV} = -\text{LHV}, \quad (8d,e)$$

where H_P and H_R are the enthalpies of product and reactant species respectively.

The fuel mass flow rate providing a desired heat transfer rate to the combustion chamber during the combustion process is calculated by

$$\dot{m}_f = \dot{Q} \cdot M_f / \text{LCV}. \quad (8f)$$

The eddy-dissipation model – In turbulent reacting flows, the Arrhenius reaction rate, the eddy-dissipation-model reaction rates given by (9b,c), or both, depending on the problem definition, are calculated. In this study, the reaction rates that appear as source terms in (1) (species transport equations) are computed by using the eddy-dissipation concept of Magnussen & Hjertager (1976). The source of chemical species i^1 due to reaction, R_{i^1} , is computed as the sum of the reaction sources over the N_R reactions that the species may participate in:

$$R_{i^1} = M_{i^1} \sum_{k=1}^{N_R} \widehat{R}_{i^1,k}, \quad (9a)$$

where $\widehat{R}_{i^1,k}$ is the molar rate of creation/destruction of species i^1 in reaction k . The reaction rate, $R_{i^1,k}$, is controlled either by an Arrhenius kinetic rate expression or by the mixing of the turbulent eddies containing fluctuating concentrations of species.

The influence of turbulence on the reaction rate is taken into account by employing the Magnussen & Hjertager model (1976). In the eddy-dissipation model, the rate of reaction $R_{i^1,k}$ is given by the smaller (i.e., limiting value) of the two expressions below:

$$\begin{aligned} R_{i^1,k} &= v_{i^1,k}^1 M_{i^1} A \rho \frac{\varepsilon}{k} \frac{m_R}{v_{R,k}^1 M_R}, \\ R_{i^1,k} &= v_{i^1,k}^1 M_{i^1} A B \rho \frac{\varepsilon}{k} \frac{\sum_P m_P}{\sum_{j^1}^N v_{j^1,k}^1 M_{j^1}}, \end{aligned} \quad (9b,c)$$

where $v_{i^1,k}^1$ is the stoichiometric coefficient for reactant i^1 in reaction k , $v_{j^1,k}^1$ is stoichiometric coefficient for product j^1 in reaction k , m_P represents the mass fraction of any product species, P , m_R represents the mass fraction of a particular reactant, R , R is the reactant species giving the smallest value of $R_{i^1,k}$, A and B are empirical constants equal to 4.0 and 0.5 respectively. The eddy-dissipation model relates the rate of reaction to the rate of dissipation of the reactant- and product-containing eddies. (k/ε) represents the time scale of the turbulent eddies following the eddy-dissipation model of Spalding (1970).

2.2c Entropy generation rate: In fluid flow, irreversibility arises due to the heat transfer and the viscous effects of the fluid. In these systems, when both temperature and velocity fields are known, the volumetric entropy generation rate (S_{gen}''') at each point in the system can be calculated as follows (Bejan 1996a),

$$S_{\text{gen}}''' = \left(S_{\text{gen}}''' \right)_{\text{heat}} + \left(S_{\text{gen}}''' \right)_{\text{fric}}, \quad (10a)$$

where $\left(S_{\text{gen}}''' \right)_{\text{heat}}$ and $\left(S_{\text{gen}}''' \right)_{\text{fric}}$ represent the entropy generation rates due to heat transfer and fluid friction, respectively, and are defined as,

$$\left(S_{\text{gen}}''' \right)_{\text{heat}} = (\lambda_{\text{eff}}/T^2) \cdot [(\partial T/\partial x)^2 + (\partial T/\partial r)^2] \quad (10b)$$

$$\left(S_{\text{gen}}''' \right)_{\text{fric}} = \mu_{\text{eff}}/T \cdot \Phi \quad (10c)$$

where Φ is

$$\Phi = 2 \cdot \left[\left(\frac{\partial u_x}{\partial x} \right)^2 + \left(\frac{\partial u_r}{\partial r} \right)^2 + \left(\frac{u_r}{r} \right)^2 \right] + \left(\frac{\partial u_x}{\partial r} + \frac{\partial u_r}{\partial x} \right)^2. \quad (10d)$$

The total entropy generation rate over the volume ($\dot{S}_{\text{gen}}$) can be calculated as follows:

$$\dot{S}_{\text{gen}} = \oint_V S_{\text{gen}}''' \partial \theta \cdot \partial r \cdot \partial x. \quad (10e)$$

Bejan number, Be , which compares the magnitude of entropy generation due to heat transfer with the magnitude of the total entropy generation, is defined by:

$$Be = (\dot{S}_{\text{gen}})_{\text{heat}} / \dot{S}_{\text{gen}}. \quad (10f)$$

When $Be \gg 0.5$, irreversibility due to heat transfer dominates, while for $Be \ll 0.5$ the irreversibility due to viscous effects dominates. For $Be \cong 0.5$, entropy generation due to heat transfer is almost of the same magnitude as that due to fluid friction.

Merit number (M) is defined as the ratio of exergy transferred to the sum of exergy transferred and exergy destroyed (Mukherjee *et al* 1987), i.e.

$$M = \dot{Q}_a / (\dot{Q}_a + \dot{I}), \quad (10g)$$

where $\dot{I}$ is defined as,

$$\dot{I} = T_{\text{amb}} \cdot \dot{S}_{\text{gen}}. \quad (10h)$$

$\dot{Q}_a$ is the rate of exergy transfer accompanying energy transfers at the rates of $\dot{Q}_w$ and $\dot{Q}_{\text{fluid}}$, and is given as (Mukherjee *et al* 1987),

$$(\dot{Q}_a)_w = \dot{Q}_w [1 - T_{\text{amb}} / (T_w)_{\text{awa}}], \quad (10i)$$

$$(\dot{Q}_a)_{\text{fluid}} = \dot{Q}_{\text{fluid}} [1 - T_{\text{amb}} / (T_{\text{out}})_{\text{mwa}}], \quad (10j)$$

and

$$\dot{Q}_a = (\dot{Q}_a)_w + (\dot{Q}_a)_{\text{fluid}}, \quad (10k)$$

where $\dot{Q}_w$ can be written as,

$$\dot{Q}_w = A_w |(q''_w)_{\text{awa}}|, \quad (10l)$$

$\dot{Q}_{\text{fluid}}$ be written as,

$$\dot{Q}_{\text{fluid}} = \dot{m}_{\text{fluid}} (C_P)_{\text{mwa}} |(T_{\text{out}})_{\text{mwa}} - T_{\text{in}}|. \quad (10m)$$

The total heat transfer rate,

$$\dot{Q}_{\text{tot}} = \dot{Q}_w + \dot{Q}_{\text{fluid}}. \quad (10n)$$

The mass-weighted average (mwa) of a quantity is computed by dividing the summation of the product of density (ρ_j), cell volume (V_j), and selected field variable (ψ_j) by summation of the product of density and cell volume:

$$(\psi)_{\text{mwa}} = \frac{\sum_{j=1}^n \psi_j \cdot \rho_j \cdot |V_j|}{\sum_{j=1}^n \rho_j \cdot |V_j|}. \quad (11a)$$

Area-weighted average (awa) of a quantity is computed by dividing the summation of the product of the selected field variable (ψ_j) and facet area (A_j) by the total area of relevant surface, (A):

$$(\psi)_{\text{awa}} = \frac{1}{A} \sum_{j=1}^n \psi_j |A_j|. \quad (11b)$$

To obtain the total entropy generation rate, first, it is necessary to solve the governing conservation equations, given in § 2.2a, with the combustion equations given in § 2.2b. Volumetric local entropy generation rate can be calculated by using the local velocities and temperatures obtained from the calculations of the governing conservation equations, and the total entropy generation rate over the volume can be obtained using numerical integration.

3. Computational procedure

3.1 Computational tools

Even the difficult general differential equations are now yielding to the approximating technique known as *numerical analysis*, whereby the derivatives are simulated by algebraic relations between a finite number of grid points in the flow field which are then solved on a digital computer. A suitable CFD computer code can be used to solve numerically the governing equations (1)–(4) along with the thermal properties equations (5a–e), the boundary condition equations (6) and the combustion equations (7)–(9). CFD is the process by which fluid flow can be predicted through arbitrary geometries giving such information as flow speed, pressures, residence times, flow patterns etc.

FLUENT 6.1 (Fluent Inc. 2003) was chosen as the CFD computer code for this work because of the ease with which the analysis model can be created, and because the software allows users to modify the code for special analysis conditions through the use of user subroutines. The FLUENT computer code uses a finite-volume procedure to solve the Navier–Stokes equations of fluid flow in primitive variables such as u -velocity, v -velocity, and pressure. It can also model the mixing and transport of chemical species by solving conservation equations describing convection, diffusion, and reaction sources for each component species. A variety of turbulence models is offered by the FLUENT computer code. A detailed description of turbulence models and its application to turbulence can be found in Fluent Inc. (2003). In the case of the k – ε models, two additional transport equations (4a,b) with sub-equations (4c–i), (for the turbulent kinetic energy and the turbulence dissipation rate) are solved, and turbulent viscosity, μ_t , is computed as a function of k and ε . The RNG k – ε model belongs to the k – ε family of turbulence models; however, unlike the standard k – ε model, the RNG k – ε model was derived using a statistical technique called renormalization group methods. These model equations are similar to the standard k – ε model, but the statistical derivation results in different values for the various constants in the equations. A more comprehensive description

of RNG theory and its application to turbulence can be found in Yakhot & Orszag (1986) and Choudhury (1993).

The RNG- $k-\varepsilon$ model was used as a turbulence model in this study. The model constants for the RNG- $k-\varepsilon$ model are $C_\mu = 0.0845$, $C_{1\varepsilon} = 1.42$, $C_{2\varepsilon} = 1.68$, and wall Prandtl number = 0.85. The solution method for this study is axisymmetric. In order to achieve higher-order accuracy at cell faces, second-order upwinding is selected. In this case, quantities at cell faces are computed using a multidimensional linear reconstruction approach (Barth & Jespersen 1989), and so higher-order accuracy is achieved at cell faces through a Taylor series expansion of the cell-centred solution about the cell centroid.

Furthermore, a computer program has been developed to calculate numerically the volumetric entropy generation rate distributions in equations (10a–d) and the other thermodynamic parameters in equations (10e–j), by using the results of the calculations performed with the FLUENT code. This program, written in FORTRAN 77 language, calculates numerically the axial and radial derivations of the temperature (T) and the components (u_x and u_r) of velocity, which are functions of the axial and radial distances, using a finite-differences approach, and thus calculates the volumetric entropy generation rate distributions, and the other thermodynamic parameters as two-dimensional. It also compares the total heat per unit mass released in the combustion with the LCV of methane which must be equal or very close to each other in the case of complete combustion.

3.2 Simulation values

Physical values are as follows:

$r_f = 0.004$ m, $r_i = 0.006$ m, $r_o = 0.01$ m, $R = 0.05$ m, $L = 0.5$ m, $T_{in} = T_{amb} = T_{ref} = 300$ K, $h_{amb} = 10$ W/m² K, $P_{op} = 101325$ Pa.

$\rho_{air} = 1.225$ kg/m³ at the air inlet. Thermal properties (C_p , λ and μ) of the methane and species are given in table 1 as functions of temperature. The density of methane at the fuel inlet and the molecular weights, enthalpies and lower heating values of reactant and product species are given in table 2. These properties except LHV are taken from the material property database given by Fluent Inc. (2003).

3.2a *Ranges of the simulation values:* Simulation values are in the ranges,

$$\begin{aligned}\dot{Q} &= 10000 \text{ W}, \\ \phi &= 0.5, 0.6, \dots, 1.0, \\ \gamma &= 10, 12, \dots, 30\%\end{aligned}$$

Inlet velocities, U_f and U_{air} can be determined as follows:

$$U_f = \frac{\dot{m}_f}{A_f \cdot \rho_f} \quad \text{and} \quad U_{air} = \frac{\dot{m}_{air}}{A_{air} \cdot \rho_{air}} \quad (12a,b)$$

where A_f and A_{air} are the areas of fuel and air inlets, respectively, and $\dot{m}_f$ and $\dot{m}_{air}$ are obtained from equations (8a–g) as dependent on γ and ϕ . Inlet velocities, U_f , U_{air} and stoichiometric air/fuel ratios, which are determined according to γ and ϕ , are given in table 3.

3.2b *Grid size:* Grid independent tests were carried out to ensure grid independence of the calculated results; consequently, grid size and grid orientation giving the grid independent

Table 1. Coefficients of polynomial functions* belonging to temperature-dependent thermal properties of species, taken from the material property database given by Fluent Inc. (2003).

		a_0	a_1	a_2	a_3	a_4
CH ₄	C_P	$4.03585 \cdot 10^{2a}$	9.05734	$-1.44200 \cdot 10^{-2}$	$1.58052 \cdot 10^{-5}$	$-6.34305 \cdot 10^{-9}$
	λ	$8.72467 \cdot 10^{2b}$	5.30547	$-2.00829 \cdot 10^{-3}$	$3.51665 \cdot 10^{-7}$	$-2.33391 \cdot 10^{-11}$
	μ	$3.32000 \cdot 10^{-2}$	0	0	0	0
O ₂		$1.08700 \cdot 10^{-5}$	0	0	0	0
	C_P	$8.34827 \cdot 10^2$	$2.92958 \cdot 10^{-1}$	$-1.49564 \cdot 10^{-4}$	$3.41389 \cdot 10^{-7}$	$-2.27836 \cdot 10^{-10}$
	λ	$9.60752 \cdot 10^2$	$1.59413 \cdot 10^{-1}$	$-3.27089 \cdot 10^{-5}$	$4.61277 \cdot 10^{-9}$	$-2.95283 \cdot 10^{-13}$
CO ₂		$3.92175 \cdot 10^{-3}$	$8.08121 \cdot 10^{-5}$	$-1.35409 \cdot 10^{-8}$	$2.22044 \cdot 10^{-12}$	$-1.41614 \cdot 10^{-16}$
	μ	$7.87943 \cdot 10^{-6}$	$4.92495 \cdot 10^{-8}$	$-9.85155 \cdot 10^{-12}$	$1.52741 \cdot 10^{-15}$	$-9.42567 \cdot 10^{-20}$
	C_P	$4.29929 \cdot 10^2$	1.87447	$-1.96649 \cdot 10^{-3}$	$1.29725 \cdot 10^{-6}$	$-3.99996 \cdot 10^{-10}$
CO		$8.41377 \cdot 10^2$	$5.93239 \cdot 10^{-1}$	$-2.41517 \cdot 10^{-4}$	$4.52273 \cdot 10^{-8}$	$-3.15313 \cdot 10^{-12}$
	λ	$1.45000 \cdot 10^{-2}$	0	0	0	0
	μ	$1.37000 \cdot 10^{-5}$	0	0	0	0
H ₂ O	C_P	$1.10160 \cdot 10^3$	$-4.80700 \cdot 10^{-1}$	$1.09600 \cdot 10^{-3}$	$-6.03400 \cdot 10^{-7}$	$7.12600 \cdot 10^{-11}$
	λ	$2.50000 \cdot 10^{-2}$	0	0	0	0
	μ	$1.75000 \cdot 10^{-5}$	0	0	0	0
N ₂	C_P	$1.56308 \cdot 10^3$	1.60376	$-2.93278 \cdot 10^{-3}$	$3.21610 \cdot 10^{-6}$	$-1.15683 \cdot 10^{-9}$
		$1.23323 \cdot 10^3$	1.41052	$-4.02914 \cdot 10^{-4}$	$5.54277 \cdot 10^{-8}$	$-2.94982 \cdot 10^{-12}$
	λ	$-7.96800 \cdot 10^{-3}$	$6.88133 \cdot 10^{-5}$	$4.49046 \cdot 10^{-8}$	$-9.09994 \cdot 10^{-12}$	$6.17331 \cdot 10^{-16}$
	μ	$-4.41894 \cdot 10^{-6}$	$4.68764 \cdot 10^{-8}$	$-5.38943 \cdot 10^{-12}$	$3.20286 \cdot 10^{-16}$	$4.91918 \cdot 10^{-22}$
	C_P	$9.79043 \cdot 10^2$	$4.17964 \cdot 10^{-1}$	$-1.17628 \cdot 10^{-3}$	$1.67439 \cdot 10^{-6}$	$-7.25630 \cdot 10^{-10}$
		$8.68623 \cdot 10^2$	$4.41630 \cdot 10^{-1}$	$-1.68723 \cdot 10^{-4}$	$2.99679 \cdot 10^{-8}$	$-2.00439 \cdot 10^{-12}$
	λ	$4.73711 \cdot 10^{-3}$	$7.27194 \cdot 10^{-5}$	$-1.12202 \cdot 10^{-8}$	$1.45490 \cdot 10^{-12}$	$-7.87173 \cdot 10^{-17}$
	μ	$7.47331 \cdot 10^{-6}$	$4.08369 \cdot 10^{-8}$	$-8.24463 \cdot 10^{-12}$	$1.30563 \cdot 10^{-15}$	$-8.17794 \cdot 10^{-20}$

*Polynomial functions are defined as $\psi(T) = a_0 + a_1 T^1 + a_2 T^2 + a_3 T^3 + a_4 T^4$; ^avalid for temperature interval 300–1000 K; ^bvalid for temperature interval 1000–5000 K

Table 2. Properties of reactant and product species.

Species	$\rho^{*,a}$ [kg/m ³]	M^a [kg/kmol]	H^a [J/kmol]	LHV^a [J/kmol]
CH ₄	0.66790	16.04303	$-7.48952 \cdot 10^7$	$-8.023 \cdot 10^8$
CO ₂	-	44.00995	$-3.93532 \cdot 10^8$	-
H ₂ O	-	18.01534	$-2.41838 \cdot 10^8$	-
O ₂	-	31.99880	-	-
N ₂	-	28.01340	-	-

*At the fuel inlet; ^ataken from the material property database given by Fluent Inc. (2003); ^bcalculated by using (8e).

results were selected, and thus a total cell number of 15000 cells (300×50 , i.e.: 250 and 50 cells at $0 \leq x \leq 0.25$ m (dense-mesh region) and $0.25 < x \leq 0.5$ m (loose-mesh region) in the axial direction respectively, and 50 cells in the radial direction) was adopted. The grid distributions are uniform within each region. In addition to this total cell number, 100 axial lines were created to more accurately calculate the derivations of temperature and velocity components.

4. Numerical results

4.1 The reaction rates

Figures 2 and 3 show the distributions of reaction rates (the rates of reactions 1 and 2) in the combustion chamber for the cases of $\phi = 0.5$ and 1.0, respectively. Reaction rates for the oxidizations of CH₄ and CO are given in (7a) and (7b) respectively. The effect of these reactions are apparent from these figures. With the increase of γ , these regions contract in

Table 3. Inlet velocities of air and stoichiometric air/fuel ratios.

γ [%]	U air [m/s]						AFR_{sto}
	$\phi = 0.5$	0.6	0.7	0.8	0.9	1.0	
10	57.511	47.926	41.079	35.944	31.951	28.756	35.420
12	48.060	40.050	34.329	30.038	26.700	24.030	29.599
14	41.310	34.425	29.507	25.819	22.950	20.655	25.442
16	36.247	30.206	25.891	22.654	20.137	18.123	22.324
18	32.309	26.924	23.078	20.193	17.950	16.155	19.898
20	29.159	24.299	20.828	18.224	16.199	14.579	17.958
22	26.581	22.151	18.987	16.613	14.767	13.291	16.371
24	24.434	20.361	17.453	15.271	13.574	12.217	15.048
26	22.616	18.847	16.154	14.135	12.564	11.308	13.929
28	21.058	17.549	15.042	13.161	11.699	10.529	12.969
30	19.708	16.423	14.077	12.318	10.949	9.854	12.138

For $\dot{Q} = 10000$ W, $U_f = 5.956$ m/s.

Figure 2. Contours of rates of reactions 1 and 2 ($\phi = 0.5$).

the axial direction whereas they expand in the radial direction. However, the reaction rate decreases significantly with the increase of ϕ .

The mass fraction distributions of species (O_2 , CO_2 , CO and H_2O) in the combustion chamber, which are related to the distributions of reaction rates, are plotted in figures 4 ($\gamma = 10\%$) and 5 ($\gamma = 30\%$) for $\phi = 0.5$ and in figures 6 ($\gamma = 10\%$) and 7 ($\gamma = 30\%$) for $\phi = 1.0$. The mass fraction distributions give the information about whether the complete combustion occurs. The influences of equivalence ratio and oxygen percentage in the air on the mass fraction distributions are apparent in these figures. As expected, in the case of $\phi < 1$ (or the air excess ratio, $\lambda > 1$), all methane molecules are completely burned into CO and

Figure 3. Contours of rates of reactions 1 and 2 ($\phi = 1.0$).

H_2O molecules, and the CO molecules are then oxidized to CO_2 molecules. At the outlet; in the case of $\gamma = 10\%$, with the increase of ϕ (from 0.5 to 1.0), while the mass-weighted averages of the mass fractions of CO_2 and H_2O , which are produced along the combustion, increase linearly from 3.95 to 6.60% and from 3.24 to 5.49% respectively, while that of O_2 decreases linearly from 4.11% to 0, and for $\gamma = 30\%$, these ranges for CO_2 , H_2O and O_2 are from 10.91 to 18.75%, 8.93 to 15.71% and 12.94% to 0 respectively. The results obtained from the figures show that in the cases of $\phi < 1$, complete combustion occurs, while in the case of $\phi = 1$ it is very close to the complete combustion state.

Figure 4. Mass fractions of species ($\phi = 0.5$ and $\gamma = 10\%$).

4.2 Temperature distributions

Heat, which is released in the chemical reaction and transferred into the flowing gas including the reactant and product molecules, increases the temperature of this gas, and hence causes the large temperature gradients that increase the local entropy generation due to the heat transfer (see (10b), in the combustion chamber. In order to view the temperature gradients in axial direction, the variations of temperature along the axis of burner are plotted in figure 8, including two sub-graphs, depending on the axial distance. As is apparent in these sub-graphs, larger temperature gradients occur in the axial direction (especially between $x = 0$ and about

Figure 5. Mass fraction of species ($\phi = 0.5$ and $\gamma = 30\%$).

0.20 m). Nonetheless, the increase of ϕ significantly reduces the gradients. Although the increase of γ gradually increases temperature profiles, it does not have much effect on the temperature gradient (especially after $x = 0.20$ m).

Two-dimensional temperature distributions within the burner for the cases of $\gamma = 10$ and 30% are shown in figure 9 for $\phi = 0.5$ and 1.0. The influences of γ and ϕ on the temperature distributions are illustrated more clearly in this figure. As expected, levels of temperature throughout the burner rises linearly with both increasing of γ and ϕ . The mass-weighted average temperature of the combustion chamber increases from 832 to 1384 K and from 1097 to 1961 K for the cases of $\phi = 0.5$ and 1.0 respectively, with the increase of γ from 10 to 30%.

Figure 6. Mass fractions of species ($\phi = 1.0$ and $\gamma = 10\%$).

As is apparent from these results, increase in γ affects the rise more than that in ϕ , i.e: the average temperature increases about 70 and 35% with the increases of γ and ϕ respectively.

Temperatures at the burner wall increase from 849 to 1427 K and from 1159 to 1962 K in the cases of $\phi = 0.5$ and 1.0, respectively, with the increase of γ from 10 to 30%. Material resistant to high temperature must be therefore selected as the burner wall material (especially in the cases of high ϕ and γ). Furthermore, the heat transfer coefficient at the burner wall should be increased to reduce the burner wall-temperature.

The heat calculations performed for the each oxygen percentage bring out that in the case of $\phi < 1$, the total heat per unit mass released in the combustion, which can be calculated

Figure 7. Mass fractions of species ($\phi = 1.5$ and $\gamma = 30\%$).

using (10l-n), is almost equal to the LCV of methane and that in the case of $\phi = 1$, they are very close to its LCV. Consequently, as emphasized also in § 4.1, this means that in the case of $\phi < 1$, complete combustion occurs, and that in the case of $\phi = 1$, it is very close to the complete combustion state.

4.3 The local entropy generation

The calculations bring out that in all investigated cases, the entropy generation rates due to the fluid friction are much lower with respect to those due to the heat transfer. In other

Figure 8. Variations of temperatures at the axis of burner depending on the axial distance.

words, the Bejan number, Be , is very close to 1 (about 0.996), and this, therefore, means that the irreversibility due to the heat transfer dominates. Variations of volumetric local entropy generation rates at the various radial planes in the cases of $\phi = 0.5$ and 1.0 are plotted versus the axial distance in figure 10 for $\gamma = 10$ and 30% . Profiles showing these variations are in an irregular form due to the very large temperature gradients. However, they take shape of a quasi-smooth line towards the burner wall. In addition to this figure, the volumetric local entropy generation rate distributions within the combustion chamber for the same cases are plotted in figure 11 as the logarithmic contours. High entropy is generated in the region, in which the reaction rates are effective, and in which the large positive and negative temperature gradients occur in the axial and radial directions. The maximum values of volumetric local entropy generation rates vary in the range of $602560 \text{ W/m}^3 \text{ K}$ (5.78 as the logarithmic) to $2951209 \text{ W/m}^3 \text{ K}$ (6.47 as the logarithmic) depending ϕ and γ . It is apparent from these figures that the variations of ϕ and γ have an irregular effect on the volumetric local entropy generation rate distribution. These values bring out that the volumetric local entropy generation rates decrease about 9 and 4% in the cases of $\phi = 0.5$ and 1.0 respectively, with an increase of γ from 10 to 30%.

Figure 12 shows the variations of entropy generation rates over the volume and merit numbers, which represent the maximum heat transfer rate to sum of the maximum heat transfer rate and the total irreversibility, with the oxygen percentage in all considered cases. On the contrary of the volumetric local entropy generation rate profiles, these total entropy generation rate profiles have a quasi-regular form and decrease exponentially with both increases of ϕ and γ . In the cases of $\phi = 0.5$ and 1.0 , they decrease from 17.55 to 5.00 W/K and from 5.56 to 1.95 W/K respectively, with increase of γ from 10 to 30%. It is apparent from these results that increase of ϕ reduces the amount of decrease in the total entropy generation rate.

Merit number profiles in the same cases of ϕ exhibit a situation contrary mentioned in the previous paragraph, i.e.: in the cases of $\phi = 0.5$ and 1.0 , they increase from 0.56 to 0.85

Figure 9. Temperature contours.

and from 0.80 to 0.93, respectively, with the increase of γ from 10 to 30%. The increase of ϕ reduces also the amount of increase in the merit number. These values indicate that the useful energy transfer rate to irreversibility rate improves as the oxygen percentage increases. Consequently, the case of $\phi = 1.0$ and $\gamma = 30\%$ is the most suitable case in terms of the entropy generation.

Figure 10. Variations of volumetric local entropy generation rates at various radial planes depending on the axial distance.

5. Conclusions

The combustion of methane with air in a burner was considered to determine numerically the local entropy generation rate in the combustion chamber. The effects of the equivalence ratio and oxygen percentage in the air on the combustion and entropy generation rate also were investigated. The resulting local entropy generation rates due to heat transfer and fluid

Figure 11. Logarithmic volumetric local entropy generation rate contours.

friction contributions were computed. The specific conclusions derived from this study can be listed briefly as follows.

- The increase of ϕ reduces significantly the reaction rate levels
- The mass-weighted averages of the mass fractions of CO_2 and H_2O increase linearly with both increases of ϕ and γ

Figure 12. Variations of entropy generation rates over the volume and merit numbers versus the oxygen percentage in the air.

- The average temperatures in the combustion chamber increase about 70 and 35% with the increases of γ (from 10 to 30%) and ϕ (from 0.5 to 1.0), respectively
- In the case of $\phi < 1$, the complete combustion occurs, and the combustion in the case of $\phi = 1$ is very close to the complete combustion state
- In all investigated cases, the Bejan number is very close to 1 (about 0.996). Therefore, the irreversibility due to the heat transfer dominates
- The volumetric local entropy generation rates decrease about 9 and 4% in the cases of $\phi = 0.5$ and 1.0, respectively, with the increase of γ from 10 to 30%
- The total entropy generation rates decrease exponentially with increase of both ϕ and γ
- The merit numbers increase with increase of both ϕ and γ . The useful energy transfer rate to irreversibility rate therefore improves as the oxygen percentage increases.

Consequently, the results of this study clearly demonstrate the numerical simulation of combustion of methane with air and the numerical solution of local entropy generation rate in the combustion chamber for various equivalence ratios and oxygen percentages in the air. Material resistant to high temperatures must be selected as the burner wall-material (especially in the cases of high ϕ and γ), and in order to reduce the burner-wall temperature, the heat transfer coefficient at the burner wall should be increased.

List of symbols

A	area;
A	empirical constant (4.0);
AFR	air/fuel ratio;
B	empirical constant (0.5);
Be	Bejan number;

$C_\mu, C_{1\varepsilon}, C_{2\varepsilon}$	coefficients in k – ε turbulence model;
CFD	computational fluid dynamics;
C_P	specific heat;
D	mass diffusion coefficient;
E	energy;
G_k	the production of turbulent kinetic energy;
h	heat transfer coefficient, sensible enthalpy;
H	enthalpy of species;
$\dot{I}$	irreversibility rate;
J	mass diffusion;
k	turbulent kinetic energy;
L	length of burner;
LCV	lower calorific value;
LHV	lower heating value;
m	mass;
m	mass fraction of species;
$\dot{m}$	mass flow rate;
M	merit number, molecular weight of species;
N	total number of species number;
N_R	reaction number;
P	pressure;
q''	heat flux per unit area;
$\dot{Q}$	heat transfer rate;
$\dot{Q}_a$	exergy transfer rate;
r	radial distance;
r_i	inner radius of air inlet;
r_o	outer radius of air inlet;
R	radius of burner;
R_{i^1}	mass rate of creation or depletion by chemical reaction;
$R_{i^1,k}$	reaction rate;
$\Re$	universal gas constant;
RNG	renormalization group;
S	modulus of the mean rate-of-strain tensor;
S_{ij}	mean strain rate;
Sc	Schmidt number;
S_{gen}'''	volumetric entropy generation rate;
$\dot{S}_{\text{gen}}$	integrated entropy generation rate;
S_h	source term;
T	temperature;
u	velocity;
U	axial inlet velocity;
v^1	stoichiometric coefficient for reactant;
v^{11}	stoichiometric coefficient for product;
V	volume;
x	axial distance;
X	mole fraction of species;

Greek symbols

α	inverse effective Prandtl number;
β	model constant;
γ	oxygen percentage in air;
χ	additional term in the ε equation;
δ_{ij}	Kronecker delta;
ε	turbulent energy dissipation rate;
ϕ	equivalence ratio;
η_0	model constant;
Φ	viscous dissipation;
λ	thermal conductivity;
λ	air excess ratio;
μ	dynamic viscosity;
θ	tangential direction;
ρ	density;
τ	stress tensor;
ψ	arbitrary variable;

Subscripts

act	actual;
air	air;
amb	ambient;
awa	area-weighted average;
eff	effective;
f	fuel;
fluid	fluid;
fric	friction;
heat	heat transfer;
i, j	indices of tensor notation;
i^1, j^1	species number;
in	inlet;
j	cell number;
k	reaction number;
max	maximum;
mwa	mass-weighted average;
op	operation condition;
out	out;
P	product species number;
R	reactant species number;
ref	reference;
r	radial;
sto	stoichiometric;
t	turbulent;
tot	total;
w	wall;
x	axial.

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