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*Cogent Environmental Science* (2017), 3: 1302543



Received: 07 December 2016  
Accepted: 24 February 2017  
First Published: 08 March 2017

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Reviewing editor:  
Geun Young Yun, Kyung Hee University,  
Republic of Korea

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## ENVIRONMENTAL CHEMISTRY, POLLUTION & WASTE MANAGEMENT | RESEARCH ARTICLE

# Numerical modelling of pollutant formation in a lifted methane–air vertical diffusion flame

Alechenu Audu Aboje<sup>1</sup>, Mohammed Umar Garba<sup>1\*</sup>, Ambali Saka Abdulkareem<sup>1</sup>, Edison Muzenda<sup>2</sup> and Aisha Abubakar Faruq<sup>1</sup>

**Abstract:** A comparison of turbulence and combustion models have been performed for predicting CO<sub>2</sub> and NO<sub>x</sub> formation from a methane diffusion flame firing vertically upwards. The flow field has been modeled using the Reynolds-Averaged Navier–Stokes equation incorporating the  $k-\epsilon$  realizable turbulence closure model, the  $k-\omega$  shear-stress transport (SST) turbulence model and the transitional SST turbulence model and the three models have been compared. Combustion was modeled using the unsteady Stationary Laminar Flamelet Model (SLFM), the Eulerian Particle Flamelet Model (EPFM), and the Pollutant Model (PM) and the three models have also been compared. Numerical predictions show good agreement with experimental data. Furthermore, the experimental data showed that the  $k-\epsilon$  realizable turbulence model and the  $k-\omega$  SST turbulence model performed better than transitional SST model in predicting the pollutant species from the flame. The result also shows that the PM performed better than flamelet models in predicting the combustion characteristics of NO<sub>x</sub> in the flame.

**Subjects:** Environmental Studies & Management; Physical Sciences; Engineering & Technology

**Keywords:** gas flares; diffusion flames; pollutant species; turbulence models



Alechenu Audu Aboje

### ABOUT THE AUTHOR

Alechenu Audu Aboje finished his PhD in 2015 from the University of Leeds in the United Kingdom where he worked on the combustion of gases, particularly methane and propane. These two gases were selected for study due to their predominance in gas flaring, a practice that is prevalent in the oil and gas fields of Nigeria and other oil- and gas-producing nations. Other areas of interest include the application of computational fluid dynamics to the prediction of pollutants and the production and applications of alternative fuels from biomass, such as biodiesels and bioethanols. He is also a University lecturer in the Department of Chemical Engineering at the Federal University of Technology, Minna, Nigeria and teaches courses in fluid mechanics, thermodynamics and unit operations of chemical Engineering.

### PUBLIC INTEREST STATEMENT

According to studies, 5% of the world's natural gas production is wasted by flaring. However, this wastage cannot be compared to the environmental and health impact of gas flaring activities. The process of gas flaring releases tonnes of toxic compounds into the atmosphere and many of these compounds have been implicated as mutagens or carcinogens. Also, the IPCC (Intergovernmental Panel on Climate Change) has established that the global warming potential of methane is 25 times that of carbon dioxide. Flaring may therefore preclude the emission of methane and other greenhouse gases, although situations may arise when the toxicity of the waste gases relative to that of the products of combustion should be taken into consideration. Methane has been widely investigated in terms of emissions characteristics. This research adds to the body of literature on methane combustion using the growing field of CFD to predict the emission of pollutants, such as nitrogen oxide in methane combustion.

## 1. Introduction

Gas flaring is the controlled combustion of waste hydrocarbon gases from oil field and oil refinery activities due to lack of infrastructure to harness the gases. This process is associated with the undesirable formation of pollutants, such as CO, NO<sub>x</sub>, unburned hydrocarbons, smoke as well as CO<sub>2</sub>. Methane constitutes more than 90% of natural gas and therefore it has been widely investigated in terms of its combustion characteristics and its emissions (Flavio, Matthias, Peter, Nikolaos, & Christian, 2011; Lawal et al., 2010; Mahmud, Sangha, Costa, & Santos, 2007). Previous experiments (Brookes & Moss, 1999) have shown that that very low concentrations of soot are present in lifted methane jet diffusion flames at atmospheric pressure. This accounts for the non-luminous appearance and higher temperature in these flames as observed by Bandaru and Turns (2000). The high temperature obtained in lifted methane diffusion flames makes NO<sub>x</sub> emission of particular concern in flaring conditions. NO<sub>x</sub> emissions have been observed to be higher in methane-air flames than in propane-air flames due to the higher flame temperatures as well as the greater entrainment of air in methane flames compared to propane flames (Lyle, Tseng, Gore, & Laurendeau, 1999; Wang, Endrud, Turns, D'Agostini, & Slavejtkov, 2002).

The advances made in computing technology have enabled researchers to model the properties of turbulent jet diffusion flames using numerical techniques. In-flame temperatures and species as well as soot have been successfully modeled by several authors with good agreements with experimental data (Mahmud et al., 2007; Norton, Smyth, Miller, & Smooke, 1993; Woolley, Fairweather, & Yunardi, 2009). A previous study of variants of the *k-ε* turbulence closure models suggested that the realizable version is superior to the other variants in modeling diffusion flames from circular pipe burners (Lawal et al., 2010). The aim of the present work is to further extend this study by comparing the *k-ε* realizable turbulence closure model with the *k-ε* shear-stress transport (SST) turbulence model and the transitional SST turbulence model with respect to their capability in predicting a methane-air vertical diffusion flame. Three combustion models have also been investigated and compared namely: the unsteady Stationary Laminar Flamelet Model (SLFM), the Eulerian Particle Flamelet Model (EPFM), and the Pollutant Model (PM). The results of the numerical investigation were validated against experimental data obtained from the work of Yap, Pourkashanian, Howard, Williams, and Yetter (1998) with reasonably good agreement between the numerical and experimental data.

## 2. Numerical method

The mathematical models available in the commercial computational fluid dynamics software, Ansys-14 (2014) were used to simulate the experimental conditions. The code solves the density-averaged form of the balance equations for mass, momentum, energy, and the relevant scalar quantities describing turbulence and combustion based on the finite volume solution method.

### 2.1. Conservation equations

A short description of the governing equations for the analysis of turbulent reacting flows is presented below in Cartesian tensor notation.

Mass conservation:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_k} (\bar{\rho} \tilde{u}_k) = 0 \quad (1)$$

Momentum conservation:

$$\frac{\partial (\bar{\rho} \tilde{u}_i)}{\partial t} + \frac{\partial}{\partial x_k} (\bar{\rho} \tilde{u}_k \tilde{u}_i) = \frac{\partial \bar{P}}{\partial x_i} + \frac{\partial \tau_{ik}}{\partial x_k} + \bar{F}_k - \frac{\partial}{\partial x_k} (\rho u_k'' u_i'') \quad (2)$$

where  $\bar{\rho}$  and  $\bar{P}$  are the unweighted mean density and pressure; the symbol  $\tilde{\phantom{x}}$  represents a Favre mean or density weighted mean quantity and the symbol  $''$  denotes a corresponding fluctuating quantity. The two terms on the left hand side of Equation (2) represent the accumulation and

convective terms, respectively. The first three terms on the right hand side represent the pressure, viscous and source terms, respectively, while the last term represents the turbulence or Reynolds stress.

Energy conservation:

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_j}(\rho h u_j) = \frac{\partial}{\partial x_j} \left( \frac{\mu}{Pr} \frac{\partial h}{\partial x_j} \right) + q_{rad} \quad (3)$$

where  $h$  and  $Pr$  are the specific enthalpy and Prandtl number of the mixture, respectively, and  $q_{rad}$  is the source term due to radiation heat loss.

## 2.2. Turbulence models

The Reynolds stresses arising from the RANS equations were closed using the realizable  $k-\varepsilon$  turbulence model, the  $k-\omega$  SST turbulence model, and the transitional SST model. The  $k-\varepsilon$  models are the most popular two-equation models for the simulation of turbulence in internal flows. The  $k$  in the equation stands for the turbulent kinetic energy, while  $\varepsilon$  stands for the turbulence frequency of the large eddies. The model is available in three forms namely: The standard  $k-\varepsilon$ , the RNG  $k-\varepsilon$ , and the realizable  $k-\varepsilon$  model. Among the reported benefit of the realizable  $k-\varepsilon$  model over, its standard version is that it more accurately predicts the spreading rate of both planar and round jets as well as providing improved predictions of the flow where boundary layers are affected by strong pressure gradients, rotation, recirculation, and separation (Shih, Liou, Shabbir, Yang, & Zhu, 1995). The modeled transport equations for  $k$  and  $\varepsilon$  in the realizable  $k-\varepsilon$  model are given by (Shih et al., 1995):

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \quad (4)$$

$$\frac{\partial(\rho \varepsilon)}{\partial t} + \frac{\partial(\rho \varepsilon u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \rho C_1 S \varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu \varepsilon}} + C_{1\varepsilon} \frac{\varepsilon}{k} C_{3\varepsilon} G_b + S_\varepsilon \quad (5)$$

where  $G_k$ ,  $G_b$ ,  $Y_M$  represent the generation due to the mean velocity gradient, the generation due to buoyancy and the contribution from fluctuating dilatation, respectively.  $S_k$  and  $S_\varepsilon$  represent the source terms for  $k$  and  $\varepsilon$ , respectively. The values for the model constants  $C_{1\varepsilon}$ ,  $C_2$ ,  $\sigma_k$  and  $\sigma_\varepsilon$  are given by Shih et al. (1995) as 1.44, 1.9, 1.0, and 1.2, respectively. These constants have been established to ensure that the model performs optimally for certain canonical flows (Ansys theory guide, 2014). In this paper, however, the model constant  $C_2$  was modified to a value of 1.8 as recommended in literature (Barlow & Frank, 1998).

The  $k-\omega$  models, first introduced by Wilcox (1988) are the second most widely used turbulence models after the  $k-\varepsilon$  models. The standard  $k-\omega$  model solves a modified version of the  $k$  equation used in the standard  $k-\varepsilon$  model and a transport equation for the turbulence frequency,  $\omega$ . The standard  $k-\omega$  model is applicable to wall-bounded flows and free shear flows and includes modifications for the effects of low-Reynolds-number flows, compressibility, and shear flow spreading. A modified version of the standard  $k-\omega$  model, known as the SST  $k-\omega$  model was developed by Menter, Langtry, and Volker (1994) to combine the reliable formulation of the  $k-\omega$  model in the near-wall region with the free-stream independence of the  $k-\varepsilon$  model in the far field. The transport equation for  $k$  and  $\omega$  is given by

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \Gamma_k \frac{\partial k}{\partial x_j} \right) + G_k - Y_k + S_k \quad (6)$$

$$\frac{\partial(\rho\omega)}{\partial t} + \frac{\partial(\rho\omega u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \Gamma_\omega \frac{\partial\omega}{\partial x_j} \right) + G_\omega - Y_\omega + D_\omega + S_\omega \quad (7)$$

where  $\Gamma_k$  and  $\Gamma_\omega$ ,  $G_k$  and  $G_\omega$ ,  $Y_k$  and  $Y_\omega$ , and  $S_k$  and  $S_\omega$  represent the effective diffusivity, generation, dissipation and source terms for  $k$  and  $\omega$ , respectively.  $D_\omega$  is the cross diffusion term. Further details on these terms are found in the ANSYS FLUENT Theory Guide.

The transition SST model is a four-equation model based on the coupling of the SST  $k$ - $\omega$  equation with two other transport equations, one for the transition onset criteria, defined by the momentum-thickness Reynolds number and one for the intermittency. The intermittency is the fraction of time that the flow is turbulent during the transition phase. This concept is used to blend the flow from laminar to turbulent regions. The transition model works with the SST turbulence model by modification of the  $k$ - $\epsilon$  equation and the model is appropriate for the prediction of laminar-turbulent transition of wall boundary layers.

### 2.3. Combustion models

The SLFM is based on the concept of a conserved scalar—the mixture fraction. In a diffusion flame comprising a fuel and oxidizer stream, the mixture fraction,  $Z$  could be defined based on the element mass fraction  $Y_i$  (Libby & Williams, 1994).

$$Z = \frac{Y_i - Y_{i2}}{Y_{i2} - Y_{i1}} \quad (8)$$

where the subscripts 1 and 2 denote the oxidant and fuel streams, respectively. Therefore, at any point in the flow of the two mixing fluids,  $Z$  can be regarded as the mass fraction of the mixture originating from the fuel stream, and  $(Z-1)$  as the mass fraction originating from the oxidiser stream. Under the assumption of equal diffusivities, which is approximately the case in many practical applications, the mixture fraction does not depend on the choice of the element used for its definition. Therefore, the mixture fraction can also describe the instantaneous temperature and composition of the mixture, i.e.

$$\phi_i = \phi_i(Z), \quad \phi = \rho, T, Y_i \quad (9)$$

where  $\phi_i$  represents the instantaneous density, temperature or mass fraction of species, respectively. The complete laminar flamelet equation consists of a one-dimensional transport equation for the conserved scalar, the mixture fraction, and temperature. The term containing the time derivative becomes important only when there are rapid changes in the scalar dissipation rate, such as what occurs at extinction. However, if the scalar dissipation rate varies slowly enough, then the time-dependent term can be neglected. This assumption and that of unity Lewis number simplifies the SLFM equations as follows (Peters, 1984):

$$\rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{w}_i = 0 \quad (10)$$

where

$$\chi = 2D \left( \frac{\partial Z}{\partial x_j} \right)^2 \quad (11)$$

$\chi$  is the scalar dissipation rate which controls the mixing and thus links the turbulence and the chemistry of the reaction.  $\dot{w}_i$  is the chemical source term,  $Y_i$  is the mass fraction of species  $i$  while  $D$  is the diffusion coefficient of the scalar.

The EPFM resolves the effect of the transient history of the scalar dissipation rate. The model accounts for the spatial evolution of the flamelet profile within the flow field by tracking sample fluid particles identified with unsteady flamelets. The method involves retaining the predicted fields of the scalar dissipation rate, mixture fraction and its variance obtained from the unsteady flamelet equations. Using these predicted fields, an improved prediction of the averaged species mass fractions and temperature are post-processed through the solution of the so-called unsteady particle marker (flamelet) equations. The unsteady flamelet equations are solved in conjunction with a transport equation for the probability of finding a fluid particle  $I_I$  at location  $x$  and time  $t$  in the flow. The equation takes the form (Barths, Hasse, Bikas, & Peters, 2000):

$$\bar{\rho} \frac{\partial \check{I}_I}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \check{u}_j \check{I}_I) = \frac{\partial}{\partial x_j} \left[ \frac{\mu_t}{\sigma_t} \frac{\partial \check{I}_I}{\partial x_j} \right] \quad (12)$$

The PM (Hughes, Tomlin, Dupont, & Pourkashanian, 2001) on the other hand uses the well-known Zeldovich, Sadovnikov, and Frank-Kamenetskii (1947) and Fenimore and Jones (1967) mechanisms to model the thermal NO and the prompt NO, respectively. Equilibrium reaction was assumed between O and O<sub>2</sub>, while partial equilibrium was assumed for the reactions involving OH. Experiments have shown that at high temperatures ( $T > 1,800$  K,  $p = 1$  atm), the reaction rates of forward and backward reactions are so fast that one obtains a partial equilibria for the reactions involving OH. However, the partial equilibrium assumption provides satisfactory results only at sufficiently high temperatures, therefore at temperatures below approximately 1,600 K, partial equilibrium may not be established because the characteristic time of combustion (given as the ratio of the flame thickness and the mean gas velocity) will be faster than the reaction time.

#### 2.4. Radiation model

To determine the fraction of heat loss due to radiation in flames, it is necessary to solve the radiative transfer equation (RTE), which appears a sink in the energy Equation (3). The governing equation for the radiative heat transfer describes the transport of incoming and outgoing radiation intensity through the computational domain and it can be expressed as (Modest, 2003):

$$\frac{dI(\vec{r}, \vec{s})}{ds} + (a + \sigma_s)I(\vec{r}, \vec{s}) = an^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(\vec{r}, \vec{s}') \Phi(\vec{s}, \vec{s}') d\Omega' \quad (13)$$

where  $\vec{r}$ ,  $\vec{s}$  and  $\vec{s}'$  are the position, direction, and scattering direction vectors, respectively.  $a$  and  $\sigma_s$  are the absorption and the scattering coefficient,  $s$  is the path length,  $n$  is the refractive index,  $I$  is the radiation intensity,  $T$  is the local temperature,  $\Phi$  is the phase function,  $\Omega'$  is the solid angle, and  $\sigma$  is the Stefan-Boltzmann constant given as  $5.672 \times 10^{-8}$  W/m<sup>2</sup>-K<sup>4</sup>.

#### 3. Computational method

The computational simulation was based on the experimental work of (Yap et al., 1998), where they investigated a methane flame firing vertically upwards from an interchangeable fuel tube of inner diameter,  $d_i$  of 1.75 mm and outer diameter,  $d_o$  of 3.18 mm at Reynolds number of 4,221. The simulation was achieved on a two-dimensional structured quad mesh generated using the ANSYS-ICEM meshing software. The mesh domain extended 2.3 m (700  $d_i$ ) in the axial direction and 0.4 m (123  $d_i$ ) in the radial direction (Figure 1), where  $d_i$  is the internal diameter of the pipe. 320 and 77 mesh nodes were used in the axial and radial directions, respectively, with the origin centered at the burner exit. The mesh distribution option was selected so as to place a finer node distribution in the pipe region and coarser nodes further away from the pipe (see Figure 2). A mesh refinement study was conducted to ensure the independence of the solution on the mesh size and density. This entailed comparing the velocity profiles for mesh sizes of  $5 \times 10^4$ ,  $1 \times 10^5$ , and  $2 \times 10^5$  cells, respectively (Figure 3). Pressure inlet boundary conditions were employed at entrainment boundaries, located 0.3 m (92  $d_i$ ) and 0.4 m (123  $d_i$ ) away from the burner exit in the axial and radial directions, respectively. A