Comparative performance study of two simple soot models for the prediction of soot level in atmospheric turbulent non-premixed flames

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Abstract. The increase of current fossil fuel consumption has led to an increase of soot emission into atmosphere. Accurate prediction of soot production and destruction in a combustion system is not only important for the purpose of the design of the system, but also vital for the operation of the combustor. Numerous soot models have been proposed to predict the soot production and destruction in a flame, categorized as empirical, semi-empirical and detailed soot models. Although the detailed model represents the highest level of soot modelling, its use has been impaired by *substantial requirement* of *resources* of *computer* and time. Therefore, empirical and semi-empirical approaches still have their position in soot modelling of practical combustors. In this study, two soot models, single-step and two-step models are examined in the simulation of atmospheric turbulent non-premixed sooting flames. The soot models are compared and evaluated for their performance in predicting soot level in methane and ethylene non-premixed flames. The commercial software Fluent 6.3 was used to perform the calculations of flow and mixing fields, combustion and soot. Standard *k-ε* and eddy dissipation models were selected as solvers for the representation of the turbulence and combustion, respectively. The two soot models used in the study are available directly from the code for evaluation. The results show that the two-step model clearly performed far better than the single-step model in predicting the soot level in both methane and ethylene non-premixed flames. With a slight modification in the constant α of the soot formation equation, the two-step model was capable of producing prediction of soot level closer to experimental data. In contrast, the single-soot model produced very poor results, leading to a significant under-prediction of soot levels in both flames.

Key words: soot, single-step model, two-step model, turbulent, non-premixed flames

Introduction

Accurate prediction of soot emission from a flame is not only important for the purpose of designing a combustion system but is also required for the purpose of operating the system. A soot model which could provide a correct description of soot formation and destruction is crucial in order to achieve the purpose. Different models describing the formation of soot have been proposed and demonstrated various level of accuracies in the estimation of soot distribution in different types of flames. The empirical soot models as reviewed in Kennedy (1997) are mainly based on model parameters which are different for different fuels. The most sophisticated soot models today, such as that proposed by Frenklach and Wang (1994) employ detailed chemical kinetic and physical models to describe each sub-process that occurs in the gas phase, solid phase, and on the surface of soot particles. Although such models are applicable over a wide range of combustion conditions, their application at present has been impaired by the excessive requirement for computer resources even for simple flames and the poor representation of soot inception chemistry, with some of the relevant reaction rates purely estimations (Wen et al., 2005). Thus, for predictions of soot in practical engineering devices, it is often necessary to use simplified models to keep the computational cost at an acceptable level without losing an acceptable degree of accuracy.

The objective of the present study is the assessment of two widely used soot models embedded in the commercial CFD code Fluent 6.3 to predicting soot levels in the atmospheric turbulent non-premixed flames of methane and ethylene. Soot formation is calculated by a single-step model and a two-step model and the results are compared with

each other as well as with experimental data of Brookes and Moss (1999) and Kent and Honnery (1987).

Soot Mathematical Modeling

The soot progression in a flame can be depicted by two participating processes, the formation and oxidation of soot. As a result, almost every soot model available at the present time incorporates these two phenomena in their model development. In this study, the single-step soot model proposed by Khan and Greeves (1974) and the two-step soot model proposed by Tesner et al. (1971) will be investigated from their performance in predicting the soot level in methane and ethylene flames operated under atmospheric pressure. The first model has been applied with some success in calculations of soot formation in diesel engines (Mehta and Das, 1992) and gas turbines (Lefebvre, 1984). With regard to the two-step model, Magnussen and Hjertager (1977) were among the first to apply the Tesner et al.'s model coupled with the eddy dissipation combustion model (EDM) to simulate soot formation in turbulent flames.

The single-step soot model of Khan and Greeves (1974) requires a solution of a transport equation soot mass fraction Y_{soot} as presented in Eq.1, of which the source term is calculated using Eq.2.

$$\frac{\partial}{\partial t}\left(\rho Y_{soot}\right)+\nabla.\left(\rho\vec{v}Y_{soot}\right)=\nabla.\left(\frac{\mu_t}{\sigma_{soot}}\nabla Y_{soot}\right)+R_{soot} \quad (1)$$

$$R_{soot} = R_{soot;form} - R_{soot;comb} \quad (2)$$

where R_{soot} = net rate of soot generation (kg/m^3.s); $R_{soot;\ form}$ = rate of soot formation (kg/m^3.s) and $R_{soot;\ comb}$ = rate of soot destruction (kg/m^3.s). The rate of soot formation is computed using a simple empirical rate expression as in Eq. 3.

$$R_{soot;form} = C_s p_{fuel} \Phi^r e^{-|E/RT} \quad (3)$$

where C_s = soot formation constant (kg/N-m-s); p_{fuel} = fuel partial pressure (Pa); Φ= equivalence ratio; r = equivalence ratio exponent; and E/R = activation temperature (K). The rate of soot combustion is the minimum of two rate expressions shown in Eq.4

$$R_{soot;comb} = \min\left[R_1;R_2\right] \quad (4)$$

The two rates are calculated in accordance to Equations 5 and 6.

$$R_1 = A\rho Y_{soot}\frac{\varepsilon}{k} \quad (5)$$

$$R_2 = A\rho\left(\frac{Y_{ox}}{\nu_{soot}}\right)\left(\frac{Y_{soot}\nu_{soot}}{Y_{soot}\nu_{soot}+Y_{fuel}\nu_{fuel}}\right)\frac{\varepsilon}{k} \quad (6)$$

where A = Constant in Magnussen model; Y_{ox}, Y_{fuel} = mass fractions of oxidizer and fuel; ν_{soot}, ν_{fuel} = mass stoichiometries for soot and fuel combustion; ε= energy dissipation; and k= kinetic energy

With respect to the two-step soot model of Tesner et al. (1971), in addition to solving the transport equation for soot mass fraction, as given in Eq. 1, the model also requires the solution of another transport equation for radical nuclei concentration using Eq. 7

$$\frac{\partial}{\partial t}\left(\rho b^*_{nuc}\right)+\nabla.\left(\rho \vec{v} b^*_{nuc}\right)=\nabla.\left(\frac{\mu_t}{\sigma_{nuc}}\nabla Y_{nuc}\right)+R^*_{nuc} \quad (7)$$

where b^*_{nuc} = radical nuclei concentration (particles x 10^{-15}/kg); σ_{nuc} = turbulent Prandtl number for nuclei transport; R^*_{nuc} = net rate of nuclei generation (particles x10^{-15}/m^3.s). The rate of soot combustion, $R_{soot;comb}$, is computed in the same way as for the single-step following Eq. 4. However, the rate of soot formation, $R_{soot;form}$, depends on the concentration of radical nuclei, as presented by Eq. 8.

$$R_{soot;form} = m_p \left(\alpha-\beta N_{soot}\right) C_{nuc} \quad (8)$$

where m_p= mean mass of soot particle (kg/particle); N_{soot}= concentration of soot particles (particles/m^3); C_{nuc}= radical nuclei concentration (particles/m^3); α = empirical constant (s^{-1}); and β = empirical constant (m^3/particle-s).

Numerical Computation

A mesh generator software GAMBIT was employed to describe the configuration of the flames being studied. The methane-air and ethylene-air jet turbulent non-premixed sooting flames of atmospheric pressure experimentally performed by Brookes and Moss (1999) and Kent and Honnery (1987) are investigated for comparing the performance of Khan and Greeves' and Tesner et al.'s models. The related references may be consulted for important characteristics, including the flame geometry, methods of data collection, and processing. The calculation of flow and mixing fields was achieved by solving the partial differential equations which describe the conservation equations for mass and momentum.

A standard *k-ε* turbulence model was used to close the above equation set, with an adjustment was made to the value of $C_{\varepsilon 1}$. The combustion calculation which solved the energy and species concentration was performed by utilizing eddy dissipation model (EDM). All the above calculations were simultaneously performed using commercial CFD software FLUENT ver. 6.3 which functions as the processor as well as post processor. The soot models calculations were implemented after the calculations of turbulence and combustion reached convergence. The soot models under the study, Khan and Greeves' and Tesner et al.'s models are readily available in the code. Adjustments were made to the soot formation constant, C_s in the Khan and Greeves' model and to the empirical constant, α in the Tesner et al.'s model during the soot calculation, respectively.

Results and Discussion

Temperature Predictions

Figure 1 presented a comparison between the centerline and radial temperature predictions of the methane flame and the experimental data. The solid line represents the temperature predictions calculated using a combination of a standard k-ε turbulence model and eddy dissipation combustion model, while the symbol of small circle represents the experimental measurements. The axial temperature predictions generally display qualitatively good results in comparison to the experimental data. The evolution of the computed axial temperature follows the trend of the axial temperature measurements. However, from quantitative point of view, from a region between 150 and 350 mm above the nozzle the temperature is over-predicted. Such over-predictions might be due to simple representation of combustion chemistry by eddy dissipation combustion model and simple radiation model selected during the combustion calculation. It is to be noted that the EDM assumes the fuel is fast burning, and the overall rate of reaction is controlled by turbulent mixing. As a consequent the chemical kinetic can be neglected, which is not the case for

other combustion models where the detailed kinetic mechanism can be included in their calculation. In addition, Fluent code provides various radiation models, ranging from simple Roseland model up to more complex models, such as Discrete Order (DO) radiation model. For the sake of simplicity in the calculation, a radiation model P1 was selected. Nonetheless, the value and location of peak temperature are well predicted by the model. With respect to the radial temperature profile, it is evidence that predictions are in reasonable agreement with the experimental as also shown in the same figure. The temperature profiles in the radial fuel-lean and fuel-rich regions are captured reasonably well.

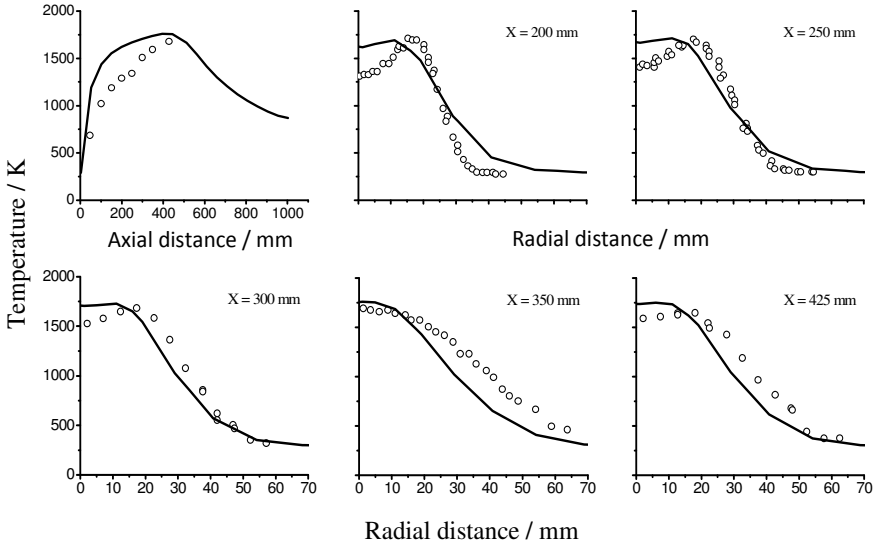

Figure 1. Axial and radial temperatures for the methane flame (symbol O measured, solid line – predictions)

Figure 2 depicted a comparison between the centerline and radial temperature predictions in the ethylene flame and the experimental data. The solid line represents the temperature predictions calculated using a combination of a standard *k-ε* turbulence model and eddy dissipation combustion model, while the symbol of small circle represents the experimental measurements. The axial temperature predictions are generally similar to those predicted in the methane flame. The model failed to capture the experimental data closer to the nozzle in the region of between 150 and 350 mm above the nozzle. This discrepancy is mainly due to the weakness of eddy dissipation combustion model which neglects the combustion kinetic as the combustion reaction is represented by one single step reaction. However, with regard to the radial profile, although the prediction in the position closer to the nozzle tip was not satisfactory, the temperature predictions were much improved at positions further downstream of the flame.

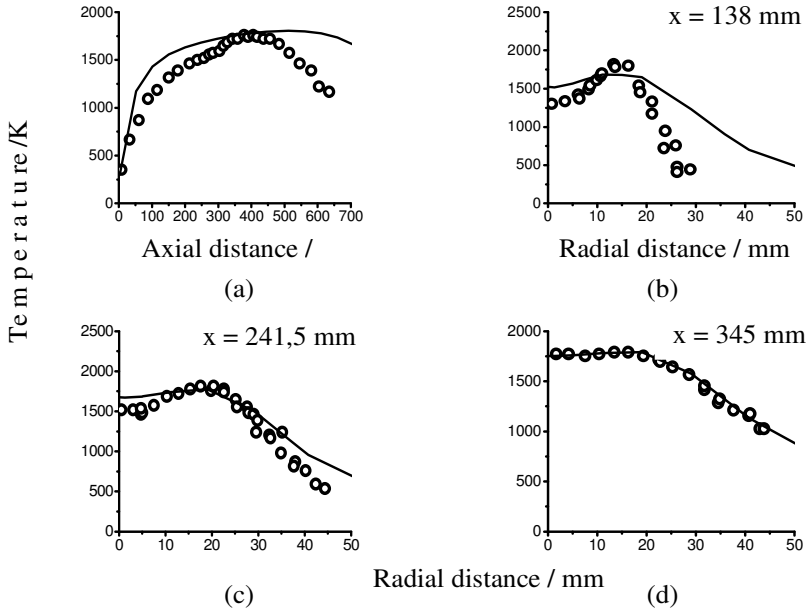

Figure 2. Axial and radial temperatures for the ethylene flame (symbol O measured, solid line – predictions)

Soot Predictions

Figure 3 presented a comparison of axial and radial predictions of soot volume fraction for the methane flame with experimental data. The symbol depicts the experimental data while solid line represents the simulations resulting from the use of Tesner et al.'s model, and the dashed line the simulations resulted from employing Khan and Greeves' model. It is clearly seen that the centreline soot volume fraction profile is very well represented by Tesner et al.'s model, when the empirical constant, α in Eq. 8 was adjusted around 3 times of the default value in the code. Although the same adjustment was made to soot formation constant, C_s in the Khan and Greeves' model, the soot predictions yielded by this model are very unrealistically low than measurements which is due to the strong role of fuel concentration in the model Zahmatkesh and Moghiman (2006). With respect to radial soot profile, although quantitatively the predictions by Tesner et al.'s model are slightly under-predicted at all axial locations, qualitatively the predicted trend is in agreement with the measurements, in which Khan and Greeves' model failed to produce. With a slight adjustment in the constant α, the current results are comparable to those produced using other semi-empirical models (Roditcheva and Bai, 2001; Kronenburg et al., 2000).

Figure 4 illustrated a comparison of axial and radial predictions of soot volume fraction for the ethylene flame with experimental data. Similar results as in the methane flame were also observed where the centreline soot volume fraction profile is very well represented by Tesner et al.'s model. The peak value of soot volume fraction was also very well captured by the model. However, it should be noted that such accurate prediction was achieved by modifying the adjustable constant α in Eq. 8 around 3 times of its default value in the code. Similar medication in the empirical constant was also performed by Roditcheva and Bai, (2001). With respect to the radial profiles, the prediction of soot in the region close to the nozzle is less satisfactory, where over-prediction and under-prediction of soot were evidence by Tesner et al.'s and Khan and Greeve's models, respectively. However,

the two-step model of Tesner et al. (1971) improved the predictions of soot in radial profiles with the progression of further downstream positions. On the contrary, the Khan and Greeve's model was unable to improve the soot predictions further downstream.

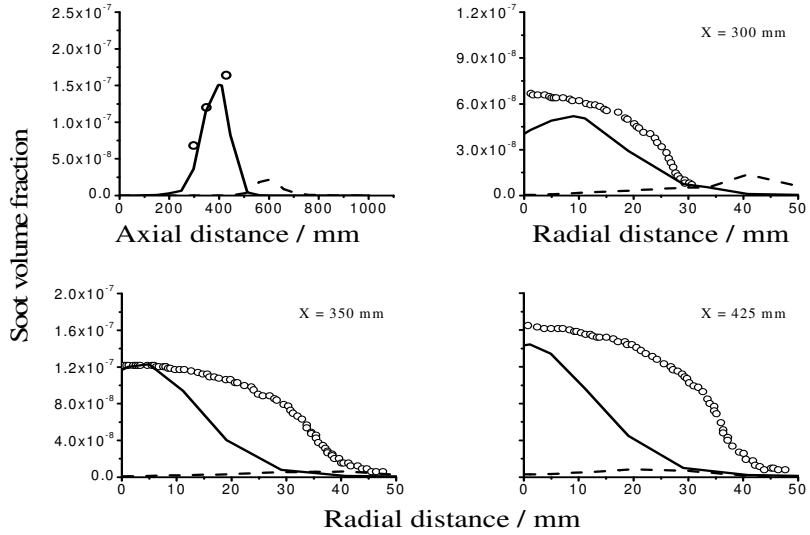

Figure 3. Axial and radial soot volume fractions for the methane flame (symbol O measured, solid line – predicted with Tesner et al.'s model, dashed line – predicted with Khan and Greeve's model).

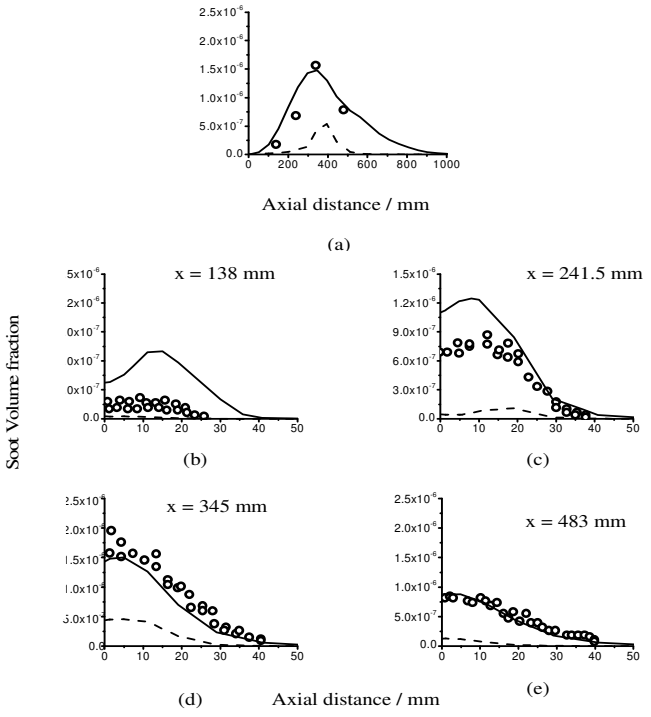

Figure 4. Axial and radial soot volume fractions for the ethylene flame (symbol O measured, solid line – predicted with Tesner et al.'s model, dashed line – predicted with Khan and Greeve's model).

Conclusions

A numerical simulation of soot formation and destruction has been adopted to study the performance of two soot models for prediction of soot levels in turbulent non-premixed flames. Soot formation is modeled by a single-step model and a two-step model as the results are compared with each other and with experimental data. The two-step soot model proposed by Tesner et al. (1971), with a light adjustment in the modeling constant, is capable of producing the predictions closer to the experimental in both methane and ethylene flames. On the contrary, the single-soot model proposed by Khan and Greeves (1974) produced very poor results, leading to a significant under-prediction of soot levels in both flames. Although the Tesner's soot model is simple in its mathematical formulation, this model is still capable of providing reasonable agreement with experimental data, allowing its application for the purpose of design and operation of an industrial combustion system.

References

Brookes S.J., Moss J.B. 1999. Measurement of soot production and thermal radiation from confined turbulent jet diffusion flames of methane, Combustion and Flame, 116:49-61.

Frenklach M., Wang H. 1994. Detailed mechanism and modelling of soot particle formation, in: Soot Formation in Combustion edited by H. Bockhorn, pp 165-190, Springer-Verlag, Berlin.

Kennedy I.M. 1997. Models of soot formation and oxidation, Progress in Energy and Combustion Science, 23: 95-132.

Kent J.H., Honnery D. 1987. Soot and mixture fraction in turbulent diffusion flames, Combustion Science and Technology, 54: 383-397.

Khan I.M., Greeves G. 1974. A method for calculating the formation and combustion of soot in diesel engines, in: Heat Transfer in Flames edited by N.H. Afgan and J.M. Beer, Chapter 25, Scripta, Washington, USA.

Kronenburg A., Bilger R.W., Kent J.H. 2000. Modeling soot formation in turbulent methane–air jet diffusion flames, Combustion and Flame, 121: 24-40.

Lefebvre A. 1984. Flame Radiation in Gas Turbine Combustion Chambers, International Journal of Heat and Mass Transfer, 27: 1493-1510.

Magnussen B.F., Hjertager B.H. 1977. On mathematical modeling of turbulent combustion with special emphasis on soot formation and combustion, Proceedings of the Combustion Insitute, 16: 719–729.

Mehta P.S., Das S. 1992. A Correlation for soot concentrations Fuel in diesel exhaust based on fuel-air mixing parameters, Fuel, 71: 689-692

Roditcheva O.V., Bai X.S. 2001. Pressure effect on soot formation on turbulent diffusion flames, Chemosphere 42: 811-821.

Tesner P.A., Snegriova T.D., Knorre V.G. 1971. Kinetics of dispersion carbon formation, Combustion and Flame, 17:253-260

Wen J.Z., Thomson M., Park S., Rogak S., Lightstone M. 2005. Proceedings of the Combustion Institute, 30: 1477-1484

Zahmatkesh I., Moghiman M. 2006. On the suitability of soot formation models in Turbulent Flame: A comparison study, EJER 11:89-98.