Soot Formation Model Performance in Turbulent Non-Premix Ethylene Flame: A Comparison Study

E Elwina¹, N Sylvia², W Wusnah², Y Yunardi³, Y Bindar⁴

¹Chemical Engineering Department, Politeknik Negeri Lhokseumawe, Aceh, Indonesia
²Chemical Engineering Dept., University of Malikussaleh, Lhokseumawe, Indonesia
³Chemical Engineering Dept., Syiah Kuala University, Banda Aceh, Indonesia
⁴Energy and of Processing System Chemical Engineering Dept., Faculty of Industrial Technology, Bandung Institute of Technology, Bandung, Indonesia

Email: elwina@pnl.ac.id

Abstract. This paper presents results obtained from the application of a computational fluid dynamics (CFD) approach to modelling of non-premixed turbulent ethylene sooting flame. The study focuses on comparing the two soot models available in the Fluent in predicting the soot level in the turbulent non-premixed ethylene flame. A standard k-ε model and Eddy Dissipation model are utilized for the representation of flow field and combustion of the flame being investigated. For performance comparison study, a single step soot model of Khan and Greeves and two-step soot model proposed by Tesner are tested. The results of calculations are compared with experimental data for a turbulent sooting flame taken from literature. The results of the study show that a combination of the standard k-ε turbulence model and eddy dissipation model is capable of producing reasonable predictions of temperature both in axial and radial profiles; although further downstream of the flame over-predicted temperatures are evidence. With regard to soot model performance study, it shows that the two-step model clearly performed far better than the single-step model in predicting the soot level in ethylene flame at both axial and radial profiles.

Keywords: soot, single-step model, two-step model, turbulent, ethylene

1. Introduction
Modelling the soot formation and destruction does not only play an important role in the design, but also essential in the operation of in a turbulent combustion process. In order to accurately predict the production and destruction of soot in such systems, an integrated model that at least represents turbulence, combustion process, soot particle production and removal, and radiation heat losses is required. The ability to apply such an integrated model, of demonstrated accuracy, to minimise soot production and emission in relation to safety and environmental considerations, and to maximize production in systems where this would be beneficial for heat transfer, would represent a major step-forward in our ability to design and manage combustion processes.

A number of soot models, ranging from empirical to detailed approaches, have been proposed in the literature, and research to develop new models and improve the existing ones is ongoing. Those approaches that have been proposed for modelling soot formation in turbulent flames have their own advantages and disadvantages. The empirical soot models as reviewed in Kennedy [1] 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 [2] 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 [3]. 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.

In this paper, the results of the application of a computational fluid dynamics (CFD) code Fluent 6.3 to modelling of ethylene non-premixed sooting flames are presented. The objective of the present work is the assessment of the two soot models available directly in the code for the prediction of soot levels in the flame. Soot formation in the flame is calculated using a single-step and tow-step models, respectively, and predicted results are compared each other. Validation is achieved by comparing the computed prediction by each soot model against available experimental data of ethylene non-premixed sooting flames [4].

2. Mathematical formulation and metode

2.1. Formatting the title

The evolution of soot in a flame can be described by two competing processes, soot formation and destruction. As a consequent, almost all soot models include these two phenomena in their mathematical development. In this study, a single-step soot model proposed by Khan and Greeves [5] and two-step soot model proposed by Tesner et al [6] will be implemented. The former model has been applied with some success in calculations of soot emissions from diesel engines [7] and gas turbines [8]. With respect to the latter model, Magnussen and Hjertager [9] were one of the first to apply the Tesner model coupled with the eddy dissipation combustion model (EDM) to simulate soot formation in flames.

The calculation of Khan and Greeves model requires a solution of a single transport equation, presented in Eq.1, in which the source term is given by Eq.2.

\[
\frac{\partial}{\partial t} (\rho Y_{soot}) + \nabla \cdot (\rho v Y_{soot}) = v \left( \frac{H}{\sigma_{soot}} Y_{soot} \right) + R_{soot}
\]

\[R_{soot} = R_{soot, form} - R_{soot, comb}\]

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 given by a simple empirical rate expression as in Eq. 3.

\[R_{soot, form} = C_s P_{fuel} \Phi e^{-E/RT}\]

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

\[R_{soot, comb} = \min \left[ R_1; R_2 \right]\]

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

\[R_1 = A \rho Y_{soot} \frac{e^r}{k}\]
\[ R_{\text{soot;comb}} = \text{Constant in Magnussen model; } Y_{\text{ox}}, Y_{\text{fuel}} = \text{mass fractions of oxidizer and fuel; } \nu_{\text{soot}}, \nu_{\text{fuel}} = \text{mass stoichiometric for soot and fuel combustion; } \varepsilon = \text{energy dissipation; and } k = \text{kinetic energy} \]

In addition to the solution of transport equation for soot mass fraction, as given in Eq. 1, Tesner model requires the solution for another transport equation for radical nuclei concentration, as shown in Eq. 7

\[ \frac{\partial}{\partial t}(\rho b_{\text{nuc}}^*) + \nabla \cdot (\rho \nabla b_{\text{nuc}}^*) = \nabla \left( \frac{\mu}{\sigma_{\text{nuc}}} \nabla Y_{\text{nuc}} \right) + R_{\text{nuc}}^* \]

where \( b_{\text{nuc}}^* = \text{radical nuclei concentration (particles x 10^{-15}/kg); } \sigma_{\text{nuc}} = \text{turbulent Prandtl number for nuclei transport; } R_{\text{nuc}}^* = \text{net rate of nuclei generation (particles x 10^{-15}/m^3.s).} \)

The rate of soot combustion, \( R_{\text{soot;comb}} \), is computed in the same way as for the single-step following Eq. 4. However, the rate of soot formation, \( R_{\text{soot;form}} \), depends on the concentration of radical nuclei, as presented by Eq. 8.

\[ R_{\text{soot;form}} = m_p (\alpha - \beta N_{\text{soot}}) C_{\text{nuc}} \]

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

The ethylene-air jet turbulent non-premixed sooting flames measured by Kent and Honnery [4] is investigated for comparing the performance of Khan and Greeves’ and Terner’s models. The related reference 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 conservation of mass and momentum. A standard \( k-\varepsilon \) turbulence model was used to close the above equation set, with an adjustment was made to the value of \( C_\varepsilon \). 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.

3. Result and discussion

3.1. Temperature Profile and contour

Figure 1 presents a comparison between the centerline and radial temperature predictions in the 1 atm ethylene flame and the experimental data. The solid line represents the temperature predictions calculated using a combination of a standard \( k-\varepsilon \) 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 (fig. 1a) 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 mechanisms 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 evident 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 2 shows the contours of temperature along the flame using the EDM model. From that, can see the colour differences to illustrate the value of the temperature, more red the contour colour, higher the temperature. The blue colour indicates the air temperature. From that picture shows that the EDM model are able to describe the contours of the flame as the actual situation, although not yet providing high accuracy, as compared with temperature data from previous experiment. But it is clear that in the middle zone the flame of temperature is higher than the rich areas of oxygen. So that the combustion phenomena can described by this model.

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

Figure 2. The Contour of the flame temperature of ethylene
3.2. Soot Profile and Contour

Figure 3 presents a comparison of axial and radial predictions of soot volume fraction for the ethylene flame with experimental data. The solid line represents the simulations resulting from the use of Tesner’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’s model, when the empirical constant, $\alpha$ 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 [10]. With respect to radial soot profile of 1 atm flame, although quantitatively the predictions by Tesner’s model are slightly under-predicted at all axial locations, qualitatively the predicted trend is agreement with the measurements, in which Khan and Greeves’ model failed to produce. With a slight adjustment in the constant $\alpha$, the current results are comparable to those produced using other semi-empirical models [11,12,13].

![Figure 3. The Comparison of experimental results and predictions for soot volume fraction in the axial and radial position in the ethylene flame KH (Ο experiments symbol, ─ two-step model prediction, ─ ─ one-step model prediction).](image-url)

In the axial profile (Fig. 3a), shows that the two-step model is able to produced satisfactory predictions. It is characterized by the conformity of prediction to the experimental data on soot growth phase and the destruction phase. The highest value of soot position can also be predicted well by two-steps model. However, it should be noted, that the accuracy is achieved by modifying the constant alpha value. This modification is performed randomly to get the results close to experimental data, considering there are no experimental data for alpha constanta value for ethylene flame. For default alpha value
represents the value for the acetylene flame. Such modifications are also mostly done by other researchers [11].

In the radial profiles, the prediction of soot in the region close to the nozzle is less satisfactory. Tesner model provides the predictions of soot which exceeds the experimental value, while the one-step model provides a prediction that is very low compared to experimental data. The Predictions which is exceed in the experimental value at position 138 mm (Figure 3b) from the surface of the nozzle is also experienced by Pitsch [14]. But, two-step model could improve the predictions of soot in radial profiles at height of 345 and 483 mm (Figure 3d and e) from the surface of the nozzle. This is possible because the prediction of temperature is more accurate in both these altitudes. The Prediction at altitude of 345 and 483 mm using by two-step soot model is better obtained by Pitsch [14]. But not so with one-step method. Although the accuracy assumption of temperature is sufficient, the one-step method predicting the soot is quite low at these two heights.

Furthermore, for two-steps model at height of 138 and 241 mm (Figure 3b and c), the deviates from the results is quite large, especially at the height of 138 mm, the simulation results none could capture the appropriate experimental data, except for one-step model obtained the simulation results close to the experimental data. In contrast to the positions 345 and 483 mm, where the two-steps model simulation is capable to capturing accordance with the experimental data, especially at a position 483 mm which is in accordance with experimental results. The Deviations that occur cannot be separated from the minimum data obtain for the kinetic reaction mechanism. However, for one-step model prediction, the results are still very far from the experimental data.

Figure 4 shows the contour of soot mass fraction which produced using two-step soot model [6] and one-step soot model [5]. The blue color indicates the minimum soot mass fraction (close to zero, or no soot), while red indicates the maximum soot mass fraction. From the pictures can be seen that the two-step model of soot begins to form in areas close to the nozzle. This is understandable because in this region rich in fuel and poor air, so that resulting a tendency to form the soot. Soot maximum is reached still in the regions rich of fuels and along with the movement direction of soot with the flow flame, the diffusion of air more higher causes the oxidation of soot comes into play. Consequently, after reaching the maximum indication, soot mass fraction decreases due to oxidation and turns into a gas phase.

Figure 4. The Contours of soot mass fraction in the flame of ethylene (a) with a two-step model and (b) with one step model

Different with two-step model, one-step model cannot predict the formation of soot in the region close to the nozzle. The soot begins to formed in areas away from the nozzle. In this area, the air is rapidly diffused into the flame. As a result, the soot is oxidized too quickly. This is evident in the mass fraction contours generated by one step model compared with the soot mass fraction contours generated by two-steps model.

The constant in both models also have an influence on outcome prediction. In the two-step model, the constanta that holds important role is an alpha value, whereas in the one-step model is the constanta
of soot formation. From Figure 4 can also see the contours of the soot in one-step model, where the rate of the soot formed is slower than the two-step model, so that the peak area on one step model are shifting. As mentioned on the theory that the one step model is a simple empirical model that the application is a little difficult to be applied to other hydrocarbons, the constanta used should be arranged so that with a certain constanta value through the sensitivity test will be obtained the accordance results with the experiments. However, the results obtained have not been close to the experimental data because in this model the soot calculation just look at the soot formation and oxidation without other processes such as the formation of soot nuclei as in the two-step model. But overall the predicted results from Tesnet et al two-step model so far has given satisfactory results that can be applied in industry because of the predictions results are not difference too much with the predicted results which is obtained by using semi-empirical soot model which more complex [14].

Pitsch [14] also conducted same simulation of the ethylene flame. The Axial temperature predictions made by Pitsch [14] reviewed on the basis of taking into account the soot and gas radiation, without the soot and gas radiation, and without soot radiation. It should be noted that Pitsch [14] using Unsteady Laminar Flamelet model with kinetics through detailed combustion. Seen that the predictions are very consistent with the experimental data when the predictions considering the soot and gas radiation. If seen the comparison results of the predicted results in this study, for height at 450 mm in terms of prediction quality in this study is slightly below with Pitsch [14] prediction results. Above 450 mm Pitsch [14] prediction is much better. From this, it can be presumed that the kinetics of combustion reaction and radiation models play an important role in generating the proper temperature predictions.

The calculated axial and radial soot volume fractions again show that better predictions can be achieved by using Tesner’s soot model. Soot volume fraction distribution in axial profile calculated using Tesner’s model is qualitatively and quantitatively in excellent agreement with the measurements, both in the soot formation and oxidation zones. It is important to note here that the Tesner’s model is capable of capturing the increase of soot level due to the increase of flame pressure which on the contrary Khan and Greeves’ model failed to produce so.

**4. Conclusion**

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 modelled 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 [6], with a light adjustment in the modeling constant, is capable of producing the predictions closer to the experimental in ethylene flames. On the contrary, the single-soot model proposed by Khan and Greeves [5] 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**

[1] I.M. Kennedy: Prog. Energ. Combust. Vol. 23 (1997), p. 95
[2] M. Frenklach and H. Wang, in: Soot Formation in Combustion edited by H. Bockhorn, Springer-Verlag, Berlin (1994).
[3] J.Z. Wen, M.Thomson, S. Park, S. Rogak, and M. Lightstone: P. Combust. Inst. Vol. 30 (2005), p. 1477
[4] Kent, J.H and Honnery, D., Soot and mixture fraction in turbulent diffusion flames. *Combustion Science and Technology* (1987), 54: 383-397.
[5] I.M. Khan and G. Greeves, in: Heat Transfer in Flames edited by N.H. Afgan and J.M. Beer, Chapter 25, Scripta, Washington, USA (1974).
[6] P.A. Tesner, T.D. Snegriova and V.G. Knorre: Combust. Flame Vol. 17 (1971), p.253
[7] P.S. Mehta and S. Das: Fuel Vol. 71 (1992), p. 689
[8] A. Lefebvre: Int. J. Heat Mass Tran. Vol. 27, p. 1493