Abstract—This paper presents the results of an application of a first-order conditional moment closure (CMC) model coupled with a semi-empirical soot model to investigate the effect of air preheat temperature on soot formation in the flames. The implementation of soot model involves the solution of two additional first-order CMC transport equations for soot mass fraction and soot particle number density. The effect of differential diffusion of soot particles on soot level predictions has been taken into account. The results of investigation showed that as the temperature of air increases the rate of soot production as well as destruction increases. As the soot is oxidised rapidly, furthermore downstream soot is almost non-existent in the flames of low- and high-preheat. The present study demonstrates that the CMC approach coupled with a semi-empirical soot model is capable of providing reliable predictions and information on soot, at different air preheat temperatures of turbulent non-premixed propane flames.

Keywords—conditional moment closure, semi-empirical model, soot, turbulent flame.

I. INTRODUCTION

Preheating the combustion air in practical combustors, such as gas turbine and diesel engines, has been adopted as an operation that could improve the combustion efficiency and productivity. The source of this heat energy is the exhaust gas stream, which leaves the process at elevated temperatures. A heat exchanger, placed in the exhaust stack or ductwork, can extract a large portion of the thermal energy in the flue gases and transfer it to the incoming combustion air. One of the merits of using the technique is to increase the flame temperature without increasing the consumption of fuel.

However, as the air temperature becomes higher, the rates of some elementary reaction steps increase, while those of other elementary steps decrease. These changes affect the distribution of species and temperature across the flame as well as soot, CO, and NO emissions.

Soot particles usually result from incomplete combustion and typically form only in fuel rich regions. When the flame temperature increases, the rate of fuel pyrolysis also enhances to form soot precursors [1]. As a consequence, the concentration of soot in the fuel rich region will also increase. However, the increase in flame temperature also enhances. However, the increase in temperature in the post flame zone leads to an increase in the soot oxidation rate and the amount of soot in the exhaust gases is drastically reduced.

First-order conditional moment closure (CMC) modelling in the form of a parabolic equation set has been performed successfully to a wide range of combustion problems, including attached non-premixed jet flames [2], [3], autoignition problems [4], bluff body flames [5] and lifted turbulent jet diffusion flames [6], [7]. In addition to these successes in modelling gas-phase combustion, CMC couple with a semi-empirical soot model has also shown promise in the calculation of soot formation in non-premixed flames [8], [9].

Even though air preheating technique has been employed for enhancing the combustion efficiency, the available literatures still lack detailed on the effect of air temperature on the formation and destruction of soot in a turbulent non-premixed flame. With this in mind, this study presents the results of an application of a first-order conditional moment closure (CMC) approach coupled with a semi-empirical soot model proposed by Leung et al. [10] and Lindstedt [11] on the effect of air preheat temperature on soot formation in air-propane turbulent non-premixed flames.

II. MATHEMATICAL FORMULATION AND CALCULATIONS

A. Target Flames and Turbulent Flow Calculations

The non-premixed air-propane and preheated-air propane flames considered in the present study have been experimentally reported by Jurng et al. [12] and Nishida and Mukohara [13], respectively. The important characteristics of each of these flames are presented in Tables 1, and further
details of the flame geometry, methods of data collection, and processing can be found in the relevant references.

| TABLE 1. OPERATING CONDITIONS FOR AIR-PROPANE AND PREHEATED-AIR PROPANE FLAMES |
|---------------------------------|-----------------|-----------------|
| Air exit temperature           | 298 K           | 323 K           | 773 K           |
| Absolute pressure/atm           | 1               | 1               | 1               |
| Fuel exit velocity/ms           | 16              | 30.0            | 30.0            |
| Reynolds number                 | 11000           | 13000           | 13000           |
| Fuel Exit temperature/K         | 298             | 298             | 298             |
| Nozzle diameter/mm              | 3.0             | 2.0             | 2.0             |
| Co-flow air velocity/ms         | 0.4             | 0.4             | 0.96            |

The calculation of flow and mixing fields was achieved by solving the Favre-averaged forms of the partial differential equations which describe conservation of mass, momentum and the transport of mixture fraction and its variance. A standard k-ε turbulence model was used to close the above equation set. Standard turbulence modelling constants appropriate to axisymmetric flows were employed, although to ensure the accurate prediction of the spreading rate of the jets, an adjustment was made to the value of ε from 1.92 to 1.86 to affect an increase in the dissipation rate of turbulence kinetic energy. A modified version of the GENMIX code [14] was implemented in the solution of the two-dimensional, axisymmetric forms of the transport equations. The code applies an implicit formula in the stream-wise direction and a hybrid-differencing scheme in the cross-stream direction for its marching integration procedure.

B. First-Order CMC-Soot Model

A general first-order, parabolic CMC equation can be obtained by averaging the instantaneous equation governing species mass fraction, \( Y_i \), in statistically stationary, turbulent reacting flow, on the condition that the instantaneous mixture fraction \( \xi \) equals an arbitrary value \( \eta \). The derivation of CMC equation can be found elsewhere [15] and in an unclosed form it can be expressed as:

\[
\frac{\partial Q_i}{\partial \xi} \langle \eta \rangle \frac{\partial \langle \eta \rangle}{\partial \xi} = \frac{1}{2} \frac{D_{\xi}}{D_{\eta}} \langle \eta \rangle \frac{\partial Q_i}{\partial \eta} + \langle \omega_i \rangle + \epsilon_{i,\eta}
\]  

[1]

For the calculation of gas-phase species mass fraction, it is assumed that both reactive and conserved scalars are diffuse equally, implying \( D_i = D_{\xi} \). As a consequence, the second and last terms on the right hand-side of Eq. 1, representing the source terms that generate differential and spatial diffusion, respectively, are cancelled. The scalar dissipation was modelled using the approach of Girimaji [16], while the remaining non-linear chemical source term \( \langle \omega_i \rangle \) was modelled as a simple first-order closure, with the mean values were obtained utilizing the CHEMKIN package [17] together with a modified full chemical kinetic scheme consisting 70 species and 463 reactions [18], supplemented with the detailed model of nitrogen chemistry of Miller and Bowman [19].

With respect to the computation of soot level in the target flames, the proposed semi-empirical soot model described in [10], [11] requires the solution of two additional transport equations for the soot mass fraction, \( Y_s \), and the soot particle number density, \( N_s \). In the case of differential diffusion being neglected, the transport equations for \( Y_s \) and \( N_s \) are obtained in a similar way as for the gas-phase species, setting \( D_{Y_s} = D_{N_s} = D_{\xi} \) for \( i = Y_s, N_s \) in Eq. 1, to give:

\[
\frac{\partial Q_s}{\partial \xi} \langle \eta \rangle \frac{\partial \langle \eta \rangle}{\partial \xi} = \frac{1}{2} \frac{D_{\xi}}{D_{\eta}} \langle \eta \rangle \frac{\partial Q_s}{\partial \eta} + \langle \omega_s \rangle + \epsilon_{s,\eta}
\]

[2]

\[
\frac{\partial Q_s}{\partial \xi} \langle \eta \rangle \frac{\partial \langle \eta \rangle}{\partial \xi} = \frac{1}{2} \frac{D_{\xi}}{D_{\eta}} \langle \eta \rangle \frac{\partial Q_s}{\partial \eta} + \langle \omega_s \rangle + \epsilon_{s,\eta}
\]

[3]

where the superscript + refers to a scalar of equal diffusivity. Considering the importance of introducing effect of differential diffusion of soot particle into the calculation as recommended in [12, 13, 23], the molecular coefficients of soot particles and nuclei are equal to zero, i.e. \( D_{Y_s} = D_{N_s} = 0 \) for \( i = Y_s, N_s \). Eq. 1 can now be simplified by neglecting the dissipation term, this being the first term on the right hand side. However, the \( \epsilon_{s,\eta} \), spatial diffusion terms seen in Eq. 1, now becomes significant. Following the work of Kronenburg et al [20] in the representation of \( \epsilon_{s,\eta} \), and the transport equations considering the effects of differential diffusion are modelled as Eqs. 4 and 5.

\[
\frac{\partial Q_s}{\partial \xi} \langle \eta \rangle \frac{\partial \langle \eta \rangle}{\partial \xi} = \left( \frac{\partial}{\partial \xi} \left( \rho D_{\xi} \frac{\partial \langle \eta \rangle}{\partial \xi} \right) \right) \langle \omega_s \rangle + \epsilon_{s,\eta}
\]

[4]

\[
\frac{\partial Q_s}{\partial \xi} \langle \eta \rangle \frac{\partial \langle \eta \rangle}{\partial \xi} = \left( \frac{\partial}{\partial \xi} \left( \rho D_{\xi} \frac{\partial \langle \eta \rangle}{\partial \xi} \right) \right) \langle \omega_s \rangle + \epsilon_{s,\eta}
\]

[5]

The source terms \( \langle \omega_s \rangle \) in Eqs. 2 and 4 account for the contribution of soot nucleation, surface growth and oxidation. Acetylene and benzene were selected as the precursor species responsible for soot nucleation [14]. However, the former species was considered as the only one governing the increase in soot mass via surface growth. The soot nucleation proceeds via \( \text{C}_2\text{H}_2 \rightarrow 2\text{C}_s + \text{H}_2 \) and \( \text{C}_6\text{H}_6 \rightarrow 6\text{C}_s + 3\text{H}_2 \). It is assumed that surface growth continues via an acetylene reaction similar to the one in soot nucleation. Soot oxidation is assumed due to the attack by \( \text{O}_2 \) and \( \text{OH} \) through \( \text{C}_s + 0.5 \text{O}_2 \rightarrow \text{CO} \) and \( \text{C}_s + \text{OH} \rightarrow \text{CO} + \text{H} \). Now, the source term for the soot mass fraction equation can be written as:
\[ \omega_s = 2k_1(Q_s)Q_{O_2}M_s + 6k_1(Q_s)Q_{C,H_4}M_s \]
\[ -2k_1(Q_s)Q_{C,H_4}M_s - k_1(Q_s)^3 Q_{O_2}M_s \]
\[ -k_1(Q_s)^3 Q_{O_2}M_s \]  \[6\]

The source terms \( \omega \) and \( \eta \) in Eqs. 3 and 5 representing the production and reduction of soot particle number density due to nucleation and agglomeration, respectively are expressed as:
\[ \omega_s = \left[ 2k_1(Q_s)Q_{O_2}M_s + 6k_1(Q_s)Q_{C,H_4}M_s \right] \frac{N_s}{v_{max}} \]
\[ -2C \left( \frac{6(Q_s)}{\rho_s Q_{O_2}} \right)^{1/6} \left( \frac{6Q_s Q_{O_2}}{\rho_s} \right)^{2} \left( \frac{\rho_s Q_{O_2}}{\rho_s} \right)^{3/2} \]  \[7\]

Reaction rate constants for nucleation, surface growth and oxidation that appear in Eqs. 6 and 7 are presented in Table 2.

<table>
<thead>
<tr>
<th>( k_1 )</th>
<th>( A )</th>
<th>( b )</th>
<th>( T_a )</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k_1 )</td>
<td>( 1.0 \times 10^4 )</td>
<td>0.0</td>
<td>21,000</td>
<td>[11]</td>
</tr>
<tr>
<td>( k_2 )</td>
<td>( 0.75 \times 10^3 )</td>
<td>0.0</td>
<td>21,000</td>
<td>[11]</td>
</tr>
<tr>
<td>( k_3 )</td>
<td>( 0.75 \times 10^3 )</td>
<td>0.0</td>
<td>12,100</td>
<td>[11]</td>
</tr>
<tr>
<td>( k_4 )</td>
<td>( 7.15 \times 10^2 )</td>
<td>0.5</td>
<td>19,680</td>
<td>[20]</td>
</tr>
<tr>
<td>( k_5 )</td>
<td>( 3.60 \times 10^{-1} )</td>
<td>0.5</td>
<td>0</td>
<td>[21]</td>
</tr>
</tbody>
</table>

Constants are in the form of the Arrhenius expression \( k = A T^b \exp(-C/aT) \) (units K, kmol, m, s).

### C. Solution of the CMC-Soot Transport Equations

Flow and mixing field data from the turbulent flow calculations employing a reacting-flow density were passed to the CMC calculation, where the set of species mass fractions, soot mass fraction, particle number density and enthalpy equations were solved in mixture fraction space. The flow and mixing field are related to the reactive scalar field through the mean density, and comparison between densities obtained from the CMC solution and prescribed equilibrium values showed little variation at the locations examined in the flames considered. Coupling of the flow field and CMC calculations was therefore deemed unnecessary for the calculations reported. Solution of the CMC equations in real space was achieved using a fractional step method, implemented using the stiff ODE solver VODE [22], which applies a backward differentiation formula approach to the solution of the nonlinear equation set. Second-order differential sample space terms were determined using a central differencing approximation. The computational grids consisted of 68 radial nodes in mixture fraction space and 38 nodes in physical space.

### III. RESULTS AND DISCUSSIONS

#### A. Propane Flame Without Air-Preheating

Fig.1 demonstrated axial and radial predictions of axial velocity for the propane flame without air preheating compared experimental data [12]. The solid line represents the simulations resulting from the use of \( k-\varepsilon \) standard turbulence model. The centre-line axial velocity predictions in the flame display qualitatively and quantitatively excellent agreement with the experimental data. The evolution of the computed axial velocity along the flame is in line with the measurements. The accuracy of such prediction was achieved by adjusting constants in the \( k-\varepsilon \) turbulence model \( C_{\varepsilon 1} \) from 1.44 to 1.54 and \( C_{\varepsilon 2} \) from 1.92 to 1.84. Similar accurate predictions were also observed for radial velocity profile at all axial positions. Overall, the \( k-\varepsilon \) standard turbulence model with slight adjustment in \( C_{\varepsilon 1} \) and \( C_{\varepsilon 2} \) is found to reproduce the flow field in the propane flame without preheating.

![Fig. 1](image1.png)

![Fig. 2](image2.png)

**TABLE 2. REACTION RATE CONSTANTS FOR SOOT FORMATION AND OXIDATION**

**Fig. 1** Axial and radial profiles of axial velocity for propane flame \( T_{air} = 298 \text{ K} \) (symbol – measured, solid line – predicted with \( k-\varepsilon \) turbulence model)

**Fig. 2** Axial and radial profiles of temperature for propane flame \( T_{air} = 298 \text{ K} \) (symbol – measured, solid line – predicted with CMC model)

The centre-line temperature predictions in the propane flame without preheating also display qualitatively and quantitatively excellence results in comparison to the experimental data. The evolution of the computed axial...
temperature is in line with the measurements along the core of
the flame. The position and value of peak temperature are very
well captured by the CMC model. This agreement is
achievable not only due to the conformity of flow field
predictions with experimental data but also due to the correct
selection radiation model and chemistry to represent the
combustion. With respect to the radial temperature
predictions, the results are not as accurate as in axial profile,
but they are still relatively in good agreement experimental
data. Although the position of off-centre peak temperature in
radial profile of $x = 200$ mm is well captured by the
prediction, its value is somewhat under-predicted. Further
downstream, under-prediction was also observed in lean fuel
region of radial profile of $x = 600$ mm.

B. Propane Flames With and Without Air Preheat

Restriction of space precludes presentation of graphs
comparing flow and temperature predictions with
experimental data for flames with air preheating. However,
treated with similar flow field calculation, it can be said that
the calculated axial mixture fraction predictions for both
propane flames with air preheating are in good agreement
with the experimental data, indicating that the mixing fields of
both the air preheated propane–air flames are well represented
by the applied $k-\varepsilon$ turbulence closure, as in the case of
propane flame without preheating. In connection with
temperature predictions, the results of centre-line mean
temperature predictions of the two air preheated flames are not
as satisfactory compared with those obtained in propane flame
without air preheating, although the temperatures in the mid-
flame region and its peak are well represented. Radial
temperature profiles along with measurements for the two air
preheated propane flames in general are in good agreement
with the experiments.

Fig. 3 compares predicted centre-line and radial
temperatures of the no-preheat flame to those of low-
and high-preheat flames. Solid, dashed and dotted lines represent
predictions of these flames, respectively. It is clearly seen that
air preheating leads to an increase of centre-line flame
temperature, particularly up to the mid-flame zone. The temperature of air preheat flames increases sharply in core of
the flame, leading to a shift of peak temperature to a lower
positions in comparison to that of no preheat flame. However,
a different trend was observed in the radial profile, where the
off-centre peak temperature for the no preheat flame is closer
to the centre-line that of air preheat flames. Further
downstream, the radial profile of temperature is significantly
different from one to another.

Fig. 4 Predicted axial and radial profiles of soot
concentrations for propane flames of $T_{\text{air}} = 298$ K (solid line), $T_{\text{air}} = 323$ K (dashed line), and $T_{\text{air}} = 773$ K (dotted line).

At this stage it is useful to compare the evolution of soot
concentration in the three flames being studied, as presented
in Fig. 4. In the axial profile, it is clearly seen that the first
soot emerged at the height of 100 mm above the nozzle of the
flame of 773 K air preheat, then at 150 mm above the nozzle of
the 323 K air preheat propane flame and finally at $x = 250$
mm in the no air preheat flame. As the temperature of the
flame increases, the rate of soot formation also increases. As
propane flame with no air preheat the soot is still evident, flames with air preheat. In contrast, further downstream of the results in no soot emission in the exhaust gases of the propane soot oxidation rate, and depletion of soot due to oxidation with the existence of high concentrations of oxygen, enhances the increase in temperature in the post flame zone, leads to an increase in the soot formation rate, leading to sharp increase in soot concentrations until they reach peak values. At the heights of 600 mm and 800 mm, soot concentrations in the 773 K and 323 K air preheat flames approach zero, respectively, as also demonstrated in the radial profiles at $x = 600$ mm and $x = 800$ mm in the same figure. However, significant soot concentration is still evident in the region further downstream for the flame without air preheat. These findings indicate that preheating combustion air in a combustion system enhances the soot formation rate, but at the same time also augments the soot oxidation rate. As a consequence, soot is almost non-existent at downstream locations in the flames of low- and high-preheat.

IV. CONCLUSION

Application of k-ε turbulence model with a slight modification in Cc1 and Cc2 successfully reproduces turbulent flow and mixing fields in the three propane flames with and without air preheat, as reflected by excellent agreement of velocity profile predictions with the experimental data. In addition the to the correct modelling of turbulent flow field, the CMC model coupled with radiation model and kinetic scheme employed play significant role in the accuracy of temperature in the three flames being studied. The use of air preheat in a combustion system promotes the increase of flame temperature. As a consequence, the temperature of flames of air preheat 323 K and 773 K increases and is higher throughout the flame compared to that of flame without air-preheat. Such increase in temperature leads to an increase in the soot formation rate, leading to sharp increase in soot concentrations until they reach peak values. However, the increase in temperature in the post flame zone, with the existence of high concentrations of oxygen, enhances the soot oxidation rate, and depletion of soot due to oxidation results in no soot emission in the exhaust gases of the propane flames with air preheat. In contrast, further downstream of the propane flame with no air preheat the soot is still evident, suggesting soot might escape oxidation process releasing pollutant into atmosphere.

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