Numerical prediction of soot emissions in ethylene flames based on DQMOM

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The main aim of the present work is to understand and determine the formation and evolution of soot particles and its effect on heat transfer from the system. The Direct Quadrature Method of Moments (DQMOM) is employed to solve in a computationally efficient manner the Population Balance Equations (PBE). Numerical simulations of turbulent ethylene-air nonpremixed flames are carried out. Gas-phase chemistry is modeled with PDF (Probability Density Function) mixture-fraction method combined with equilibrium chemistry. As many as 20 chemical species are considered in the equilibrium chemistry calculations. Turbulent-chemistry interactions are through presumed $\beta$-PDF. The particle phase is computed with PBE.

The evolution of the soot particles is described by nucleation, surface growth, aggregation and oxidation, the most important processes in the evolution of soot. The kinetic models for nucleation, growth, oxidation are shown below along with aggregation model.

Nucleation: In the present numerical approach acetylene is considered responsible for soot nucleation. The corresponding rate equation from Moss et al. [1995] is:

$$J = N_A \rho^2 T^6 \times 10^6 \exp \left( -\frac{46100}{T} \right) X_{C_2H_2}$$

Molecular growth: acetylene molecules are considered to be responsible for the molecular growth and the corresponding rate expression is given by Liu et al. [2003]:

$$G_{mg} = \frac{6}{D_f \rho_s} \left( \frac{R_{c1}}{R_{c0}} \right)^{3-D_f} 2M_s 6 \exp \left( -\frac{6038}{T} \right) [C_2H_2]$$

Oxidation: Oxidation kinetic model proposed by Said et al. [1997] is used.

$$G_{ox} = \frac{P}{D_f \rho_s} T^{\frac{3}{2}} 6.5 \exp \left( -\frac{26500}{T} \right) Y_{O_2}$$

Aggregation: Widely used Fuchs interpolation formula of Brownian kernel is considered for the aggregation (see Zucca et al. [2006]).

$$\beta_{12} = 4\pi(D_1 + D_2)(R_{c1} + R_{c2}) \left[ \frac{R_{c1} + R_{c2}}{R_{c1} + R_{c2} + (g_1^2 + g_2^2)^{\frac{3}{2}}} + \frac{4(D_1 + D_2)}{R_{c1} + R_{c2} + (c_1^2 + c_2^2)^{\frac{3}{2}}} \right]^{-1}$$

Where, $c_i = \sqrt{\frac{8k_bT}{\pi m_i}}$, $D_i = \frac{k_b T}{6\pi \mu R_{c1}} \left[ \frac{5+4Kn_i+6Kn_i^2+18Kn_i^3}{5-Kn_i+(8+\pi)Kn_i^2} \right]$, $l_i = \frac{8D_i}{\pi c_i}$, $g_i = \frac{(2R_{c1} + l_i)^3 - (4R_{c1}^3 + l_i^3)}{6R_{c1}^{3l_i}} - 2R_{c1}$

Here, $X$ is mole fraction, $Y$ is mass fraction, $k_b$ is Boltzmann constant, $m$ is particle mass, $M_s$ is soot molecular weight, $N_A$ is Avogadros number and $[C_2H_2]$ represents the acetylene concentration.
Mono-variate population balance modeling is considered with particle diameter as the internal co-ordinate. With the DQMOM approach one needs to solve a limited number of scalar transport equations (typically 4-6) coupled with the Navier-Stokes equations. It is relatively easy to implement DQMOM in commercial CFD solvers (here Ansys-Fluent) and it can be extended for multivariate PBE. The DQMOM algorithm is coupled to Ansys-Fluent through a complex User Defined Function (UDF). In the literature, many experimental results can be found concerning soot formation in turbulent nonpremixed flames burning ethylene. Three different flames have been chosen for our simulations, involving different flow conditions and a wide range of Reynolds numbers as shown in Table 1.

<table>
<thead>
<tr>
<th>Flame</th>
<th>Fuel</th>
<th>Re (mm)</th>
<th>$u_i$ (m/s)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>C$_2$H$_4$</td>
<td>14600</td>
<td>3.0</td>
<td>52.0</td>
</tr>
<tr>
<td>II</td>
<td>C$_2$H$_4$</td>
<td>13500</td>
<td>4.56</td>
<td>25.8</td>
</tr>
<tr>
<td>III</td>
<td>C$_2$H$_4$</td>
<td>5700</td>
<td>9.0</td>
<td>6.3</td>
</tr>
</tbody>
</table>

Table 1: Different experimental test conditions considered for simulation

The comparison of simulation results with the experimental data demonstrates that the developed modeling approach can describe accurately the formation and evolution of soot particles in turbulent flames. Analysis of results shows that heat loss from the system is highly significant and there is a clear need for better radiation models in future investigations. Further tests involving other conditions and different fuels will be carried out in the near future.

References


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Introduction

Due to the adverse effects of soot on human health (lung cancer) and the environment (global warming) it has attracted great attention of researchers from many years. The research still has high significance due to the adverse effects of soot on human health and environment its detailed understanding is necessary.


Analyse different factors affecting soot-particles formation.

Assess detailed physical and chemical processes involved.

Objectives

There are four important mechanisms involved in soot formation and its subsequent evolution:

1. Nucleation
2. Molecular growth
3. Aggregation and
4. Oxidation

Soot evolution

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Result and Discussions

• DQMOM is a moment-based method to solve PBE

• In the DQMOM approach the distribution function is represented as a summation of a finite number, N, of multi-dimensional Dirac delta functions [2] as shown below.

\[
 f(\xi, x, t) = \sum_{i=0}^{N} w_i(\xi, x, t) \delta(\xi - \xi_i, x, t)
\]

• Here, N is the number of delta functions, \( w_i(\xi, x, t) \) is the weight of node \( i \).

• Substituting Eq. (2) in Eq. (1) and after subsequent manipulations and moment transformation, one obtains greatly simplified coupled equations

\[
 (1 - \Gamma) \sum_{a=0}^{N} \sum_{i=0}^{N} a_i a_{a,i} = \bar{S}_0 + \bar{C}_0
\]

\[
 \frac{\partial w_i}{\partial t} + \frac{\partial}{\partial x} \left( \bar{u} w_i + \bar{\alpha} \right) - \frac{\partial}{\partial x} \left( \bar{\xi}_i w_i \right) = a_i
\]

\[
 \frac{\partial a_i}{\partial t} + \frac{\partial}{\partial x} \left( \bar{u} a_i + \bar{\alpha} a_i \right) - \frac{\partial}{\partial x} \left( \bar{\xi}_i a_i \right) = \bar{b}_i
\]

• For \( N = 2 \), monotonous PBE results in 4 transport equations (easy to implement in CFD solver) and set of 4 algebraic equations which can be solved easily.

Conclusions

• Due to the adverse effects of soot on human health and environment its detailed understanding is necessary.

• Coupled processes leading to soot are extremely complex.

• Considerable heat-loss due to soot radiation.

• Results demonstrate potential of DQMOM in solving PBE at acceptable computational cost.

• Study of individual mechanisms on soot production shows that nucleation and aggregation are the most important mechanisms.

• First comparisons with experimental data are acceptable, but not perfect.

References

