Revision to Modeling Soot Derived from Pulverized Coal

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The purpose of this paper is to address a number of concerns that researchers have expressed when implementing the soot model of Brown and Fletcher (10.1021/ef9702207).† A more common notation is presented here along with a table of units for clarification. It is the hope of the authors that this notation and associated clarifications will facilitate implementation of this model.

Alexander J. Josephson and David O. Lignell have been added as authors in this revision. Some equation and notation changes are presented in this revision. These changes are meant to reflect the original implementation of this model and correct a few minor inconsistencies in the original print. As a result, a reader may find the original paper.

For clarification, the steady-state Reynolds-averaged Navier–Stokes equations for the conservation of soot mass, tar mass, and soot particle number (eqs 4–6 in the original paper) are changed by assimilating the gas density into the transport source terms.

\[
\bar{V}(\rho \bar{u} Y_C) = \bar{V}
\left(\frac{\mu}{\sigma} \nabla Y_C + S_{\nabla Y_C}\right)
\]

(1)

\[
\bar{V}(\rho \bar{u} Y_T) = \bar{V}
\left(\frac{\mu}{\sigma} \nabla Y_T + S_{\nabla Y_T}\right)
\]

(2)

\[
\bar{V}(\rho \bar{u} N_C) = \bar{V}
\left(\frac{\mu}{\sigma} \nabla N_C + S_{\nabla N_C}\right)
\]

(3)

Definitions of variables and their units, in these and subsequent equations, are given in Tables 1 and 2. Source terms in eqs 1–3 are defined by

\[ S_{\nabla Y_C} = \dot{\Gamma}_{FC} - \dot{\Gamma}_{OC} \]

(4)

\[ S_{\nabla Y_T} = \dot{\Gamma}_{FT} - \dot{\Gamma}_{FC} - \dot{\Gamma}_{GT} - \dot{\Gamma}_{OT} \]

(5)

\[ S_{\nabla N_C} = (N_C/M_{C, min}) \dot{\Gamma}_{FC} - \dot{\Gamma}_{AN} \]

(6)

where the \( \dot{\Gamma} \) terms refer to formation (F), oxidation (O), gasification (G), and aggregation (AN) of either soot (C) or tar (T). Equations 4–6 are consistent with equations presented by Brown. Rates are defined as follows:

\[
\dot{\Gamma}_{FT} = S_{\nabla Y_T}
\]

(7)

\[
\dot{\Gamma}_{OT} = (\rho \bar{u} Y_T)(\rho \bar{u} Y_O) A_{OT} e^{-E_{OT}/RT}
\]

(8)

\[
\dot{\Gamma}_{GT} = (\rho \bar{u} Y_T) A_{GT} e^{-E_{GT}/RT}
\]

(9)

\[
\dot{\Gamma}_{FC} = (\rho \bar{u} Y_T) A_{FC} e^{-E_{FC}/RT}
\]

(10)

Table 1. Transport Equation Source Terms

<table>
<thead>
<tr>
<th>term</th>
<th>A</th>
<th>( E ) (kJ/mol)</th>
<th>source</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \dot{\Gamma}_{OT} )</td>
<td>( 6.77 \times 10^7 ) m^2 kg^{-1} s^{-1}</td>
<td>N/A</td>
<td>source term for tar</td>
</tr>
<tr>
<td>( \dot{\Gamma}_{GT} )</td>
<td>( 9.77 \times 10^{18} ) s^{-1}</td>
<td>52.3</td>
<td>Shaw et al.³</td>
</tr>
<tr>
<td>( \dot{\Gamma}_{FC} )</td>
<td>( 5.02 \times 10^{18} ) s^{-1}</td>
<td>286.9</td>
<td>Ma¹</td>
</tr>
<tr>
<td>( \dot{\Gamma}_{OC} )</td>
<td>( 1.09 \times 10^7 ) kg K^{1/2} m^{-3} atm^{-1} s^{-1}</td>
<td>198.9</td>
<td>Ma¹</td>
</tr>
<tr>
<td>( \dot{\Gamma}_{AN} )</td>
<td>N/A</td>
<td>164.5</td>
<td>Lee et al.⁴</td>
</tr>
</tbody>
</table>

Table 2. Table of Units Given for Clarification

<table>
<thead>
<tr>
<th>term</th>
<th>description</th>
<th>unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C )</td>
<td>collision frequency constant</td>
<td>unitless</td>
</tr>
<tr>
<td>( C_{\text{mass}} )</td>
<td>number of carbon atoms per incipient soot particle</td>
<td>unitless</td>
</tr>
<tr>
<td>( d_p )</td>
<td>soot particle diameter</td>
<td>m</td>
</tr>
<tr>
<td>( \epsilon )</td>
<td>Boltzman constant</td>
<td>J/K</td>
</tr>
<tr>
<td>( M_C )</td>
<td>molecular weight of carbon</td>
<td>kg/kmol</td>
</tr>
<tr>
<td>( N_A )</td>
<td>Avogadro’s number</td>
<td>kmol⁻¹</td>
</tr>
<tr>
<td>( N_C )</td>
<td>soot particles per unit mass</td>
<td>kg⁻¹</td>
</tr>
<tr>
<td>( p_{O2} )</td>
<td>partial pressure of oxygen</td>
<td>atm</td>
</tr>
<tr>
<td>( R )</td>
<td>ideal gas constant</td>
<td>kJ mol⁻¹ K⁻¹</td>
</tr>
<tr>
<td>( S_{A,C} )</td>
<td>surface area of soot per volume</td>
<td>m²/m³</td>
</tr>
<tr>
<td>( S_{N_C} )</td>
<td>source term for the number of particles</td>
<td>m⁻³ s⁻¹</td>
</tr>
<tr>
<td>( S_{\text{tar}} )</td>
<td>source term for tar</td>
<td>kg m⁻³ s⁻¹</td>
</tr>
<tr>
<td>( S_{\text{C}} ) and ( S_{\text{C}} )</td>
<td>source term for the mass fraction of soot and tar, respectively</td>
<td>kg m⁻³ s⁻¹</td>
</tr>
<tr>
<td>( T )</td>
<td>temperature</td>
<td>K</td>
</tr>
<tr>
<td>( \epsilon )</td>
<td>gas velocity</td>
<td>m/s</td>
</tr>
<tr>
<td>( \mu )</td>
<td>mass fractions of soot, tar, and O₂, respectively</td>
<td>unitless</td>
</tr>
<tr>
<td>( \rho )</td>
<td>turbulent viscosity</td>
<td>kg m⁻³ s⁻¹</td>
</tr>
<tr>
<td>( \rho_{C} )</td>
<td>density of soot</td>
<td>kg/m³</td>
</tr>
<tr>
<td>( \rho_{C} )</td>
<td>solid density of soot</td>
<td>kg/m³</td>
</tr>
<tr>
<td>( \sigma )</td>
<td>turbulent Schmidt number</td>
<td>unitless</td>
</tr>
</tbody>
</table>
\[
\dot{r}_{OC} = S_{A_{\nu,C}} \frac{P_{OC}}{T^{1/2}} \frac{A_{OC} e^{-E_{OC}/RT}}{2}
\]  
(11)

\[
S_{A_{\nu,C}} = (N_{\nu p}) \pi d_p^2 = (N_{\nu p}) \pi \left( \frac{6Y_{C}}{\pi N_C \rho_C} \right)^{2/3}
\]  
(12)

\[
\dot{r}_{AN} = 2C_4 \left( \frac{6M_C}{\pi \rho_C} \right)^{1/6} \left( \frac{6kT}{\rho_C} \right)^{1/2} \left( \frac{\rho_{g} Y_{C}}{M_C} \right)^{1/6} \left( \rho_{g} N_{C} \right)^{11/6}
\]  
(13)

Equations 7–13 include changes to accommodate the assimilation of gas density into the overall respective source terms, clarify the calculation of the surface area, and correct for some unit inconsistencies. In these equations, the solid soot density is assumed to be 1950 kg/m³ and \(S_{P_{tar}}\) should be calculated from a separate coal devolatilization model. Table 1 shows Arrhenius constants and activation energies for the source terms in the transport equations (eqs 4–6), reproduced from the original table published by Brown and Fletcher (10.1021/ef9702207), with a few clarifications to match the units and equations presented here, along with corrected references and a misprinted exponential.

While this addendum amends and clarifies some of the equations and parameters originally published, to the authors’ knowledge, simulation results published in the original document are still accurate.

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### REFERENCES