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Addition/Correction
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Revision to Modeling Soot Derived from Pulverized Coal

Alexander J. Josephson,[†] David O. Lignell,[†] Alexander L. Brown,[‡] and Thomas H. Fletcher[*,†]

[†]Department of Chemical Engineering, Brigham Young University, 350 CB, Provo, Utah 84602, United States

[‡]Sandia National Laboratories, Albuquerque, New Mexico 87185, United States

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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).[1] 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 orginal print. As a result, a reader may implement this model from the information given in this revision alone. Validation and simulation results have not changed from 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.

$$\vec{\nabla}(\rho_g \vec{u} Y_C) = \vec{\nabla}\left(\frac{\mu}{\sigma}\vec{\nabla} Y_C\right) + S_{Y_C} \quad (1)$$

$$\vec{\nabla}(\rho_g \vec{u} Y_T) = \vec{\nabla}\left(\frac{\mu}{\sigma}\vec{\nabla} Y_T\right) + S_{Y_T} \quad (2)$$

$$\vec{\nabla}(\rho_g \vec{u} N_C) = \vec{\nabla}\left(\frac{\mu}{\sigma}\vec{\nabla} N_C\right) + S_{N_C} \quad (3)$$

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

$$S_{Y_C} = \dot{r}_{FC} - \dot{r}_{OC} \quad (4)$$

$$S_{Y_T} = \dot{r}_{FT} - \dot{r}_{FC} - \dot{r}_{GT} - \dot{r}_{OT} \quad (5)$$

$$S_{N_C} = (N_a/M_C C_{min})\dot{r}_{FC} - \dot{r}_{AN} \quad (6)$$

where the $\dot{r}$ 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:

$$\dot{r}_{FT} = SP_{tar} \quad (7)$$

$$\dot{r}_{OT} = (\rho_g Y_T)(\rho_g Y_{O_2}) A_{OT} e^{-E_{OT}/RT} \quad (8)$$

$$\dot{r}_{GT} = (\rho_g Y_T) A_{GT} e^{-E_{GT}/RT} \quad (9)$$

$$\dot{r}_{FC} = (\rho_g Y_T) A_{FC} e^{-E_{FC}/RT} \quad (10)$$

Table 2. Table of Units Given for Clarification

term	description	unit
C_a	collision frequency constant	unitless
C_{min}	number of carbon atoms per incipient soot particle	unitless
d_p	soot particle diameter	m
k	Boltzman's constant	J/K
M_C	molecular weight of carbon	kg/kmol
N_a	Avogadro's number	$kmol^{-1}$
N_C	soot particles per unit mass	kg^{-1}
p_{O_2}	partial pressure of oxygen	atm
R	ideal gas constant	$kJ\ mol^{-1}\ K^{-1}$
$SA_{v,C}$	surface area of soot per volume	m^2/m^3
S_{N_C}	source term for the number of particles	$m^{-3}\ s^{-1}$
SP_{tar}	source term for tar	$kg\ m^{-3}\ s^{-1}$
S_{Y_C} and S_{Y_T}	source term for the mass fraction of soot and tar, respectively	$kg\ m^{-3}\ s^{-1}$
T	temperature	K
$\vec{u}$	gas velocity	m/s
Y_C, Y_T, and Y_{O_2}	mass fractions of soot, tar, and O_2, respectively	unitless
μ	turbulent viscosity	$kg\ m^{-1}\ s^{-1}$
ρ_g	density of gas	kg/m^3
ρ_C	solid density of soot	kg/m^3
σ	turbulent Schmidt number	unitless

Table 1. Transport Equation Source Terms

term	A	E (kJ/mol)	source
	N/A	N/A	source term for tar
$\dot{r}_{OT}$	$6.77 \times 10^5\ m^3\ kg^{-1}\ s^{-1}$	52.3	Shaw et al.[2]
$\dot{r}_{GT}$	$9.77 \times 10^{10}\ s^{-1}$	286.9	Ma[3]
$\dot{r}_{FC}$	$5.02 \times 10^8\ s^{-1}$	198.9	Ma[3]
$\dot{r}_{OC}$	$1.09 \times 10^5\ kg\ K^{1/2}\ m^{-2}\ atm^{-1}\ s^{-1}$	164.5	Lee et al.[4]
$\dot{r}_{AN}$	N/A	N/A	Fairweather et al.[5]

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$$\dot{r}_{OC} = SA_{v,C}\frac{p_{O_2}}{T^{1/2}}A_{OC}e^{-E_{OC}/RT} \quad (11)$$

$$SA_{v,C} = (N_C\rho_g)\pi d_p^{\ 2} = (N_C\rho_g)\pi\left(\frac{6Y_C}{\pi N_C\rho_C}\right)^{2/3} \quad (12)$$

$$\dot{r}_{AN} = 2C_a\left(\frac{6M_C}{\pi\rho_C}\right)^{1/6}\left(\frac{6kT}{\rho_C}\right)^{1/2}\left(\frac{\rho_g Y_C}{M_C}\right)^{1/6}(\rho_g N_C)^{11/6} \quad (13)$$

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/m^3 and SP_{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.

■ AUTHOR INFORMATION

Corresponding Author

*E-mail: tom_fletcher@byu.edu.

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