



# Modeling soot formation from solid complex fuels<sup>☆</sup>

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## ARTICLE INFO

### Article history:

Received 26 February 2018

Revised 15 June 2018

Accepted 18 June 2018

### Keywords:

Soot formation

Coal

Biomass

Method of moments

## ABSTRACT

A detailed model is proposed for predicting soot formation from complex solid fuels. The proposed model resolves two particle size distributions, one for soot precursors and another for soot particles. The precursor size distribution is represented with a sectional approach while the soot particle-size distribution is represented with the method of moments and an interpolative closure method is used to resolve fractional methods. Based on established mechanisms, this model includes submodels for precursor coagulation, growth, and consumption, as well as soot nucleation, surface growth, agglomeration, and consumption. The model is validated with comparisons to experimental data for two systems: coal combustion over a laminar flat-flame burner and biomass gasification. Results are presented for soot yield for three coals at three temperatures each, and for soot yield from three types of biomass at two temperatures each. These results represent a wide range of fuels and varying combustion environments, demonstrating the broad applicability of the model.

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## 1. Introduction

The formation of soot is a well-studied phenomena but still an active area of research [1]. Most research in soot formation processes have focused on soot formed from gaseous fuels, and sophisticated detailed-models have been developed to predict soot concentrations in these types of systems [2–9]. Soot models tend to follow a series of observed mechanism steps: particle nucleation, coagulation, surface growth, aggregation, and oxidation.

In gaseous fuels, poly-cyclic aromatic hydrocarbons (PAH) act as soot precursors. PAHs are formed in fuel-rich regions where radical gas species are in high enough concentrations to facilitate the formation of aromatic rings [10]. Small aromatics grow through various chemical mechanisms to form larger PAHs. Once PAHs are of sufficient size, they nucleate forming soot nuclei. Once nuclei are formed, particles grow through surface-gas reactions and particle-particle coagulation [4,11]. Small particles are roughly spherical; but as particles grow larger, they will begin to aggregate into chain-like structures [12].

Soot formation processes for solid fuel combustion differ from gaseous fuel [13]. This is because during the primary pyrolysis of complex solid fuels, such as wood or coal, a large variety

of volatile species are released from the parent fuel into the surroundings. Some of these species, often referred to as tars, are large molecules and aromatic in nature. These tars have a tendency to serve as primary soot precursors [14]. As opposed to PAHs from gaseous fuels, tar molecules may have aliphatic portions and inorganic elements attached to the aromatic clusters reflecting the composition of the parent fuel, thus altering the fundamental chemistry of the molecule [15]. The soot formation processes in these solid-complex fuel environments are not as well studied as for gaseous fuels, and there exist only a few predictive models for these systems [16–19]. These existing models contain system-specific and fuel-specific empirical calibrations and are limited in their extended application.

This study presents a physics-based detailed model for predicting soot formation from complex-solid fuels along with two validation cases, one using coal and the other using biomass. Effects of soot on combustion systems (radiative properties, combustion efficiency, etc) are most closely linked to the soot volume fraction which may be derived from a particle size distribution (PSD) resolved by this model. Results of the proposed model are compared against measured soot concentrations.

## 2. Model development

As described in the introduction, soot formation is dependent on the presence of soot precursors and the transformation of soot particles throughout a system. The proposed model describes PSDs and their time-evolution for both soot precursors and soot

<sup>☆</sup> As applied to wood and coal combustion.

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## Nomenclature

Variable	Meaning	Units	Equations
$A_{CO_2}$	Pre-exponential constant for gasification via $CO_2$	$\frac{kg\ K^{1/2}}{Pa^{1/2}\ m^2\ s\ K^2}$	(26)
$A_{H_2O}$	Pre-exponential constant for gasification via $H_2O$	$\frac{kg\ K}{Pa\ m^2\ s}$	(26)
$A_{O_2}$	Pre-exponential constant for oxidation via $O_2$	$\frac{kg\ K^{1/2}}{Pa\ m^2\ s}$	(25)
$A_{OH}$	Pre-exponential constant for oxidation via OH	$\frac{kg\ K}{Pa\ m^2\ s}$	(25)
$C_a$	Soot particle collision diameter constant	$m$	(13), (15), (41)
$C_{(d)}$	Soot collision radius proportionality constant	–	(15)
$C_h$	Precursor collision diameter constant	$m$	(10), (11), (13), (41)
$C_s$	Soot particle spherical diameter	$\frac{m^{1/3}}{kg}$	(13), (14), (40), (39), (41), (48)
$Cg_i$	Rate at moment change due to coagulation	$\frac{kg}{s}$	(28), (30), (32), (33), (35), (36), (38), (50), (52)
$Cn_i$	Rate at moment change due to consumption	$\frac{kg}{s}$	(28), (45)
$\langle d \rangle$	Particle shape factor	–	(15), (40), (43), (44), (45), (46), (47), (49), (48), (50), (52)
$d_A$	Diameter of a single aromatic ring	$m$	(11)
$d_i$	Collision diameter of species $i$	$m$	(8), (10)
$Dp_i$	Rate at moment change due to precursor deposition	$\frac{kg}{s}$	(28), (41), (45), (47)
$E_{CO_2}$	Activation energy for gasification via $CO_2$	$\frac{J}{mole}$	(26)
$E_{H_2O}$	Activation energy for gasification via $H_2O$	$\frac{J}{mole}$	(26)
$E_{O_2}$	Activation energy for oxidation via $O_2$	$\frac{J}{mole}$	(25)
$f_i^{(x,y)}, g_i, h_i$	Grid functions defined within the text	–	(35), (36), (37), (48), (49), (50), (51), (52)
$Gr_i$	Rate at moment change due to surface growth	$\frac{kg}{s}$	(28), (40), (45), (48)
$[i]$	Concentration of species $i$	$\frac{kmol}{m^3}$	Table 1, (16), (17), (21)
$k_B$	Boltzmann constant (1.38064852e-23)	$\frac{m^2\ kg}{s^2\ K}$	(8), (13), (41), (47)
$k_s$	Rate of a surface reaction	$\frac{kg}{m^2\ s}$	(39), (40)
$K_c$	Computed constant for the continuum regime of particle coagulation	$\frac{m^3}{s}$	(31), (32), (33), (50), (51)
$K'_c$	Another computed constant for the continuum regime of particle coagulation	$\frac{kg^{1/3}}{m^{1/3}}$	(31), (32), (33), (50), (51)
$K_f$	Computed constant for the free-molecule regime of particle coagulation	$\frac{m^3}{skg^{1/6}}$	(34), (35), (36), (52)
$k_i$	Kinetic rate constant	$\frac{m^3}{kmol\ s}$	Table 1, (17), (21)
$Kn$	Knudsen number	–	(38)
$m_i$	Molecular mass of species $i$	$kg$	(2), (6), (9), (10), (11), (13), (17), (22), (24), (27), (29), (30), (31), (34), (37), (39), (40), (42), (43), (46), (48), (51)
$M_i$	Moment $i$ of a PSD	$\frac{kg^r}{m^3}$	(2), (3), (4), (13), (28), (32), (33), (40), (41), (42), (43), (45), (48), (49), (50)
$n_{bins}$	Number of resolved discrete sections	#	(1), (7), (29), (42)
$N_i$	Particles/molecules of species $i$	$\frac{\#}{m^3}$	(1), (2), (5), (7), (13), (16), (22), (23), (24), (27), (29), (30), (37), (39), (42), (43), (51)
$Nu_i$	Rate at moment change due to nucleation	$\frac{kg}{s}$	(28), (29), (45), (46)
$P_i$	Partial pressure of species $i$	$Pa$	(25), (26)
$r_{consume_i}$	Rate of oxidation/gasification for precursor species $i$	$\frac{\#}{m^3\ s}$	(5), (27)
$r_{crack_i}$	Rate of thermal cracking for precursor species $i$	$\frac{\#}{m^3\ s}$	(5), (16)
$r_{depo_i}$	Rate of deposition for precursor species $i$ onto soot particles	$\frac{\#}{m^3\ s}$	(5), (13)
$r_{form_i}$	Rate of formation for precursor species $i$	$\frac{\#}{m^3\ s}$	(5), (6)
$r_{growth_i}$	Rate of surface growth for precursor species $i$	$\frac{\#}{m^3\ s}$	(5), (22)
$r_{nucl_i}$	Rate of coagulation for precursor species $i$	$\frac{\#}{m^3\ s}$	(5), (7)
$R$	Ideal gas constant	$\frac{mole\ K}{kg}$	Table 1, (25), (26)
$R_{HACA}$	Rate of surface growth through the HACA mechanism	$\frac{\#}{m^3\ s}$	(17), (22), (39), (40), (48)
$R_{gasification}$	Rate of gasification	$\frac{kg}{m^2\ s}$	(26), (27), (48)
$R_i$	Reaction rate $i$	$\frac{\#}{m^3\ s}$	Table 1, Eq. (16)
$R_{oxidation}$	Rate of oxidation	$\frac{kg}{m^2\ s}$	(25), (27), (48)
$R_{pyrene}$	Rate of pyrene molecules created	$\frac{\#}{m^3\ s}$	(6)
$R_{pyrolysis}$	Rate of precursor release from primary pyrolysis	$\frac{kg}{m^2\ s}$	(6)
$S_i$	Surface area of species $i$	$m^2$	(22), (23), (27), (39), (43)
$t$	Time	$s$	(5), (28), (39), (45)
$T$	Local temperature	$K$	Table 1, (8), (13), (19), (20), (25), (26), (41), (47)
$x_{phe}, x_{naph}, x_{tol}, x_{ben}$	Fraction of precursors characterized under a type	–	(16)
$\alpha$	Fraction of surface sites kinetically available for reaction	–	(17), (18)
$\beta_{i,j}$	Frequency of collision between species $i$ and $j$	$\frac{m^3}{s}$	(7), (8), (29), (30), (31), (34)
$\Delta m$	Change of mass resulting from a single reaction	$kg$	(39), (40), (49)
$\mu_i$	Reduced moment $i$ ( $\frac{M_i}{M_C}$ )	$kg^i$	(18), (44)
$\mu_{i,j}$	Reduced mass of species $i$ and $j$ ( $\frac{m_i m_j}{m_i + m_j}$ )	$kg$	(8), (9)
$\rho_s$	Soot density	$\frac{kg}{m^3}$	(14)
$\chi_i$	Number of species $i$ on particle surface	$\frac{\#}{m^2}$	(17), (21)

particles; however, the method used to depict each PSD will be different. We use the abbreviation of PSD to describe the distribution of soot precursors for convenience despite the size of precursors being too small to be considered particles.

The precursor PSD is represented using a sectional method. In the sectional method, a series of pseudo-chemical species are used to represent all precursors that are within a section of the full PSD. Each section is a subset of the PSD with different size

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