



## Soot predictions in premixed and non-premixed laminar flames using a sectional approach for PAHs and soot

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### ABSTRACT

A new soot model is presented, which has been developed for CFD applications, combining accuracy and efficiency. While the chemical reactions of small gas phase species are captured by a detailed chemical kinetic mechanism, polycyclic aromatic hydrocarbons (PAHs) and soot particles are represented by sectional approaches. The latter account for important mechanisms such as the formation of sections, their oxidation, the condensation of acetylene, and the collisions between sections. The model has been designed to predict soot for a variety of fuels with good accuracy at relatively low computational cost. Universal model parameters are applied, which require no tuning in dependence of test case or fuel. Soot predictions of ethylene, propylene, kerosene surrogate, and toluene flames are presented, which show good agreement with the experimental data. Furthermore, the importance of the correct choice for thermodynamic data of PAHs and soot is highlighted and the impact of heat radiation is discussed.

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### 1. Introduction

Soot can be found in a variety of combustion applications despite the fact that it is known to be an important pollutant. Not only does it affect the environment but also human health [1–4]. In addition, it may cause technical problems such as locally elevated heat loads for the combustor walls due to heat radiation [5–7]. Although soot has been studied over the last decades by a variety of research groups, it is still far from being completely understood [8]. During combustion of hydrocarbons it is formed in fuel-rich regions of the flame within a given temperature range. However, fuel rich conditions are very difficult to avoid, especially in the case of liquid fuels. Hence, it is important to better understand soot formation and the involved chemical processes in order to decrease soot emissions in practical applications.

Various soot models have been published in the past. The simplest among them are empirical models, which are usually restricted to the choice of fuel and to specific operating conditions. Nevertheless, once correctly tuned, they allow sensitivity analyses at low computational cost [9,10].

Semi-empirical models include PAH and soot chemistry in a simplified way. Their chemical mechanisms take major soot growth species such as acetylene or even aromatics into account. The flamelet approach, for example, where species concentrations are linked to scalars such as mixture fraction, allows reasonable

predictions in non-premixed flames [11–14]. However, in combustion systems where premixing effects and strong turbulence-chemistry interactions are involved the applicability of this approach is limited.

More analytical but computationally expensive methods use detailed finite-rate chemistry for molecular species, while soot particles are lumped in one way or another. For the interface between gas phase and soot different techniques exist. While in simplified models soot is directly formed from acetylene [11,12,15–17], more detailed models use aromatic species such as benzene [18,19], naphthalene [20], or even pyrene [21,22].

One of the most basic ways of lumping soot is found in two equation soot models, where soot is represented by two variables only, e.g. soot mass fraction and soot number density [16,19,23–26]. Although these models contain no information about the soot size distribution, they allow predictions in soot volume fraction, number density, and mean particle size. Depending on the underlying chemical mechanism, promising CFD results have been achieved in the past with these models even for complex 3D configurations [27,28].

A more detailed lumping technique is the method of moments [15,29,30]. Here the soot size distribution is described by its moments, for which transport equations are solved. Although the correct description of the physical size distribution function includes an infinite number of moments, the moments of most interest are usually only those of low order [31–33]. Moreover, assuming a logarithmic size distribution, already the first three moments suffice for a complete description [34]. But this assumption is not generally valid [35–39]. Instead, a priori information about the

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### Nomenclature

$A$	surface area	$T$	temperature
$c$	stoichiometric coefficient	$T_a$	activation temperature
$C$	concentration	$u$	axial velocity
$d$	diameter	$Y$	mass fraction
$fv$	soot volume fraction	$\alpha$	exponent of Arrhenius reaction rate
$k$	Arrhenius reaction rate	$\beta$	collision frequency
$k_0$	constant of Arrhenius reaction rate	$\eta$	oxidation efficiency
$k_B$	Boltzmann constant	$\phi$	premixing ratio
$m$	mass	$\gamma$	collision efficiency
$M$	molecular mass	$v$	stoich. coeff.: forward (') and backward (")
$N_a$	Avogadro constant	$\rho$	density
$N_r$	number of reactions		
$N_{sp}$	number of species		
$O'$	reaction order of educt	<i>sub- and superscripts</i>	
$S_x$	chemical source term of species $x$	$i, j, k$	general index for sections
$S_r$	chemical source from reaction $r$	$s$	soot
		$\alpha, \beta$	general species index

shape of the distribution function is needed in order to determine the required number of moments.

One of the most detailed lumping techniques is the sectional approach [20–22,40,41]. Here soot particles are lumped into sections, which are then treated as “virtual” species with averaged properties. The great advantage of this technique is that any kind of size distribution can be captured and that different sized particles may have different properties like reactivity, for example. Furthermore, sections can be treated in analogy to real species in many regards. Especially in combination with other models, such as heat radiation or turbulence chemistry interaction, this analogy is a great advantage as far as the effort of implementation is concerned. However, such methods are mostly applied to rather simple test cases like laminar flames because the involved computational effort is usually relatively high.

Particle tracking techniques [35,42], where soot particles are not lumped by properties but by number, may reach an even higher degree of detail depending on the number of stochastic particles used.

The model described in this work features a sectional approach, so that soot size distributions can be predicted at any point of the flame without a priori knowledge of the shape of the distribution function. In order to reduce the computational effort, PAH molecules are also captured by a sectional approach. Furthermore, PAH and soot sections with radical branches are not treated separately, resulting in a skeletal global reaction formulation.

The model is applied to a variety of fuels and flames showing its capability to predict soot with good accuracy at acceptable computational cost without the need of any tuning. With respect to the combination of accuracy and efficiency, this model bridges the gap between very detailed and computationally low cost models. In this regard, it is not the purpose of this work to show higher accuracy than very detailed soot models when applied to laminar flames but to significantly reduce the computational cost in order to be able to calculate more complex test cases.

## 2. Numerical model

All presented results have been obtained by means of steady state simulations using the DLR in-house Code THETA – an incompressible flow solver for finite-volume grids, which has been optimized for combustion problems. It features a multigrid algorithm, dual grid technique, a stiff-chemistry solver, and parallelization via domain decomposition.

The soot model consist of three sub models describing molecular gas phase species, polycyclic aromatic hydrocarbons (PAHs), and soot. In order to improve the compatibility with other models and to reduce the computational cost, the chemical source term is represented in a global Arrhenius like formulation in all sub models

$$S_x = M_x \sum_{r=1}^{N_r} (v''_{x,r} - v'_{x,r}) S_r. \quad (1)$$

with

$$S_r = k_0 T^\alpha \exp(-T_a/T) \prod_{\beta=1}^{N_{sp}} C_\beta^{O'_{\beta,r}}. \quad (2)$$

All sub models respect mass conservation also regarding their interaction.

### 2.1. Gas phase chemistry

The chemical kinetic mechanism of the gas phase consists of the base mechanism mentioned in [43], which has mainly been derived from the works by Slavinskaya et al. [44,45]. It considers molecular species up to the first aromatic ring including benzene, toluene, and their radicals. For the kerosene surrogate flame, consisting of volumetric 12% toluene (C<sub>7</sub>H<sub>8</sub>), 23% isooctane (C<sub>8</sub>H<sub>18</sub>), and 65% *n*-decane (C<sub>10</sub>H<sub>22</sub>), a sub mechanism is added, which has been derived from another work by Slavinskaya et al. [46], where this surrogate has first been proposed.

The base mechanism as well as the kerosene surrogate sub mechanisms have already extensively been validated in the past by different authors [43,47,46]. The conjunction of the two mechanisms has been validated for ignition delay with respect to Jet A-1 fuel.

### 2.2. PAH chemistry

All aromatic molecules with a molecular mass between 100 and 800 g/mol are considered PAHs (Polycyclic Aromatic Hydrocarbons). They are represented by three logarithmically spaced PAH sections with a scaling factor of two as demonstrated in Fig. 1. For reasons of computational efficiency, radical PAHs are not considered separately but a global formulation is chosen.

During the current work the intra sectional mass distribution function, describing the mass distribution within one PAH section,

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