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A simplified model for soot formation and oxidation in CFD simulation of non-premixed hydrocarbon flames

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Abstract

A new approach to modeling soot formation and oxidation in non-premixed hydrocarbon flames has been developed and subjected to an initial calibration. The model considers only the phenomena essential for obtaining sufficiently accurate predictions of soot concentrations to make CFD calculations of fire radiation feasible in an engineering context. It is generalized to multiple fuels by relating the peak soot formation rate to a fuel's laminar smoke point height, an empirical measure of relative sooting propensity, and applying simple scaling relationships to account for differences in fuel stoichiometry. Soot oxidation is modeled as a surface area independent process because it is controlled by the diffusion of molecular oxygen into the zone of active soot oxidation rather than being limited by reaction of OH· radicals with the available soot surface area. The soot model is embedded within a modified version of NIST's Fire Dynamics Simulator and used for a comparison of predicted and measured temperatures, soot volume fractions, and velocities in laminar ethylene, propylene, and propane flames. The

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Nomenclature

A_f	flame surface area (m^2)
B_R	soot constant (dimensionless)
c_p	constant-pressure specific heat (kJ/kg K)
C_2	Planck's second constant (m K)
$C_{\kappa R}$	constant relating f_v and T to κ_s [$(m\,K)^{-1}$]
D	diffusivity (m^2/s)
f	mixture fraction soot formation function ($kg/m^3\,s$)
f_v	soot volume fraction (m^3 soot/m^3 mixture)
g	temperature soot oxidation function (dimensionless)
$\boldsymbol{g}$	acceleration of gravity vector (m/s^2)
h	sensible enthalpy (kJ/kg)
h°	enthalpy of formation (kJ/kg)
h_T	total enthalpy ($h + h^\circ$) (kJ/kg)
ΔH_c	heat of combustion (kJ/kg)
k	thermal conductivity (W/m K)
ℓ_s	laminar smoke point height (m)
ℓ_f	flame height (m)
L	pathlength, mean bean length (m)
M	molecular weight of a single species (kg/mol)
$\overline{M}$	mean molecular weight of a gas mixture; $\overline{M} = (\Sigma Y_i/M_i)^{-1}$ (kg/mol)
N	soot number density (particles/m^3)
p°	reference pressure (101,300 Pa)
p_0	background pressure (Pa)
Pr	Prandtl number (dimensionless)
$\dot{Q}$	heat release rate (W or kW)
Q	volumetric flow rate (cm^3/s)
R	universal gas constant (8.314 J/mol K)
S	Stoichiometric oxidant to fuel mass ratio (dimensionless)
Sc	Schmidt number (dimensionless)
T	temperature (K)
$\boldsymbol{u}$	velocity vector (m/s)
V	velocity (m/s)
X	mole fraction (dimensionless)
Y	mass fraction (dimensionless)
Z	mixture fraction (dimensionless)

Greek symbols

κ	emission/absorption coefficient (m^{-1})
λ	wavelength (μm)
μ	viscosity (kg/m s)
ν	Stoichiometric coefficient (dimensionless)