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A fully coupled fluid/solid model for open air combustion of horizontally-oriented PMMA samples

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ABSTRACT

The predictive capability of computational fluid dynamics (CFD) fire models is highly dependent on the accuracy with which the source term due to fuel pyrolysis can be determined. The pyrolysis rate is a key parameter controlling fire behavior, which in turn drives the heat feedback from the flame to the fuel surface. The main objectives of the present study were twofold. First, an in-depth pyrolysis model of a semi-transparent solid fuel (here, clear poly-methyl-methacrylate or PMMA) with in-depth radiation and a moving gas/solid interface was coupled with a CFD code which included turbulence, combustion and radiation for the gas phase. Second, experiments were conducted in order to validate coupled model results. A combined genetic algorithm/pyrolysis model was used with Cone Calorimeter data from a non-flaming pyrolysis experiment to estimate a unique set of kinetic parameters for PMMA pyrolysis. Flaming experiments were conducted on square slabs of PMMA with side dimensions of 10, 20 and 40 cm. From data collected at the center of the slabs, it was found that i) for any sample size, the experimental regression rate remains almost constant with time, with average values of 5.8, 8.6 and 10.9 $\mu m\, s^{-1}$ for the PMMA slabs with side lengths of 10, 20 and 40 cm respectively, and ii) although the radiative and total heat transfers increase significantly with sample size, the radiative contribution to the total heat flux remains almost constant (∼80%). Coupled model results show a fairly good agreement with the literature and with current measurements of the heat fluxes, gas temperature and regressing surface rate at the center of the slabs. Predicted flame heights based on a threshold temperature criterion were found to be close to those deduced from the correlation of Heskestad. However, discrepancies between predicted and measured total pyrolysis rates are observed, which result from the underestimation of the flame heat feedback at the edges of the slab, as confirmed by the comparison between predicted and observed topography of burned samples.

1. Introduction

One of the major issues in fire safety studies is the development of predictive numerical tools for the characterization of fire behavior in terms of heat release rate, wall heat fluxes and temperature levels. “Predictive” means that model inputs must be independent of the event which is to be predicted. Fuel parameters and ventilation conditions meet this requirement, while the pyrolysis rate does not. Indeed, fire behavior depends on the rate at which the fuel can vaporize, which in turn is highly dependent on the heat feedback from the flame to the fuel surface. The feedback loop, or in other words the coupling between the condensed and gas phases, must be described accurately in order to increase the predictive capability of computational fluid dynamics (CFD) fire models.

Regarding thermal degradation of semi-transparent materials, various pyrolysis models have been developed ([1–7], to name but a few). They differ mainly with regard either to the physics involved, depending on whether pyrolysis occurs only at the sample surface (ablation or surface pyrolysis models) or inside the solid (volume pyrolysis models), or to the assumptions used regarding in-depth radiation or radiative fuel properties. Only a few of them take into account spectral variations of in-depth radiation absorption [1,3] and polymer surface regression [2,6,7]. A more detailed description of pyrolysis models is presented by Pizzo et al. [2].

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Nomenclature

A_b	surface of burning sample (m^2)
A_s	pre-exponential Arrhenius coefficient (s^{-1})
c_p	specific heat at constant pressure ($J\,kg^{-1}\,K^{-1}$)
D	diffusion coefficient ($m^2\,s^{-1}$)
$E_{b\nu}$	spectral blackbody emissive power ($W\,s\,m^{-2}$)
E_s	activation energy ($J\,mol^{-1}$)
G	incident radiation ($W\,m^{-2}$)
$\boldsymbol{g}$	gravitational field ($m\,s^{-2}$)
H_f	flame height (m)
H_g	heat of gasification ($J\,kg^{-1}$)
h	enthalpy ($J\,kg^{-1}$), heat exchange coefficient ($W\,m^{-2}\,K^{-1}$)
I, $\boldsymbol{I}$	radiative intensity ($W\,m^{-2}$), unit tensor
k	turbulent kinetic energy (TKE) ($m^2\,s^{-2}$)
L	initial thickness of slab (m)
$\dot{m}''_s$	local pyrolyzate mass flux ($kg\,s^{-1}\,m^{-2}$)
$\dot{m}'''_s$	generation rate of pyrolysis products per unit sample volume ($kg\,s^{-1}\,m^{-3}$)
n	refractive index
Pr	Prandtl number
p	pressure (Pa)
q, $\boldsymbol{q}$	heat flux, heat flux vector ($W\,m^{-2}$)
$\dot{Q}'''$	heat production per unit volume ($W\,m^{-3}$)
$\boldsymbol{r}$	position vector (m)
R_u	universal gas constant ($J\,mol^{-1}\,K^{-1}$)
Re	Reynolds number
s	stoichiometric oxygen-to-fuel weight ratio
T	temperature (K)
t	time (s)
u_x	gas velocity component in the x-direction ($m\,s^{-1}$)
u_{reg}	regression velocity of the slab surface ($m\,s^{-1}$)
$\boldsymbol{u}$	gas velocity ($m\,s^{-1}$)
W_k	molecular weight of gaseous species k ($kg\,mol^{-1}$)
x	space coordinate along the slab thickness (m)
Y	mass fraction
Z	mixture fraction
Δh_c	effective heat of combustion ($J\,kg^{-1}$)
Δh_f^0	standard heat of formation ($J\,kg^{-1}$)
ε	dissipation of TKE ($m^2\,s^{-3}$), emissivity
κ	absorption coefficient (m^{-1})
λ	conductivity ($W\,m^{-1}\,K^{-1}$)
μ	viscosity ($kg\,m^{-1}\,s^{-1}$)
ν	frequency (Hz)
ρ	intrinsic density ($kg\,m^{-3}$)
σ	Stefan–Boltzmann constant ($\sigma = 5.67 \times 10^{-8}\,W\,m^{-2}\,K^{-4}$)
σ_k, σ_t, σ_ε	turbulent Prandtl/Schmidt numbers
$\boldsymbol{\Omega}$	unit vector in a given direction

Subscripts

0	initial
b	blackbody
ch	chemical
$cond$	conduction
$conv$	convection
ext	external
e	effective
F	fuel
g	gas phase
I	gas/solid interface
k	gaseous species k
L	lower face
rad	radiative
reg	regressing surface
s	solid phase
$soot$	soot
t	turbulent
η	wavenumber
∞	ambient

Superscripts

+	upward direction (positive x)
−	downward direction (negative x)

Acronyms

CFD	Computational fluid dynamics
DNS	Direct numerical simulation
EDC	Eddy dissipation concept
LES	Large eddy simulation
MLR	Mass loss rate
MMA	Methyl methacrylate
NIST	National Institute of Standards and Technology
PMMA	Polymethyl methacrylate
RANS	Reynolds averaged Navier–Stokes
TKE	Turbulent kinetic energy

While many experimental studies have been performed on the burning of vertically-oriented or inclined slabs of PMMA (see for example [2]), their burning in the horizontal configuration has been the subject of little investigation. In [7], Linteris and co-workers burned $10 \times 10 \times 2.54\,cm^3$ black PMMA samples in the cone calorimeter at imposed radiant heat fluxes from 0 to $75\,kW\,m^{-2}$. The data available from the experiments were flame visual images, heat release rate and mass loss rate as a function of time. The sample final mass and the surface topography of the burned samples were also recorded. They observed that the samples did not burn uniformly over their exposed surface, and that the effect was more pronounced at the lower heat flux, especially at $0\,kW\,m^{-2}$ (as is the case here for flaming experiments). They used the burned sample thickness as a function of position over the sample surface to estimate the burning rate variations, and thus the total net heat flux, over the surface of the samples. In their study, on the effect of oxygen on flame heat flux in horizontal and vertical orientations, Beaulieu and Dembsey [8] used embedded heat flux gages at the pyrolyzing surface of black PMMA samples to measure the total heat flux, as well as the radiative and convective components. They also measured the flame height and flame temperature. Results from small-scale experiments using 10.2 cm diameter samples, in the horizontal orientation and in atmospheric oxygen concentration (20.9%), were: a steady state flame heat flux of $20 \pm 3\,kW\,m^{-2}$, with a radiative part of $12 \pm 3\,kW\,m^{-2}$ and a convective part of $8 \pm 3\,kW\,m^{-2}$, a mass loss flux of $5.8 \pm 1\,g\,m^{-2}\,s^{-1}$, a flame height of 17.8 ± 0.64 cm, and a flame temperature of 1184 ± 100 K. Other results were obtained for large-scale samples, ranging from 17.8 to 122 cm in diameter, showing no scalability for the flame heat flux. A total heat flux of $31 \pm 3\,kW\,m^{-2}$ and a mass loss flux of $7.7 \pm 1\,g\,m^{-2}\,s^{-1}$ were recorded for the 17.8 cm sample. It is noteworthy that, as observed by Linteris et al. [7], the total heat flux was found to vary considerably across the diameter of the sample with higher values near the center and lower values near the edge. Pure pyrolysis (non-flaming) experiments on $10 \times 10 \times 3\,cm^3$ horizontally-oriented clear PMMA samples were conducted by Pizzo et al. [2], where the slabs were exposed to radiant heat flux levels of 14 and $18\,kW\,m^{-2}$ from a cone calorimeter. They reported data on the time evolution of the regressing surface at the center of the slab and temperatures at two depths within the solid. Those obtained at $18\,kW\,m^{-2}$ are