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Upward Flame Spread Simulations by Coupling an Enthalpy-Based Pyrolysis Model with CFD

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ABSTRACT

In simulations of developing fires in enclosures, a correct prediction of flame spread is crucial in the prediction of the fire growth rate. The simulation of this phenomenon requires two different kinds of solvers: one that deals with the solid phase, to determine the thermal degradation and volatile release (pyrolysis); a second one that calculates the combustion process in the flame formed by mixing of the volatiles with the ambient air. The processes in the solid and the gas phase require proper modeling. Moreover, an adequate coupling strategy at the interface between the solid and the gas phase is an important point of interest. The paper focuses on a method to successfully combine these two types of calculations. Two types of flame spread (upward and downward) demonstrate the possibilities of this approach. We conclude that the coupling between the two phases works fine, providing a mechanism of simulating flame spread with two different codes. It is found, however, that the prediction of the gas phase requires finer grids or more accurate models than used in this study, to obtain quantitatively better results, particularly in case of upward flame spread.

KEYWORDS: pyrolysis, flame spread, CFD.

NOMENCLATURE LISTING

A	pre-exponential factor (m^3/kgs)	Greek	
c_p	specific heat (J/kgK)	ε	turbulent dissipation rate (m^2/s^3)
f	stoichiometric O/F ratio	ϕ	generic variable
h	specific enthalpy (J/kg)	Γ	generic diffusivity (m^2/s)
k	thermal conductivity (W/mK)	ν	thermal diffusivity (m^2/s)
k	turbulent kinetic energy (m^2/s^2)	ρ	density (kg/m^3)
m''	mass flux ($\text{kg/m}^2\text{s}$)	Subscripts	
M	molecular weight (kg/kmol)	act	activation
p	pressure (Pa)	c	char
q''	heat flux (W/m^2)	cond	conductive
Q_{pyr}	heat of pyrolysis (J/kg)	conv	convective
S	generic source term	f	front
t	time (s)	F	fuel
T	temperature (K)	in	incident
u	velocity (m/s)	pyr	pyrolysis (gas)

V	volume (m ³)	s	surface
x	space coordinate (m)	v	virgin
Y	mass fraction	0	ambient

INTRODUCTION

In simulations of developing fires in enclosures, it is crucial to correctly predict the rate of flame spread over combustible surfaces. This phenomenon involves chemical reactions in the solid and the gas phase. In the solid phase, upon external heat input, the virgin material degrades at higher temperatures, releasing combustible volatiles. This *pyrolysis* process thus consumes an amount of heat and generates an amount of fuel. In the gas phase, these volatiles mix with the ambient air and a combustion reaction takes place, with the formation of a flame. This process thus provides an amount of heat and consumes an amount of fuel. The spread of a flame is controlled by the timescale of the mechanism described above. In order to correctly predict flame spread, both the solid and the gas phase require proper modeling. Moreover, an adequate coupling strategy at the interface between the solid and the gas phase is an important point of interest. In the present paper, we focus on the coupling strategy and describe the models invoked. It will appear that better models are needed if one wants to quantitatively study upward flame spread phenomena.

Two types of flame spread are intensively studied in literature. The driving mechanism is in both cases the heat input from the flame to the solid. In the case of upward flame spread, the heat transfer from the flame to the virgin material happens primarily by radiation. A correct prediction of flame height is therefore essential for the correct prediction of flame spread. The flame height prediction depends on the kinetics of the chemical reaction considered and to a greater extent, especially in the case of a turbulent flow, on the (turbulent) mixing between fuel and oxidizer. In the case of downward flame spread, the heat transfer between the flame and the virgin solid is established by gas phase conduction. Since the virgin material does not really *see* the flame, radiation can be neglected (cf. [1]).

From the above, it can be expected that downward flame spread simulations are not that dependent on the models (radiation, soot) invoked in the gas phase. Therefore, particularly in laminar flows, they suit as the ideal test cases for checking the quality of the solid phase model and the coupling between the two phases. In practice, downward flame spread is not encountered that often and is far less severe in terms of fire hazards than upward flame spread, which happens a lot faster. Therefore, the future focus is on upward flame spread simulations. In this paper, we also show that the coupling strategy works fine for upward flame spread simulations, but, because of the gas phase models, the flame height is not correctly predicted. More precisely, as will be demonstrated further down, it is the position of the flame's leading edge that is wrongly predicted.

Upward flame spread simulations have mostly been performed with PMMA as solid material (e.g. [2]). Its properties are well known and much experimental work is available to validate the results. PMMA is categorized as a non-charring material: during the pyrolysis process, all virgin material transforms into volatiles. A charring

material (pine wood for example) does not transform completely in volatiles, but leaves behind char, allowing for higher surface temperatures. The solid phase model has the property that it is a unified code that can handle both charring and non-charring materials. Upward flame spread simulations are performed on both types of materials.

The focus of this paper is to show that the coupling strategy between the gas phase and the solid phase is able to simulate upward and downward flame spread for charring and non-charring materials. With respect hereto, especially in upward flame spread scenarios, a comparison with experimental data is not made. This will be the topic of future research.

SOLID PHASE MODEL

The solid phase is described by an enthalpy model. This means that one transport equation for static enthalpy is solved:

$$\frac{\partial \rho h}{\partial t} = - \frac{\partial \dot{q}_{conv}''}{\partial x} - \frac{\partial \dot{q}_{cond}''}{\partial x} \quad (1)$$

The enthalpy level changes because conduction takes place in the material and an amount of enthalpy is convected outwards with the volatile release. Conduction can be described in all directions by Fourier's law, whereas the model assumes that the transport of gases is perpendicular to the exposed surface. Pyrolysis is described as a phase change at the pyrolysis temperature T_{pyr} and requires an amount of heat Q_{pyr} per mass unit of volatiles produced.

Since we use a discretization of Eq. 1 on a fixed mesh, the temperature field is represented as a piecewise linear function (linear from node to node or from node to pyrolysis front location). If a piecewise constant temperature representation were to be used, as is standard in a finite volume formulation, the mass flow rate of volatiles would become discontinuous, which is not favorable for coupling with a CFD-code.

From the enthalpy, the temperature field and pyrolysis front location are reconstructed by expressing that

$$\rho h V = \int_{cell\ volume} \rho(x) h(T(x)) . dx \quad (2)$$

and

$$(\rho_v - \rho_c) \frac{dx_{f,pyr}}{dt} Q_{pyr} = -k_c \left. \frac{\partial T}{\partial x} \right|_c + k_v \left. \frac{\partial T}{\partial x} \right|_v \quad (3)$$

Expression (3) states that the pyrolysis front is allowed to move, if more heat is provided than goes through by conduction. In Eq. 2, $h(T)$ consists of the sensible

enthalpy and the formation enthalpy of virgin/char material. Full details on the solution procedure can be found in [3,4].

Generally speaking, the solid phase pyrolysis code can be seen as a black box solver (S), providing a solution for the solid phase in the form

$$(\dot{\mathbf{m}}''_{pyr}, \mathbf{T}_s) = S(\dot{\mathbf{q}}''_{in}) \quad (4)$$

with $\dot{\mathbf{m}}''_{pyr} = (\rho_c - \rho_v) d\mathbf{x}_{f,pyr} / dt$ the mass flow rate vector at the gas-solid interface and \mathbf{T}_s the surface temperature vector. $\dot{\mathbf{q}}''_{in}$ is the incident heat flux vector, coming from the flame. Note that, for non-charring materials, the surface temperature cannot reach values higher than T_{pyr} . Also, in that case, $-k_c \partial T / \partial x|_c$ is replaced by \dot{q}''_{in} , since no char exists.

GAS PHASE MODEL

The gas phase is simulated with the commercial package Ansys Fluent. Conservation equations of mass, species mass fractions, momentum and energy are solved. In case of turbulent flows, two extra equations are solved (conservation of turbulent kinetic energy and turbulent dissipation rate). We describe some specific features of the sub models below.

Generally speaking, the gas phase CFD code can be seen as a black box solver (G), providing a solution for the gas phase in the form

$$(\dot{\mathbf{q}}''_{in}) = G(\dot{\mathbf{m}}''_{pyr}, \mathbf{T}_s). \quad (5)$$

Conservation equations

In general, the conservation equations of mass, momentum and energy take the form

$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho u_i \phi}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\rho \Gamma \frac{\partial \phi}{\partial x_i} \right) + S \quad (6)$$

with ϕ equal to $\{1, u_x, u_y, h, Y_F, Y_{O_2}, Y_{CO_2}, Y_{H_2O}\}$. The diffusivities are calculated as a function of the mixture, with constant thermal conductivity $k=0.0454 \text{ W/m}^2\text{K}$ and constant species diffusivity $D=2.88e-5 \text{ m}^2/\text{s}$. Specific heat is calculated with a mixing law, and each component uses polynomial functions for specific heat as a function of temperature. Viscosity is calculated using Sutherland's Law for the different species.

If MMA is considered as a fuel, the same properties are given as air at that temperature, apart from the specific heat and the density. The specific heat of MMA is considered constant $c_p=1183 \text{ J/kgK}$. All appearing species are treated as an incompressible ideal gas, which means that density is given by

$$\rho_\alpha = \frac{p_0 M_\alpha}{RT} \quad (7)$$

Source terms S include chemical source terms in species and energy equation and, if radiation is taken into account, a radiant heat source in the energy equation. In the momentum equation, gravity acts as a source term as well.

Chemical reactions

Chemistry is treated as a single-step reaction, depending on the fuel:



The chemical source term in laminar flow calculation is determined by the Arrhenius expression

$$S_{MMA} = -A\rho^2 Y_{MMA} Y_{O_2} \exp(T_{act}/T) \quad (9)$$

with pre-exponential factor $A=5.928e+9 \text{ m}^3/\text{kgs}$ and activation temperature $T_{act} = 1.07e+4 \text{ K}$. The heat of combustion of MMA is taken as $\Delta h=25.9 \text{ MJ/kg}$ [5].

In turbulent flows, the reaction is not controlled by the chemical kinetics. It rather is the mixing between fuel and oxidizer that controls the reaction rate. We use the Eddy Break-Up model to determine the reaction as a function of the turbulent mixing time scale:

$$S_{MMA} = -4\rho \frac{k}{\varepsilon} \min(Y_{MMA}, Y_{O_2} / f) \quad (10)$$

with $f=1.92$ the stoichiometric oxygen to fuel mass ratio. In case of propane as a fuel, Eq. 10 remains similar, with a different value for f .

Turbulence

Turbulence is modeled here with the RNG k - ε model. We checked that the obtained results were similar to results obtained with the standard k - ε model. The turbulence model includes two extra transport equations, for the turbulent kinetic energy k and the turbulent dissipation rate ε . Extra terms are introduced in the equations to include the effect of buoyancy on turbulence generation. At the wall, enhanced wall treatment was used to model the boundary layer. This wall treatment predicts correct results for a broad range of normalized distances of the first cell to the wall.

Radiation

Radiation requires solving the radiative transfer equation (RTE). Here, we adopt the Discrete Ordinates Method (DOM), which discretizes the RTE in a number of directions (4 θ -divisions, 2 ϕ -divisions). The gases are treated as grey gases, meaning that the spectral dependency is neglected.

Numerics

The conservation equations are discretized using first-order upwind for the convective terms, second-order central for the diffusive terms and backward Eulerian discretization for the time derivatives. A SIMPLE procedure is used to couple the equations.

COUPLING BETWEEN SOLID AND GAS PHASE

The coupling between the solid and gas phase solvers is done by solving the implicit system (4-5) with Gauss-Seidel iterations. More precisely, this means:

$$\begin{aligned}(\dot{\mathbf{q}}_{in}^{\prime\prime})^{n+1,k+1} &= G(\dot{\mathbf{m}}_{pyr}^{\prime\prime}, \mathbf{T}_s)^{n+1,k} \\ (\dot{\mathbf{m}}_{pyr}^{\prime\prime}, \mathbf{T}_s)^{n+1,k+1} &= S(\dot{\mathbf{q}}_{in}^{\prime\prime})^{n+1,k+1}\end{aligned}\tag{11}$$

The loop is considered to be converged if

$$\|(\dot{\mathbf{m}}_{pyr}^{\prime\prime}, \mathbf{T}_s)^{n+1,k+1} - (\dot{\mathbf{m}}_{pyr}^{\prime\prime}, \mathbf{T}_s)^{n+1,k}\| < 0.01\tag{12}$$

where $\|\cdot\|$ means the L_2 -norm of the vector.

IGNITION AND DOWNWARD FLAME SPREAD

First, we simulate a laminar test case. A plate of PMMA, isolated at one side, is exposed to an external radiative heat flux. The incoming heat causes the material to pyrolyse. In the gas phase, a flame is not readily established once pyrolysis starts. It takes some time to ignite. The ignition delay time not only depends on the Arrhenius parameters of the reaction, but also on the behavior of the flow to obtain favorable circumstances for reaction (high temperature at a near stoichiometric mixture). Once a flame appears, it spreads in two directions. In this case, we are not interested in the upward flame spread behavior. Therefore, the radiation model was switched off. Focusing on the downward flame spread, a flame spread velocity could be obtained numerically.

Consider a gas phase calculation domain of 2 cm by 8 cm. At the bottom boundary, a constant uniform velocity is imposed. The top boundary is defined as a pressure-outlet. At the left boundary, symmetry conditions apply. The domain has a uniform mesh with grid size 0.4 mm. The right boundary is the solid PMMA material, which has a thickness of 0.82 cm. The solid grid has a mesh size in y-direction equal to the

gas phase. In x-direction, the solid is divided into 10 cells. The time step is taken equal to 0.01 seconds.

The external radiation is imposed at 2 cm below the top corner and has a Gaussian distribution with a width of 2 cm and a peak value of 50 kW/m².

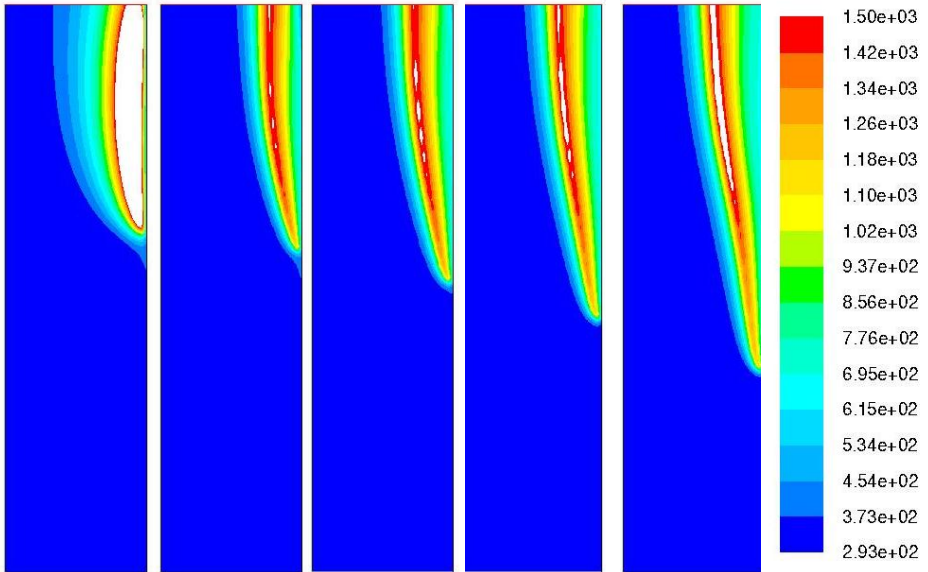


Figure 1. Downward flame spread (0.3 m/s, 293 K). Contours of temperature at 5.6 s, 10 s, 20 s, 40 s, 80 s.

For an inlet velocity of 0.3 m/s and an inlet temperature of 293 K, ignition takes place 5.6 seconds after radiation is switched on. A relatively big flame with high flame temperatures suddenly appears at the moment of ignition. From then on, the front moves slowly downwards at a speed of 0.08 mm/s.

The given numerical results are only preliminary. A finer, non-uniform grid and higher-order discretizations will favor results that are more in line with e.g. [1]. Results for ignition delay times at different inlet temperatures and velocities are summarized in Table 1. The trend that ignition time increases with increasing velocity and decreasing temperature is confirmed also numerically. To illustrate that the phenomenon of downward flame spread is well captured, Fig. 1 shows contour plots of the temperature field at certain moments.

	0.7 m/s	0.3 m/s
293 K	5.9 s	5.6 s
340 K	4.3 s	4.1 s

Table 1. Ignition delay times as a function of inlet velocity and temperature.

UPWARD FLAME SPREAD

The upward flame spread test cases are simulated using a turbulence model. In this case, it is also important to take radiation heat fluxes into account.

In a first test case, we consider a charring solid of 3 mm thick and 10 cm high. This solid is exposed to an external constant heat flux of 40 kW/m^2 up to 6 mm high from the bottom. Initially, the entire set-up is at 295 K. The CFD-domain is 20 cm wide and 30 cm high. The solid interface is at the right boundary, which is composed of three pieces: the bottom and top 10 cm are treated as an adiabatic wall; the pyrolysing solid is placed in the middle 10 cm. The bottom, left and top boundaries of the CFD-domain are considered open. A pressure outlet boundary condition is applied, imposing a linearly varying pressure to incorporate the buoyancy. Where the pressure-outlet is in fact an inlet, the gas enters the domain normal to the boundary, having a turbulence intensity of 10% and a length scale based on a hydraulic diameter of 5 cm. A uniform Cartesian grid with spacing 2 mm is used in the gas phase. In the solid phase, the vertical grid spacing is 2 mm as well, resulting in a continuous grid at the interface. The grid spacing in horizontal direction is smaller (0.5 mm). The time step is equal to 0.1 s.

In the solid phase, we use the properties of white pine [6]: $\rho_v=380.0 \text{ kg/m}^3$, $\rho_c =76.0 \text{ kg/m}^3$, $c_v=1196.0 \text{ J/kgK}$, $c_c =986.8 \text{ J/kgK}$, $k_v =0.36 \text{ W/mK}$, $k_c =0.2 \text{ W/mK}$, $Q_{\text{pyr}}=1.2 \text{ MJ/kg}$, $T_{\text{pyr}}=658 \text{ K}$. The volatile gases are modeled as propane, with default properties.

Although the results differ somewhat from experimental observations, the coupling algorithm can be assessed because a flame appears, giving feedback to the solid material. Figure 2 shows the flame at $t=50 \text{ s}$. Contours of temperature indicate that it takes some time for the fuel, generated at the surface exposed to external heat flux, to mix with the oxygen and react. Because of this artifact, a 'dead zone' of unburnt solid appears (Fig. 3).

A second test case consists of a non-charring material. The plate of pine wood in the above case is replaced by a plate of PMMA of 10 cm by 2.5 cm (similar to [2]). The horizontal grid spacing in the solid is 2.5 mm. An external heat flux of 50 kW/m^2 is applied at the bottom. A typical figure is provided in Fig. 4. It is clear that the flame height is predicted far too long. More importantly, the leading edge of the flame appears too high, causing in this case no other material to pyrolyse than the part receiving the external heat flux. Further research is needed here. A major point of attention will be the grid extent and resolution in the gas phase.

In order to completely validate the numerical results, we mention that a correct choice of models for radiation and soot is important. However, these are not responsible for the incorrect prediction of the flame's leading edge.

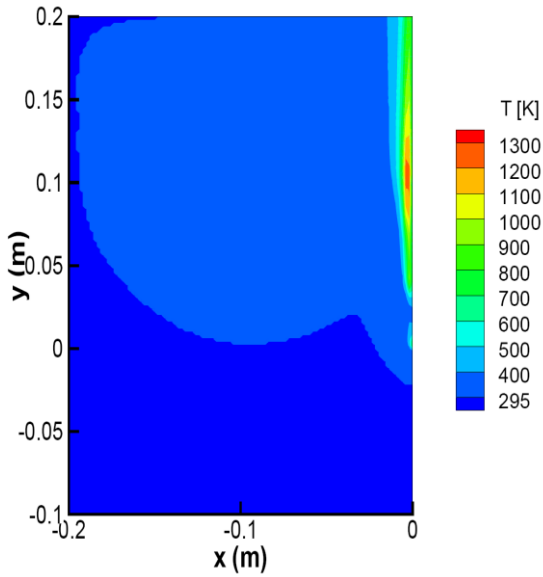


Figure 2. Upward flame spread. Contours of temperature at 50 s.

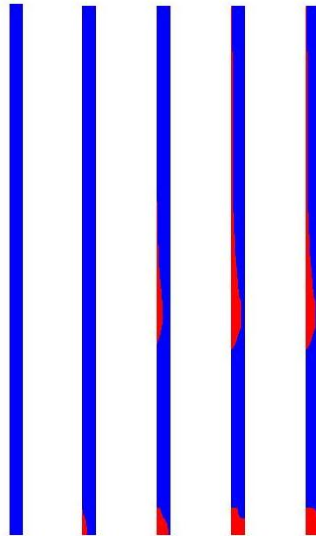


Figure 3. Char/virgin material distribution inside the solid at $t=0$ s, 50 s, 100 s, 150 s and 200 s.

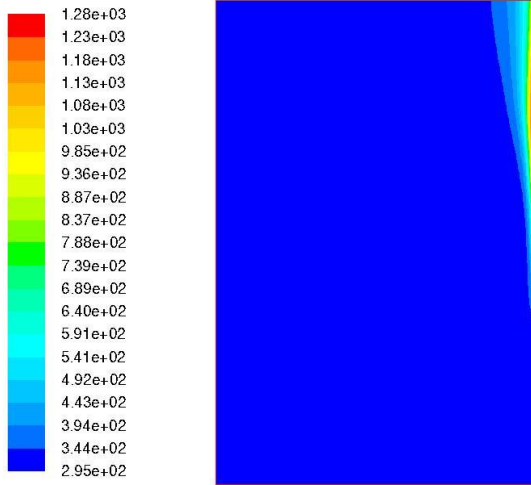


Figure 4. Upward flame spread for non-charring solid. Temperature contours reveal that the flame is predicted too high.

CONCLUSION

In this paper, we described how the coupling between the gas phase and the solid phase is dealt with for the prediction of upward or downward flame spread. We chose to use two different simulation packages: a self-written code for the solid pyrolysis and a commercially available package for the gas phase combustion. The pyrolysis code has the advantage that it uses a fixed mesh and can deal with both charring and non-charring materials. The use of a commercially available package has the advantage that it is well documented and organized and that it consists of many models and material properties. The coupling is stabilized with Gauss-Seidel iterations.

Two types of flame spread demonstrate the possibilities of this approach. The laminar downward flame spread simulation predicted good results, although some grid refinement studies are needed to be conclusive. The upward flame spread simulations were not satisfactory. The flame position, particularly the position of the leading edge of the flame, was wrongly predicted, causing the entire simulation result to be quantitatively incorrect. Better gas predictions are needed through grid refinements and extensions or even model changes. It was found, however, that the coupling between the two phases works fine, providing a mechanism of simulating flame spread with two different codes.

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