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Multiphase CFD Model of Wildland Fire Initiation and Spread

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Introduction

Wildland fires are extremely complex and destructive phenomena and their behavior depends on the state of vegetation, meteorological conditions and ground terrain. Experimental studies of wildfire behavior are expensive and challenging tasks. This makes the development of robust and accurate models of wildfire behavior an extremely important activity. There are various types of wildland fire models: statistical, empirical, semi-empirical and physics-based. This paper is devoted to the development and validation of a physics-based multiphase Computational Fluid Dynamics (CFD) model of wildland fire initiation and spread and smoke dispersion.

Over the past 30 years, a significant progress in the development of physics-based wildfire models has been achieved. In particular, fully physical multiphase wildfire models have been developed by Grishin *et al.* (1986), Grishin 1997, Porterie *et al.* 1998, 2000, Morvan and Dupuy 2001, Mell *et al.* 2007. According to a review by Morvan 2011, one of the most advanced models of this type is the three-dimensional (3D) model, WFDS (Wildland-urban interface Fire Dynamics Simulator), developed by the National Institute of Standards and Technology (NIST) and the U.S. Forest Service. The validation of WFDS is ongoing: its recent validation was conducted by Menage *et al.* 2012 with using the experimental data of Mendes-Lopes *et al.* 2003 on surface fire propagation in a bed of *Pinus pinaster* needles. The same set of data was also used by Porterie *et al.* 2000 in validating their multiphase model.

In the present study, a fully physical multiphase 3D model of wildland fire behavior was developed and incorporated into the commercial general-purpose CFD software, PHOENICS, employed as a framework and a solver. The model contains the main features proposed by previous researchers, i.e. Grishin 1997 and Porterie *et al.* 1998, 2000, and it accounts for all the important physical and physicochemical processes: drying, pyrolysis, char combustion, turbulent combustion of gaseous products of pyrolysis, exchange of mass, momentum and energy between gas and solid phase, turbulent gas flow and convective, conductive and radiative heat transfer. It has been validated using the experimental data of Mendes-Lopes JMS *et al.* 2003. The predicted rate of spread (ROS) of wildfire compares quantitatively well with its experimental values obtained at various wind speeds (from 1 to 3 m/s). The use of PHOENICS software as a framework for modeling allows model applications by potential users (students, researchers, fire management teams, etc.) without any special CFD background due to availability of user-friendly software interface, documentation and technical support. Moreover, an open and general structure of software enables users to modify the model, test various built-in models of turbulence and radiation, try various numerical schemes and import geometries from CAD packages in order to model complex shapes of objects in wildland-urban interface (WUI).

Physical and Mathematical Formulation

Following a multiphase modeling approach proposed by Grishin 1997 and Porterie *et al.* 2000 the forest is considered in this paper as a chemically reactive multiphase medium containing gas phase with a volume fraction of ϕ_g and condensed phase with a volume fraction of ϕ_s (liquid water, dry organic matter, solid pyrolysis products and mineral part of fuel). The interaction between phases is modeled by two sets of phase governing equations linked with proper source terms expressing the gas flow resistance, multiphase heat transfer and chemical reactions. The model accounts for drying, pyrolysis, char combustion, turbulent combustion of gaseous products of pyrolysis, turbulent gas flow and heat transfer. In this study, the radiative heat transfer is approached with a simple radiation model similar to widely used P1 – approximation and soot formation is ignored. The Arrhenius-type kinetics is used for heterogeneous reactions (drying, pyrolysis and char combustion) and the eddy dissipation concept (EDC) of Magnussen and Hjertager 1976 is applied for modeling the gaseous combustion. Turbulence is modeled by using the renormalization group (RNG) k-ε model. Figure 1 shows the 3D domain containing the gas flow region, a fuel bed representing the forest and an ignition line. The specific sizes of domain and fuel bed vary in various case studies.

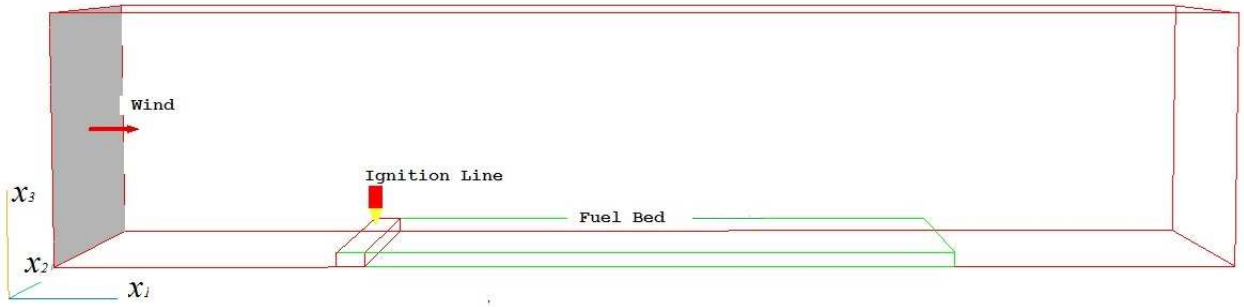

Figure 1: Computational domain: wind, ignition line and fuel bed

The gas phase governing equations are written in a generic form as follows:

$$\frac{\partial}{\partial t}(\rho\Phi)+\frac{\partial}{\partial x_i}\left(\rho u_i\Phi-\Gamma_\Phi\frac{\partial\Phi}{\partial x_i}\right)=S_\Phi \qquad (1)$$

Here, t is the time; x_i is the spacial coordinate (i=1, 2, 3); ρ is the gas mixture density; u_i is the velocity component in x_i direction and the specific expressions for dependent varibale, Φ, diffusive exchange coefficient, Γ_Φ, and source term, S_Φ, are given in Table 1 below. The gas phase volume fraction, ϕ_g, is taken equal to unity in equation (1) as $\phi_g = 1-\phi_s$, where the volume fraction of condensed phase, ϕ_s, is very small in the present study (ϕ_s <0.016). The gas density is calculated from the ideal gas law equation of state for mixture of gases: $p = \rho RT\sum_{\alpha=1}^{3}\frac{c_\alpha}{M_\alpha}$, where p is the gas pressure; T is the absolute gas temperature; R is the universal gas constant; c_α is the mass fraction of α- species of gas mixture; index α = 1,2,3, where 1 corresponds to oxygen, 2 - to carbon monoxide, 3 - to all other components of gas mixture ($\sum_{\alpha=1}^{3}c_\alpha=1$); M_α is the molecular weight of α-component of gas phase.

Table 1. Dependent variables, effective exchange coefficients and source terms in equation (1)

Conservation of	Φ	Γ_Φ	S_Φ
Mass	1	0	$\dot{m}$
x_i – momentum	u_i	$\mu + \mu_t$	$-\frac{\partial p}{\partial x_i} + \rho g_i - \frac{1}{8} A_s C_d \rho u_i \lvert \vec{u} \rvert$
Enthalpy	h	$\frac{\mu}{\mathrm{Pr}} + \frac{\mu_t}{\mathrm{Pr}_t}$	$m_5 q_5 - A_s h_s (T - T_s) + 4\varepsilon_1 \sigma (T_3^4 - T^4)$
Mass of α – species	c_α	$\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t}$	$m_{5\alpha}$
Turbulent kinetic energy	k	$\mu + \frac{\mu_t}{\sigma_k}$	$\rho(P_k + W_k - \varepsilon)$
Dissipation rate of turbulent kinetic energy	ε	$\mu + \frac{\mu_t}{\sigma_\varepsilon}$	$\rho \frac{\varepsilon}{k}(C_{\varepsilon 1} P_k - C_{\varepsilon 2}\varepsilon + C_{\varepsilon 3} W_k - R_{RNG})$

Here, h is the gas enthalpy; k is the turbulent kinetic energy; ε is the dissipation rate of turbulent kinetic energy; μ and μ_t are the dynamic molecular and turbulent viscosities calculated from equations: $\mu = \frac{1.479 \cdot 10^{-6} T^{1.5}}{(T + 116.275)}$, $\mu_t = C_\mu \rho k^2 / \varepsilon$; *Pr*, *Sc*, Pr_t and Sc_t are the molecular and turbulent Prandtl and Schmidt numbers; σ_k, σ_ε,, C_μ,, $C\varepsilon_1$, $C\varepsilon_2$, $C\varepsilon_3$ are the empirical constants of turbulent model; g_i is the gravity acceleration component ($\vec{g} = (0,0,-g)$); $\vec{u}$ is the gas velocity vector having three velocity components u_1, u_2, u_3; A_s is the specific wetted area of fuel bed ($A_s = \phi_s \sigma_s$); σ_s is the surface-area-to-volume ratio of solid particle; C_d is a particle drag coefficient ($C_d = 24(1+0.15\, Re_{es}^{0.687})/ Re_{es}$, Re_{es}<800) depending on the effective particle Reynolds number, $Re_{es} = \rho \lvert \vec{u} \rvert d_{es}/\mu$,which is calculated using the equivalent spherical particle diameter, $d_{es}=6/\sigma_s$; h_s is the particle heat transfer coefficient ($h_s = \lambda Nu_s / d_s$) depending on the heat conductivity of gas, λ, particle Nusselt number, Nu_s , and equivalent diameter of cylindrical particle, $d_s = 4/\sigma_s$; Nu_s is a function of particle Reynolds number, $Re_s = \rho \lvert \vec{u} \rvert d_s/\mu$: $Nu_s = 0.683 \mathrm{Re}_s^{0.466}$; q_5 is the heat release rate of gas phase combustion of carbon monoxide (q_5 =1.E+7 J/kg); σ is the Stephan-Boltzman constant; T_S is the absolute temperature of solid phase; T_3 is the 'radiosity temperature' defined as $(R_I/(4\sigma))^{1/4}$,where R_I is the incident radiation (Wm^{-2}); ε_1 is the absorption coefficient of gas phase; P_k, W_k are the turbulent production terms; R_{RNG} is an additional term proposed in the RNG *k*-ε model (R_{RNG} = 0 in *k*-ε model). The mass rates $\dot{m}$, m_5 , m_{51} and m_{52} are defined as (see Grishin 1997 and Porterie *et al.* 2000)

$$\dot{m} = (1-\alpha_c) R_1 + R_2 + \frac{M_C}{M_1} R_3, \; m_5 = \frac{4\rho\varepsilon}{k} \min(c_2, \frac{c_1}{0.5}), \; m_{51} = -\frac{1}{2}\frac{M_1}{M} m_5 - R_3 \qquad (2)$$

$$m_{52} = \nu_g (1-\alpha_c) R_1 - m_5, \quad R_1 = k_1 \rho_1 \varphi_1 \exp(-E_1 / RT_S), R_2 = k_2 \rho_2 \varphi_2 T_S^{-0.5} \exp(-E_2 / RT_S)$$

$$R_3 = \frac{3}{8} k_3 \rho \varphi_3 \sigma_s c_1 \exp(-E_3 / RT_S)$$

Here M, M_1 and M_C are the molecular weights of gas mixture, oxygen and carbon; α_c and ν_g are the coke number and the fraction of combustible gaseous products of pyrolysis defined by Grishin *et al.* 1986 and Grishin 1997 (α_c = 0.06, ν_g = 0.7); R_1 , R_2 and R_3 are the mass rates of chemical reactions (pyrolysis, evaporation and char combustion) approximated by Arrhenius laws whose parameters, i.e. pre-exponential constants k_i and activation energies E_i, are available from Grishin *et al.* (1986) and Porterie *et al.* 2000: k_1 = 3.63E+4 s^{-1}, k_2 = 6.E+5 $K^{1/2}$ s^{-1}, k_3 = 430 ms^{-1}, E_1 / R = 7250 K, E_2 / R = 5800 K, E_3 / R = 9000 K.

The rates of degradation of condensed phase are computed from the equations (Grishin 1997):

$$\rho_1 \frac{\partial \varphi_1}{\partial t} = -R_1, \rho_2 \frac{\partial \varphi_2}{\partial t} = -R_2, \rho_3 \frac{\partial \varphi_3}{\partial t} = \alpha_C R_1 - \frac{M_C}{M_1} R_3, \rho_4 \frac{\partial \varphi_4}{\partial t} = 0, \sum_{i=1}^{5} \varphi_i = 1, \varphi_S = \sum_{i=1}^{4} \varphi_i . \quad (3)$$

As suggested by Grishin 1997 and Porterie *et al*. 2000, the solid particles are considered thermally thin and their temperature is computed from the following conservation equation:

$$\sum_{i=1}^{4} \rho_i C_{pi} \varphi_i \frac{\partial T_S}{\partial t} = -q_1 R_1 - q_2 R_2 + q_3 R_3 + 4\varepsilon_2 \sigma (T_3^4 - T_S^4) + A_s h_s (T - T_S) \quad (4)$$

Here and above ρ_i, φ_i and C_{pi} are the density, volume fraction and specific heat of a phase component (1 – dry organic substance, 2 – liquid water, 3 – condensed products of pyrolysis, 4 – mineral component of fuel, 5 – gas phase); q_i are the heat release rates of chemical reactions. In this study, for i = 1, 2, 3 and 4, ρ_i = 680, 1000, 200 and 200 kgm^{-3}; C_{pi} = 2.0, 4.18, 0.9 and 1.0 $kJkg^{-1}K^{-1}$; q_1 = 418 Jkg^{-1} and q_3 = 1.2E+7 Jkg^{-1} as in Porterie *et al*. 2000 and q_2 = 3.E+6 Jkg^{-1} as in Grishin *et al.* (1986)). The initial volume fractions of condensed phase are calculated from equations (Grishin *et al.* (1986)):

$$\varphi_{1e} = \frac{\rho_0 (1 - \nu_{ash})}{\rho_1}, \varphi_{2e} = \frac{W \rho_0 (1 - \nu_{ash})}{100 \rho_2}, \varphi_{3e} = 0, \varphi_{4e} = \frac{\rho_0 \nu_{ash}}{\rho_4} \quad (5)$$

Here, ρ_0 is the bulk density of fuel; ν_{ash} is the ashes content (ν_{ash} = 0.04); W is the fuel moisture content (%). In the first validation study (see next section), ρ_0 = 10 kgm^{-3}, W = 10%, and equations (5) result in the following initial values of φ_i: φ_{1e} = 0.014, φ_{2e} = 9.1E-4, φ_4 = 8.E-4.

The radiative transfer equation (RTE) is written with use of a PHOENICS variable, T_3:

$$\frac{\partial}{\partial x_i}\left(\lambda_3 \frac{\partial T_3}{\partial x_i} \right) = 4\varepsilon_1 \sigma (T_3^4 - T^4) + 4\varepsilon_2 \sigma (T_3^4 - T_S^4); \ \lambda_3 = 4\sigma T_3^3 / (0.75 (\varepsilon_1 + \varepsilon_2) + 1 / W_{gap}) \quad (6)$$

Here, ε_1 and ε_2 are the absorption coefficients of gas and solid phases; ε_1, which depends on gas temperature and mass fractions of products of gaseous combustion, was taken equal to a constant value of 0.1 for simplicity in this study; $\varepsilon_2 = \phi_s \sigma_s / 4 = \phi_s / d_s$ according to Porterie *et al.* 1998.

Equation (6) is a formulation similar to RTE in P1-approximation used by Porterie *et al.* 1998

with the only difference that an additional term, $1/W_{gap}$, is included as proposed in PHOENICS documentation on IMMERSOL radiation model (W_{gap} is the gap between the solid walls).

Results and Discussion

The model described in the previous section was validated in a case, which was studied experimentally by Mendes-Lopes JMS *et al.* 2003 and numerically by Porterie *et al.* 1998, 2000 and Menage *et al.* 2012. In this case, the fuel bed has the following input parameters (according to Porterie *et al.* 1998, 2000): a height of 5 cm, a fuel load value of 0.5 kg/m^2 , a needles density of 680 kg/m^3 , a bulk fuel density of 10 kg/m^3, an initial moisture content of 10% and a surface-area-to-volume ratio of needles of about 5511 m^{-1}. A 2.2 m x 1 m x 0.05 m fuel bed was considered within a 4.2 m x 1 m x 0.9 m domain (see Figure 1). For the sake of simplicity, a 2D formulation was applied by ignoring the gas flow and transport of mass and energy in x_2 direction. A computational grid of 190x40 cells was used based on grid sensitivity study. The ignition source was located at the beginning of fuel bed (at 1 m distance from the origin) and the ignition was simulated by introducing a volumetric heat source of 0.1 m length over the whole fuel bed width and height (its temperature was linearly increased from 700°K to 1000°K during the first 8 seconds of simulation). The three wind speeds of 1, 2 and 3 m/s were considered. The focus of our study was on the model capabilities to predict the fire rate of spread (ROS) measured by Mendes-Lopes JMS *et al.* 2003 and to reproduce the main flow patterns predicted numerically by Porterie *et al.* 1998, 2000. The ROS was calculated (in accordance with Porterie *et al.* 1998, 2000) as a speed of propagation of the isotherm T_s = 600°K (or 500°K) at the ground level. Figure 2 shows the transient propagation of pyrolysis front defined with use of isotherm T_s = 600°K for three wind speeds of 1, 2 and 3 m/s. The quasi-steady values of ROS defined as rates of change of front positions with time are 1.2, 2.5 and 4.3 cm/s respectively. These values are well compared with the experimental ROS values of Mendes-Lopes JMS *et al.* 2003 (measured at zero slope of bed): 1.04, 2.08 and 4.92 cm/s respectively.

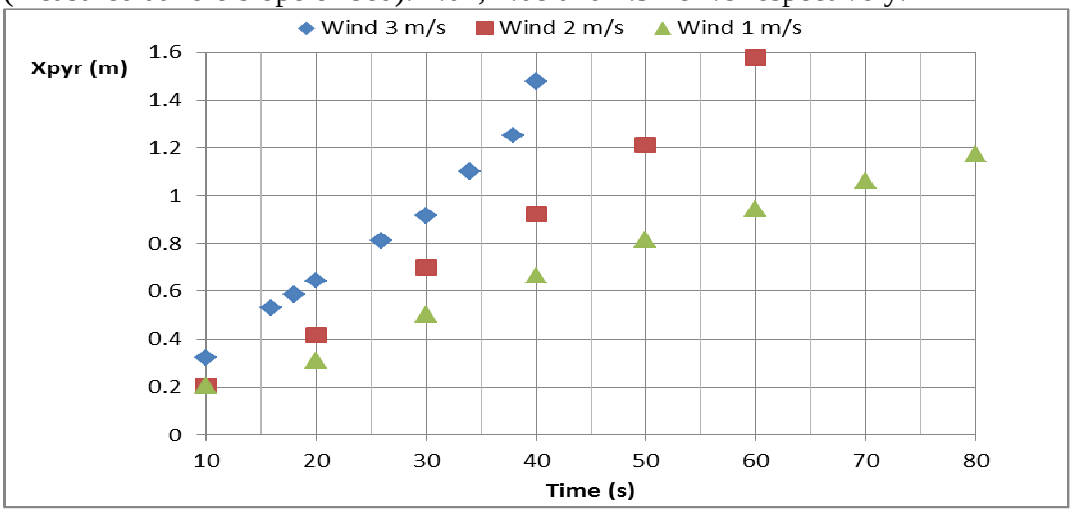

Figure 2. Pyrolysis front propagation for three wind speeds of 1, 2 and 3 m/s

Figure 3 shows the distributions of solid phase temperature, T_s, and mass fractions of oxygen (C1) and carbon monoxide (C2) (a gaseous product of pyrolysis) predicted for a wind speed of 1

m/s at x_3 = 0 m and t = 20 s. The fuel bed heating from propagating fire causes water evaporation, pyrolysis (between 400°K and 500°K) and char combustion (at about 700°K). The carbon monoxide, which is released during pyrolysis, participates in gaseous combustion and its mass fraction drops to zero. The oxygen mass fraction reduces in pyrolysis zone due to creation of CO in that zone and then it drops to zero within the combustion zone due to oxygen consumption.

Figure 4 shows the distributions of gas temperature and velocity predicted at t = 40 s for wind speeds of 1 and 2 m/s (top and bottom respectively). At a wind speed of 1 m/s, a large clockwise eddy is formed ahead of strong buoyant plume and the plume is oscillating with time. As wind speed increases from 1 to 2 m/s, a transition from buoyancy-dominated regime to wind-driven regime is observed and the plume becomes more stable. These flow patterns were also reported by Porterie *et al*. 2000.

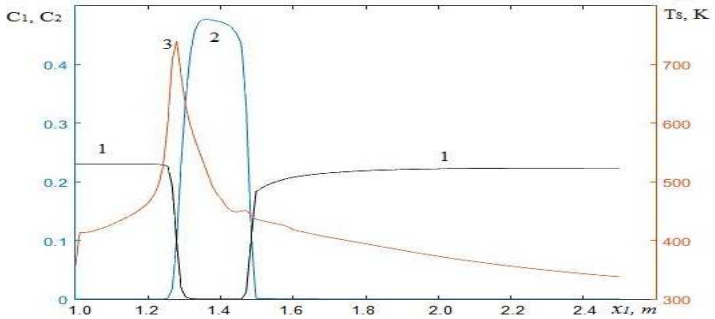

Figure 3. Solid phase temperature (3) and mass fractions of oxygen (1) and carbon monoxide (2) for wind speed of 1 m/s at t = 20 s

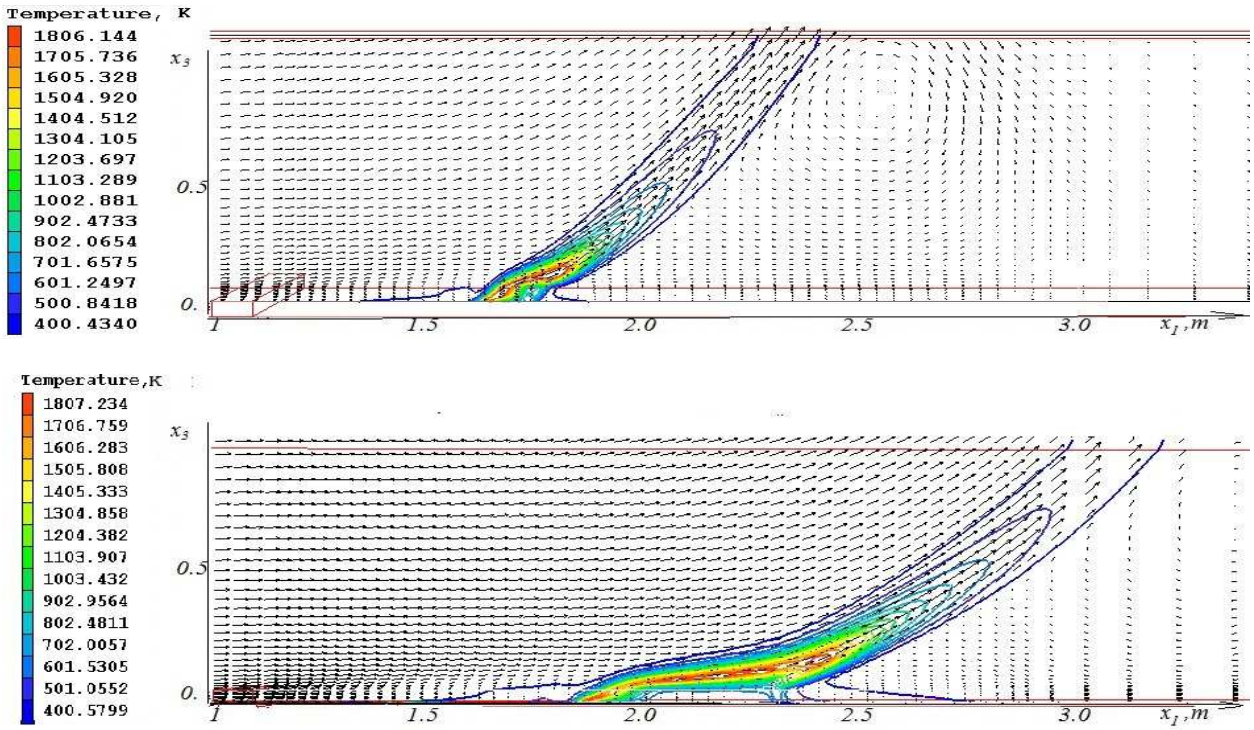

Figure 4. Gas temperature and velocity vectors at wind speeds of 1 m/s (top) and 2 m/s (bottom) at t = 40 sec

Conclusions

A multiphase CFD model of wildfire initiation and spread has been developed and incorporated into the multi-purpose CFD software, PHOENICS. The model accounts for all the important physical and physicochemical processes: drying, pyrolysis, char combustion, turbulent combustion of gaseous products of pyrolysis, exchange of mass, momentum and energy between gas and solid phase, turbulent gas flow and convective, conductive and radiative heat transfer. Turbulence is modeled by using the RNG k-ε model and the radiative heat transfer is approached with a model similar to P1-approximation. The Arrhenius-type kinetics is used for heterogeneous reactions (drying, pyrolysis and char combustion) and the eddy dissipation concept is applied for modeling the gaseous combustion. The model was validated using the experimental data of Mendes-Lopes *et al.* 2003 on surface fire propagation in a bed of *Pinus pinaster* needles studied in a wind tunnel. The predicted rate of spread (ROS) is well agreed with experimental values obtained at various wind speeds (from 1 to 3 m/s). The model is being further developed by modifying the radiative heat transfer model and it will be validated using the data on large forest fires including crown fires.

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