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Multiphase CFD Model of Wildland Fire Initiation and Spread

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Presentation Overview

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- Modeling Approach
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Objective

- **Experimental studies of wildfire behavior are expensive and challenging.**
- **It makes the wildfire model development extremely valuable.**
- **There are various types of models: statistical, empirical, semi-empirical and physics-based.**
- **The objective of this paper is to develop and validate a fully physical multiphase 3D model of wildfire behavior and smoke dispersion, which is both advanced and pragmatic.**

Introduction

- Over the **past 30 years**, **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 and others.
- According to Morvan 2011, one of the most advanced physical models is **WFDS** (Wildland-urban interface Fire Dynamics Simulator), developed by the National Institute of Standards and Technology (NIST) and the U.S. Forest Service. Its validation is ongoing but far from complete.
- **Our model** is based on combining the approaches proposed by Grishin 1997 and Porterie *et al.* 1998, 2000 and using the Computational Fluid Dynamics (CFD) software, PHOENICS, as a framework and a solver.
- **PHOENICS** is the commercial multi-purpose CFD software, which has been developing by **CHAM** Limited (UK) since 1981. Our company, **ACFDA**, is North American CHAM's Agency since 1998.

Modeling Approach - Summary

- The forest is considered as a **chemically reactive multiphase medium containing gas phase and condensed phase** (liquid water, dry organic matter, solid pyrolysis products and mineral part of fuel).
- 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.
- 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**.
- The **radiative heat transfer** is approached with a simple radiation model similar to widely used **P1 – approximation**.
- **Soot formation is ignored**.

Modeling Approach - Geometry

- **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 cases. In the first validation case (surface fire), the fuel bed height was 5 cm. In a case of crown fire, it is a few meters.**

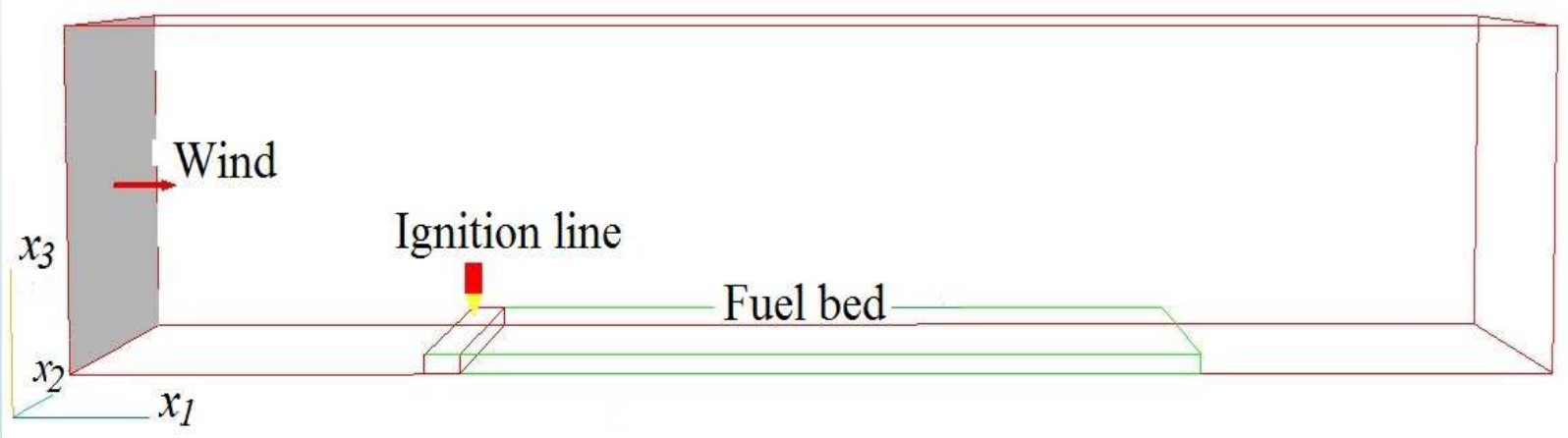


Figure 1. Computational Domain (wind, fuel bed and ignition line)

Modeling Approach – Gas-Phase Equations

- The **gas-phase governing equations** are written in a generic form:

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

- 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 variable, Φ, diffusive exchange coefficient, Γ_Φ, and source term, S_Φ,** are given in Table 1 below.

- 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.

Modeling Approach – Gas-Phase Equations

(Expressions for Φ, Γ_Φ, S_Φ)

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	$\mu + \frac{\mu_t}{\sigma_\varepsilon}$	$\rho \frac{\varepsilon}{k}(C_{\varepsilon 1} P_k - C_{\varepsilon 2}\varepsilon + C_{\varepsilon 3} W_k - R_{RNG})$

Modeling Approach - Nomenclature

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:

$$\mu = \frac{1.479 \cdot 10^{-6} T^{1.5}}{(T + 116.275)}, \qquad \mu_t = C_\mu \rho k^2 / \varepsilon$$

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 ($\vec{g} = (0,0,-g)$);

$\vec{u}$ - the gas velocity vector having three velocities components u_1, u_2, u_3 ;

A_s - the specific wetted area of fuel bed $A_s = \phi_S \sigma_S$;

σ_s - surface-area-to-volume ratio of solid particle; ϕ_S - volume fraction of condensed phase;

- ***Cd*** is a particle drag coefficient ($C_d=24(1+0.15\ Re_{es}^{0.687})/\ Re_{es}$, $Re_{es}<800$);
- h_s is the particle heat transfer coefficient ($h_s=\lambda Nu_s/d_s$, $Nu_s=0.683Re_s^{0.466}$);
- 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 $(R_I/(4\ \sigma))^{1/4}$ (R_I is incident radiation in 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 ;

Modeling Approach – Chemical Reaction Rates

- $\dot{m}, m_5, m_{51}, m_{52}$ - mass rates of production of gas mixture, oxygen and carbon monoxide:

$$\dot{m} = (1-\alpha_c)R_1 + R_2 + \frac{M_C}{M_1}R_3, m_{51} = -\frac{1}{2}\frac{M_1}{M}m_5 - R_3, m_{52} = \nu_g(1-\alpha_c)R_1 - m_5 \quad (2)$$

$$m_5 = \frac{4\rho\varepsilon}{k}\min(c_2, \frac{c_1}{0.5})$$ - carbon monoxide combustion rate – EDC model,

α_c and ν_g are coke number and fraction of combustible products of pyrolysis (0.006 and 0.7);

R_1, R_2 and R_3 are the mass rates of pyrolysis, evaporation and char combustion approximated by Arrhenius laws with pre-exponential constants k_i and activation energies E_i available from Grishin *et al.* 1986 and Porterie *et al.* 2000:

$$R_1 = k_1\rho_1\varphi_1\exp(-E_1/RT_S), R_2 = k_2\rho_2\varphi_2T_S^{-0.5}\exp(-E_2/RT_S), R_3 = \frac{3}{8}k_3\rho\varphi_3\sigma_s c_1\exp(-E_3/RT_S) \quad (3)$$

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

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

The temperature of solid particles, that are considered thermally thin, is computed from the energy conservation equation:

$$\sum_{i=1}^{4} \rho_i C_{pi} \varphi_i \frac{\partial T_S}{\partial t} = -q_1 R_1 - q_2 R_2 + q_3 R_3 + 4\varepsilon_2 \sigma (T_3^4 - T_S^4) + A_s h_s (T - T_S) \quad (5)$$

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.

The initial volume fractions of condensed phase components are calculated from equations (Grishin *et al.*, 1986):

$$\varphi_{1e} = \frac{\rho_0 (1 - \nu_{ash})}{\rho_1}, \varphi_{2e} = \frac{W \rho_0 (1 - \nu_{ash})}{100 \rho_2}, \varphi_{3e} = 0, \varphi_{4e} = \frac{\rho_0 \nu_{ash}}{\rho_4} \quad (6)$$

Here ρ_0 - is the bulk density of fuel; ν_{ash} - is the ashes content ; W is the fuel moisture content (%).

The radiative transfer equation (RTE) is written with use of 'radiosity temperature' T_3, which is $(R_I/(4\,\sigma))^{1/4}$ (R_I is incident radiation in Wm^{-2}):

$$\frac{\partial}{\partial x_i}\left(\lambda_3 \frac{\partial T_3}{\partial x_i}\right) = 4\varepsilon_1\sigma(T_3^4 - T^4) + 4\varepsilon_2\sigma(T_3^4 - T_S^4), \quad \lambda_3 = 4\sigma T_3^3/(0.75(\varepsilon_1+\varepsilon_2)+1/W_{gap}) \qquad (7)$$

where ε_1 and ε_2 are the absorption coefficients of gas and condensed phases; $\varepsilon_2 = \phi_s\sigma_s/4 = \phi_s/d_s$ according to Porterie *et al.* 1998; ε_1 depends on gas temperature and mass fractions of products of gaseous combustion (ε_1 = 0.1 for simplicity in this study); W_{gap} is the gap between the solid walls, which is introduced in the IMMERSOL radiation model of PHOENICS.

Equation (7) 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.

Results and Discussion

Model Validation – Input Conditions

- **The model was incorporated into PHOENICS and validated for surface fire propagation in a bed of *Pinus pinaster* needles 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 well-defined 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 for three wind speeds of 1, 2 and 3 m/s.**
- **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).**

Model Validation – Rate of Spread

- **2D formulation was applied for the sake of simplicity 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 focus of validation 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 (pyrolysis front).**
- **The quasi-steady values of ROS calculated as rates of change of front positions with time were 1.2, 2.5 and 4.3 cm/s for three wind speeds of 1, 2 and 3 m/s respectively. These values are well compared with the experimental ROS values of Mendes-Lopes JMS *et al.* 2003: 1.04, 2.08 and 4.92 cm/s.**

Model Validation – Pyrolysis Front Propagation

- 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 predicted slope increases significantly with a wind speed increase from 1 to 3 m/s.

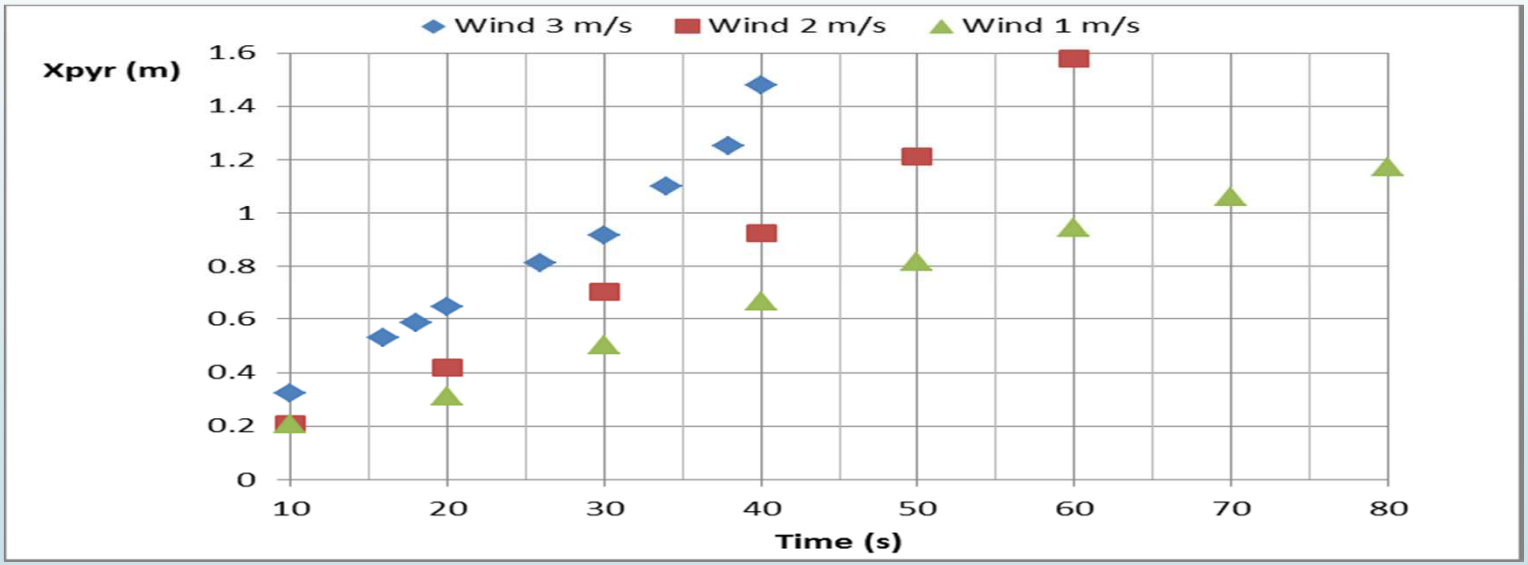


Figure 2. Pyrolysis front propagation for wind speeds of 1, 2 and 3 m/s

Discussion – Processes in Fuel Bed Region

- **Figure 3 shows the distributions of solid phase temperature, T_s, mass fractions of oxygen (C1) and carbon monoxide (C2) predicted for a wind speed of 1 m/s at the ground level (x_3 = 0 m) and at t = 20 s.**
- **The fire propagation 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.**

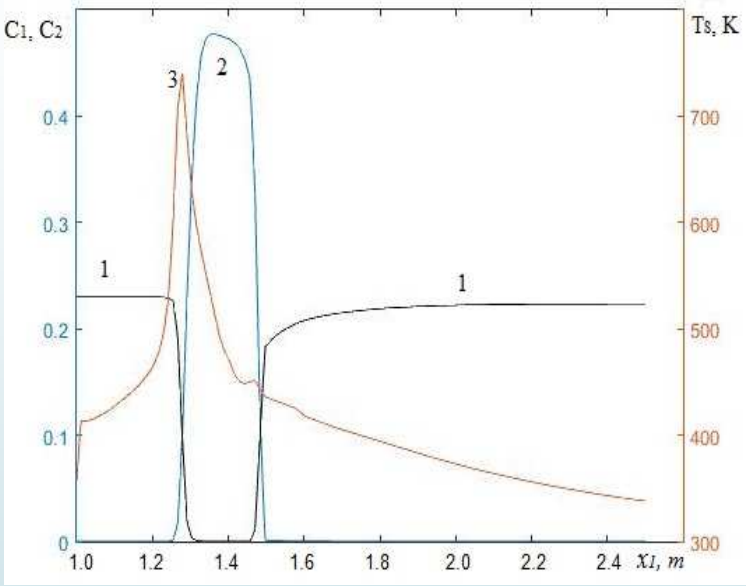


Figure 3. Solid phase temperature (3) and mass fractions of oxygen (1) and carbon monoxide (2) for wind speed of 1 m/s

Discussion – Plumes at Winds of 1 and 2 m/s

Figure 4 shows the distributions of gas temperature and velocity predicted at t = 40 s for wind speeds of 1 and 2 m/s (left and right respectively). At a wind speed of 1 m/s, a large clockwise eddy is formed ahead of strong buoyant plume. 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.

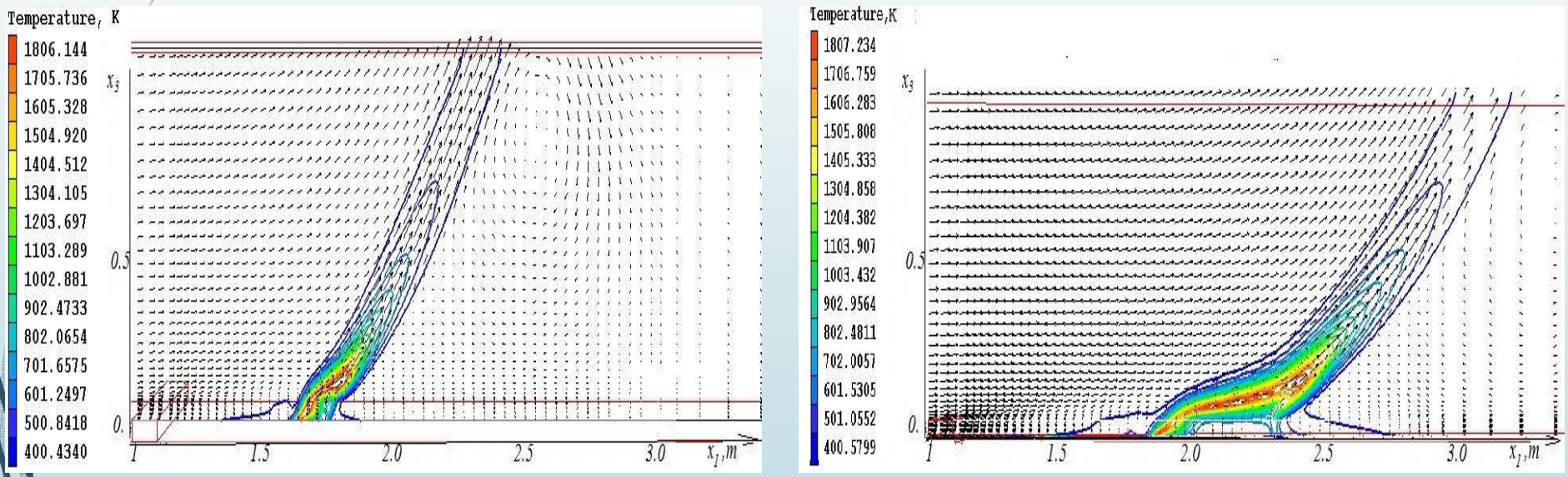
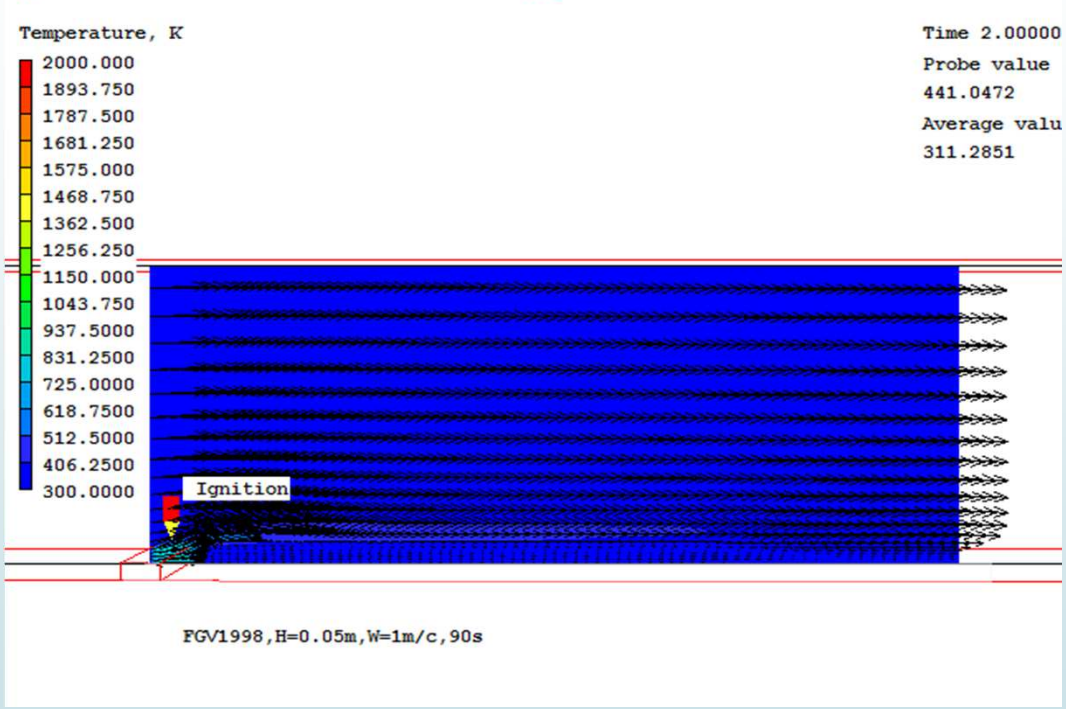


Figure 4. Gas temperature and velocity vectors at wind speeds of 1 m/s (left) and 2 m/s (right) at t = 40 sec

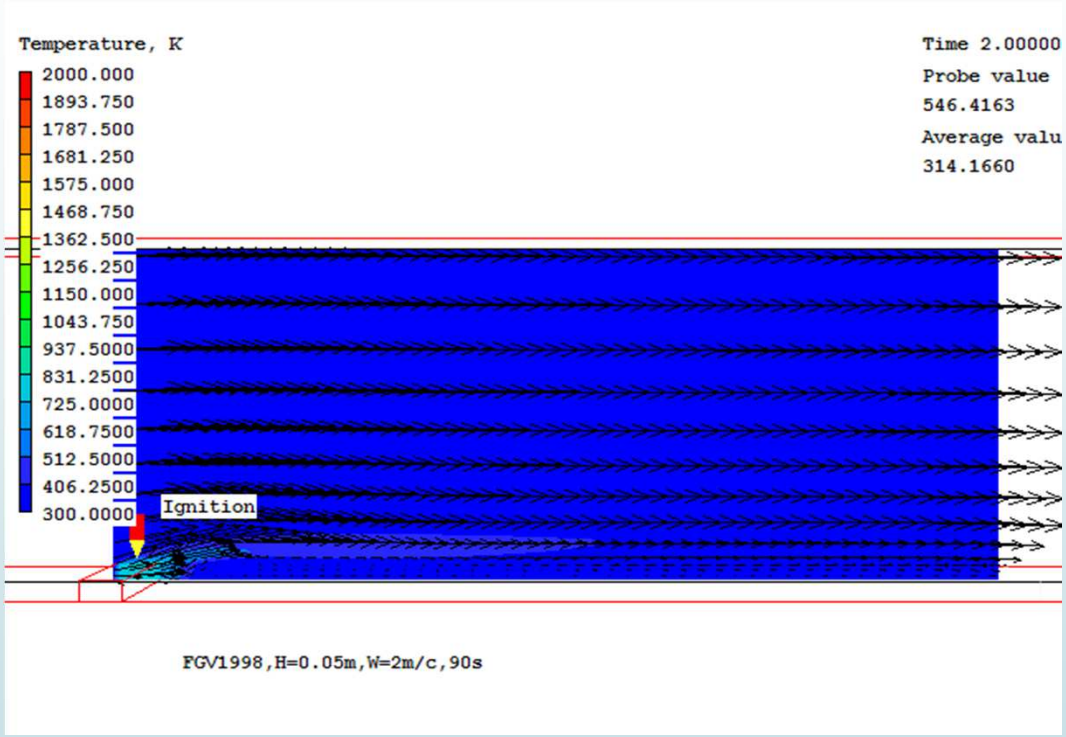
Discussion - Fire Propagation at 1 m/s wind

Buoyancy-dominated and oscillating plume behavior at a wind speed of 1 m/s



Discussion - Fire Propagation at 2 m/s wind

Wind-dominated and more stable plume behavior at a wind speed of 2 m/s



Conclusions

- **A fully physical multiphase model of wildfire behavior 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.**
- **The model was validated using the experimental data of Mendes-Lopes *et al.* 2003 for surface fire propagation in a bed of *Pinus pinaster* needles.**
- **The predicted fire rate of spread (ROS) is well agreed with experimental data obtained at various wind speeds (from 1 to 3 m/s).**
- **The model is recommended for wildfire research and analyses and it is available from ACFDA (www.acfda.org).**

Future Work

- Improving radiative heat transfer sub-model
- Testing various models of turbulence and chemical kinetics
- Model validation for large forest fires including crown fires
- Applying the model for complex geometries (Wildland-urban interface)
- Seeking a collaboration with researchers and organizations interested in developing/applying physical wildfire models (info@acfda.org).

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THANK YOU!

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