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Authors
Ghabi, Chekib
Rein, Guillermo
Ben Ticha, Hmaied
et al.

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BIDIMENSIONNAL NUMERICAL MODEL FOR POLYUERETHANE SMOLDERING IN A FIXED BED

Chekib GHABI[1], Guillermo REIN[2], H. BenTICHA[1]. Mohamed SASSI[3]
[1] Laboratoire d'Eudes des Systèmes Thermiques et Energétiques,
Ecole Nationale d'Ingénieurs de Monastir, 5000 Tunisie
[2] Department of Mechanical Engineering, University of California at Berkeley, USA
[3] The Petroleum Institute, P.O. Box 2533, Abu Dhabi, UAE
E-mail : ghabichekib@yahoo.fr

ABSTRACT

Smoldering combustion is described as an exothermic superficial heterogeneous-reaction that can propagate in the interior of porous fuels. Smoldering is generally an incomplete combustion reaction, which leaves behind a porous char that contains significant amounts of unburned fuel. If compared to flaming combustion, the heat release and the temperature characteristics of smoldering are low and its propagation is a slow process. Besides its characteristics of a weak combustion process, smoldering poses serious risk to fire safety; it is a common fire initiation scenario, because it is difficult to detect as, it can go unnoticed for long periods of time, It yields a high conversion of fuel to toxic products, and it can suddenly switch to flaming combustion. The propagation of the smoldering front is usually controlled by two factors: oxygen availability and heat losses. However it's the result of several interacting mechanisms, such as chemical reactions (pyrolysis and oxidation), convection and diffusion of heat and oxygen, heat transfer between the gas and the solid phases, heat losses to the surrounding and flow in a porous media.

The developed axisymmetric two-dimensional model solves the governing equations for forward propagation of smoldering in a porous fuel bed. The conservation equations for energy in the solid and the gas phases are considered separately but interact through an interfacial heat exchange. Species conservation in the solid and the gas phases, and overall mass conservation are numerically solved. The heterogeneous chemical kinetics include pyrolysis of the fuel, and oxidation of the fuel and of the carbonaceous residual. The second oxidation is accompanied by the formation of solid ash and gas products, which pose the potential risk of transition from smoldering to flaming combustion. The obtained numerical results feature the gas and solid temperature evolutions, the char mass fraction evolution, and the smoldering propagation velocity. The finite volume method was used for the spatial discretization, and the implicit one for time. The obtained equations were solved by the Bi-Conjugate Gradient Stabilized (BI-CGSTAB) technique.

NOMENCLATURE

A	Frequency factor
Y	Mass fraction
	Greek Symbols
ΔH	Reaction Enthalpy
ε	Porosity
$\dot{w}$	Mass reaction rate
	Subscripts
a	Char oxidation
ox	Fuel oxidation
c	Char
eff	Effective
g	Gas
s, f	Solid
py	Fuel pyrolysis
gs	Gas-solid
sg	Solid-gas
w, g	Wall-gas
w, s	Wall-solid

INTRODUCTION

Smoldering is a self-sustaining reaction in which the heat released by surface oxidation causes pyrolysis of the unaffected fuel adjacent to the reaction zone, which in turn yields a rigid char, which that subsequently undergoes surface oxidation. The availability of heat, oxygen and fuel is sufficient to maintain a continuous reaction but not enough for a flaming fire to grow. The smoldering process produces a variety of gases that can be toxical, and the smoldering transition to combustion is a dangerous fire problem.

Smoldering is usually controlled by two main parameters: availability of oxygen to the smoldering front and heat losses to the surroundings [1].

Several works on smoldering of polymeric and biomass materials have been reported in the literature. A discussion of one-dimensional forward smoldering was presented by Buckmaster and Lozinski [2]. Summerfield et al. [3] developed a 1D model for steady draw smoldering of a cigarette. Dosanjh et al., [4] in their work on the analytic modeling of propagation of a smoldering front through a porous solid fuel examined the conditions for a steady smolder-front and for the transition to extinction. Leach et al. [5] extended this 1D model to transient cases. Separated gas and solid phase energy equations were considered and two equations for oxygen conservation, in the bulk and at the solid surface. The resulting equations were solved numerically using a finite-difference technique. Di Blasi [6, 7] refined the kinetic model for the smoldering of wood slabs under thermal radiation on one face. Effects of variable properties, unsteady gas phase processes, pressure and velocity variations and convective transport of tar species were accounted for. The secondary reactions from tar to char and gas were also included in the model. Most of the modeling works mentioned above used the kinetic data provided by Kashiwagi and Nambu [8] for a cellulose paper. Other sources of kinetic data are also available [9, 13]. Bar-Ilan et al. [10] conducted smoldering experiments of polyurethane under microgravity conditions, and presents unique data to assess and improve the performance of a mathematical model of smoldering combustion. The photographs of the smoldered samples show significant radial effects on the propagation of the smoldering front.

Despite the contributions of above works to the understanding and treatment of the smoldering process, there is still a need for 2D models able to predict the radial effects observed in experiments.

In this paper, a fixed bed of polyurethane foam is considered for smoldering analysis. A two-dimensional cylindrical model for predictions of flow, heat transfer and chemical kinetics in the smoldering of the porous media. Furthermore, oxygen transport and combustion product in the porous material as well as heat transfer from the lateral surface is accounted for. The gas and solid phases are treated separately. The bi-conjugate gradients method is used to solve the discretised equations [11].

MATHEMATICAL MODEL

In this study, we adopt a transient bi-dimensional model of energy and mass conservation in the solid and gas phases. The air flow is introduced at the left base, and ignition is initialized from the heating of this surface to a well specified temperature. The reaction of smoldering reaction propagates then from the left to the right base.

Governing equations

Energy equation in the solid phase

$$\frac{\partial(\rho_s C_{p_s} T_s)}{\partial t} =$$

$$\frac{1}{r}\frac{\partial}{\partial r}(rk_{s,ef}\frac{\partial}{\partial r}(T_s)) + \frac{\partial}{\partial z}(k_{s,ef}\frac{\partial}{\partial z}(T_s)) + div(\vec{q}_{rad}) \quad (1)$$

$$-\dot{w}_{ox}\Delta H_{ox} - \dot{w}_{py}\Delta H_{py} - \dot{w}_a\Delta H_a + h_{gs}S(T_g - T_s)$$

Species conservation equations in the solid phase.

$$\frac{\partial(\rho_s Y_{char})}{\partial t} = \dot{\omega}_{ox}n_{c1} + \dot{\omega}_{py}n_{c2} - \dot{\omega}_a \quad (2)$$

$$\frac{\partial(\rho_c Y_a)}{\partial t} = \dot{\omega}_a n_a \quad (3)$$

Energy conservation equation in the gas phase

$$\frac{\partial(\varepsilon\rho_g Cp_g T_g)}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(r\varepsilon\rho_g Cp_g u_{r,g} T_g) +$$

$$\frac{\partial}{\partial x}(\varepsilon\rho_g Cp_g u_{z,g} T_g) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\varepsilon k_{g,eff}\frac{\partial T_g}{\partial r}\right) + \quad (4)$$

$$\frac{\partial}{\partial z}\left(\varepsilon k_{g,eff}\frac{\partial T_g}{\partial z}\right) + h_{gs}S(T_s - T)_g$$

Continuity equation in the gas phase

$$\frac{\partial(\varepsilon\rho_g)}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(r\varepsilon\rho_g u_{r,g}) + \frac{\partial}{\partial z}(\varepsilon\rho_g u_{x,g}) = \quad (5)$$

$$\varepsilon(\dot{w}_{py}v_{g2} + \dot{w}_{ox}(v_{g1} - v_{o1}) + \dot{w}_{ox}(v_{g3} - v_{o3}))$$

Oxygen conservation equation on the gas phase

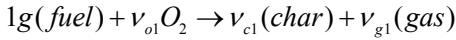$$\frac{\partial(\varepsilon \rho_g Y_{o2})}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}(r\varepsilon \rho_g u_{r,g}Y_{o2})+$$

$$+\frac{\partial}{\partial z}(\varepsilon \rho_g u_{x,g}Y_{o2})=\frac{1}{r}\frac{\partial}{\partial r}\left(r\varepsilon D_{eff}\frac{\partial Y_{o2}}{\partial r}\right) \qquad (6)$$

$$+\frac{\partial}{\partial z}\left(\varepsilon D_{eff}\frac{\partial Y_{o2}}{\partial z}\right)+h_m S(Y_{o2s}-Y_{o2})$$

Oxygen equation on the solid surface

$$\frac{\partial(\varepsilon_s \rho_{gs}Y_{o2s})}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}\left(r\varepsilon_s \rho_{gs}u_{rs}Y_{o2s}\right)+$$

$$\frac{\partial}{\partial z}\left(\varepsilon_s \rho_{gs}u_{zs}Y_{o2s}\right)=\frac{\partial}{\partial r}\left(r\varepsilon_s D_{eff}\frac{\partial}{\partial r}(Y_{o2s})\right)+$$

$$\qquad (7)$$

$$\frac{\partial}{\partial z}\left(\varepsilon_s D_{eff}\frac{\partial}{\partial z}(Y_{o2s})\right)+h_m S(Y_{o2}-Y_{o2s})-$$
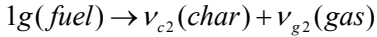
$$\dot{w}_{ox}\nu_{o1}-\dot{w}_a\nu_{o3}$$

The gas mass volume is calculated assuming ideal gas. Equations (6) and (7) are considered to determine the flux of oxygen to the solid surface. Coefficients of convective heat transfer and mass transfer between the solid and the gas phases are considered, and adopted by analogy.
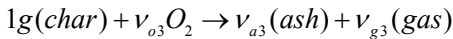
Reaction kinetics

Exothermic oxidation
$$1g(fuel)+\nu_{o1}O_2 \rightarrow \nu_{c1}(char)+\nu_{g1}(gas)$$
Endothermic pyrolysis
$$1g(fuel) \rightarrow \nu_{c2}(char)+\nu_{g2}(gas)$$
Exothermic char oxidation
$$1g(char)+\nu_{o3}O_2 \rightarrow \nu_{a3}(ash)+\nu_{g3}(gas)$$

The rates of production and consumption of mass are similar to those given by Kashiwagi and al. [8] and are written as follows:

Fuel oxidation

$$\dot{\omega}_{ox}=\left(1-Y_c-Y_a\right)^f \rho_s A_{ox}(Y_{o2})^m \exp\left(\frac{-E_{ox}}{RT_s}\right) \qquad (8)$$

Fuel pyrolysis

$$\dot{\omega}_{ox}=\left(1-Y_c-Y_a\right)^g \rho_s A_{py} \exp\left(\frac{-E_{py}}{RT_s}\right) \qquad (9)$$

Char Oxidation

$$\dot{w}_{ox}=Y_c \rho_{char} A_{ash}(Y_{o2})^h \exp(\frac{-E_{ash}}{RT_s}) \qquad (10)$$

Char oxidation takes place at high temperature and has been identified as a key mechanism for transition to flaming [12, 14].

Transfer coefficients and physical properties

The heat transfer coefficient is calculated as a function of Reynolds and Prandtl numbers. Many authors proposed a correlation for the internal coefficient of heat transfer between a gas and a stationary solid bed.

$$Nu=\frac{h_{gs}d_p}{k_g}=2+1.1\mathrm{Re}^{2/3}\mathrm{Pr}^{1/3} \qquad (11)$$

Where d_p is the pore diameter and λ_g is the gas thermal conductivity. The specific surface of exchange between the solid and the gas is defined by: $S=\frac{4(1-\varepsilon)}{d_p} \qquad (12)$

By analogy, Incropera and Dewitt [12] present a correlation to determine the mass transfer coefficient:

$$\frac{h_{gs}}{h_m}=\rho_g C_{p_g} Le^{(1-n)} \qquad (13)$$

Where Le is the Lewis number, defined as (α/D). For most applications it is reasonable to assume n = 1/3.

We used the mass fractions of char and ash to calculate the mass fraction of the solid, and to determine the variation of the physical properties. The char oxidation to ash takes place at high temperatures that can induce inflammation of the material. For simplicity, we consider that the physical properties of char and ash are identical [5].

The radiation is important in the burning of porous materials. It is modeled by the Rosseland approximation, and is expressed according to a radiative conductivity. Therefore, the total thermal conductivity of the solid is given by:

$$k_{efs}=k_s+k_{rad} \qquad (14)$$

$$k_s=(Y_c+Y_a)k_c+(1-Y_c-Y_a)k_s \qquad (15)$$

$$k_{rad}=16\sigma d_p T_s^3/3 \qquad (16)$$

Figure 1
Forward smoldering configuration
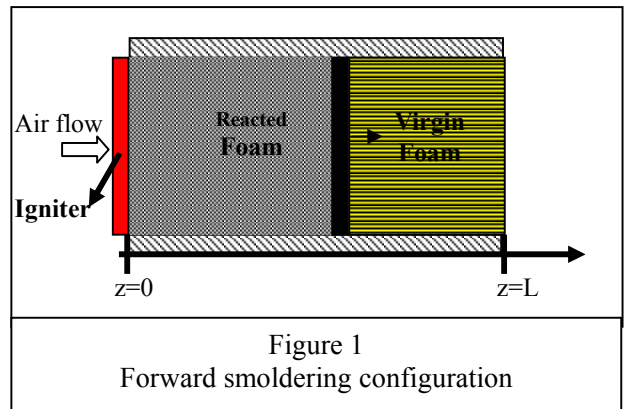
INITIAL AND BOUNDARY CONDITIONS

The igniter is located at the left face. Air is introduced through the left face and it crosses the material exiting with the gas product at the right base. In this configuration, named forward smoldering, the smolder front propagates from the left to the right in the direction of the airflow. On the right face we consider a fully developed in the hot gas that leaves through this surface to the outside where the gradients are set to zero.

At the inlet (z=0):

$$T_s = T_{ig}, \; T_g = T_{gin},$$
$$Y_{o2} = Y_{o2in}, \; U_g = U_{gin} \quad \text{before igniter shutdown} \quad (17)$$

$$k_{efs} \frac{\partial T_s}{\partial x} = h_s \left(T_s - T_{amb} \right) \quad \text{after igniter shutdown} \quad (18)$$

The ignition protocol is the following. Heating the left face during 500s from 300 K to 680 K exponentially initializes the smolder front, and then temperature is maintained fixed at this value until the smolder front begins to self-propagate. When the front moves 2.3 cm from the initial position, then igniter is shut off. In the right face, hot gases leave the sample to the outside and gradients are null during the whole process.

On the lateral surfaces of the cylindrical sample, exchange between gas and solid phases with the wall and the external air are considered. The wall will be impermeable for mass transfer. We assumed that the energy flux to the wall and the external air to be:

$$k_{s,eff} \left. \frac{\partial T_s}{\partial r} \right|_{r=R} = h_{w,s} (T_w - T_{s,R}),$$

$$k_g \left. \frac{\partial T_g}{\partial r} \right|_{r=R} = h_{w,g} (T_w - T_{g,R}), \quad (19)$$

$$\left. \frac{\partial Y_{o2}}{\partial r} \right|_{r=R} = 0$$

At t=0s the solid bed is unreacted, and temperature of gas and the solid are constant and equal to the ambient temperature.

$$T_s = T_{amb}, \; T_g = T_{gin} = T_{amb},$$
$$Y_{o2} = Y_{o2in}, \; Y_c = Y_a = 0 \quad (21)$$

RESULTS AND DISCUTIONS

In this section, results are presented for the case of an inlet air velocity fixed at 5.3 mm/s. With this code we can simulate the bi-dimensional smoldering phenomena.

Table 1
Input parameters of the simulation

Properties	Value
L	15 cm
R	7.5 cm
ε	0.75
ε_s	$5 \; 10^{-3}$
ρ_s	26.5 kg/m^3
k_g	$2.58 \; 10^{-2} \text{ W/mK}$
k_{s0}	$6.3 \; 10^{-2} \text{ W/mK}$
d_p	$5 \; 10^{-5} \text{ m}$
ΔH_{ox}	-5700 J/g
ΔH_{py}	570 J/g
ΔH_a	-25,000 J/g
U_{in}	5.3 mm/s

In this numerical simulation the inlet air velocity is fixed at 5.3 mm/s during the whole process. Dosanjoh et al. [4] indicated that to maintain the propagation of the smoldering front it is necessary to increase or decries the heat removal from the reaction zone by increasing or decreasing the air velocity. Thus, a complete model analysis is presented to address several aspects related to smoldering propagation. In this simulation we consider an exchange of heat transfer between the solid and ambient gas after igniter shutdown. With this code we can simulate the bi-dimensional smoldering phenomena.
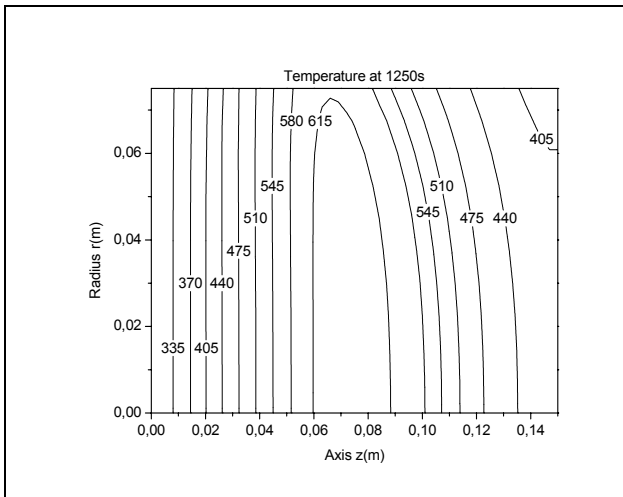

Figure 2
Distribution of the temperature of the solid (in K) at t = 1100s
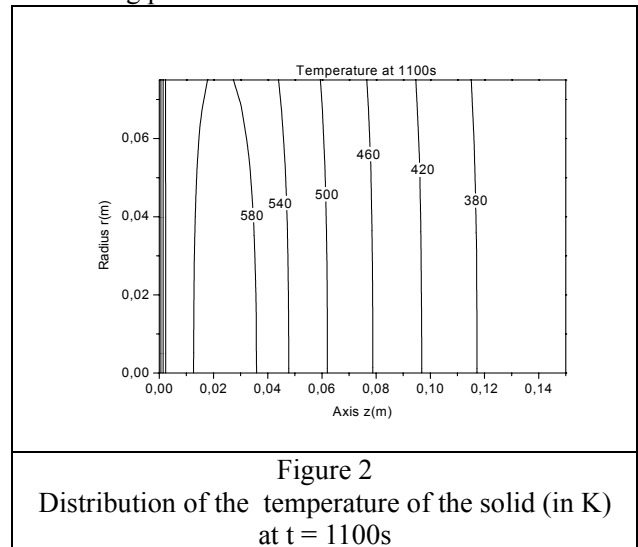
Figure 3
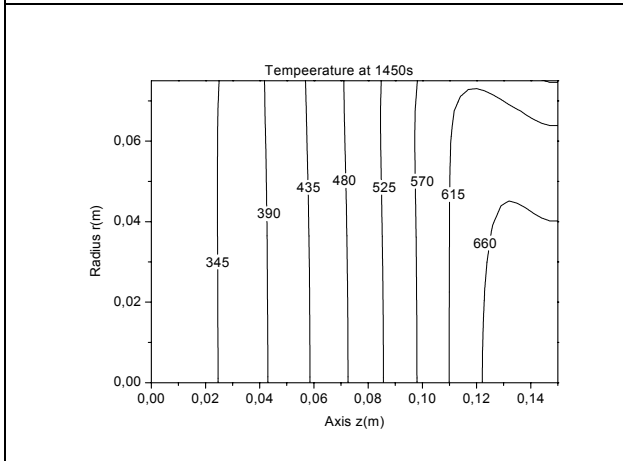Distribution of the temperature of the solid (in K) at t = 1250s

Figure 4
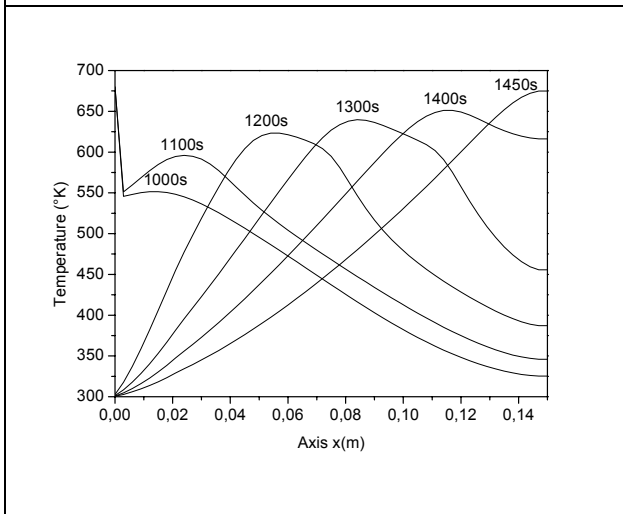Distribution of the temperature of the solid (in K) at t = 1450s

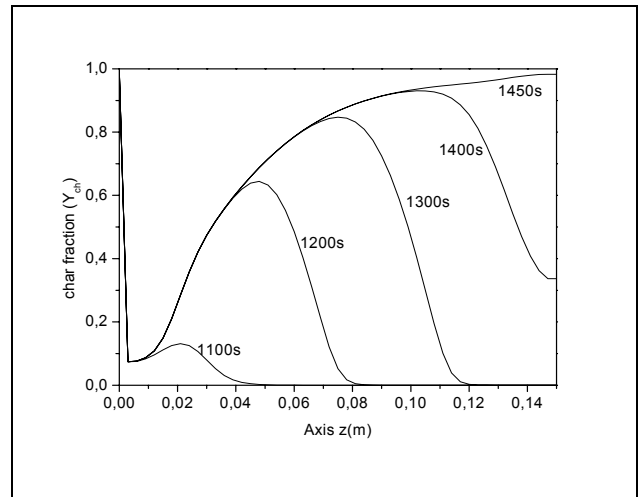Figure 5
Solid temperature evolution with time at r = 0m

Figure 6
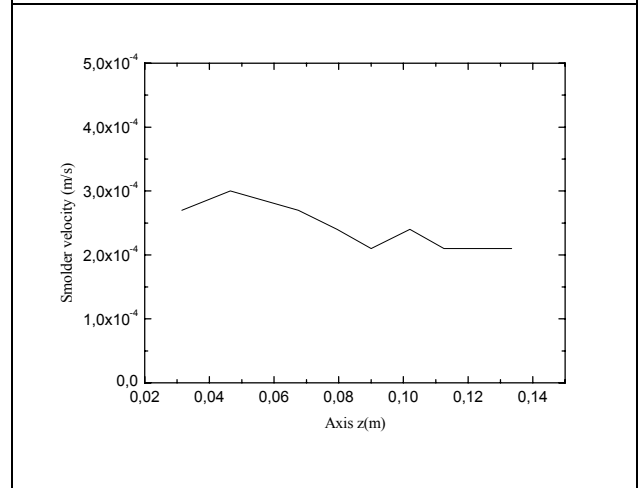Char mass fraction evolution with time at r = R

Figure 7
Smolder velocity as a function of axial distance from the igniter.

In this section, the results from the two-dimensional numerical simulations of forward smoldering are presented. The geometry of the studied configuration is shown in fig. 1, and the input parameters of the simulations are summarized in table 1. The effects of flow in porous media, chemistry, and convective and radiative heat transfer in our two-phase system are considered. Only few results concerning the solid and the gas temperature temporal evolutions, the char mass fraction evolution, and smolder velocity distribution are presented and discussed.

Figure 1, 2, and 3 show the solid temperature field at different instants of time after the self smolder propagation at t= 1100s, t= 1250s, and t= 1450s ; respectively. Anon flaming smolder zone is observed. The heat produced at the reactions zone

contributes, mainly, to the smolder wave propagation from left to right, while a small part of it is lost to the cold side wall, the smolder wave propagates perpendicular to the bed axis accelerates in the beginning and then shows down toward the right end (see fig. 4) leaving the burned char and reacted foam behind.

Figure 5 shows the axial char mass fraction temporal evolution. Initially, and because of incoming cold air very little char is formed near the ignition end. Then, as the smolder waves propagates toward the right end, all the foam is converted to char. From fig. 5 and 6, the smolder wave velocity is deduced and shown in fig. 6 as noted earlier, an initial acceleration is observed, and the velocity decreases slightly toward the right end. The observed average smolder velocity is of the order of 0.25 mm/s.

CONCLUSIONS

In this contribution an axisymmetric two-dimensional model solves the governing equations for forward propagation of smoldering in a porous fuel bed. The conservation equations for energy in the solid and the gas phases are considered separately but interact through an interfacial heat exchange. Species conservation in the solid and the gas phases, and overall mass conservation are numerically solved. The heterogeneous chemical kinetics includes pyrolysis of the fuel, and oxidation of the fuel and of the carbonaceous residual. The second oxidation is accompanied by the formation of solid ash and gas products, which pose the potential risk of transition from smoldering to flaming combustion. The obtained numerical results feature the gas and solid temperature evolutions, the char mass fraction evolution, and the smoldering propagation velocity. The finite volume method was used for the spatial discretization, and the implicit one for time. The obtained equations were solved by the Bi-Conjugate Gradient Stabilized (BI-CGSTAB) technique.

Thus, a comprehensive model analysis is presented to address several aspects related to fix fuel bed smoldering.

KEYWORDS
Smoldering; fuel bed; combustion modeling; porous media; two dimensions; Bi-CGStab.

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