18èmes Journées Internationales de Thermique (JITH 2017)
Monastir (Tunisie), 25 - 27 Octobre 2017

Computational Model of Smoldering Combustion

Saida CHATTI, Chekib GHABI, Abdallah Mhimid
Ibn El Jazzar Avenue 5000 Monastir TunisiaAdresse des auteurs
Chatti_saida@yahoo.com
ghabichekib@yahoo.fr
Abdmhimid@yahoo.fr

Abstract: Smoldering phenomenon is described as a flameless form of combustion. It deriving its heat from heterogeneous reactions happening on the surface of a solid fuel when heated in an oxidizer medium. In this work a computational study has been carried out to explain smoldering ignition and propagation in polyurethane foam. The two-dimensional, transient, governing equations for smoldering combustion in a porous fuel are established accounting for improved solid-phase chemical kinetics. The model describes opposed and forward propagation. The solid-phase kinetics suitable for numerical simulation has been developed and applied to the investigation of smoldering combustion. The numerical simulation has been effected using the lattice Boltzmann method. It predicts the reaction-front thermal and species structure, the onset of smoldering ignition, and the propagation rate. The results reproduce the features of the smolder process and represent a significant step in smoldering combustion modeling.

Key words:

Smoldering combustion, polyurethane foam, chemical kinetics, numerical simulation

Introduction

Smoldering is a surface combustion reaction that propagates through a porous combustible material [1, 2]. The heat released in the reaction is characteristically low [3]. Smoldering involves complex processes related to fluid flow and heat and mass transfer in porous media. This phenomenon is studied both theatrically and experimentally. Indeed, Ohlemiller provides two extensive reviews [1, 4] studies present in the literature. The problem of combustion is so complex. It involves fluid mechanical process and heat transfer. The complexity of the reaction limits our ability to handle such phenomena without numerical simulation. The numerical techniques for combustion become essential for engineers and research scientists [5, 6].

Recently, the lattice Boltzmann method (LBM) has emerged as an efficient alternative method for numerical simulation [7]. It is a mesoscopic technique that closed the gap between macroscopic and microscopic scale. The principle of LBM is the kinetic theory of fluid motion. It is derived from the Boltzmann transport equation. This method interests in the behavior of a cluster of particles as a unit. In fact, the simulation with LBM consists of following the evolution of fluid particle in discretized space, speed and time [8]. LBM received considerable attention due to many advantages: the convection operator of the equation is linear. It's adapted to parallel processes computing. Solving the Laplace equation is not necessary at each time step to satisfy the continuity equation. The Lattice Boltzmann method is used to model flow behavior in complex geometries thanks to its easy implementation under complex fluid–solid boundary conditions. In comparison with conventional CFD methods, the LBM has simple calculation procedure [9-11]. The main advantage of this method is the simple implementation of boundary conditions. These benefits motive the simulation of incompressible fluid flow in porous media.

In present paper, we apply the LBM to study the lattice the smoldering combustion. The kinetic process is composite of three equations. The char and the temperature profiles are presented; they describe the evolution of the phenomenon.

1. Problem presentation

The geometry of interest that was studied is shown in figure 1. It consists of a fixed bed of foam with a length and width of 15 cm. Initially, the entire foam fuel is unreacted. Air is forced to flow into the left face of the foam material. The combustion process is initiated by holding a high temperature or a high heat flux at the front during a period of time until self sustaining is obtained. The reaction zone propagates from the left to right side of the medium.

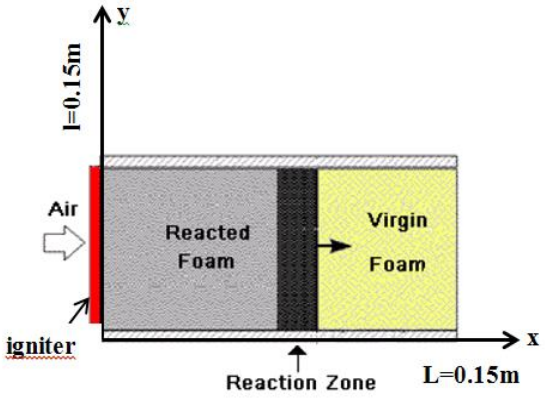

Figure 1: Forward smoldering of fixed bed of foam

2. Mathematical model

The mathematical model treats the two-dimensional time-dependent conservation equations for the solid and the gas. The computational domain follows the forward smoldering combustion. Indeed forced airflow and ignition are imposed at the same boundary. The reaction front moves in the same direction as the airflow (from right to left). The model includes the following equations [12, 13]:

2.1 Assumptions

In this simulation we adopt the following assumptions:

- The gaseous species have identical diffusion coefficients.
- The reactions didn't cause the shrinkage of volume.
- We account for the diffusion of the heat and the oxygen from the solid surface to the bulk gas.
- The porous media and the flowing gas properties are homogeneous and isotropic
- The porous matrix is rigid
- The gas is incompressible and the properties of the fluid and solid phases are constant.
- Gas-phase and condensed-phase are in thermal equilibrium.
- No homogeneous gas-phase reactions occur.
- Unit Schmidt number

2.2 Kinetic processes

The chemical reactivity of the solid is modeled with a 3 step chemical mechanism. Indeed, the fuel decomposes through endothermic pyrolysis giving gaseous products and solid char. The solid fuel undergoes also oxidation. The second step is the char oxidation; it is highly exothermic reaction in which it is converted to gaseous products and ash. The kinetic model is given as follow [14]:

The fuel pyrolysis:

$$1g\ fuel \longrightarrow n_{c2}\ char + n_{g2}\ gas$$

The fuel oxidation:

$$1g\ fuel + n_{o1}\ O_2 \longrightarrow n_{c1}\ char + n_{g1}\ gas$$

The char oxidation:

1g char + n_{o3} O_2 $\longrightarrow$ n_{a3} ash + n_{g3} gas

The mathematical expressions of the reactions rate are [14]:

2.2.1 Thermal oxidation

$$\omega_{ox} = (1 - Y_c - Y_a)^f \rho_s \, A_{ox} \left(Y_{o_2}\right)^m exp^{-\frac{E_{ox}}{RT}} \quad (1)$$

2.2.2 Pyrolysis

$$\omega_{py} = (1 - Y_c - Y_a)^g \rho_s \, A_{py} exp^{-\frac{E_{py}}{RT}} \quad (2)$$

2.2.3 Char oxidation

$$\omega_a = Y_c \, \rho_c \;\; A_a \left(Y_{o_2}\right)^h exp^{-\frac{E_a}{RT}} \quad (3)$$

The coefficients f, g, h, m represent the reaction order

2.3 conservations equations

2.3.1 Solid phase species conservation

$$\frac{\partial(\rho_s Y_c)}{\partial t} = n_{c1}\omega_{ox} + n_{c2}\omega_{py} - \omega_a \; (4)$$

$$\frac{\partial(\rho_c Y_a)}{\partial t} = n_{a3}\omega_a \quad (5)$$

2.3.2 Gas phase mass conservation

$$\frac{\partial \rho_g}{\partial \mathrm{t}} + \nabla.\left(\rho_g u\right) = \left(n_{g1} - n_{o1}\right)\omega_{ox} + n_{g2}\omega_{py} + \left(n_{g3} - n_{o3}\right)\omega_a \quad (6)$$

3.3.3 Momentum conservation

$$\frac{\partial \rho_g}{\partial t} + (u.\nabla)\left(\frac{u}{\varepsilon}\right) = -\frac{1}{\rho_g}\nabla(\varepsilon p) + \upsilon_e \nabla^2 u + F \quad (7)$$

$$F = -\frac{\varepsilon \upsilon}{K}u - \frac{\varepsilon F_\varepsilon}{\sqrt{K}}|u|u + \varepsilon G \quad (8)$$

3.3.4 Oxygen conservation in the bulk gas

$$\frac{\partial\left(\rho_g Y_{o_{2_B}}\right)}{\partial \mathrm{t}} + \nabla\left(\rho_g u Y_{o_{2_B}}\right) = \nabla\left(\rho_g D_g \nabla\left(Y_{o_{2_B}}\right)\right) + \frac{h_m S}{\varepsilon_B}\left(Y_{o_{2_S}} - Y_{o_{2_B}}\right) (9)$$

3.3.5 Oxygen conservation at the surface

$$\frac{\partial\left(\rho_g Y_{o_{2_s}}\right)}{\partial \mathrm{t}} + \nabla\left(\rho_g u_s Y_{o_{2_s}}\right) = \nabla\left(\rho_g D_g \nabla\left(Y_{o_{2_s}}\right)\right) + \frac{h_m S}{\varepsilon_s}\left(Y_{o_{2_B}} - Y_{o_{2_s}}\right) - \frac{n_{o1}}{\varepsilon_s}\omega_{ox} - \frac{n_{o3}}{\varepsilon_s}\omega_a \quad (10)$$

3.3.6 The energy conservation

$$\frac{\partial\left(\rho_s C_{ps} T\right)}{\partial t} = \nabla(\lambda_s \nabla T) + \nabla(\lambda_{rad}\nabla T) - \omega_{ox}\Delta H_{ox} + \omega_{py}\Delta H_{py} + \omega_a \Delta H_a \quad (11)$$

3. Numerical method: Lattice Boltzmann method for smoldering combustion

The lattice Boltzmann method is characterized by: simple numerical codes, easy parallel implementations and clear physical pictures. The lattice Boltzmann method is recognized as an efficient alternative for numerical simulation of complex flows. We present a lattice Boltzmann model for simulation of smoldering. It includes reaction, diffusion, and convection. The chemical reaction does not affect the flow field. Temperature, flow and concentration fields are decoupled and solved separately. The simulation of the combustion fields involves the reaction term modeling heat release and mass rate of production. We use the double-distribution-function model proposed by Shan et al. [15]. Its main feature is that the flow, temperature, and species fields are treated by two sets of distribution functions.

3.1 Flow fields

For incompressible flow, the evolution equation of the density can be written as [11]:

$$f(x + \delta t\, c_i, t + dt)_i - f(x,t)_i = \frac{f(x,t)_i - f(x,t)^{eq}}{\Gamma_\nu} + \delta t F_i \quad (12)$$

The discrete velocities of the D2Q9 model are given by:

$$\begin{cases} c_0 = 0 \\ c_i = c\left(cos\left((i-1)\frac{\pi}{2}\right), sin\left((i-1)\frac{\pi}{2}\right)\right) \quad for\ i = 1{,}4 \\ c_i = c\left(cos\left((i-1)\frac{\pi}{2} + \frac{\pi}{4}\right), sin\left((i-1)\frac{\pi}{2}\right) + \frac{\pi}{4}\right) for\ i = 5{,}8 \end{cases} \quad (13)$$

The equilibrium distribution function is [16]:

$$f_i^{eq} = \omega_i \rho\left[1 + \frac{3c_i u}{c^2} + \frac{9(c_i u)^2}{2\varepsilon^4} - \frac{3u^2}{2\varepsilon c^2}\right] (14)$$

Where the weight are: $\begin{cases} \omega_0 = \frac{4}{9} \\ \omega_i = \frac{1}{9}\ for\ i = 1{,}4 \\ \omega_i = \frac{1}{36}\ for\ i = 5{,}8 \end{cases}$

The macroscopic quantities are related to the distribution functions in many references such as [17]:

$$\rho(x,t) = \sum_{i=1}^{8} f(x,t)_i \quad (15)$$

$$u(x,t) = \sum_{i=0}^{8} \frac{c_i f(x,t)_i}{\rho} + \frac{F\delta t}{2} \quad (16)$$

3.2 Temperature and species field

The temperature is described using the diffusion convection equation. It is followed by an appropriate distribution function $g(x,c,t)$. Its evolution is given by [18]:

$$g(x + c_i\delta t, t + \delta t)_i - g(x,t)_i = -\frac{g(x,t)_i - g(x,t)_i^{eq}}{\Gamma_c} + \omega_i Q_T \delta t \quad (17)$$

The thermal equilibrium distribution function is given by [16]:

$$\begin{cases} g_0^{eq} = -\dfrac{2\rho\Sigma u^2}{3c^2} \\ g_0^{eq} = \dfrac{\rho\Sigma}{9}\left[\dfrac{3}{2} + \dfrac{3c_i u}{2c^2} + \dfrac{9(c_i u)^2}{2c^4} - \dfrac{3u^2}{2c^2}\right] \; for\; i = 1{,}4 \\ g_0^{eq} = \dfrac{\rho\Sigma}{36}\left[3 + \dfrac{6c_i u}{c^2} + \dfrac{9(c_i u)^2}{2c^4} - \dfrac{3u^2}{2c^2}\right] \; for\; i = 5{,}8 \end{cases} \quad (18)$$

The temperature using the D2Q9 LBE model is given by this equation:

$$T(x,t) = \frac{1}{\rho}\sum_{i=0}^{8} g(x,t)_i \quad (19)$$

In order to follow the species production or disappearance we define the distribution function $h(x,c,t)$ which is similar to the $g(x,c,t)$ function.

4. Simulation results

Using the lattice Boltzmann method, the temperature and the char profiles are presented at different section of the medium. For a specific time, the temperature and the char production are followed along the medium.

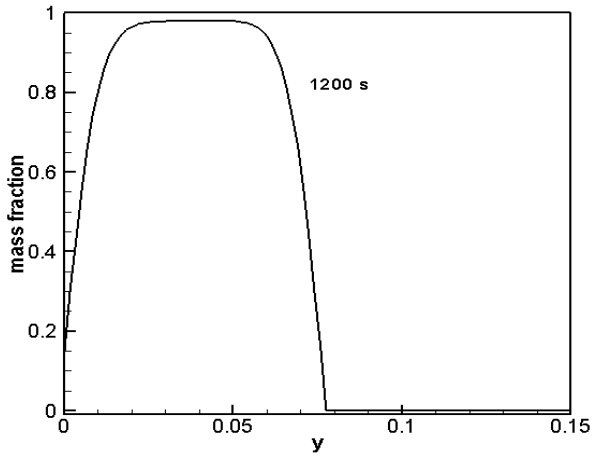

Figure 2: Char mass fraction evolution

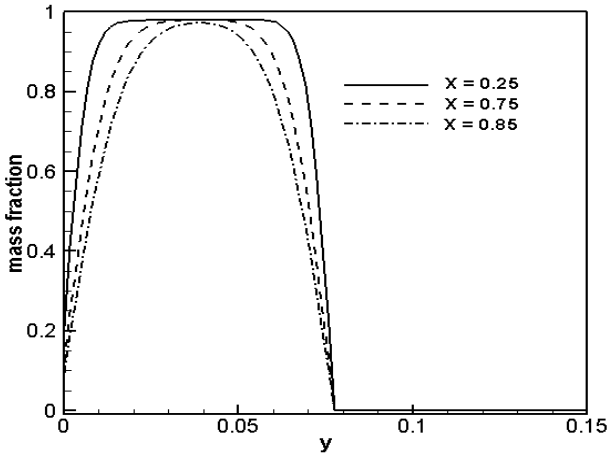

Figure 3: Char mass fraction at different cross section

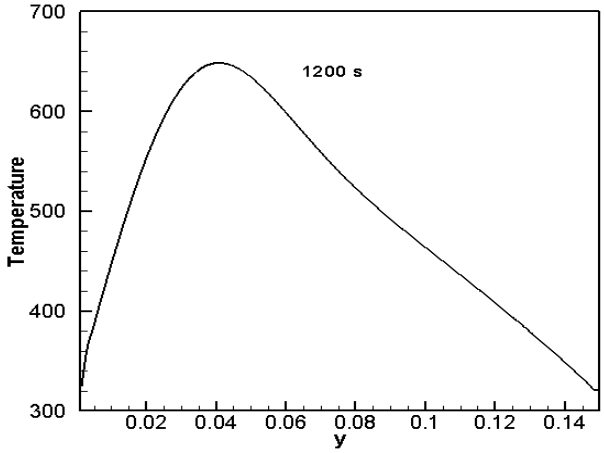

Figure 4: Temperature profile

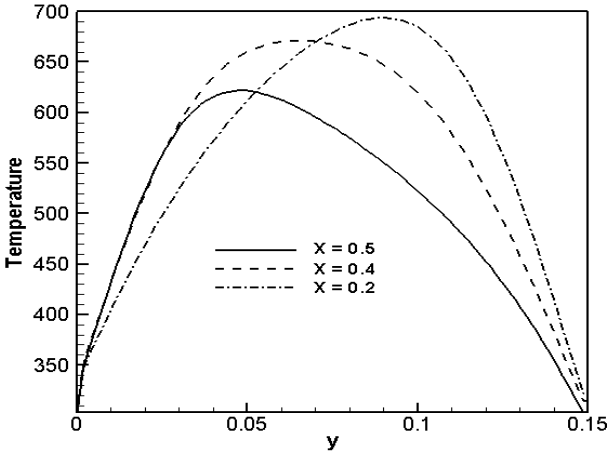

Figure 5: Temperature profile at different cross section

Conclusion

The smoldering combustion is slow flameless combustion. The reaction is heterogeneous and occurs in the interior or on the surface of the porous fuel.

The modulation of the phenomenon needs the application of particular assumptions. It is governed by the conservations equations. The resolution of these equations is complex due to the multidisciplinary aspect. The numerical simulation based on the lattice Boltzmann method is an efficient tool. It allows the control of the smoldering reaction propagation. The temperature variation and the species production are studied along the computational domain.

The LBM is used to study smolder velocity, heat released and species fractions.

Nomenclature

variable	signification	value
A_{ox}, A_{py}, A_a	Frequency factor	$5.69*10^{11}$, $2*10^{17}$, $5*10^{8}$
E_{ox}, E_{py}, E_a	Activation energy	159.88, 220.215, 159.88 K
C_{ps},C_{pc}, C_{pg}	Solid char and gas specific heat capacity	1.7 $KJKg^{-1}K^{-1}$, 1.1 $KJKg^{-1}K^{-1}$, 1.004 $KJKg^{-1}K^{-1}$
D_g, D_s	gas and solid diffusivity coefficients	
D_{g_0}, D_{s_0}	gas and solid diffusivity coefficients	$4.53*10^{-5}$
d_p	Pore diameter	5.10^{-5} m
n_{c1}, n_{c2}, n_{o1}, n_{o3}, n_{a3}, n_{g1}, n_{g2}, n_{g3}	Stoichiometric coefficient	0.21, 0.24, 0.41, 1.65, 0.03
Q_{cond}, Q_{conv}, Q_{ch}, Q_r	Heat released by conduction, convection, chemical reaction and radiation	
R	Ideal gas constant	8.31 $Jmol^{-1}K^{-1}$
T	Temperature	
T_0	Initial temperature	300 K
Y_a, Y_c, Y_{o_2}	Mole fraction	
Geek letters		
ε	Porosity	0.975
λ_g	Gas thermal conductivity	
λ_{g_0}	Initial gas thermal conductivity	
λ_s	Solid thermal conductivity	
λ_{s_0}	Initial solid thermal conductivity	
λ_{rad}	Radiation conductivity	
λ_{rad0}	Initial radiation conductivity	
ρ_c	Char density	
ρ_{c_0}	Initial char density	

ρ_g	Gas density	
ρ_{g_0}	Initial gas density	
ρ_s	Solid density	
ρ_{s_0}	Initial solid density	
ΔH_{ox}	Foam oxidation enthalpy	
ΔH_{py}	Pyrolysis enthalpy	
ΔH_a	Char oxidation enthalpy	
ω_{ox}	Foam oxidation enthalpy	
ω_{py}	Pyrolysis enthalpy	
ω_a	Char oxidation enthalpy	

References

[1] T. J. Ohlemiller, *Prog. Energ. Combust. Sci*., Volume 11, 277-310, 1986.
[2] D. Drysdale, An Introduction to Fire Dynamics, *Wiley New York*, 256, 1987.
[3] M. Summerfield and N. Mesina, *Prog. Astronaut*., Volume 73, 129-194,1981.
[4] T. J. Ohlemiller, The SFPE handbook of fire protection engineering, 3rd ed., 2.171–2.179, 1995.
[5] N. Peters, Turbulent Combustion, *Cambridge University Press*, Cambridge, 2000.
[6] T. Poinsot and D. Veynante, Theoretical and Numerical Combustion, *R.T. Edwards Inc*., Philadelphia, 2001.
[7] L. Li, R. Mei, J. F. Klausner, Boundary conditions for thermal lattice Boltzmann equation method, *Journal of Computational Physics*, Volume 237, 366–395, 2013
[8] G.H Tang , W. Q. Tao, and Y. L. He, Simulation of fluid flow and heat transfer in a plane channel using the lattice Boltzmann method, International journal of modern physics B, Volume17, 183-187, 2003
[9] T. Seta, E. Takegoshi, K. Kitano, K. Okui, Thermal lattice Boltzmann model for incompressible flows through porous media, *Journal of Thermal Science and Technology*, Volume 1, 90-100, 2006
[10] Z. Guo and T. S. Zhao, *Lattice Boltzmann model for incompressible flows through porous media*, Physical review, Vol.66, 036304-1-036304-9, 2002
[11] S. Chatti, C. Ghabi, A.Mhimid, Effect of Obstacle Presence for Heat Transfer in Porous Channel, *Springer International Publishing Switzerland*, 823-832, 2015.
[12] S. V. Leach, G. Rein, J. L. Ellzey, and O. A. Ezekoye, J. L. Torero, Kinetic and Fuel Property Effects on Forward Smoldering Combustion, *combustion and flame*, Volume 120, 346–358, 2000.
[13] A.B. Dodd, C. Lautenberger, A.C. Fernandez-Pello, Numerical examination of two-dimensional smolder structure in polyurethane foam, *Proceedings of the Combustion Institute*, Volume 32, 2497–2504, 2009.
[14] C. Ghabi, H. Benticha and M. Sassi, Parametric study of the heat transfer coefficient in bi-dimensional smoldering simulation, *Thermal science* Volume 11, 95-112, 2007.
[15] K. Yammamoto, X. He, G. D Doolen, Combustion simulation using the lattice Boltzmann method, JSME International journal Serie B, Volume 47, 403- 409, 2004.
[16] S. CHATTI, C. GHABI, A.MHIMID, fluid flow and heat transfer in porous media and post heated obstacle: Lattice Boltzmann simulation, *International journal of heat and technology*, Volume 38, 377-385, 2016.
[17] M.A Mussa, S. Abdullah, C.S. Nor Azwadi, N. Muhamad, Simulation of natural convection heat transfer in an enclosure by the lattice-Boltzmann method, *computers and fluids*, Volume 44, 162- 168, 2011.
[18] K. Yamamoto, X. He and G. D. Doolen, Simulation of Combustion Field with Lattice Boltzmann Method, *Journal of Statistical Physics*, Volume 107, 367- 383, 2002.