ISSN 2176-5480

22nd International Congress of Mechanical Engineering (COBEM 2013)
November 3-7, 2013, Ribeirão Preto, SP, Brazil

A LEVEL SET MODEL FOR MULTIDIMENSIONAL SIMULATIONS OF FLAMES IN POROUS MEDIA

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Abstract. *The simulation of multidimensional premixed flames within porous media demands the solution of a complex set of conservation equations, including the solid phase heat diffusion, solid to solid radiation and interphase surface heat transfer. For the momentum equation additional terms should be included in order to model the heat loss induced by the solid matrix. Since the numerical solution of such set of equations is computationally demanding there is interest in simplified models that are able to predict the main thermal characteristics of porous burners with reduced computational cost. The objective of the present work is to compare a conventional model for flames in porous media with a model based on the level set formulation. The conventional model is the one that solves the entire set of conservation equations while in the level-set model the species equations are replaced by G-equation, which describes the dynamics of an infinitely thin flame front. The problem considered for the analysis is a two-dimensional slot burner with prescribed fields of inlet speeds and outlet pressure. The numerical methodology used to solve the set of conservation equations is the finite element method with a Cartesian coordinate system. The advantages and limitations of the proposed model are discussed.*

Keywords: *combustion in porous media; level-set method; multidimensional simulation*

The rapid advance in technology and improvement in living standards required the use abundant fossil fuels which brogth two important challenges for any nation (Abdul Mujeebu et al., 2009). One is the rapid reduction of fossil fuel sources, and the other is the environmental pollution. According to the authors, the combustion in porous media is one of the new technologies that will help in facing such challenges.

Combustion in porous inert media is characterized by a mechanism of recirculation of heat from the combustion products to the incoming reactants. This heat recirculation extends the flame stability and allows for the burning of fuels with low heat content (Wood and Harris, 2008). As noted by many authors (Brenner et al., 2000, Talukdar et al. 2004, Mishra et al. (2006), Wood and Harris 2008 and Abdul Mujeebu et al. 2009), the combustion in porous media has an interesting advantages compared with the free flame combustion due to higher firing rates, the increased turn-down ratio, the exteded n limits of flammability and low emission of pollutants, such as , carbon monoxide (CO) and nitrogen oxides (NO_x).

Brenner et al. (2000), Moraga et al. (2008) and Harris and Wood (2008) report that the porous burners are already commercially available and are applications in various fields including heat and water environments, heating and pre-heaters for cars, metal heat treatment , coating and paint drying, chemical processing, glass manufacturing, wood and paper drying and food processing.

When dealing with engineering problems each application requires different solutions in terms of power, operational temperature and burner shapes. Then, the multiple scale nature of the problem, the stiffness and nonlinearity of the chemical reaction terms, combined with the nonlinearity of the flow in porous media and the 3D geometries of interest, bring difficulties in building useful design tools to the development of new burners because of the large computational effort involved. Simplified models that could predict the most important thermal aspects of the combustion within porous media, with reduced computational effort, would be of great interest for engineering applications.

The objective of the present work is to construct a simplified model, based on the level set formulation, for the simulation of multidimensional premixed flames in porous inert media able to predict the main thermal characteristics of porous burners with reduced computational time.

ISSN 2176-5480

1. MATHEMATICAL FORMULATION

1.1 The level set model

Duchamp de Langeneste and Pitsh (2002) describe that the method of level set has been used to describe the dynamic evolution of the fronts and discontinuities. According to Pereira (2009), the level set method is based on a transport equation for a scalar non-reactive G, which describes the propagation of the flame front. The thickness of the flame is assumed to be small and the problem is reduced to a thin reactive layer separating the exhaust of unburned.

According to Poinsot and Veynante (2000), the transport equation describing the evolution of a continuous field of which in a particular iso-level provides the location of the forward reaction, or the flame is located on the iso-surface $G = G_o$. According to Duchamp de Langeneste and Pitsh (2000) and Pitsh and Duchamp de Langeneste (2002), this level is the advection velocity field outside $\vec{U}$, while this iso-surface normal propagates itself with the laminar flame speed s_L. Duchamp de Langeneste and Pitsh (2000), Pitsh and Duchamp de Langeneste (2002) and Pereira (2009) argue that shifting flame front depends on the local balance between the flow velocity and the velocity of flame propagation and the dynamics this reactive layer is described by the equation-G.

The flame is located at the isosurface G = G0, and the dynamics of this iso-surface is described by the G equation defined in Eq. (1). It is a kinematic equation stating that a point at an isosurface remains at this isosurface for any time (i.e., the material derivative normal to the flame front – lefte hand side - is equal to the propagation term – right hand side). The local variation of the scalar G is the result of the balance between the convection term and the propagation term.

$$\frac{\partial G}{\partial t} + \underbrace{\vec{U}.\vec{\nabla} G}_{\text{Convection}} = \underbrace{s_L \left|\vec{\nabla} G\right|}_{\text{Propagtion}} . \tag{1}$$

At the flame surface jump conditions may be written relating the reactants and the combustion products. For combustion in porous media it is more convenient to define a heat release term at the flame front to be included in the energy conservation equation. The advantage of using the level set formulation is that the species mass conservation may be neglected and all the kinetic information needed is the flame speed in Eq. (1). Thid results in a much fast solution since a simplified set of equationsmay be considered. On the other hand details of the reaction region are lost and the reaction sheet approximation implies a an infinite velocity for the propagation of any perturbation (e.g. heat losses) through the reaction front. For the solution of steady state problems these limitations don't seem to be much important.

1.2 Reinitialization step

The G-equation have a meaning only at the flame front where the flame velocity is defined. Then, to solve Eq. (1) is convenient to keep the G field as a signed distance function, i.e., to keep gradient module G equal to the one. In other words it is useful to replace the level-set function by a better behaved function which has the same zero level set of the original function. This condition needs to be enforced, which is commonly called reinitialization. Russo and Smereka (2000) state that a reinitialization is important because in many applications the level set function obtained by solving the G-equation may become distorted due to too large gradients near the interface (flame).

The reinicialization method is based on the transient solution of the following equation:

$$\frac{\partial G}{\partial t} = \text{sgn}_{i,j}\left(1 - \left|\vec{\nabla} G\right|\right), \tag{2}$$

where $\text{sgn}_{i,j}$ is sign function given by:

$$\text{sgn}_{i,j} = \frac{G_0}{\sqrt{G_0^2 + \left|\vec{\nabla} G\right|^2 \Delta x^2}} . \tag{3}$$

Sussman, Smereka and Osher (1994), Chen et al. (1997) and Russo and Smereka (2000) report that Eq. (1) written in the form discretized into a two-dimensional problem is given by:

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$$G_{i,j}^{n+1} = G_{i,j}^{n} - \Delta t.\mathrm{sgn}_{i,j}.G(G)_{i,j}, \tag{4}$$

where:

$$G(G)_{i,j} = \begin{cases} \sqrt{\max\left(a_{+}^{2}, b_{-}^{2}\right) + \max\left(c_{+}^{2}, d_{-}^{2}\right)} & se\ G_{0_{i,j}} > 0 \\ \sqrt{\max\left(a_{-}^{2}, b_{+}^{2}\right) + \max\left(c_{-}^{2}, d_{+}^{2}\right)} & se\ G_{0_{i,j}} < 0 \end{cases}, \tag{5}$$

where: Δt is the time interval, i and j are the positions in the mesh (respectively x e y), max is the maximum value among the values described, Δx is the difference between two values x on the horizontal axis, Δy is the difference between two values y on the axis of ordinates and a, b, c and d are third-order ENO approximations to the gradient of G in each direction. This ENO method allows one to extend first-order accurate upwind diferencing to higher-order spatial accuracy by providing better numerical approximations to G^{-} or G^{+}.

1.3 Numerical methodology

The physical-mathematical model of the porous burner described in this paper was solved numerically using a FORTRAN code. The numerical model is based on the finite volume method and finite differences, besides the use of the SIMPLE algorithm to solve the pressure-velocity coupling. To ensure that the pressure field satisfies the equation of continuity mating components of velocity and pressure through the use of outdated elements for the velocity field. The combustion was treated with a global model of reactions (chemical kinetics) of a step. To solve the convective and diffusive terms in the conservation equations adopted the hybrid differential scheme which combines the Upwind scheme with the scheme of central differences. To solve the source term of the G-equation, and the procedure of its reinitialization, adopted the scheme of Godunov as Duchamp de Langeneste and Pitsh (2002), which discretizes the derivatives with ENO scheme. The proposed model is under construction and only the results for the reinitialization procedure will be shown.

1.4 Phisical and mathematical modeling

The set of conservation equations for reacting flows in porous media is based on the semi-heuristic formulation presneted by Kaviany (1995), where the equations a presented in a volume averaged form. Below it is shown the conservation equations for the mass, momentum, energy for the fluid phase, the energy for the solid phase and the chemical species:

$$\frac{\partial \left\langle \rho_f \right\rangle^f}{\partial t} + \vec{\nabla}.\left(\left\langle \rho_f \right\rangle^f \left\langle \vec{u}_D \right\rangle^f \right) = 0, \tag{6}$$

$$\frac{\left\langle \rho_f \right\rangle^f}{\varepsilon}\left(\frac{\partial \left\langle \vec{u}_D \right\rangle}{\partial t} + \left\langle \vec{u}_D \right\rangle.\vec{\nabla}\left\langle \vec{u}_D \right\rangle \right) = -\vec{\nabla}\left\langle p \right\rangle^f + \frac{\mu_f}{\varepsilon}\nabla^2\left\langle \vec{u}_D \right\rangle - \frac{\mu_f}{\mathbf{K}}\left\langle \vec{u}_D \right\rangle - \frac{C_E}{\sqrt{\mathbf{K}}}\left\langle \rho_f \right\rangle^f \left|\left\langle \vec{u}_D \right\rangle\right|\left\langle \vec{u}_D \right\rangle, \tag{7}$$

$$\varepsilon\left\langle \rho_f \right\rangle^f \left\langle c_{p,f} \right\rangle^f \frac{\partial \left\langle T_f \right\rangle^f}{\partial t} + \varepsilon\left\langle \rho_f \right\rangle^f \left\langle c_{p,f} \right\rangle^f \vec{u}_D.\vec{\nabla}\left\langle T_f \right\rangle^f = \varepsilon\vec{\nabla}.\left(\left\langle k_f \right\rangle^f.\vec{\nabla}\left\langle T_f \right\rangle^f \right) + \\ + \frac{A_{sf}}{V}h_c\left(\left\langle T_s \right\rangle^s - \left\langle T_f \right\rangle^f \right) - \varepsilon\sum_{k=1}^{N_{sp}}\left\langle \dot{\omega}_k \right\rangle^f M_k h_k, \tag{8}$$

$$(1-\varepsilon)\left\langle \rho_s \right\rangle^s \left\langle c_{p,s} \right\rangle^s \frac{\partial \left\langle T_s \right\rangle^s}{\partial t} = (1-\varepsilon)\vec{\nabla}.\left(\left\langle k_s \right\rangle^s.\vec{\nabla}\left\langle T_s \right\rangle^s \right) - \frac{A_{sf}}{V}h_c\left(\left\langle T_s \right\rangle^s - \left\langle T_f \right\rangle^f \right) + \vec{\nabla}.\left\langle \vec{q}_r \right\rangle, \tag{9}$$

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$$\varepsilon \left\langle \rho_f \right\rangle^f \left(\frac{\partial \left\langle Y_k \right\rangle^f}{\partial t} + \left\langle \vec{u}_D \right\rangle . \vec{\nabla} \left\langle Y_k \right\rangle^f \right) = \varepsilon \vec{\nabla} . \left[\left\langle \mathbf{D}_{m,k} \right\rangle^f \left\langle \rho_f \right\rangle^f \right] \vec{\nabla} \left\langle Y_k \right\rangle^f + \varepsilon \left\langle \dot{\omega}_k \right\rangle^f M_k$$

$$\text{with } k = 1,2,...,N_{sp} - 1 . \qquad (10)$$

Where the symbol $\langle\ \rangle$ means a volume averaged over a representative elementary volume. The parameters ρ_f is the density of the fluid, $\vec{u}_D$ is the Darcy velocity vector, ε is the porosity, p is the pressure, C_E is the Ergun constant, μ_f is the fluid viscosity, $\mathbf{K}$ is the permeability tensor of the porous medium V is the total volume, $c_{p,f}$ is the specific heat at constant pressure of the fluid, T_f is the fluid temperature, A_{sf} the area between solid and fluid, h_c is the heat transfer coefficient by convection, T_s is the temperature of the solid, N_{sp} is the number of chemical species, $\dot{\omega}_k$ is the volume mass production rate of chemical species k due to chemical reaction, M_k the molecular weight and the chemical species k, h_k is the specific enthalpy of the chemical species k, $c_{p,s}$ is the specific heat at constant pressure of the solid, $\mathbf{k}_{e,s}$ is a tensor effective thermal conductivity of the solid, $\vec{q}_r$ is the radiant heat flux vector, $\mathbf{D}_{m,k}$ is the mass diffusivity of chemical species k and Y_k is the mass fraction of chemical species k.

For the level set model the equation for the species is not solved and the heat release term at the energy equation is replaced by a term derived from the *G* field. For the solution of the G-equation, an analytical expression is used for the laminar flame speed s_L within porous media (Pereira, 2009).

1.5 Numerical methodology

The physical-mathematical model of the porous burner described in this paper was solved numerically using a FORTRAN code. The numerical model is based on the finite volume method and finite differences, besides the use of the SIMPLE algorithm to solve the pressure-velocity coupling. To ensure that pressure field satisfies the equation of continuity mating components of velocity and pressure through the use of outdated elements for the velocity field. The combustion was treated with a global model of reactions (chemical kinetics) of one step. To solve the convective and diffusive terms in the conservation equations it was adopted the hybrid differential scheme which combines the Upwind scheme with the scheme of central differences. To solve the source term of the equation-G, and the procedure of its reinitialization, adopted the scheme of Godunov as Duchamp de Langeneste and Pitsh (2002), which discretizes the derivatives with ENO scheme.

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1.7 Results for the reinitialization of a two-dimensional distorted field

To evaluate the ability of this method to maintain the initial position of the zero level-set, while changing the G fiel to a signed distance function, two test problems containing regions of low and high gradients near the zero level-set interface is solved (Russo and Smereka (2000) and Duchamp de Langeneste and Pitsh (2002)):

$$G_0(x, y, 0) = \sqrt{x^2 + y^2} - 4 , \qquad (11)$$

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$$G_0(x, y, 0) = \left[0{,}1 + (x - 3{,}5)^2 + (y - 2)^2\right]\left[\sqrt{\left(\frac{x}{4}\right)^2 + \left(\frac{y}{2}\right)^2} - 1\right], \tag{12}$$

where Eq.(11) represents a G field in with the zero level set is a circumference and Eq. (12) represents a G field in with the zero level set is an ellipse. To reinitialize these fields we used a uniform grid with17x17 volumes for the circunference case and 50x50 volumes for the ellipse case. In both cases, the contours ranging from -1 to 0.6 and are spaced by 0.2 and the results were obtained using the reset function equation signal defined by equation (4). To solve numerically the reset procedure of the G-equation adopted the scheme of Godunov as Duchamp de Langeneste and Pitsh (2002).

Figure 1 shows the reconstruction of the two-dimensional distance function using equation (3) with the initial condition given by equation (11) the following numbers of iterations: 0, 50, 160 and 320.

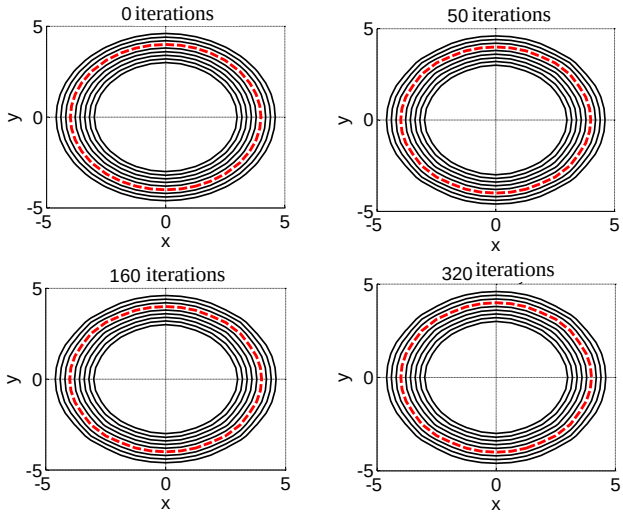

Figure 1. Reconstruction of two-dimensional distance function using equation (3) with the initial condition given by equation (11) the following numbers of iterations: 0, 50, 160 and 320

Figure 2 shows the reconstruction of the two-dimensional distance function using equation (3) with the initial condition given by equation (12) the following numbers of iterations: 0, 10, 25 and 50.

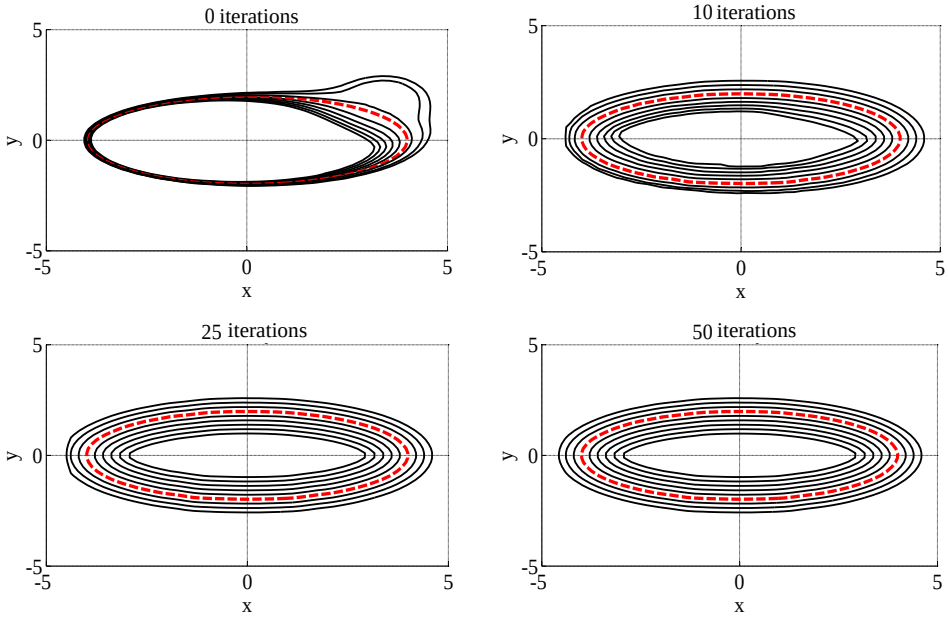

Figure 2. Reconstruction of two-dimensional distance function using equation (3) with the initial condition given by equation (12) the following numbers of iterations: 0, 10, 25 and 50

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The zero level curve is shown in Figures 1 and 2 by the dotted line in red. This means that our choice of initial conditions given by the equations (11) and (12) have low and high gradient near zero contour as viewed in Figure 2.

Figure 3 shows the curves of zero G to the circumference of the following numbers of iterations: 0, 50, 160 and 320 while Figure 4 shows the contour of zero G for the ellipse to the following number of iterations: 0, 10, 25 and 50. These figures show that the the zero level of the G field is preserved during the reinitialization procedure as required.

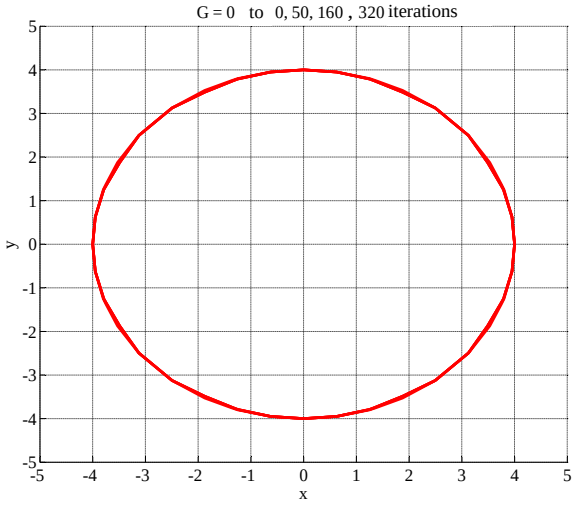

Figure 3. Zero level curves G of the circumference to the following numbers of iterations: 0, 50, 160 and 320

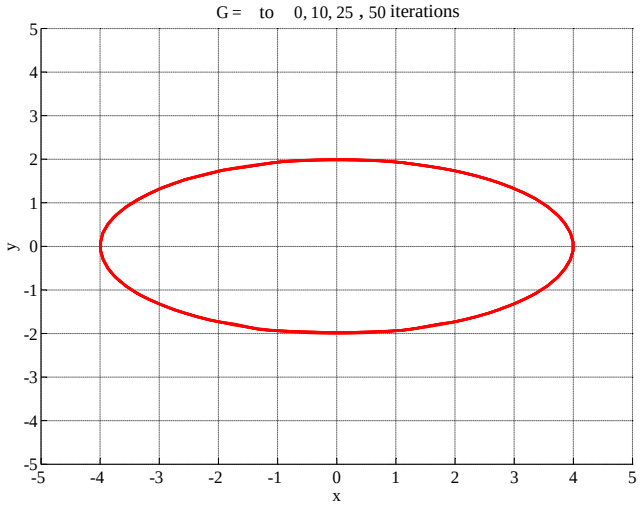

Figure 4. Contours of zero G for the ellipse to the following number of iterations: 0, 10, 25 and 50

It appears in Figures 3 and 4 that with the use of equation (3) the lines of the zero level G for different numbers of iterations performed practically overlap, i.e. the zero-level interface G hardly move. Finally, it is concluded that the results correspond to those found in the literature consulted.

2. CONCLUSION AND NEXT STEPS

The results obtained for the reinitialization procedure is in accordance with those present in literature. A next step to be done, will be the implementation of the source term with an analytical expression for the laminar flame speed in porous media and to obtain the numerical solution of a two-dimensional burner.

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