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A Numerical Solution of a Model for Heat Transfer in Moving Beds

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This article aims to study the heat transfer in the pyrolysis of oil shale in a diluted and concurrent moving bed reactor. It was developed a numerical solution for a non-linear heat transfer (convective and radiant) model through the orthogonal collocation method. In this method the particle interior temperature profile is approximated by an orthogonal polynomial of an arbitrary degree that is replaced into the model equations generating a system of ordinary differential equations. The results obtained were compared with an existing analytical solution of the quasi-linearized heat transfer model. The comparison shown an excellent agreement in the range of the parameters analyzed.

KEYWORDS: Orthogonal collocation method, numerical solution, pyrolysis, heat transfer, oil shale.

1. Introduction

Brazil owns the second largest reserves of oil shale in the world. The main oil shale deposits are located less than 100 meters deep and are distributed in layers of variable thickness and distinct levels of kerogen. Generally, the content of organic matter in the deposits of oil shale ranges between 5% and 25%, as in the Irati formation of oil shale at São Mateus do Sul – PR, Brazil, which has a 9% average in oil. Under this perspective of research, aiming new sustainable ways of composing the global energy matrix, the decomposition of oil shale and gas has been studied in various aspects, and largely in the field of Chemical Engineering. Because it is a non-renewable resource and generates hazardous products for to the environment, it has been largely invested in research in order to achieve technologies combining energy efficiency with environmental sustainability. In this way, other works have developed analytical solutions for heat transfer models of pyrolysis in diluted moving beds: Bertoli (1989, 2000) using the Laplace Transform and the Duhamel theorem; Meier et al. (2009) through the self-adjoint operator method. Those solutions incorporate a quasi-linearized radiant heat transfer coefficient between the wall and the particle:

$$hr = \varepsilon_P \sigma \left(Tw^2 + Tps^2\right)\left(Tw + Tps\right). \tag{1}$$

With the aim of to evaluate the nonlinear radiant effects, in the present work a numerical solution by the orthogonal collocation method is given. The results obtained are compared with an existent analytical solution (Bertoli, 1989, 2000).

2. Model Equations

The main assumptions in the present analysis are the same as described in Bertoli (1989, 2000). The equation of the model differs only by the fact that now the radiant term isn´t linearized. The equations for the fluid and the particle are:

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$$\frac{dT_f}{dt} = \frac{h_w A_w u_p}{V \rho_f C_f u_f} \left(T_w - T_f\right) - \frac{n_v h_p A_p u_p}{V \rho_f C_f u_f} \left(T_f - T_{ps}\right) \quad ; \tag{2}$$

$$\frac{\partial T_p}{\partial t} = \frac{\alpha}{\xi^2} \frac{\partial}{\partial \xi} \left[\xi^2 \frac{\partial T_p}{\partial \xi} \right] \quad . \tag{3}$$

With the following initial and boundary conditions:

$$T_p \left(\xi, 0\right) = T_f(0) = T_i \quad ; \tag{4}$$

$$\frac{\partial T}{\partial \xi}\Big|_{\xi=0} = 0 \quad ; \tag{5}$$

$$-\frac{\partial T_p}{\partial \xi}\Big|_{\xi = R_p} = \frac{h_p}{k_p}\left(T_{ps} - T_f\right) + \frac{\varepsilon_p \sigma}{k_p}\left(T_{ps}{}^4 - T_w{}^4\right) \quad . \tag{6}$$

Defining the dimensionless variables:

$$\theta_f \equiv \frac{T_f}{T_i} \quad , \quad \theta_p \equiv \frac{T_p}{T_i} \quad , \quad r \equiv \frac{\xi}{R_p} \quad , \quad \tau \equiv \frac{\alpha_p t}{R_p^2} \quad ,$$

$$\theta_w \equiv \frac{T_w}{T_i} \quad , \quad \beta_1 \equiv \frac{h_p R_p}{k_p} \quad , \quad \beta_2 \equiv \frac{\varepsilon_p \sigma R_p T_i{}^3}{k_p} \quad ,$$

$$\beta_3 \equiv \frac{h_w A_w u_p R_p{}^2}{V \rho_f C_f u_f \alpha_p} \quad , \quad \beta_4 \equiv \frac{n_v h_p A_p u_p R_p{}^2}{V \rho_f C_f u_f \alpha_p} \quad ,$$

the following equations are identified:

$$\frac{d\theta_f}{d\tau} = \beta_3 \left(\theta_w - \theta_f\right) - \beta_4\left(\theta_f - \theta_p|_1\right) \quad , \tag{7}$$

$$\frac{\partial \theta_p}{\partial \tau} = \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \frac{\partial \theta_p}{\partial r} \right] \quad , \tag{8}$$

$$\theta_p\left(r, 0\right) = \theta_f\left(0\right) = 1 \quad , \tag{9}$$

$$\frac{\partial \theta_p}{\partial r}\Big|_{r=0} = 0 \quad , \tag{10}$$

$$-\frac{\partial \theta_p}{\partial r}\Big|_{r=1} = \beta_1\left(\theta_p|_1 - \theta_f\right) + \beta_2\left(\theta_p^4\big|_1 - \theta_w^4\right) \quad . \tag{11}$$

Also, with the variable change, $u = r^2$, it follows that:

$$\frac{d\theta_f}{d\tau} = \beta_3\left(\theta_w - \theta_f\right) - \beta_4\left(\theta_f - \theta_p|_1\right) \quad , \tag{12}$$

$$\frac{\partial \theta_p}{\partial \tau} = 4\left\{ u \; \frac{\partial^2 \theta_p}{\partial u^2} + \frac{3}{2} \; \frac{\partial \theta_p}{\partial u} \right\} \quad , \tag{13}$$

$$-2\frac{\partial \theta}{\partial u}\Big|_{u=0} = \sqrt{u}\,\frac{\partial \theta}{\partial u}\Big|_{u=0} = 0 \quad , \tag{14}$$

$$-2\frac{\partial \theta_p}{\partial u}\Big|_{u=1} = \beta_1\left(\theta_p|_1 - \theta_f\right) + \beta_2\left(\theta_p^4\big|_1 - \theta_w^4\right). \tag{15}$$

3. Polynomial Approximation

The following polynomial approximation is introduced:

$$\theta_p(u,\tau) \cong \overset{n+1}{\theta_p}(u,\tau) = \sum_{j=1}^{n+1} \ell_j(u)\,\theta_{pj}(\tau) + a(\tau)(u-1)\overset{(1,1/2)}{Pn}(u) \tag{16}$$

or

$$\overset{n+1}{\theta_p}(u,\tau) = \sum_{j=1}^{n+1} \ell_j(u)\,\theta_{pj}(\tau) + b(\tau)(\mathrm{u}-1)\frac{\overset{(1,\,1/2)}{Pn}(u)}{\overset{(1,\,1/2)}{Pn}(1)} \cdot \tag{17}$$

Where:

$\ell_j(\mathrm{u}) = \mathrm{j_{th}}$ Lagrange interpolating polynomial ,

$\overset{(1,\,1/2)}{Pn}(u) =$ a Jacobi polynomial of order n ,

$b(\tau) = a(\tau)\,P_{n\,(1)}^{(1,\,1/2)}.$

Now defining,

$$p_{NT}(u) \equiv (u-1)\,\overset{(1,\,1/2)}{P_n}(u) \quad . \tag{18}$$

It follows that:

$$u\,\frac{d^2 p_{NT}}{du^2} + \frac{3}{2}\,\frac{dp_{NT}}{du} = (n+1)(n+3/2)\overset{(1,1/2)}{P_n(u)} \quad . \tag{19}$$

By the orthogonal collocation method, the collocation points are chosen as the zeros of a Jacobi polynomial; in this case, $\overset{(1,1/2)}{P_n(u)}$, then,

$$u\,\frac{d^2 p_{NT}}{du^2} + \frac{3}{2}\,\frac{dp_{NT}}{du} = \begin{cases} 0 & i = 1, \ldots\ldots\ldots n \\ (n+1)(n+3/2)\,\overset{(1,\,1/2)}{P_n}(1) & i = n+1 \end{cases}$$

where i = 1, ... n are internal collocation points.

Therefore, from Eq. (2) – (5) we have

$$\frac{d\theta_f}{d\tau} = \beta_3 \left(\theta_w - \theta_f\right) - \beta_4 \left(\theta_f - \theta_{pN+1}\right) \quad , \tag{20}$$

$$\frac{d\theta_{pi}}{d\tau} = 4 \sum_{j=1}^{n+1} \left[u_i B_{ij} + \frac{3}{2} A_{ij} \right] \quad i = 1, \ldots n \quad , \tag{21}$$

$$\frac{d\theta_{pN+1}}{d\tau} = 4 \sum_{j=1}^{n+1} \left[u_{N+1} B_{N+1,j} + \frac{3}{2} A_{N+1,j} \right] \theta_{pj} + 4 \, (n+1) \, (n + 3/2) \, b(\tau) \tag{22}$$

$$-2 \sum_{j=1}^{n+1} A_{n+1} \theta_{pj} - 2b(\tau) \left\{ \frac{d}{du} (u-1) \ell_{n+1} (u) \right\}_{u=1} = \beta_1 \left(\theta p \Big|_1 - \theta f \right) + \beta_2 \left(\theta_p^4 \Big|_1 - \theta_w^4 \right) \tag{23}$$

The term in brackets in the last equation is equal 1. Also,

$$Aij = \frac{d\ell j}{du}\Big|_{u_i} \quad and \quad Bij = \frac{d^2 \ell j}{du^2}\Big|_{u_i}$$

The resulting system is:

$$\frac{d\theta_{pi}}{d\tau} = \sum_{j=1}^{n+1} C_{ij} \, \theta_{pj} \quad i = 1, \ldots n \quad , \tag{24}$$

$$\frac{d\theta_{N+1}}{d\tau} = \sum_{j=1}^{n+1} C_{N+1,j} \, \theta_{pj} + 4 \, (n+1)(n+3/2) \, b(\tau) \quad , \tag{25}$$

$$\frac{d\theta_f}{d\tau} = \beta_3 \left(\theta_w - \theta_f\right) - \beta_4 \left(\theta_f - \theta_{pN+1}\right) \quad , \tag{26}$$

$$\theta_{po} = \theta_{fo} = 1 \qquad i = 1, \ldots n + 1 \quad . \tag{27}$$

Where:

$$C_{ij} = 4 \left\{ u_i B_{ij} + \frac{3}{2} A_{ij} \right\} \quad , \tag{28}$$

$$a(\tau) = -\sum_{j=1}^{n+1} A_{N+1,j} \theta_{pj} - \frac{\beta_1}{2} \left(\theta_{N+1} - \theta_f\right) - \frac{\beta_2}{2} \left(\theta_{N+1}^4 - \theta_w^4\right) \quad . \tag{29}$$

Also, the mean temperature of the particle is given by

$$\overline{\theta_p}(\tau) = \frac{3}{2} \int_0^1 u^{1/2} \, \theta_p^{(n+1)}(u,\tau) du = \sum_{j=1}^{n+1} w_j \, \theta_{pj} \tag{30}$$

Were, w_j = weight of the quadrature (Radau quadrature with inclusion of u = 1).
More details in the collocation method are given by Villadsen *et al.* (1978).

4. Results

For the integration of the system of Eq. (6)–(9) we choose as initial step, $h_0 = 1,0 \times 10^{-5}$ and as precision, $\varepsilon = 1 \times 10^{-6}$. Also, the following parameters were obtained from Bertoli (1989, 2000) (thermal test Nº 5).

$$\beta_1 = 0.04823\,;\ \beta_2 = 1.663\,x\,10^{-4}\ ;$$

$$\beta_3 = 0.09250\ ;\ \beta_4 = 0.4260.$$

For $\tau = 0$, the Jacobian of the system of Eq. (6) – (9) is ($N = 2$; $\varepsilon = 1 \times 10^{-6}$; $h_o = 1 \times 10^{-5}$; $\alpha = 1$; $\beta = ½$):

$$J = \begin{bmatrix} -15.70 & 20.03 & -4.36 & 0 \\ 9.965 & -44.33 & 34.36 & 0 \\ -8.700 & 137.7 & -130.05 & 1.013 \\ 0 & 0 & 0.4537 & -0.546 \end{bmatrix}.$$

This Jacobian matrix has the following eingenvalues:

$$\lambda_1 = -169.22\ ;\ \lambda_2 = -20.71\ ;\ \lambda_3 = -0.033$$

$$\lambda_4 = -0.6769\ .$$

in this case, the problem is stiff. So, for integration of the system formed by Eq. (6) - (9) we use a third order semi-implicit Runge Kutta method STIFF 3 (Villadsen et al., 1978). The Figure (1) and Figure (2) were generated to demonstrate the variation of the mean temperatures of the particle and of the fluid along the reactor, respectively. The set of conditions were those of the thermal test Nº 5 presented in Bertoli (2000) (except for the wall temperature and the temperatures at the reactor entrance).

The results of the Figures (1) and (2) were obtained at *Tw* = 500 ° C and *Tfi* = *Tpi* = 150 ° C; they shown excellent agreement in the numerical solution of this non-linear model and the analytical solution presented in Bertoli (1989). This agreement is possible because in the region where the greater flow of radiant heat transfer occurs for the particle (near the entrance of the reactor) the quasi-linearization of the radiant contribution is an adequate approximation if the temperature of the particle surface does not vary significantly; that probably is due to the high heat capacity of the solid, associated with the convective heat transfer between the fluid and the particle. Furthermore, in the region where the temperature of the particle surface is high, the temperature difference *(Tw - Tps)* is small and therefore at this point, the radiation is a small portion of the total heat transferred to the particle in the reactor. It is important to note that although the wall temperature is 500ºC, radiant on the surface of the particles $(Qrad\ /\ Qtotal)_{ps}$ flow is in the range 60-80% by analytical solution (Bertoli, 1989).

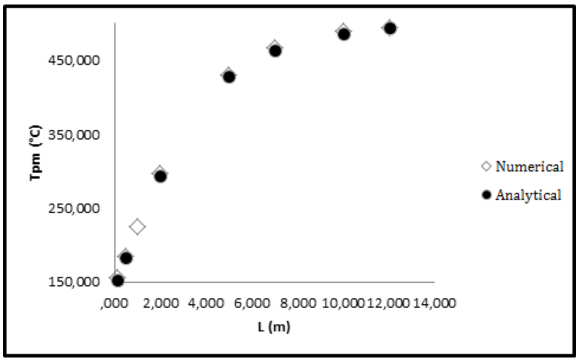

Figure 1: Variation of average particle temperature along the reactor

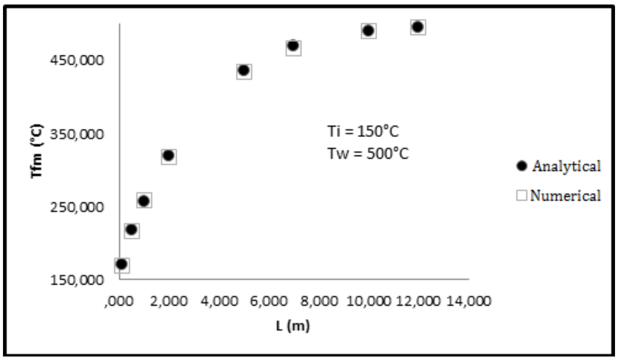

Figure 2: Changes in mean temperature of fluid along the reactor.

5. Conclusion

The agreement between the numerical and analytical solutions demonstrates the capability of the orthogonal collocation method in to handle the problem of heat transfer in moving beds. Also in the present work it was possible to confirm several results from the literature obtained with the analytical solution of the equivalent linearized heat transfer model for moving beds: In Bertoli (1989, 2000) it was pointed that radiant heat transfer between the particle and the wall plays an important role and cannot be neglected in comparison with the fluid–particle convective heat transfer; in Bertoli et al. (2012) a discussion was made relative to the time scales involved in the thermal radiation phenomena; in Meier et al. (2009) it was defined a radiation Biot number where a temperature inversion between the fluid and particle occurs. All these results are now supported considering the non-linear nature of the thermal radiation phenomena, through the numerical solution obtained. The numerical solution is particularly interesting at low values of τ, where the analytical solution has difficulties in convergence (Bertoli, 1989).

Nomenclature

A_w	wall differential area, $2\pi R\ \mathrm{dx}$
A_p	surface area of single particle, $= \pi\, d_p^2$
C	specific heat at constant pressure
h_p	fluid to particle heat transfer coefficient
h_r	radiant heat transfer coefficient between the wall and the particle
h_w	wall heat transfer coefficient
n_v	number of solid particles in the volume *V*
R_p	particle radius
T	temperature
T_{ps}	particle surface temperature
V	pipe differential volume, $= \pi R^2\ \mathrm{dx}$
T_w	wall temperature
u	axial velocity
x	axial distance
α	thermal diffusivity
ε	void fraction
ε_p	surface emissivity of particles
ξ	radial position inside a particle
ρ	density
σ	Stefan-Boltzmann constant

Subscripts

f	fluid
p	particle

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