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MODELLING THE DRYING OF A PARALLELEPIPEDIC OIL SHALE PARTICLE

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Abstract - A numerical model is proposed to describe the process of drying a parallelepipedic oil shale particle. Assuming Fick's law, the diffusion equation for the shape of the particle was used. The objective of the study was to develop a computer program in Fortran to estimate the moisture content of an oil shale particle undergoing drying as a function of time and position. The average moisture content was also obtained. The model takes into account the migration of water by diffusion within the solid and its loss at the interface. The model results were compared to experimental data from an apparatus which measured the mass loss of a particle. The apparatus comprised an electronic balance attached by a thin wire to the particle placed inside an incubator.
Keywords: Oil shale; Drying; Mathematical modelling.

INTRODUCTION

Oil shale is a sedimentary rock that contains organic matter scattered throughout a mineral matrix. Thermal decomposition, also known as retorting, pyrolysis or devolatilization, converts the solid organic material of the shale into liquid and gaseous fractions and a solid carbonaceous residue. Oil shale moisture consumes the available heat for pyrolysis. Little is known about the kinetics of moisture removal from oil shale.

The particles used were obtained from the Petrosix process feedstock. Petrosix is the retorting process developed by Petrobras, a Brazilian oil company, which has been operating for almost fifteen years. The retorting process particles, which measure between 1.2 cm and 7.5 cm, have an approximately parallelepipedic shape. This work complements previous work on modelling the pyrolysis of Petrosix particles by Lovo Jr. (2003), which also addressed parallelepipedic particles. In their work on Petrosix, Rajagopal et al. (1986) concluded that "the thermodynamic efficiency of the retort and the overall process will be improved by predrying and/or preheating the shale rock".

The aim of this work was to develop a three-dimensional numerical model to estimate the moisture content of an oil shale particle undergoing drying as function of time and position and the average moisture content of the particle.

MODEL DEVELOPMENT

The mathematical model is based on the diffusional model. A three-dimensional model is proposed to describe the drying of parallelepipedic oil shale particles. The model is based on the following assumptions:

- the moisture content is uniformly distributed throughout the particle.

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- the diffusion coefficient is constant.
- the environmental conditions are constant.

The diffusion model is given by Equation 1.

$$\frac{\partial X}{\partial t} = D \left(\frac{\partial^2 X}{\partial x^2} + \frac{\partial^2 X}{\partial y^2} + \frac{\partial^2 X}{\partial z^2} \right) \quad (1)$$

with the following boundary and initial conditions, for a Cartesian coordinate system with its origin placed at the particle center are:

x axis

$$x = 0 \quad \frac{\partial X}{\partial x} = 0, \qquad x = L_x \quad -k\frac{\partial X}{\partial x} = k_C \left(X - X_E \right),$$

$$t = 0 \quad X = X_0$$

y axis

$$y = 0 \quad \frac{\partial X}{\partial y} = 0, \qquad y = L_y \quad -k\frac{\partial X}{\partial y} = k_C \left(X - X_E \right),$$

$$t = 0 \quad X = X_0$$

z axis

$$z = 0 \quad \frac{\partial X}{\partial z} = 0, \qquad z = L_z \quad -k\frac{\partial X}{\partial z} = k_C \left(X - X_E \right),$$

$$t = 0 \quad X = X_0$$

The solution of the three-dimensional Equation 1 is obtained as the product of one-dimensional problems. In dimensionless variables (defined below):

$$\psi\left(\xi_x, \xi_y, \xi_z, \tau_x, \tau_y, \tau_z\right) =$$

$$= \psi_x\left(\xi_x, \tau_x\right) \; \psi_y\left(\xi_y, \tau_y\right) \; \psi_z\left(\xi_z, \tau_z\right)$$

in which ψ_i, $i = x, y, z$ are obtained by solving Equation 2:

$$\frac{\partial \psi_i}{\partial \tau_i} = D \left(\frac{\partial^2 \psi_i}{\partial \xi_i^2} \right) \quad (2)$$

with the following boundary and initial conditions:

x axis

$$\xi_x = 0 \quad \frac{\partial \psi_x}{\partial x} = 0, \qquad \xi_x = 1 \quad \frac{\partial \psi_x}{\partial x} = -Bi_x \; \psi_x,$$

$$\tau_x = 0 \quad \psi_x = 1$$

y axis

$$\xi_y = 0 \quad \frac{\partial \psi_y}{\partial y} = 0, \qquad \xi_y = 1 \quad \frac{\partial \psi_y}{\partial y} = -Bi_y \; \psi_y,$$

$$\tau_y = 0 \quad \psi_y = 1$$

z axis

$$\xi_z = 0 \quad \frac{\partial \psi_z}{\partial z} = 0, \qquad \xi_z = 1 \quad \frac{\partial \psi_z}{\partial z} = -Bi_z \; \psi_z,$$

$$\tau_z = 0 \quad \psi_z = 1$$

The dimensionless variables are given below:

y axis

$$\xi_y = \frac{y}{L_y}, \qquad \tau_y = \frac{D}{L_y^2} t, \qquad \psi_y = \frac{X - X_E}{X_0 - X_E}$$

x axis

$$\xi_x = \frac{x}{L_x}, \qquad \tau_x = \frac{D}{L_x^2} t, \qquad \psi_x = \frac{X - X_E}{X_0 - X_E}$$

z axis

$$\xi_z = \frac{z}{L_z}, \qquad \tau_z = \frac{D}{L_z^2} t, \qquad \psi_z = \frac{X - X_E}{X_0 - X_E}$$

in which X_E is the moisture content at equilibrium with the environmental conditions and X_0 is the initial moisture content:

The solution of Equation 2 is given as an infinite series (Crank, 1975):

$$\psi_i = \sum_{n=1}^{\infty} \frac{4 \; \text{sen}\,\lambda_n}{(2\lambda_n + \text{sen}\,2\lambda_n)} \cos\left(\lambda_n \xi_i\right) \; e^{-\lambda_n^2 \tau_i} \quad (3)$$

in which each λ_n is a root of Equation 4:

$$\tan\lambda_n + \frac{Bi_i}{\lambda_n} = 0 \quad (4)$$

Bi_i is defined for each direction, as shown below.

$$Bi_x = \frac{k_C L_x}{D}, \qquad Bi_y = \frac{k_C L_y}{D}, \qquad Bi_z = \frac{k_C L_z}{D}$$

The average moisture content of the parallelepipedic particle ($\bar{\Psi}$) may be obtained by averaging the moisture values at points on a tridimensional grid established within the limits L_x, L_y, L_z.

EXPERIMENTAL PROCEDURE

Samples

Oil shale particles were supplied by Petrobras from its mine in the city of São Mateus do Sul. Samples had approximately parallelepipedic shapes. The particle sizes were 0.06 m x 0.05 x 0.03 m for the run at 60 ºC and 0.08 m x 0.04 m x 0.02 m for the run at 90 ºC.

Experimental Apparatus

An incubator was used to dry the particle as shown in the schematic setup (Figure 1). The particle was placed in the incubator, hanging by a wire, which was attached to the bottom of an electronic balance. The particle was partially shielded by a metal wall to avoid the effect of air circulation. Mass loss was monitored continuously. The drying temperature was monitored by two thermocouples, one near the sample and the other in the incubator chamber. Before starting the drying, the particle was weighed. The experimental results on mass loss were collected until constant weight was obtained. Drying conditions were maintained constant throughout the runs. Mass loss during drying was recorded.

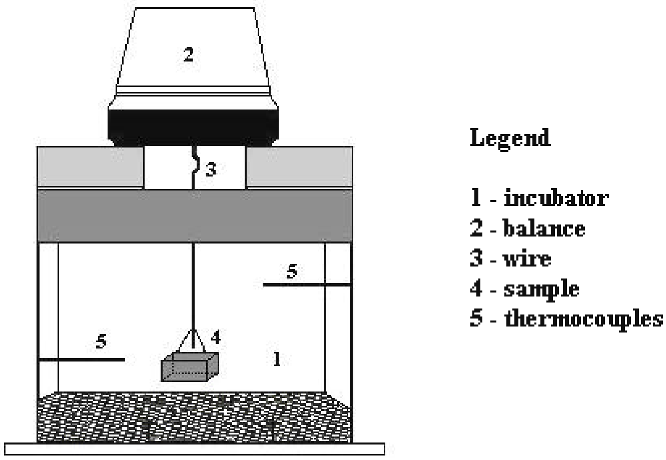

Figure 1: Schematic setup.

RESULTS AND DISCUSSION

The experiments were carried out at 60 ºC and 90 ºC. The drying of the oil shale particles was described by plotting the moisture content versus time, as shown in Figure 2. The rate of moisture removal increased when the air temperature increased from 60 ºC to 90 ºC. The drying run at 60 ºC ended before equilibrium was reached (more than 3 days).

The drying rate curve was calculated by numerical differentiation of the moisture content with respect to time. Data were plotted against moisture content, as shown in Figure 3. This curve indicates that the drying occurs in the falling rate period, with no constant rate period.

Table 1 compares the experimental and theoretical results for the runs at 60 ºC and 90 ºC. The theoretical results were obtained by averaging local values at points on a 11x11x11 grid. Figures 4 and 5 show numerical and experimental curves at 60 ºC and 90 ºC, respectively. The agreement between experimental and predicted results is satisfactory.

Table 2 shows values for the diffusion coefficient for oil shale, obtained from the literature.

The effective diffusivity of water vapor within the shale and the mass coefficient of water vapor from slab surface to the incubator had to be assumed in the model. The diffusion coefficient value for the Brazilian oil shale was assumed to be $8x10^{-8}$ m^2/s, within the range found in the literature (Table 2). The mass transfer coefficient values assumed to calculate the Biot number were $12x10^{-8}$ m/s (run at 60º C) and $25x10^{-8}$ m/s (run at 90 ºC). The Biot numbers calculated were in the same range as those found by Lane et al. (1988).

Table 3 indicates that increasing the grid points from 11x11x11 to 31x31x31 had little influence on the results.

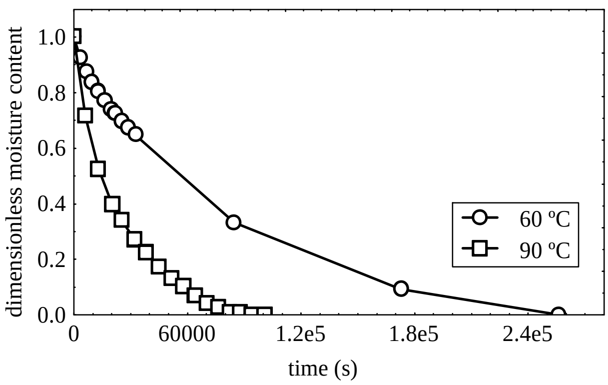

Figure 2: Dimensionless moisture content curves

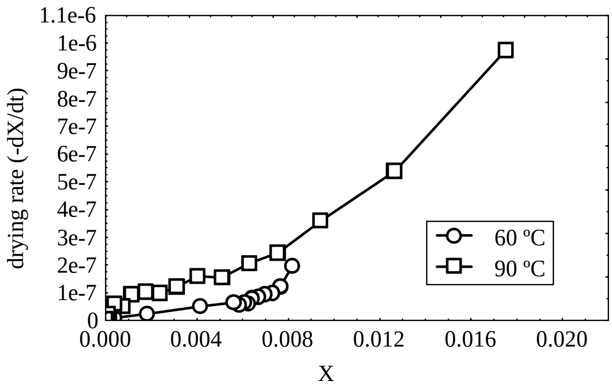

Figure 3: Drying rate curves.

Table 1: Dimensionless moisture obtained experimentally and by the mathematical model at 60 ºC and 90 ºC.

T = 60 ºC				T = 90 ºC			
Experimental		**Model**		**Experimental**		**Model**	
time (s)	y	**time (s)**	y	**time (s)**	y	**time (s)**	y
0	1.0000	0	1.0000	0	1.0000	0	1.0000
3240	0.9248	3240	0.9541	6000	0.7143	6000	0.7701
6600	0.8764	6600	0.9064	13200	0.5245	13200	0.5658
9900	0.8391	9900	0.8597	20400	0.3978	20400	0.4152
12900	0.8068	12900	0.8171	25200	0.3401	25200	0.3378
16200	0.7739	16200	0.7704	31800	0.2738	31800	0.2543
19800	0.7405	19800	0.7193	38400	0.2236	38400	0.1915
21600	0.7277	21600	0.7003	45000	0.1721	45000	0.1442
25200	0.6993	25200	0.6638	51600	0.1326	51600	0.1086
28800	0.6759	28800	0.6273	58200	0.1013	58200	0.0818
32400	0.6487	32400	0.5909	64200	0.0704	64200	0.0632
84720	0.3318	84720	0.3104	70200	0.0428	70200	0.0488
172800	0.0919	172800	0.0890	76200	0.0272	76200	0.0377
256320	0.0000	256320	0.0062	82200	0.0099	82200	0.0291
-	-	-	-	88200	0.0078	88200	0.0225
-	-	-	-	94200	0.0008	94200	0.0174
-	-	-	-	100800	0.0000	100800	0.0131

Table 2: Diffusion coefficient values found in the literature.

Type	T, ºC	D, m^2/s	References
Stuart oil shale	100 - 250	2.1×10^{-7}	Lane et al., (1988)
Stuart oil shale	22	7.3×10^{-8}	Duffy and Haynes, (1992)
Condor oil shale	22	9.5×10^{-8}	Duffy and Haynes, (1992)

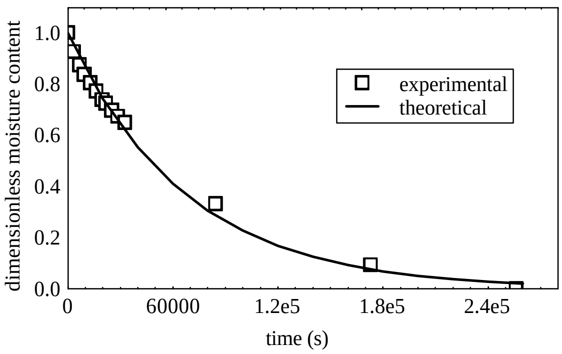

Figure 4: Theoretical and experimental dimensionless moisture content at 60 ºC.

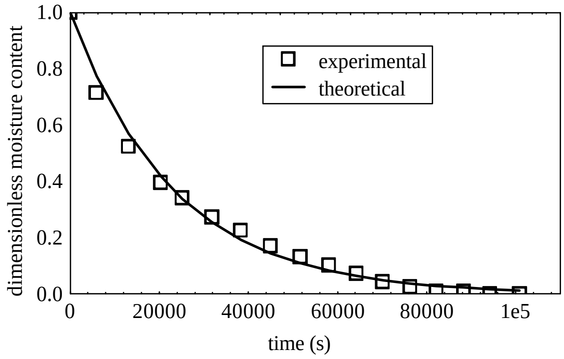

Figure 5: Theoretical and experimental dimensionless moisture content at 90 ºC.

Table 3: Effect of number of grid points on theoretical results, run at 90 ºC.

Experimental		Theoretical		
		11x11x11	**21x21x21**	**31x31x31**
time (s)	y	y	y	y
0	1.0000	1.0000	1.0000	1.0000
6000	0.7143	0.7710	0.7717	0.7719
13200	0.5245	0.5658	0.5663	0.5664
20400	0.3977	0.4152	0.4155	0.4157
25200	0.3401	0.3378	0.3381	0.3382
31800	0.2738	0.2543	0.2546	0.2546
38400	0.2235	0.1915	0.1917	0.1917
45000	0.1721	0.1442	0.1443	0.1444
51600	0.1326	0.1086	0.1087	0.1087
58200	0.1013	0.0818	0.0819	0.0819
64200	0.0704	0.0632	0.0633	0.0633
70200	0.0428	0.0488	0.0489	0.0489
76200	0.0272	0.0377	0.0378	0.0378
82200	0.0099	0.0291	0.0292	0.0292
88200	0.0078	0.0225	0.0225	0.0225
94200	0.0008	0.0174	0.0174	0.0174
100800	0.0000	0.0131	0.0131	0.0131

CONCLUSIONS

The mathematical model developed enables prediction of the distribution of moisture within parallelepipedic oil shale particles undergoing drying. Results indicate that the predicted and measured moisture content profiles agree satisfactorily. Further studies are necessary to obtain accurate values for the effective diffusion coefficient of moisture within the oil shale particle. The model may be integrated with a general pyrolysis model.

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NOMENCLATURE

Bi	Biot number	(-)
D	effective diffusivity	m^2/s

L_x, L_y, L_z	particle half-thickness	m
k	thermal conductivity	W/m K
k_C	mass transfer coefficient	m/s
t	time	s
T	temperature	ºC
X	moisture content	kg H_20/ kg dry solid
x,y,z	space coordinates	m

Greek Symbols

τ	dimensionless time	(-)
ξ	dimensionless coordinates	(-)
$\psi = \frac{X - X_E}{X_0 - X_E}$	dimensionless moisture	(-)
$\bar{\Psi} = \frac{\bar{X} - X_E}{X_0 - X_E}$	average dimensionless moisture	(-)

Subscripts

0	initial condition	(-)
E	equilibrium condition	(-)

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