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SIMULATING LIGHT OIL EVAPORATION IN A STEFAN TUBE

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Abstract. *This work deals with the numerical simulation of the evaporation process that results from the passage of nitrogen in a Stefan tube initially filled with a liquid-vapor mixture of light oil hydrocarbons (represented here by pentane and methane) at equilibrium at 101 bar abs and 38.5°C. Results are presented for concentration fields in both phases and for the transient evolution of the liquid-vapor interface.*

Keywords: *Ternary diffusion, Transient diffusion, Oil recovering.*

1. INTRODUCTION

At the end of the primary exploitation phase of fractured petroleum reservoirs, a great deal of oil (60%, in some cases) is still trapped in the pores of the solid matrix. One technical solution to continue the production is to have a “dry” gas circulating through the fissures, leading to the evaporation of the light fractions of the oil (represented here by methane, C1, and pentane, C5). However, for this procedure to be feasible, it is necessary to know the effect of several operational parameters, such as the nature of the injected gas and its optimal injection flow, a task that can be more easily accomplished with the aid of numerical simulations of a suitable model of transport in porous media (Morel et al, 1990).

The methane produced in place is usually the gas selected for the extraction, but another convenient alternative is simply to use atmospheric air (represented by nitrogen, N2). The 3-component evaporation process associated with this latter case (C5-C1-N2), at the microscopic level, is the scope of the present work. Inside the liquid and vapor phases, ternary diffusion takes place and these two processes are connected via thermodynamical equilibrium at the liquid-vapor interface. Ternary diffusion can be modeled with an extension of Fick´s law for two components, but, unlike the binary case, ternary coefficients present a strong dependence on the molar concentrations of the components. Besides, such dependence is greatly increased by the thermodynamical corrections associated with the high pressures normally encountered in real situation. The characterization of this evaporation process is completed with ternary equilibrium at the liquid-vapor interface, also highly dependent on molar concentrations, which turns ternary evaporation into an essentially transient process.

In this work, the finite volume technique is used to solve the system of partial differential equations governing this evaporation process, in the specific case of a Stefan tube filled with a mixture of pentane and methane (C5-C1), initially at 101 bar abs and 38.5°C, subjected to a flux of nitrogen (N2). The geometry was intentionally left as simple as possible, in order to concentrate on the understanding of the phenomenological details. This study can be viewed as the simulation of the evaporation of *one pore* of an actual petroleum reservoir (normally, a rocky matrix), a necessary step before the simulation of the porous media at the macroscopic level (see, for example, Laurindo and Prat, 1998).

2. DESCRIPTION OF THE PROBLEM

Figure 1 shows the problem to be solved. From an initial condition of liquid-vapor equilibrium in a mixture C5-C1 in a Stefan tube, at 101 bar abs and 38.5°C, nitrogen (N2) diffuses through the vapor and liquid phases, eliminating the hydrocarbons.

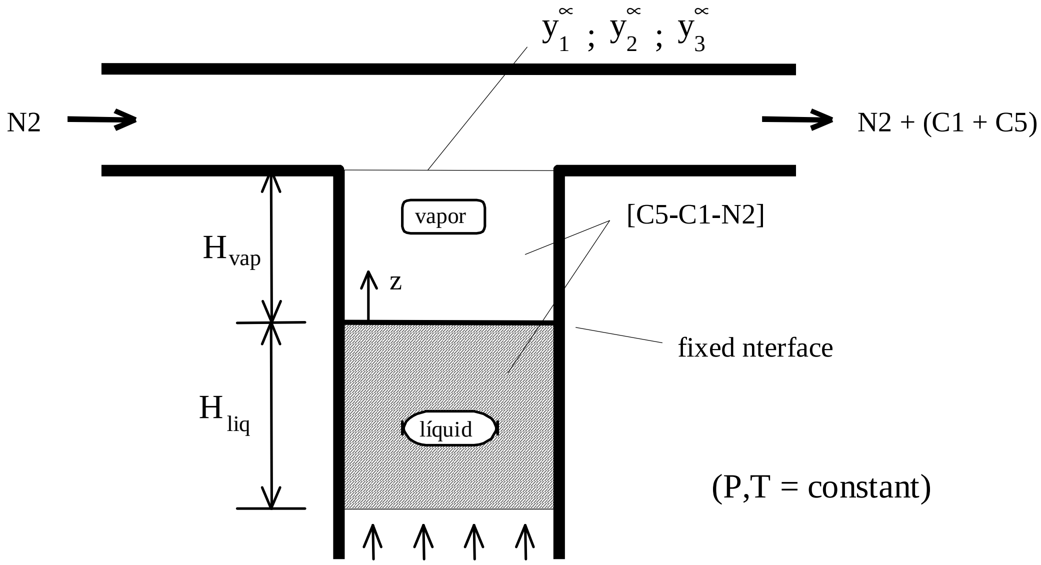

Figure 1 - Light oil evaporation in a Stefan tube.

In both phases, the ternary mixture C5-C1-N2 was modeled according to the "non-ideal" model discussed in Freitas and Prat (1999). The condition at the interface follows the ternary diagram of equilibrium, for the given values of pressure and temperature, which means that it varies with time as the quantity of N2 diffused in the system increases. Because of this transient characteristic of the interface, both vapor and liquid phases must be modeled as transient. The interface is kept immobile and the interior face of the tube is open, to allow liquid flux. The effect of the viscosity is neglected, so the model can be implemented in 1-D.

3. TERNARY DIFFUSION

In both phases, the governing equations for transient ternary diffusion can be written, for the 3 components (i=1 for C5, i=2 for C1 and i=3 for N2) as (Bird et al., 1960):

$$\frac{\partial c_i}{\partial t} = -\frac{\partial N_i}{\partial z} \tag{1}$$

where the total molar flux of each species "i" is given by:

$$N_i = J_i + c_i u = J_i + x_i N_t \tag{2}$$

The diffusive flux can be written as:

$$J_i = -c_t D_{ii} \frac{\partial x_i}{\partial z} - c_t D_{i1} \frac{\partial x_1}{\partial z} \tag{3}$$

where D_{ii} and D_{i1} represent Fick’s coefficients for ternary diffusion, corrected to take into account the non-idealities of this problem (see Taylor and Krishna, 1993, and Freitas and Prat, 1999). Then, defining $\gamma_{ij} = c_t D_{ij}$, Eq. (1) can be written in a more convenient form for the numerical treatment as:

$$\frac{\partial (c_t x_i)}{\partial t} + \frac{\partial}{\partial z}(c_t u x_i) = \frac{\partial}{\partial z}\left(\gamma_{ii} \frac{\partial x_i}{\partial z}\right) + S \tag{4}$$

where the diffusion part of "i" due to other components’ gradients is confined in a source-term:

$$S = \frac{\partial}{\partial z}\left(\gamma_{i1} \frac{\partial x_1}{\partial z}\right) \tag{5}$$

3.1 Numerical discretisation

Equation (4) is solved by the finite volume method (Patankar, 1980). To the typical volume shown in Fig. 2, Eq. (4) can be written as:

$$a_P (x_i)_P = a_N (x_i)_N + a_S (x_i)_S + b_P \tag{6}$$

where:

$$a_N = \frac{\gamma_n}{\delta z_n} A\left[\left|(Pe_i)_n\right|\right] + max\left[-(c_t u)_n, 0\right] \tag{7}$$

$$a_S = \frac{\gamma_s}{\delta z_s} A\left[\left|(Pe_i)_s\right|\right] + max\left[(c_t u)_s, 0\right] \tag{8}$$

$$a_P = a_N + a_S + \left[(c_t u)_n - (c_t u)_s\right] + (c_t)_P \frac{\Delta z}{\Delta t} \tag{9}$$

$$\begin{aligned} b_P = {} & \frac{(c_t)_P^0 (x_i)_P^0 \Delta z}{\Delta t} + \\ & \left\{ (\gamma_{i1})_n \left[\frac{(x_1)_N - (x_1)_P}{\delta z_n}\right] B\left[(Pe_1)_n, (Pe_2)_n\right] - (\gamma_{i1})_s \left[\frac{(x_1)_P - (x_1)_S}{\delta z_s}\right] B\left[(Pe_1)_s, (Pe_2)_s\right] \right\} \end{aligned} \tag{10}$$

In the expressions above, Pe is the Peclet number for the mesh, $Pe_i = c_t u(\delta z)/(\gamma_{ii})_{front}$, for a γ_{ii} evaluated at the boundary.

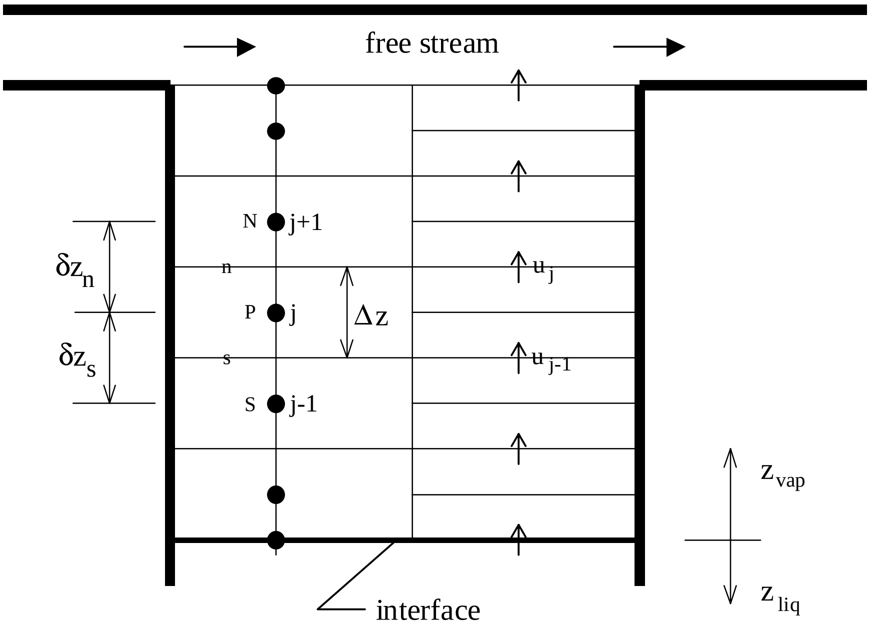

Figure 2 - Typical finite volume for both phases.

3.2 "Power-law" scheme in a ternary system

In the expressions for the coefficients, Eqs. (4) to (10), the following functions appear:

$$A(Pe) = \max\left[0, (1 - 0.1Pe)^5\right] \tag{11}$$

$$B(Pe_1, Pe_2) = \frac{A(Pe_2)Pe_1 - A(Pe_1)Pe_2}{Pe_1 - Pe_2} \tag{12}$$

Eqs. (11) and (12) result from an adaptation of the "power law" scheme (Patankar, 1980) to the specific case of ternary diffusion. This scheme allows the finite volume method to perform a more correct evaluation of the balance between the effects of diffusion and convection. The adaptation shown above is a complement of this scheme, including the effect of the crossed coefficients from Eq. (3) in the evaluation of the situation at the boundaries of the volumes.

3.3 Method of solution

The algebraic system of equations represented by Eq. (6) was solved by a combination of Gaussian Elimination (implemented as the Tridiagonal Matrix Algorithm - TDMA) with the iterative method of Gauss-Seidel, to consider the non-linear condition of the equations.

4. INDUCED CONVECTION

The convective part of each component's flux, given by Eq. (2), is associated to a velocity field that can be directly calculated from global conservation of mass, given by:

$$\frac{\partial c_t}{\partial t} = -\frac{\partial N_t}{\partial z} = -\frac{\partial (c_t u)}{\partial z} \tag{13}$$

where "u" is the molar average of the mixture velocity. According to Eq. (13), the velocity field "u" can be calculated parabolicaly from the interface, as a result of the variation of the total concentration ($c_t = c_1 + c_2 + c_3$), in an iterative process.

4.1 Pressure formulation

Another way of solving the same problem is to assume that the velocity u is linked to a pressure field by means of the expression for the mean velocity in a Poiseuille flow between parallel plates, given by:

$$u = -K \frac{\partial P}{\partial z} = -\frac{\mathrm{L}^2}{12\mu} \frac{\partial P}{\partial z} \tag{14}$$

where "L" corresponds to the distance between plates (m), μ is the viscosity (Pa.s) and K ($= \mathrm{L}^2 / 12\mu$) is a constant, characteristic of the problem. This transformation is extremely convenient for a subsequent implementation of the simulation in porous media.

Substituting Eq. (14) in Eq. (13), it is obtained:

$$\frac{\partial c_t}{\partial t} = K \frac{\partial}{\partial z}\left(c_t \frac{\partial P}{\partial z} \right) \tag{15}$$

with boundary conditions of total molar flux prescribed at the interface, to both phases, prescribed pressure (101 bar abs) to the vapor phase and pressure fixed in an arbitrary value for the boundary opposed to the interface in the liquid phase.

Equation (15) was also submitted to discretisation by the finite volume method and the resulting algebraic system of equations is solved simultaneously with Eq. (6).

4.2 Boundary condition for P

For both phases, the boundary condition at the interface can be put in the following form:

$$P_I = P_2 + \frac{u^I (\delta z_s)_2}{K} \tag{16}$$

where "2" corresponds to the second grid point, just after the interface.

5. LIQUID-VAPOR INTERFACE IN A TERNARY SYSTEM

The condition that defines the interface is the continuity of local molar fluxes:

$$N_1^L = -N_1^V \quad \text{and} \quad N_2^L = -N_2^V \tag{17}$$

where the minus sign stands for the opposed sense of the coordinates, indicated in Fig. 2. Besides, global continuity must be respected ($N_t^L = -N_t^V$), what guarantees flux continuity for the third component.

Taking into account the expressions for the interpolations at the boundaries of the computational volumes, Eqs. (11) and (12), the vapor molar fluxes at the interface ("I") can be written as:

$$N_1^V = \gamma_{11}^V \left[\frac{(y_1)_I - (y_1)_2}{\delta z_n^V} \right] A\left(Pe_1^V\right) + (y_1)_I \, N_t^V \tag{18}$$

$$N_2^V = \gamma_{22}^V \left[\frac{(y_2)_I - (y_2)_2}{\delta z_n^V} \right] A\left(Pe_2^V\right) + \gamma_{21}^V \left[\frac{(y_1)_I - (y_1)_2}{\delta z_n^V} \right] B\left(Pe_1^V, Pe_2^V\right) + (y_2)_I \, N_t^V \tag{19}$$

Equivalent expressions can be obtained for the liquid, as functions of the properties evaluated at the interface by the liquid side (L) and the molar concentrations of the liquid (x).

Peclet numbers shown above are given by:

$$Pe_i^V = \frac{N_t^V \delta z_n^V}{\gamma_{ii}^V} \quad \text{and} \quad Pe_i^L = \frac{-N_t^V \delta z_n^L}{\gamma_{ii}^L} \tag{20}$$

The substitution of the fluxes into Eq. (17) leads to two expressions for the total flux N_t^V. Equating these two expressions, the following relation is obtained:

$$\begin{aligned}
\left(N_t^V\right)_I &= \left\{ \gamma_{11}^V \left[\frac{y_1^{eq} - (y_1)_2}{\delta z_n^V} \right] A\left(Pe_1^V\right) + \gamma_{11}^L \left[\frac{x_1^{eq} - (x_1)_2}{\delta z_n^L} \right] A\left(Pe_1^L\right) \right\} \frac{1}{\left(x_1^{eq} - y_1^{eq}\right)} = \\
&= \left\{ \gamma_{22}^V \left[\frac{y_2^{eq} - (y_2)_2}{\delta z_n^V} \right] A\left(Pe_2^V\right) + \gamma_{21}^V \left[\frac{y_1^{eq} - (y_1)_2}{\delta z_n^V} \right] B\left(Pe_1^V, Pe_2^V\right) \right\} \frac{1}{\left(x_2^{eq} - y_2^{eq}\right)} + \\
&\quad + \left\{ \gamma_{22}^L \left[\frac{x_1^{eq} - (x_2)_2}{\delta z_n^L} \right] A\left(Pe_2^L\right) + \gamma_{21}^L \left[\frac{x_1^{eq} - (x_1)_2}{\delta z_n^L} \right] B\left(Pe_1^L, Pe_2^L\right) \right\} \frac{1}{\left(x_2^{eq} - y_2^{eq}\right)}
\end{aligned} \tag{21}$$

Equation (21) has only one unknown, since all six equilibrium molar fractions can be written as functions of only one among them (for example, x_2^{eq}). This equation completes the problem formulation.

6. RESULTS

The solution method as described above was applied to the problem shown in Fig. 1, to the following set of parameters:

- $P = 101$ bar abs and $T = 38.5\,°C$
- $H_{vap} = 0.5$ mm and $H_{liq} = 1$mm
- $y_1^{\infty} = 0$; $y_2^{\infty} = 0$ and $y_3^{\infty} = 1$

The results for a transient analysis, performed from the moment when the tube contains only a binary mixture of C5-C1, until the instant t=3s, are shown in Figs. 3 to 7.

Figures 3 and 4 show the evolution of the interface. At each instant, the 6 curves shown give values that figure over the corresponding ternary diagram of equilibrium for C5-C1-N2 (see Freitas and Prat, 1999). It can be observed a very fast augmentation of the quantity of nitrogen and a marked lowering of the methane at the interface. In fact, according to the diagram of equilibrium, the system tends, as a result of the addition of N2, to the binary equilibrium C5-N2.

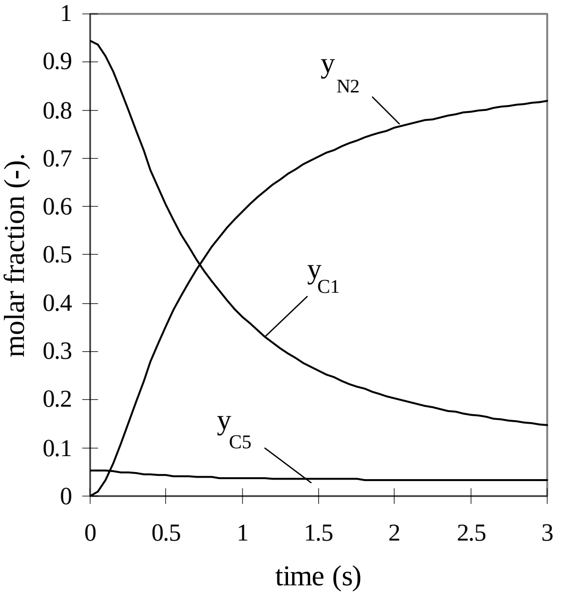

Figure 3. Evolution of the vapor molar fractions at the interface. (h_{vap}= 0.5 mm ; $h_{líq}$ = 1 mm) and ($y_1^\infty = 0$; $y_2^\infty = 0$).

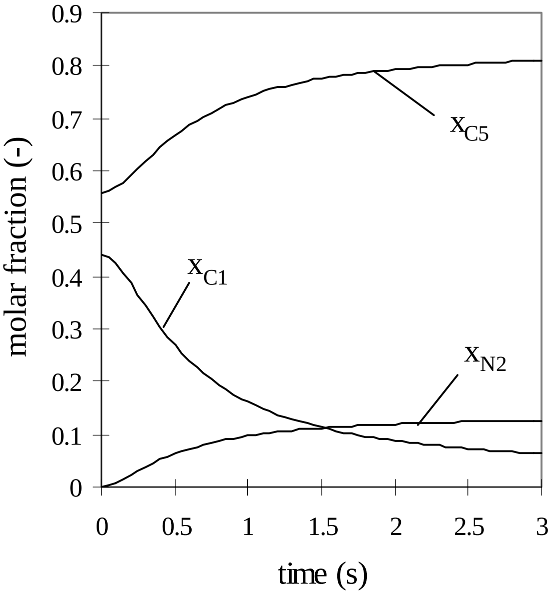

Figure 4. Evolution of the liquid molar fractions at the interface. (h_{vap}= 0.5 mm ; h_{liq}= 1 mm) and ($y_1^\infty = 0$; $y_2^\infty = 0$).

To the given values of the parameters, the effect of imposing a nitrogen flux at the free boundary is rapidly propagated to the system as a whole . Figures 5 and 6 show that, after just 3 seconds, there is almost no more pentane in the vapor and the diffusion in the liquid already touched the bottom of the tube (the distance from interface is adimensionalized over the size of the domain).

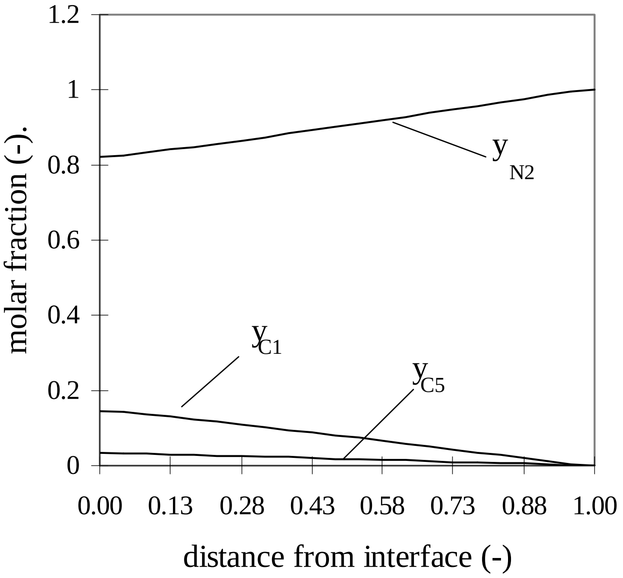

Figure 5. Concentration fields at the vapor phase at t=3 s. (h_{vap}= 0.5 mm ; h_{liq}= 1 mm) and ($y_1^{\infty} = 0$; $y_2^{\infty} = 0$).

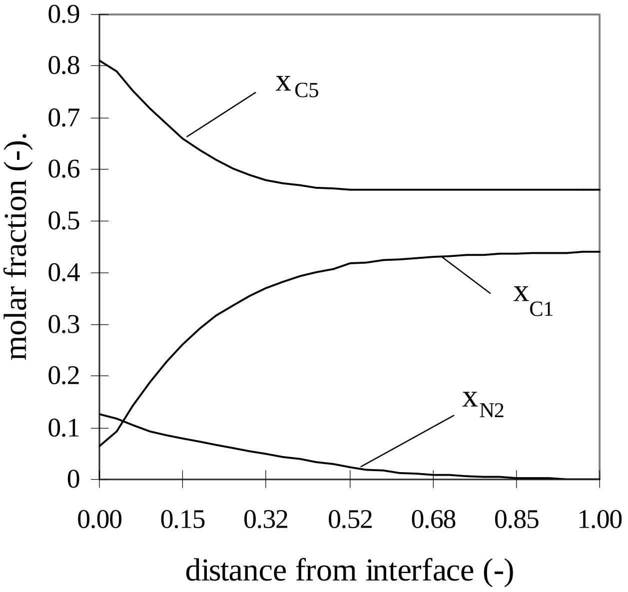

Figure 6. Concentration fields at the liquid phase at t=3 s. (h_{vap}= 0.5 mm ; h_{liq}= 1 mm) and ($y_1^{\infty} = 0$; $y_2^{\infty} = 0$).

Figure 7 is associated to the fluxes that cross the interface liquid-vapor. It can be observed that, even with a strong injection of N2, the total flux is positive, which can be explained by the intense elimination of methane. The curves have the expected behavior, but the flux of pentane presents the particularity of becoming negative during a short period, right after the beginning of the process. It is justified by the fact that the addition of N2 leads the molar fraction of C5 to *increase*. At the beginning, the quantity of C5 brought to the interface by the liquid is not enough to satisfy this condition and the vapor must supply the necessary complementation. As long as the total flux increases, the quantity of C5 brought by convection from the liquid to the interface becomes more important and the tendency changes.

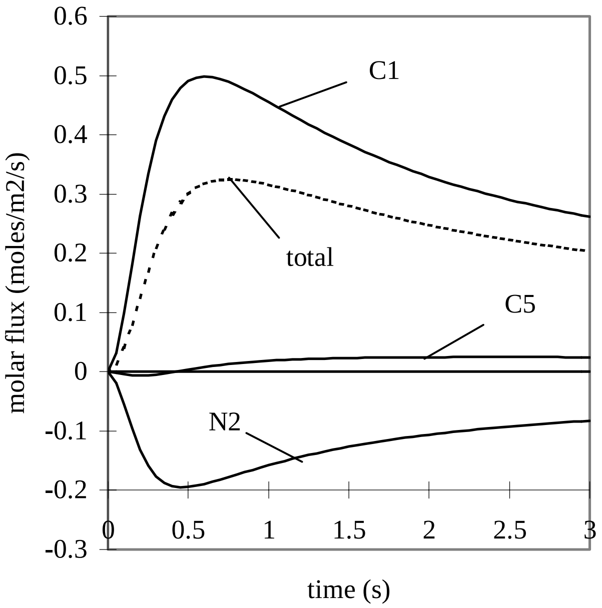

Figure 7. Evolution of the local molar fluxes at the interface.
(h_{vap}= 0.5 mm ; h_{liq}= 1 mm) and ($y_1^{\infty} = 0$; $y_2^{\infty} = 0$).

7. CONCLUSION

A methodology for the numerical simulation of the ternary evaporation in a Stefan tube was presented. This simulation is the basis for the more involved simulation of ternary evaporation in a porous media, a subject of interest in the field of petroleum engineering. Ternary evaporation in a Stefan tube is a complex transient process, because the condition at the liquid-vapor interface changes all the time, until the complete elimination of one of the components (in this case, C1 is eliminated first). Furthermore, diffusion fluxes of a certain component depend not only on the component itself, but also on the others, by means of "crossed coefficients". In the context of a porous media, such an analysis is further complicated by issues concerning the topology and morphology of the solid matrix. So, it is evident that a fundamental point to the simulation of ternary evaporation of light oil from a petroleum reservoir is the thorough understanding of the evaporation at the pore level. The situation studied in the present work corresponds to 1-D simulation of a binary mixture C5-C1, at high pressure (101 bar abs) and 38.5°C, subjected to a stream of nitrogen, as an extraction agent. The methodology revealed efficient and stable and can be used to the determination of concentration fields and fluxes, as a basis for a macroscopic simulation or for the simulation of a porous media as a network (as in Laurindo and Prat, 1998).

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