Two Dimensionnal Model for Extraction Packed Column Simulation using Finite Element Method

N. Outili, A-H. Meniai

Abstract—Modeling transfer phenomena in several chemical engineering operations leads to the resolution of partial differential equations systems. According to the complexity of the operations mechanisms, the equations present a nonlinear form and analytical solution became difficult, we have then to use numerical methods which are based on approximations in order to transform a differential system to an algebraic one. Finite element method is one of numerical methods which can be used to obtain an accurate solution in many complex cases of chemical engineering. The packed columns find a large application like contactor for liquid-liquid systems such solvent extraction. In the literature, the modeling of this type of equipment received less attention in comparison with the plate columns. A mathematical bidimensionnal model with radial and axial dispersion, simulating packed tower extraction behavior was developed and a partial differential equation was solved using the finite element method by adopting the Galerkine model. We developed a Mathcad program, which can be used for a similar equations and concentration profiles are obtained along the column. The influence of radial dispersion was prooved and it can't be neglected, the results were compared with experimental concentration at the top of the column in the extraction system: acetone/toluene/water.

Keywords—finite element method, Galerkine method, liquid-liquid extraction modelling, packed column simulation, two dimensional model

I. INTRODUCTION

THE modeling of polyphasic transfer phenomena in many chemical engineering operations led to the resolution of partial differential equations systems. According to the complexity of the mechanisms involved, the equations generally present a nonlinear character and it is rare to determine an analytical solution, there is then recourse to numerical methods founded on approximations which transform the differential system into an algebraic one.[1] The basic idea of this method is to simplify the complex problem and replace it by another simpler whose solution is easier to obtain since its field is discredited by several under fields called finite elements. This will make it possible to find an approximation, near the exact solution. [2]

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II EXTRACTION COLUMN MODELING

A material balance by applying the dispersion model ([3,4]) on a differential element of the column (fig 1) and in the absence of any reaction, leads to the transient global differential equation that models the column behavior, taking into account axial and radial dispersions:

$$-\phi V_d \frac{\partial y}{\partial z} + E_z \phi \frac{\partial^2 y}{\partial z^2} + E_r \phi \frac{\partial}{\partial r}\left(r \frac{\partial y}{\partial r}\right) - K_{od} a \left(y - y^*\right) = \phi V_d \frac{\partial y}{\partial t} \quad (1)$$

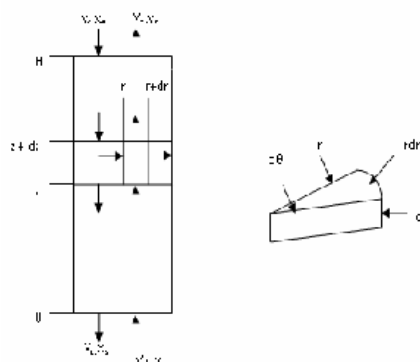With equilibrium equation: $y^* = m\,x$ (2)
m equilibrium slope

Fig. 1 Column scheme and a differential element

A material balance on the lower part of the column gives:

$$(1-\phi)\,V_c\,x + \phi\,V_d\,y_e = \phi\,V_d\,y + (1-\phi)\,V_c\,x_s\,\phi \quad (3)$$

And $x = \dfrac{\phi}{1-\phi}\dfrac{V_d}{V_c}(y - y_e) + x_s$ (4)

By replacing equations (2) and (4) in (1) we have:

$$-\phi V_d \frac{\partial y}{\partial z} + E_z \phi \frac{\partial^2 y}{\partial z^2} + E_r \phi \frac{\partial}{\partial r}\left(r \frac{\partial y}{\partial r}\right) - K_{od} a \left(\alpha\, y + \beta\right) = \phi V_d \frac{\partial y}{\partial t} \quad (5)$$

With: $\alpha = 1 - m \dfrac{\phi}{1-\phi}\dfrac{V_d}{V_c}$ et $\beta = m\dfrac{\phi}{1-\phi}\dfrac{V_d}{V_c}y_e - m\,x_s$ (6)

Boundary conditions used to solve the differential equation are:

At $z = 0$, $y = y_e$ and at $z = H$, $\dfrac{\partial y}{\partial z} = 0$ (7)

The axial symmetry imposes the following boundary conditions in the radial direction:

At $r = 0$, $\frac{\partial y}{\partial r} = 0$ (8)

On the wall, at $r = R$, $\left.\frac{dy}{dr}\right|_{r=R} = -\frac{K_{od}}{E_r}(y - y_\infty)$ (9)

With y_∞ : fraction obtained at an infinite height of the column

III NUMERICAL METHOD

The finite element method is a numerical method that can be used to obtain a fairly accurate solution of complex problems in science and engineering. Initially the method was developed in 1956 by Turner, Clough, Martin and Topp for problems of aviation [5].

Over the years this method has been shown, the ability to solve different problems of applied science or engineering. It is now considered one of the best tools for solving many practical problems.

The basic idea of this method is to find a solution to a complex problem by replacing it by a simpler one, where the solution domain is discredited by several subdomains called finite elements. This will find an approximate solution, close to the exact one. Generally if this method can be adapted, some well-defined steps can be followed and which are:([1,2,5,6]

- Discretization of the problem domain: in one-dimensional cases, linear elements are used and in two dimensional analysis, the isosceles triangle is the basic most adopted element.
- Selecting an interpolation model to represent the variable fields in each element: the polynomial functions are the most used models.
- Derivation of characteristic matrices and vectors of the element: Different procedures are used to derive the equations of the element, including the method of Galerkine. After integration we write the characteristic equation of the element e in the form:

$$\left[K^{(e)}\right]\overline{\varphi}^{(e)} = \overline{P}^{(e)}$$ (10)

Where K(e) is the characteristic matrix of element e, P (e) is the characteristic vector and φ is the vector of unknowns at the nodes.

- Assembly of matrices and characteristic vectors for the global equations: Once the matrices and vectors obtained, the next step is to establish the equations defining the overall system:

$$[K] = \sum_{e=1}^{E}\left[K^{(e)}\right] \quad et \quad \overline{P} = \sum_{e=1}^{E}\overline{P}^{(e)}$$ (11)

E is the total number of elements in the system

- Solving the system of equations: After assembly, we can solve the system of equations after incorporation of boundary conditions. One of the direct methods used for solving such a system of equations is the Gauss elimination method.

IV RESULTS AND DISCUSSION

Solving the differential equation of a particular case is obtained using the finite element method and a Mathcad code was used. We will therefore study the effect of dispersion on the concentration profiles along the column.

The results obtained in this work are compared with those obtained experimentally by Seibert and Humphrey [7] in their study of an extraction packed column in the treatment of the system: acetone-toluene-water, we used the same data and same operating conditions of their column: a packed column of 1.524 m height and 10.2 cm diameter, filled with Raschig rings of 1.27 cm diameter with an interfacial area of 347.72 m^2/m^3 and a void fraction of 0.64. The experimental results of Seibert and Hamphrey [7], gives only the mole fraction at the outlet of the column ys, which will be used to validate the simulation results

A.Axial dispersion effect

We solve the differential equation obtained for the permanent case taking into account axial dispersion, which can be summarized in the following differential equation:

$$-\phi V_d \frac{\partial y}{\partial z} + E_z \phi \frac{\partial^2 y}{\partial z^2} - K_{od} a(\alpha y + \beta) = 0$$ (12)

Ez: the coefficient of axial dispersion in the dispersed phase expressed as a dimensionless number of Pe_d calculated according to the operating point considered: V_c, V_d The boundary conditions used are as follows:

At $z = 0$, $y = ye$ and at $z = H$, $\frac{\partial y}{\partial z} = 0$ (13)

We use 12 linear elements with two nodes per element (Fig 2) and a Lagrange polynomial of degree one. In steady state, the change in mole fraction along the column is shown on the graph in Figure 3. It decreases with the height of the column.
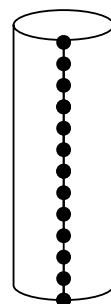

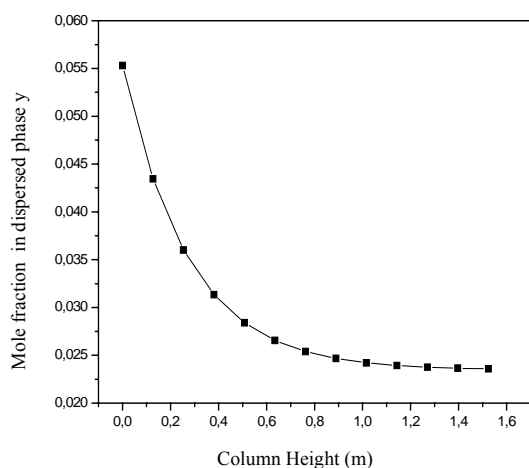Fig 2 Discretization of the field with 12 linear elements

Fig 3 Variation of the along the column (Vc=2.10mm/s, Vd=4.75mm/s Ez = 1.66 10^{-3} m^2/s or Ped=0.023)

To study the effect of axial dispersion on the profile of the mole fraction along the column, we compare the results obtained without the effect of dispersion. For the latter case the differential equation is simplified and an analytical solution giving the variation of mole fraction as a function of the column height is given by:

$$y = \left(y_e + \frac{\beta}{\alpha} \right) \exp\left(-\frac{K_{od}\, a\, \alpha}{V_d\, \phi}\, z \right) - \frac{\beta}{\alpha}$$

(14)

The values obtained are given in Table 1. From these results, the mole fractions increase slightly in the presence of axial dispersion along the column, but its effect is considered negligible and even vanishes when approaching the exit of the column. The relative error between experimental value of the mole fraction and calculated one at the column outlet is: 28%

TABLE I
EFFECT OF AXIAL DISPERSION ON THE AXIAL PROFILE OF THE MOLE FRACTION

Height (m)	Mole fractions of solute in the dispersed phase	
	Without dispersion (analytic)	Axial dispersion
0	0,0553	0,0553
0,127	0,04339062	0,04344338
0,254	0,03593471	0,03600168
0,381	0,03126692	0,03132914
0,508	0,02834463	0,02839757
0,635	0,02651512	0,02655552
0,762	0,02536976	0,02540146
0,889	0,02465269	0,02467429
1,016	0,02420378	0,02422119
1,143	0,02392273	0,02393264
1,27	0,02374678	0,02375658
1,397	0,02363662	0,02363985
1,524	0,02356766	0,02357419
ys (exp)	0.0328	

B. Effect of radial dispersion

The treatment of two-dimensional problem allows us to study the effect of radial dispersion on the concentration profile along the column. The differential equation to be solved:

$$-\phi V_d \frac{\partial y}{\partial z} + E_z \phi \frac{\partial^2 y}{\partial z^2} + E_r \phi \frac{\partial}{\partial r}\left(r \frac{\partial y}{\partial r} \right) - K_{od}\, a(\alpha\, y + \beta) = 0$$

(15)

The radial dispersion Er has often been neglected because the radial profiles obtained were flat, and this result was attributed by [9] in their modeling of a distillation column, to the fact that used boundary conditions on concentration gradients at the wall and at the axis of the column was equal to zero:

By performing numerical experiments and assigning the gradient at the wall values different from zero (no physical sense), these authors found that the radial profile was flatter and the radial concentration changed according to the values of the limit imposed .In the case of liquid-liquid extraction the gradient at the wall is nonzero and is given by some authors [7, 8] by equation (9)The column is discredited by linear triangular elements in natural coordinates to simplify the differentiation and integration of terms of matrices and characteristic vectors of elements. It was used 36 linear triangular elements (3 elements for the radius and 7 for the height) and 48 elements (we increased the number of elements used radially). Figure 4 shows the mesh used to discretize the column.
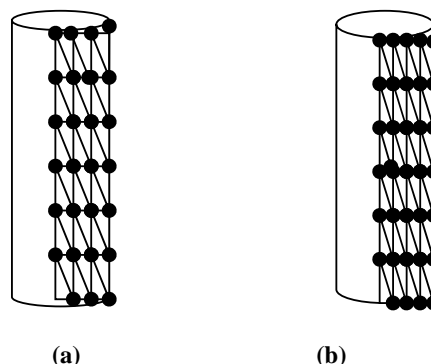

(a) (b)

Fig. 4 Discretization mesh : a) 36 elements et b) 48 elements

In Tables 2 and 3 are shown the results obtained using a non-zero gradient for the boundary condition at the wall of the column for the two meshes shown above. The radial variation is small but it is more important than the zero gradient case (fig 6), and in addition there is also a difference by increasing the number of elements radially. Dimensional profile as a function of mole fraction (Fig. 5) is almost flat compared to that of Figure 7, a slight variation occurs near the wall and the outlet of the column.
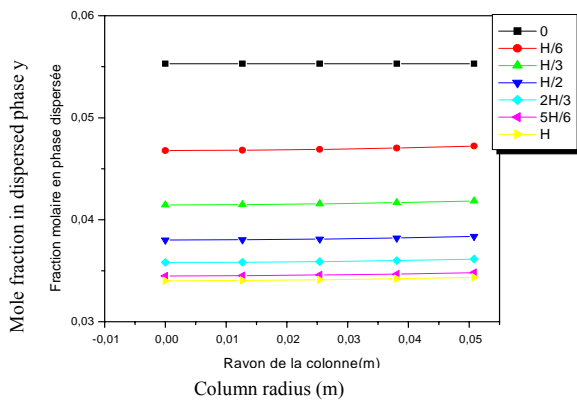
Fig 5 Profile of the mole fraction with nonzero gradient at the wall (48 elements)
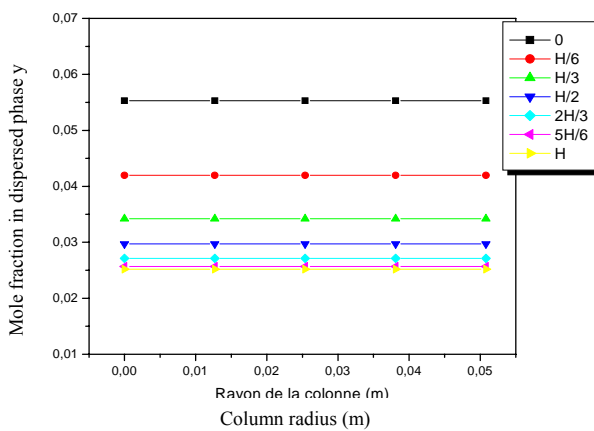

Fig 6 Profile of the mole fraction with zero gradient at the wall (48 elements)

By plotting the variation of this last fraction versus radius of the column, a difference from the flat profile appears and it is more pronounced in the case of non-zero gradient as in the zero gradient fig 7 et 8.
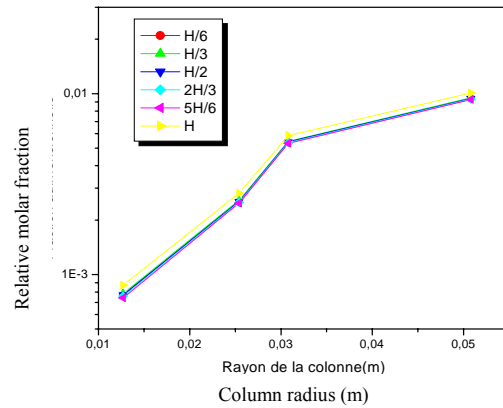

Fig 7 Profile of the relative fraction with nonzero gradient at the wall (48 elements)
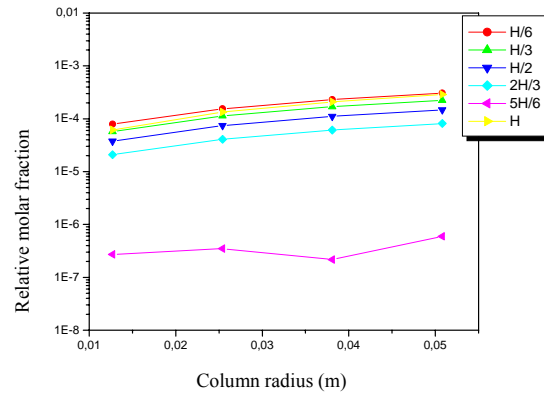

Fig 8 Profile of the relative fraction with zero gradient at the wall (48 elements)

TABLE II
VARIATION OF THE MOLE FRACTION WITH NONZERO GRADIENT AT THE WALL (36 ELEMENTS)

Height (m)	Mole fraction analytic	Mole fraction at :			
		0	R/3	2R/3	R
0	0.0553	0.0553	0.0553	0.0553	0.0553
0.254	0.03593	0.046771	0.046835	0.04698	0.04722
0.508	0.02833	0.041437	0.041494	0.041626	0.041839
0.762	0.02536	0.037995	0.038048	0.038167	0.038361
1.016	0.02419	0.035798	0.035846	0.035957	0.03614
1.270	0.02374	0.034484	0.034529	0.034636	0.034811
1.524	0.02356	0.033997	0.03405	0.034167	0.034353
ys (exp)	0.0328				

TABLE III
VARIATION OF THE MOLE FRACTION WITH NONZERO GRADIENT AT THE WALL (48 ELEMENTS)

Height (m)	Mole fraction analytic	Mole fraction at :				
		0	R/4	R/2	3R/4	R
0	0.0553	0.0553	0.0553	0.0553	0.0553	0.0553
0.254	0.0359	0.04678	0.046820	0.046902	0.047034	0.047227
0.508	0.0283	0.04145	0.041481	0.041555	0.041674	0.041841
0.762	0.0254	0.03800	0.038035	0.038102	0.038211	0.038363
1.016	0.0242	0.03581	0.035834	0.035897	0.035999	0.036141
1.270	0.0237	0.03449	0.034517	0.034578	0.034675	0.034812
1.5240	0.0236	0.03401	0.034039	0.034105	0.034209	0.034352
ys(exp)	0.0328					

To further verify the influence on the radial profile we defined a relative molar fraction:

$$\frac{y|_r - y|_{r=0}}{y|_{r=0}} \qquad (16)$$

Thus, we note that the influence of radial dispersion is important on the values of mole fraction at the axe of the column and the relative error between the value of mole fraction at the output given by this model and experimental one reduces to 3.6% (Table III).We thus arrive at the

following result: the two-dimensional model with non-zero gradient at the wall boundary condition is best which governs the behavior of the column, even if the effect of radial dispersion is not manifested much radially, it must be taken into account when modeling the columns because it has considerable influence on the axial profile, this result is shown on the graph in fig 9.
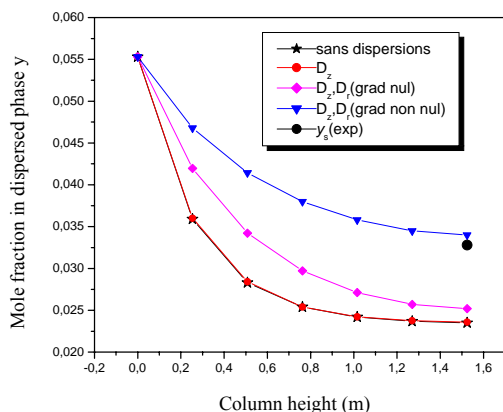

Fig 9 Influence of dispersions: axial and radial on the axial profile of the molar fraction of dispersed phase

V. CONCLUSION

In this work we presented a numerical model that simulates a packed column of liquid-liquid extraction using the finite element method, the results are similar to those obtained analytically or experimentally and also shows that the assumption of negligible radial dispersion is not always reliable, because even if the radial profile is almost flat, radial dispersion influences the axial profile and thus can not be neglected for a more accurate resultThe mathcad code developed offers the ability to change systems to process, properties and dimensions of columns used.

NOTATION

a : interfacial area (m^2/m^3)

E_r : radial dispersion coefficient (m^2/s)

E_z : axial dispersion coefficient (m^2/s)

E : total number of elements

H : column height (m)

K_o: global mass transfer coefficient (m / s)

m : distribution coefficient

r : radial coordinate (m)

R : column radius (m)

t : time (s)

V : phase superficial velocity (m/s)

x : continuous phase mole fraction

y dispersed phase mole fraction

z : axial coordinate (m)

Greek letters

α : constant

β : constant

ϕ : dispersed phase holdup

Indices

c : continuous phase

e : at inlet

d : dispersed phase

s : at outlet

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