UTILIZATION OF THOMAS MODEL TO PREDICT THE BREAKTHROUGH CURVES FOR ADSORPTION AND ION EXCHANGE

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ABSTRACT

Fixed bed sorption processes such as adsorption and ion exchange do not operate at steady state. The design equations are differential that usually require numerical methods to solve. Thomas gives a general analytical solution for these equations. It is based on second-order reaction kinetics and the assumption of Langmuir isotherm. Computer program for the solution of Thomas model was designed using MATLAB 7.0. Four sets of experimental data are tested to show the capability of Thomas model to predict the breakthrough curves for adsorption and ion exchange processes. These data represent the sorption of o-cresol from water by activated carbon, acetic acid from air by activated carbon, phenol from water by natural zeolite, and trichloroethylene from air by zeolite-5A.The results show that there are a good agreement between the experimental data and the model.

الخلاصة

أن عمليات الامتزاز والتبادل الايوني للطور الثابت تكون متغيرة ، فالمعادلات الخاصة بالتصاميم هي معادلات تفاضلية تحتاج الى حلول بالطرق العددية.

توماس استطاع أن يعطي حل عام تحليلي لهذه المعادلات مستندا على ديناميكية التفاعل من الدرجة الثانية ومعادلة لانكمير عند التوازن. تم اعداد برنامج رياضي لموديل توماس بأستخدام **MATLAB 7.0** .

أستخدمت اربعة نماذج من التجارب لغرض أظهار مقدرة موديل توماس للتنبأ بمنحنيات الامتزاز والتبادل الايوني. البيانات مثلت امتزاز الاورثوكريسول من الماء بواسطة الفحم المنشط ، وحامض الخليك من الهواء بواسطة الفحم المنشط، والفينول من الماء بواسطة الزيولايت، وثلاثي كلوروالاثلين من الهواء بواسطة الزيولايت. النتائج بينت ان هناك تطابق جيد بين البيانات العملية والموديل.

KEY WORDS

Fixed bed, adsorption, ion exchange, breakthrough curves, Thomas model.

-INTRODUCTION

Rigorous fixed bed models, usually cast in the form of partial differential equations, allow a realistic mathematical description of the sorption column dynamics. When the equilibrium relationship is linear, an analytical solution for the fixed bed dynamic behavior can always be obtained. For nonlinear systems the governing equations are usually solved numerically. Thomas model gives a general analytical solution for these equations based on second-order reaction kinetics and the assumption of non linear equilibrium relationship of Langmuir isotherm. Thomas neglects the axial dispersion [Chu, 2010].

Thomas model is employed by many researchers to predict the breakthrough curves for adsorption and ion exchange [Chu, 2010, Han, et.al. 2009, Vijayaraghavan and Yun, 2008, Han, et.al, 2007, and Han, et.al, 2007].

Sorption from water or gas on a fixed bed of adsorbent is a process of unsteady state mass transfer between the liquid or gas and solid phase. The concentration of adsorbed substance in both phases is a function of both time and location in bed [Wolborska, 1999].In simple fixed-bed adsorption, the solute undergoing adsorption is removed continually from the carrier liquid or gas and accumulates upon the surface of the solid phase. Such transfer proceeds until the concentration on the solid reaches a value corresponding to equilibrium with the concentration in the feed stream, and the column effluent reaches the feed concentration. Ion exchange is a case of exchange adsorption in which ions chemically bound in the resin phase are displaced in essentially stoichiometric proportions by ions initially in the liquid phase. In either adsorption or ion exchange, the step of accumulation in the solid phase is termed saturation. Sorption is commonly performed in a packed bed where a granular adsorbent such as granular activated carbon or natural zeolite is held stationary in a column and the contaminated water is contacted with the adsorbent by its continuous passage through the bed. In a typical saturation operation, the column effluent is practically free of solute until a state of complete saturation of the entire column is approached. From then on, the effluent concentration increases rapidly toward the original feed concentration. The solute concentration in the effluent may be plotted against the cumulative volume or against the elapsed time; such a plot is termed the concentration history for adsorption or exchange. The point in the concentration history at which solute concentration just reaches a detectable level is known as the breakthrough volume or breakthrough time. The portion of effluent concentration history in which the solute concentration increases from breakthrough to nearly complete saturation has been termed the breakthrough curve, the adsorption wave or the exchange zone. This region is of major practical importance, and the ensuring derivations will be carried out in order especially to calculate this portion of the entire concentration history [Hiester and Vermeulen, 1952 McCabe, et.al, 2001].

In both operations (adsorption and ion exchange) the concentrations in fluid and solid phase inside the bed depend both on position and time, it is unsteady state rate controlled process, therefore sorption occurs only in a particular region of the bed, known as the mass transfer zone, which moves through the bed with time [Thomas and Crittenden, 1998].

The location of the breakpoint and the shape of the breakthrough curve (degree of concavity) are influenced by many parameters pertaining to the nature of the adsorption equilibrium isotherm and the mass transfer rate [Basheer and Najjar, 1996].

Sorption processes are differential; they usually require numerical methods to solve [Tan, 1984]. The general analytical solution is that of Thomas [Thomas, 1944], it is based on second-order reaction kinetics, but can also apply to diffusion-limited system, as demonstrated by Hiester and Vermeulen [Hiester and Vermeulen, 1952].

The aim of this study is to show the capability of Thomas model to predict the breakthrough curves for both adsorption and ion exchange processes. Four sets of experimental data represent adsorption and ion exchange for liquid and gas are used to test the model.

FIXED BED PROCESS MODEL

Methods of second-order kinetics

The following reactions for ion exchange and for physical adsorption will be considered [Hiester and Vermeulen, 1952, Smith, 1988].

$$A + B.Resin \rightarrow B + A.Resin \qquad (ion\ exchange)$$

$$A + Sorbent \rightarrow A.Sorbent \qquad (adsorption)$$

The rate for ion exchange at the particle surfaces, in the case of ions of the same valence, may be expressed as:

$$\frac{d(A.Resin)}{dt} = K_{kin}\left[(A)(B.Resin) - \left(\frac{1}{\bar{k}}\right)(B)(A.Resin)\right] \qquad (1)$$

Where the parentheses denote concentration, t is the time, K_{kin} is the rate constant for reaction, and $\bar{k}$ is equilibrium constant for the reaction.

Since the resin has a finite capacity, then the sum of the concentrations of $B.Resin$ and $A.Resin$ is equal to a constant [Sherwood, et.al, 1975].

$$(B.Resin) + (A.Resin) = \bar{Q} \qquad (2)$$

Similarly in the solution phase outside the resin, the sum of concentrations of A and B is constant:

$$(A) + (B) = (C_o) \qquad (3)$$

The following substitutions may then be made:

$$\left.\begin{array}{l} (A) = (C) \\ (B) = (C_o - C) \\ (A.Resin) = (q) \\ (B.Resin) = (\bar{Q} - q) = (q_\infty - q) \end{array}\right] \qquad (4)$$

Here q is the amount of A combined per unit weight of dry resin; $\bar{Q}$ is the ultimate capacity of dry adsorbent per unit weight; q_∞ is the capacity of adsorbent that is reached at saturation. For ion exchange, only, $q_\infty = \bar{Q}$ and eq. (1) becomes:

$$\left[\frac{dq}{dt}\right] = K_{kin}\left[C(q_\infty - q) - \frac{1}{k}q(C_o - C)\right] \qquad (5)$$

Assuming Langmuir equilibrium under practically isothermal reaction conditions, the rate for adsorption at the solid surfaces may be written [Keinath and Weber, 1968].

$$\frac{d(A.Sorbent)}{dt} = K_{kin}\left[(A)(Sorbent) - \left(\frac{1}{k}\right)(A.Sorbent)\right]$$

Let:

$$\left.\begin{array}{l} (A) = (C) \\ (A.Sorbent) = (q) \\ (Sorbent) = (\bar{Q} - q) \end{array}\right] \qquad (6)$$

$$\left[\frac{dq}{dt}\right] = K_{kin}\left[C(\bar{Q} - q) - \frac{1}{k}q\right] \qquad (7)$$

Equations of transport

The material balance on the fluid and solid phase for an infinitesimal thickness of bed at any given cross section (neglecting the axial dispersion) is given by [Sherwood, et.al, 1975]:

$$\varepsilon \frac{\partial c}{\partial t} + \rho_b \frac{\partial q}{\partial t} + U \frac{\partial c}{\partial z} = 0 \qquad (8)$$

Eq. (8) must be coupled with the following equation [Sherwood, et.al, 1975]:

$$\rho_b \frac{\partial q}{\partial t} = KaF(C,q) \qquad (9)$$

This equation expresses the rate of addition of solute to the solid phase in terms of the interface mass transfer coefficient Ka and a driving force $F(C,q)$ to be selected [Sherwood, et.al, 1975]. K is the kinetic coefficient based on a unit of exterior particle surface and a is the total surface in a unit volume of packed bed.

The design of a fixed bed device for adsorption or ion exchange requires solution of these two equations.

Thomas solution for sorption breakthrough curves

The most useful treatment of the sorption design problem is that of Thomas [Thomas, 1944]. Thomas assumed that the rate of adsorption on the right hand side of eq. (9) can be represented by an expression suggested by the stoichiometry of the monovalent ion exchange reaction then:

$$\rho_b \frac{\partial q}{\partial t} = Ka \left[C(q_m - q) - \frac{1}{\bar{k}} (C_o - C) q \right] \qquad (10)$$

Eq. (10) is expressed in terms of a kinetic coefficient K and the two Langmuir isotherm constants (q_m and $\bar{k}$)

The expression in square brackets is called the “kinetic driving force” and K is the corresponding “kinetic coefficient”. It is possible to relate K to individual mass transfer coefficients representing diffusion resistance in fluid and solid phase. Eq. (10) is simplified for further use by redefining the time scale by [Sherwood, et.al, 1975]:

$$\theta = t - \frac{\varepsilon Z}{U}$$

Then equations (8 and 10) become:

$$\rho_b \frac{\partial q}{\partial \theta} + U \frac{\partial c}{\partial z} = 0 \qquad (11)$$

$$\rho_b \frac{\partial q}{\partial \theta} = Ka \left[C(q_m - q) - \frac{1}{\bar{k}} (C_o - C) q \right] \qquad (12)$$

Thomas model can be used to reduce equations (11 and 12) to a linear equation by introducing a transformation of the dependent variables. His solution for adsorption boundary conditions on $C(Z,\theta)$ and $q(Z,\theta)$, such that $C(0,\theta) = C_o = constat$ and $q(Z,0) = 0$, can be expressed by following the nomenclature of Vermeulen et al. [Vermeulen, et.al, 1973]:

$$X = \frac{J(\bar{R}N,\ N\bar{T})}{J(\bar{R}N,\ N\bar{T}) + \left(1 - J(N,\bar{R}N\bar{T})\right)\exp\left((\bar{R}-1)N(\bar{T}-1)\right)} \qquad (13)$$

Where:

$$\left.\begin{aligned} J(u,v) &= 1 - \varphi_1(u,v) \\ \varphi_1(u,v) &= \int_0^u \varphi_o(\lambda,v)\,d\lambda \\ \varphi_o(\lambda,v) &= \exp(-\lambda - v)\, I_o(2\sqrt{\lambda v}) \end{aligned}\right] \qquad (14)$$

I_o is the modified Bessel function of zero order, and the approximate calculation of the J function is:

$$J(u,v) = \frac{1}{2}\left[1 - \operatorname{erf}\left(\sqrt{u} - \sqrt{v}\right) + \frac{exp\left[-(\sqrt{u}-\sqrt{v})^2\right]}{\sqrt{\pi}\left[\sqrt{v} + (u*v)^{\ 1/4}\right]}\right] \qquad (15)$$

Tan [Tan, 1980 and Tan, 1984] modified the work of Hiester and Vermeulen [Hiester and Vermeulen, 1952] by placing the dimensionless eq. (13) of the breakthrough curve, in a new form suitable for microcomputer application:

$$\frac{1}{X} = 1 + \exp(G) \qquad (16)$$

$$G = ln[\varphi_1(N,\bar{R}N\bar{T})] - ln[J(\bar{R}N,N\bar{T})] + (\bar{R}-1)N(\bar{T}-1) \qquad (17)$$

$$\left.\begin{aligned} \varphi_1(N,\bar{R}N\bar{T}) &= J(\bar{R}N\bar{T},N)\left[1 - \frac{\varphi_o(\bar{R}N\bar{T},N)}{J(\bar{R}N\bar{T},N)}\right] \\ \varphi_o(u,v) &= \frac{exp\left[-(\sqrt{u}-\sqrt{v})^2\right]}{2\sqrt{\pi}(u*v)^{1/4}} \end{aligned}\right] \qquad (18)$$

The integral error function erf was approximated as follows [Forbes and Underhill, 1986]:

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$$\operatorname{erf}x = 1 - (a_1 t + a_2 t^2 + a_3 t^3 + a_4 t^4 + a_5 t^5)e^{-x^2} \qquad (19)$$

Where:

$$t = \frac{1}{1+BX} \qquad (20)$$

$a_1 = 0.254829592,\ a_2 = -0.284496736,\ a_3 = 1.421413741, a_4 = -1.453152027$

$a_5 = 1.061405429, \qquad B = 0.3275911$

The number of transfer unit N , the separation factor $\bar{R}$ and the throughput parameter $\bar{T}$ can be calculated as follows [Tan, 1984, Sherwood et.al, 1975]:

$$\left.\begin{aligned}
N &= \frac{KaZ}{U} \\
\bar{R} &= \frac{1}{\bar{\bar{k}}} \\
\bar{T} &= \frac{UC_o\theta}{q_m\, Z\rho_b} \\
a &= \frac{4}{d_p}(1-\varepsilon) \quad \text{For spherical particles} \\
\bar{\bar{k}} &= 1 + \bar{k}C_o \\
\theta &= t - \frac{\varepsilon Z}{U}
\end{aligned}\right] \qquad (21)$$

K can be estimated for liquid sorption as follows [Treybal, 1985]:

$$\left.\begin{aligned}
\frac{1}{K} &= \frac{(\bar{\bar{k}}+1)}{2\bar{\bar{k}}}\left[\frac{C_o/q_m\,\rho_b}{K_s} + \frac{1}{K_f}\right] \\
K_s &= \frac{15D_s}{(1-\varepsilon)d_p}
\end{aligned}\right] \qquad (22)$$

D_s is the surface diffusivity ,can be estimated experimentally.

K_f Can be estimated from the semi empirical correlation shown below [Sherwood et.al, 1975]:

$$K_f = \frac{D_o}{d_e}\left[2 + 1.45\, R_e^{1/2}\, S_c^{1/3}\right] \qquad (23)$$

Where d_e is the equivalent diameter for non spherical particle of adsorbent.

The equations, that are used to estimate K for sorption of gases, are listed below [Sherwood et.al, 1975]:

$$\left.\begin{aligned}
&\frac{1}{K}=\frac{(\bar{\bar{k}}+1)}{2\bar{\bar{k}}}\left[\frac{1}{K_p}+\frac{1}{K_f}\right]\\
&K_f=\frac{J_D\,U}{(Sc)^{2/3}}\\
&J_D=1.175(Re)^{2/3}\\
&K_p=\frac{60\,D_p}{S_o(1-\varepsilon)d_p^2}\\
&S_o=\frac{particle\ surface\ area}{volume\ of\ particle}\\
&\frac{1}{D_p}=\frac{\tau}{x}\left[\frac{1}{D_k}+\frac{1}{D_f}\right]\\
&D_k=\frac{19400x}{S_g\rho_p}\sqrt{\frac{T}{M}}
\end{aligned}\right]\qquad(24)$$

$$\bar{\bar{k}}=1+\bar{k}p$$

A computer program was constructed using MATLAB 7.0 software to calculate the outlet concentration at any time, in order to plot the breakthrough curves. Figure (1) shows the flow chart for MATLAB 7.0 program.

Resistance to mass transfer between phases

The precise design of fixed bed units should allow for several sources of mass transfer resistance. The transport and subsequent adsorption of adsorbate onto adsorbent particle consists of three main mechanisms [Scott and Paul, 1987], they are, transport through the fluid boundary layer to the external surface of the adsorbent particle, Interparticle diffusion in the liquid phase (pore diffusion) and/or in the adsorbed state along the pore walls (surface diffusion), and adsorption to the solid surface of the pore.

For eq. (10) to be employed in the design calculations, Thomas kinetics coefficient K must be found from individual phase mass transfer coefficients as mentioned.

In pores of diameter much greater than the mean free path of a molecule diffusion occurs by process of molecular collisions in the gas phase within the pore (Max William or bulk diffusion), but if the molecular mean free path is much greater than the pore diameter diffusion occurs by molecules colliding with the pore walls (Knudsen diffusion) [Smith, 1988].

Both molecular and Knudsen diffusion may occur in the same porous medium when the porous medium contains both macro pores and micro pores. The mean free path in liquids is so small that Knudsen diffusion is not significant.

Surface diffusion coefficient can be obtained by using the procedure described by Foo and Carmen [Foo and Rice, 1979, Carman and Haul, 1954].

RESULTS AND DISCUSSION

Four sets of experimental data [Maghazachi, 1989, Ebrahim, 2010, Mustafa, 1992, and Ibrahim, 1992] are adopted and compared with Thomas model.

The first data applied sorption of acetic acid from air onto activated carbon; the second applied sorption of phenol onto natural zeolite; the third applied sorption of o-cresol from water by activated carbon; and the final data applied the sorption of trichloroethylene from air by zeolite-5A.

Table (1) shows the values of system parameters for the four sets. The breakthrough curves for experimental and theoretical data were plotted in Figures (2 to 5).

Figures (2 and 3) show a comparison between Thomas model and experimental data for the first and second sets, the average absolute errors was 6% and 5% respectively, a good agreement can be observed, and R^2 were 0.930 and 0.963 respectively.

Figure (4) shows a comparison between theoretical and experimental data for the third set. The deviation of Thomas model from the experimental curve is due to that: the number of transfer unit (N) is equal to one for this set of data as shown in Table (1), and R^2 equal to 0.881. High numbers of transfer unit ($N \geq 10$) will give less deviation, [Thomas and Crittenden, 1998].

Figure (5) shows the comparison between theoretical and experimental data for the fourth set. It can be observed that Thomas model is in almost good agreement with the experimental data above 400 second of time, and the deviation widen below this value .This is because that, Thomas model did not account for axial dispersion which is important in this case (low velocity and high concentration) see Table (1). A special consideration may be needed to include the axial dispersion within the resin particle, because axial dispersion for porous particle may be important when flow rates are low and the sorption is fast and strong, this can be seen in gases of low Reynolds number. R^2 was equal to 0.713 [Thomas and Crittenden, 1998].

CONCLUSIONS

The following points can be concluded from the present research:

- Thomas model can be used to some extent predict the breakthrough curve for adsorption and ion exchange for gases and liquids.
- Thomas model gives a general analytical solution that allows for nonlinear equilibrium relationship.
- Less deviation between the experimental data and Thomas model can be obtained for high number of transfer unit (N) and for the case when the axial dispersion have no effect.

Table (1): Values of the systems parameters

Symbol	Units	1st Set [Maghazachi, 1989]	2nd Set [Ebrahim, 2010]	3rd Set [Mustafa, 1992]	4th Set [Ibrahim, 1992]
ρ_b	g/cm^3	0.4	0.58	0.4	0.714
ρ_p	g/cm^3	1.4	2.12	1.4	1.044
d_p	cm	0.068×0.26	0.05	0.068×0.26	0.02
ε	-	0.714	0.3	0.714	0.315
T	K	303	303	313	305
Z	cm	20	10	6	17.5
U	cm/s	157.2	0.142	0.4	2.32
C_o	g/cm^3	43.7×10^{-6}	150×10^{-6}	100×10^{-6}	578×10^{-6}
q_m	g/g	0.488	0.076	0.271	0.045
$\bar{k}$	cm^3/g	$236\ x10^{3}$	$70.85\ x10^{3}$	$12.2\ x10^{3}$	$3.45x10^{3}$
K	cm/s	4.3	5.2×10^{-4}	4.1×10^{-3}	0.06
N	-	9	3	1	8

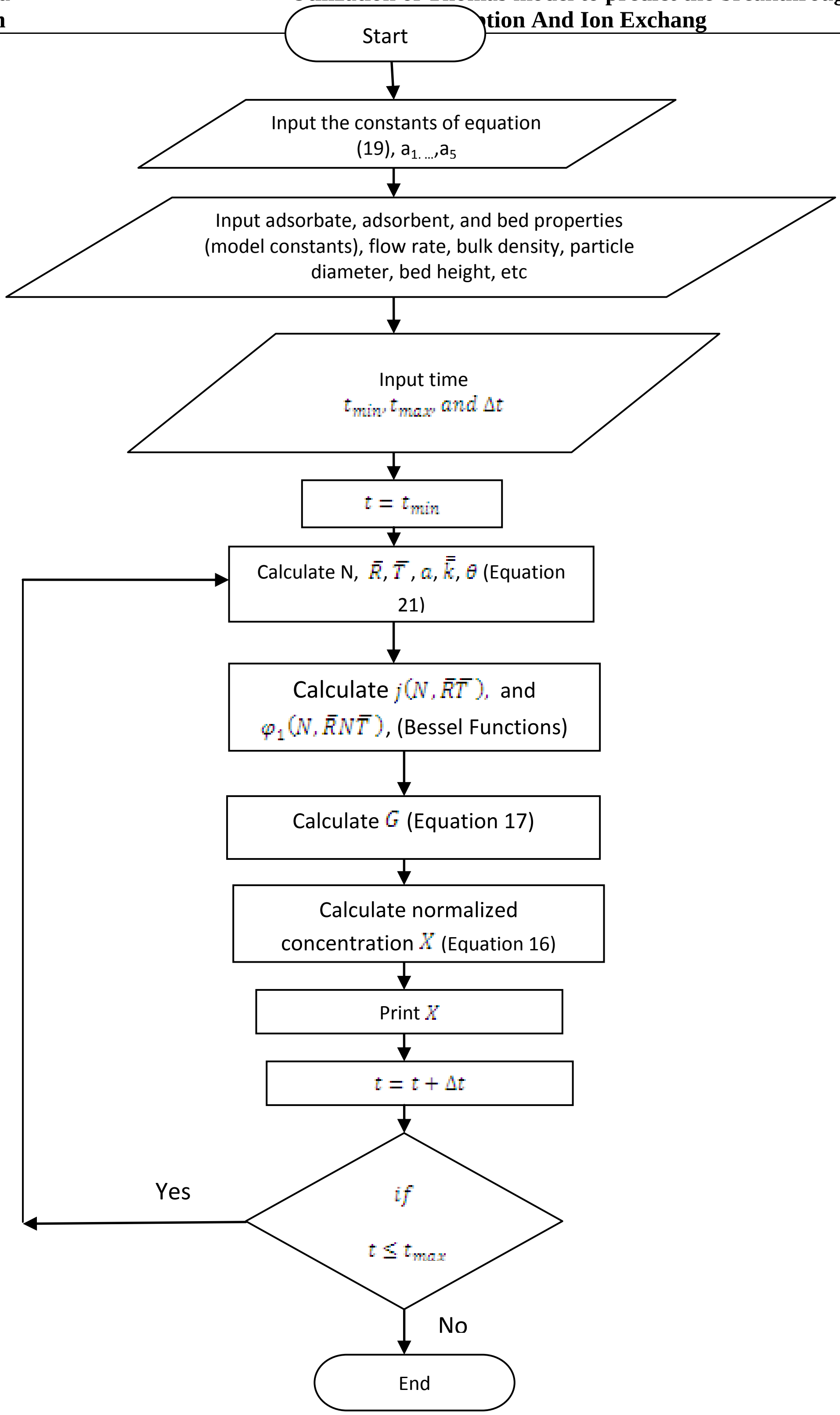

Fig. 1: Flow chart of the program in MATLAB 7.0

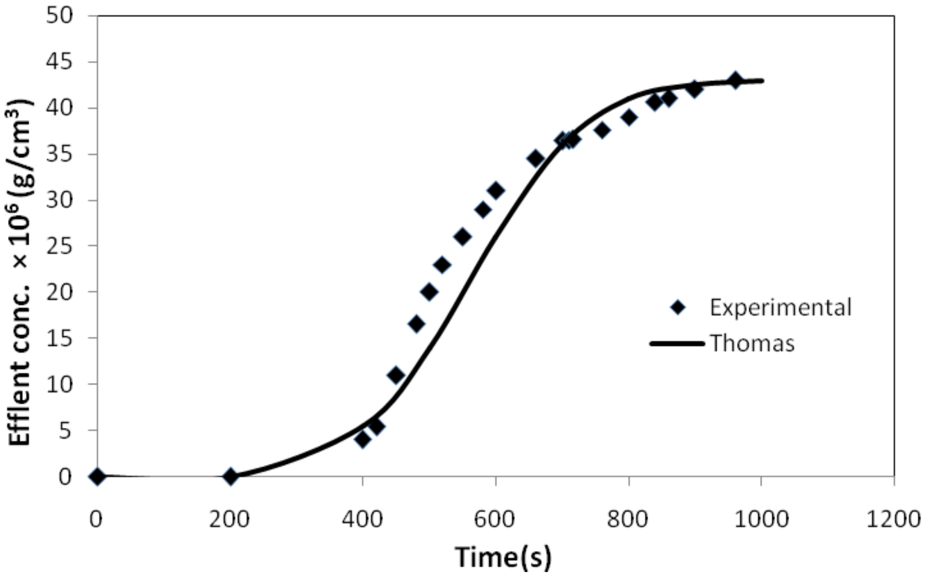

Fig. 2: Experimental and predicted breakthrough curves for sorption of acetic acid from air by activated carbon.

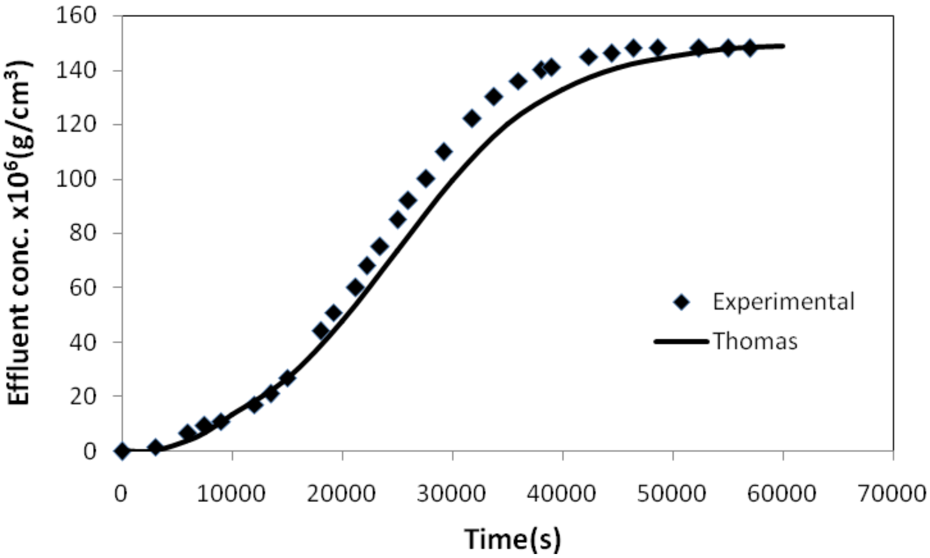

Fig. 3: Experimental and predicted breakthrough curves for sorption of phenol from water by natural zeolite.

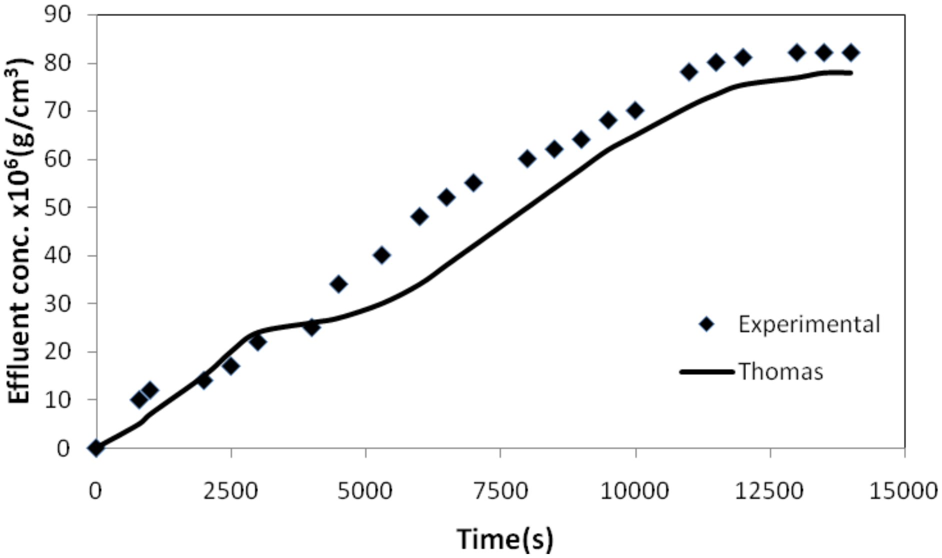

Fig. 4: Experimental and predicted breakthrough curves for sorption of o-cresol from water by activated carbon.

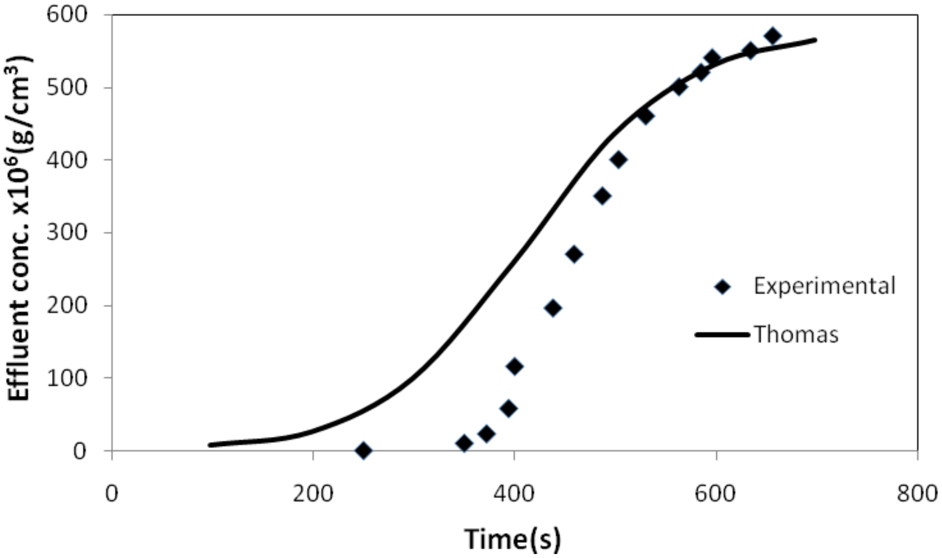

Fig. 5: Experimental and predicted breakthrough curves for sorption of trichloro ethylene from air by zeolite-5A.

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Nomenclature

A	Solute species
a	Interfacial area of solid phase per volume of bed, m^2/m^3
B	Solute species
C	Concentration of fluid, g/cm^3
Co	Initial concentration, g/cm^3
Ce	Concentration of solute at equilibrium, g/cm^3
Do	Molecular diffusivity, cm^2/s
D_f	Fluid phase diffusivity, cm^2/s
D_p	Particle phase diffusivity, cm^2/s
D_k	Kundsen diffusion coefficient, cm^2/s
D_s	Surface diffusion coefficient, m^2/s
de	Equivalent diameter of the particle, cm
d_p	Particle diameter, cm
K	Kinetic mass transfer coefficient for Thomas model, cm/s
K_f	Mass transfer coefficient for fluid phase, cm/s
K_p	Mass transfer coefficient in pore phase, cm/s
$\bar{k}$	Equilibrium constant or Langmuir constant, cm^3/g
$\bar{\bar{k}}$	$\bar{\bar{k}}=1+\bar{k}c_o$ or $\bar{\bar{k}} = 1 + \bar{k}\,p$
M	Molecular weight, g/gmol
N	Number of transfer units
P	Adsorbate partial pressure, Kpa
P_o	Adsorbate partial pressure in the feed gas mixture, Kpa
$\bar{Q}$	Ultimate capacity of dry adsorbent, g/g
Q	Fluid flow rate, cm^3/s
q	Adsorbate phase concentration (capacity), g/g
q_m	Maximum solid phase concentration value corresponding to complete coverage of surface by a monolayer, g/g
q_∞	Adsorbed phase concentration at saturation, g/g
R	Gas constant, 8.3143 kJ/kmol K
$\bar{R}$	Separation factor
S_o	External surface area per unit volume of particle, 1/cm
T	Temperature, K
T_o	Standard temperature,273K
$\bar{T}$	Throughput parameter
t	Time, s
U	Superficial fluid velocity, cm/s
X	C/Co, Normalized concentration
Z	Bed height, cm
ε	Porosity in packed bed
θ	Contact time, s

ρ_b	Bulk density of bed, g/cm^3
ρ_p	Particle density, g/cm^3
τ	Tortuosity factor
x	Fraction void space inside the porous particles
R_e	Reynolds number
S_c	Schmidt number