SORPS: SORption Process Simulation Software

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Abstract—**Nowadays, sorption is one of the fastest growing techniques for the treatment of wastewaters, due to availability of large variety of biomaterials. A lot of experimentation has been done for finding effective biomaterials. The mechanism and effectiveness of sorption is done by comparative study of experimentation results and theoretical models.**

A computer tool SORPS (SORption Process Simulation) is developed by using MATLAB 7.11. This tool divides sorption process in two categories i.e. batch and column studies. In batch kinetic, intra-particle diffusion, isotherm (equilibrium), thermodynamics and energy studies can be performed and in column, breakthrough curve of sorbent can be determined. More than sixty comparative studies can be performed for variable operational variables. Its interface is user friendly and with self-explanatory steps. It also has flexibility to perform comparison between experimental results and theoretical models; and it is helpful in saving time and cost. Thus, SORPS is preferred over other sorption study tools and it has potential to become a useful tool for industry.

Index Terms—**sorption, biomaterials, comprehensive tool, SORPS, batch and column studies**

I. INTRODUCTION

Due to tremendous industrialization and metropolitan growth over the few decades, the water pollution has grown dramatically [1]. The adulteration of industrial wastewater is a particular and major concern due to its toxic effects on aquatic life, plants and human beings [2].

Thus, the removal of toxic contaminants by cheaper and more effective way is a real challenge of the present modern World. Pollutants of wastewater are usually treated by physical or chemical treatment processes. These processes may include coagulation, flocculation, precipitation, ozonation, adsorption, oxidation, irradiation, ion exchange and membrane processes [3]. Currently, the use of sorbents for the treatment of wastewaters is now days largely used due to availability of large variety of biomaterials. The main advantages of sorption are high selectivity, low operational cost, no wastage sludge and good removal performance [4].

For understanding the mechanism, nature, suitability and sustainability of sorption process, the kinetic models, intra-particle diffusion models, equilibrium isotherm models and thermodynamics parameters are evaluated [5]. Continuous sorption process is very important with respect to industrial application and for this; sorption process is studied in packed and fluidized columns [6-7]. The continuous sorption is abundantly carried out in packed columns. For the design and satisfactory operation of packed column, the study of breakthrough curves and column parameters is necessary [8].

For effective commercial application the sorption process needs to be optimized and it can be done effectively by simulating different mathematical models on computer [9]. Mathematical models and computer simulation of sorption process together form prevailing computer tools for performing various tasks of diverse altitudes. For sorption process design and optimization, batch and column studies are very important; these studies cannot be utilized and handled without appropriate models and computer tools [10]. Furthermore, a range of experimentation and laboratory work is required for determining the effectiveness of sorbent for

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sorbate at various operational conditions. These experiments are quite time consuming and costly. In order to make them economical, use of computer tools is valuable.

II. BACKGROUND

Adsorption is a process in which molecules strew from the fluid to the surface of the solid adsorbent forming a discrete adsorbed phase; in other words adsorption is a surface phenomenon [11]. Like other unit operations (e.g. distillation and absorption etc.), adsorption depends on the mass transfer of individual species. The design of adsorption equipment depends on mechanism, equilibrium data, represented by kinetic and isotherm models respectively, as well as on transient mass balances for the adsorbate, represented by the so-called breakthrough curves [12].

Normally, adsorption process studies are divided in two categories: batch adsorption studies and column adsorption studies.

A. Batch Adsorption Studies

In batch adsorption process, kinetic studies, intra-particle diffusion studies, isotherm (equilibrium) studies, thermodynamics and energy studies are carried out. The batch sorption models involved in these studies are illustrated in Table I to Table IV.

Kinetics data is necessary for the design of an adsorption system. The knowledge of rate equation(s) is necessary for studying the mechanism of adsorption and for time versus concentration profile [13-14]. Normally, the pseudo first order kinetic model, pseudo second order kinetic model and Elovich kinetic model are used for finding the mechanism of adsorption. These models are shown in Table I.

Along with other factors, intra-particle diffusion controls the rate of adsorption by means of sequential processes [15-16]. The sequence of these processes is: (i) diffusion of solute from solution to particles surrounding film; (ii) diffusion from film to particle surface, (iii) diffusion from particle surface to inner sites (pores) and (iv) uptake (involvement of several processes). The intra-particle diffusion models are shown in Table II.

Isotherm data are necessary for the design of adsorption systems. Furthermore, study of adsorption isotherms is significant to develop model which correctly represents the results for design purposes [10, 17]. Isotherm also evaluates feasibility of the adsorption process for a given usage [16]. The most widely used isotherm models are shown in Table III.

The adsorption thermodynamics and energy relate to the process mechanism. There are two types of thermodynamic properties: directly measureable properties (temperature and equilibrium constant) and indirectly measureable properties (entropy, enthalpy and free energy); and further energy is determined by using Arrhenius equation [18-20]. The thermodynamics and energy models are shown in Table IV.

TABLE I.
DIFFERENTIAL AND INTEGRATED FORM OF SORPTION KINETIC MODELS

Kinetic Model	Differential	Integrated Form	Plot
Pseudo First Order [21]	$\dfrac{dq_t}{dt} = k_1(q_e - q_t)$	$\log(q_e - q_t) = \log q_e - \dfrac{k_1 t}{2.303}$	$\log(q_e - q_t)\ vs\ t$
Pseudo Second Order [13-14]	$\dfrac{dq_t}{dt} = k_2(q_e - q_t)^2$	$\dfrac{t}{q_t} = \dfrac{1}{k_2 q_e^2} + \dfrac{t}{q_e}$	$\dfrac{t}{q_t}\ vs\ t$
Elovich [22]	$\dfrac{dq_t}{dt} = \alpha\, e^{-\beta q_t}$	$q_t = \dfrac{1}{\beta}\ln(\alpha\,\beta) + \dfrac{1}{\beta}\ln t$	$q_t\ vs\ \ln t$

TABLE II.
NON-LINEAR AND LINEAR FORM OF SORPTION INTRA-PARTICLE DIFFUSION MODELS

Intra-particle Diffusion Model	Non-Linear Form	Linear Form	Plot
Weber–Morris [23]	$R_{WM} = k_{id} t^a$	$\log R_{WM} = \log k_{id} + a \log t$	$\log R_{WM}\ vs\ \log t$
Mckay–Poots [24]	-	$q_t = X_i + k_i t^{\frac{1}{2}}$	$q_t\ vs\ t^{\frac{1}{2}}$
Igwe–Abia [25]	-	$\ln(1-\propto) = -k_p t$	$\ln(1-\propto)\ vs\ t$

TABLE III.
NON-LINEAR AND LINEAR FORM OF SORPTION ISOTHERM MODELS

Isotherm Model	Non-Linear Form	Linear Form	Plot
Freundlich [26]	$q_e = K_F C_e^{(1/n_F)}$	$\log(q_e) = \log(K_F) + (1/n_F)\log(C_e)$	$\log(q_e)\ vs\ \log(C_e)$
Hill [27]	$q_e = \dfrac{q_s C_e^{n_{Hl}}}{K_D + C_e^{n_{Hl}}}$	$\log\left(\dfrac{q_e}{q_s - q_e}\right) = n_{Hl}\log(C_e) - \log(K_D)$	$\log\left(\dfrac{q_e}{q_s - q_e}\right)\ vs\ \log(C_e)$

Models	Non-Linear Form	Linear Form	Plot
Langmuir [28]	$q_e = q_{max} \dfrac{K_L C_e}{1 + K_L C_e}$	$\dfrac{C_e}{q_e} = \dfrac{1}{q_{max}} C_e + \dfrac{1}{K_L q_{max}}$	$\dfrac{C_e}{q_e}$ vs C_e
		$\dfrac{1}{q_e} = \left(\dfrac{1}{K_L q_{max}}\right)\dfrac{1}{C_e} + \dfrac{1}{q_{max}}$	$\dfrac{1}{q_e}$ vs $\dfrac{1}{C_e}$
		$q_e = q_{max} - \left(\dfrac{1}{K_L}\right)\dfrac{q_e}{C_e}$	q_e vs $\dfrac{q_e}{C_e}$
		$\dfrac{q_e}{C_e} = K_L q_{max} - K_L q_e$	$\dfrac{q_e}{C_e}$ vs q_e
Brunauer-Emmett-Teller [10, 29]	$q_e = \dfrac{BQC_e}{(C_s - C_e)[1 + (B-1)(C_e/C_s)]}$	$\dfrac{C_e}{(C_s - C_e)q_e} = \dfrac{(B-1)}{BQ}\dfrac{C_e}{C_s} + \dfrac{1}{BQ}$	$\dfrac{C_e}{(C_s - C_e)q_e}$ vs $\dfrac{C_e}{C_s}$
Tempkin [30]	$q_e = \dfrac{RT}{b_T}\ln(K_T C_e)$	$q_e = \dfrac{RT}{b_T}\ln(K_T) + \dfrac{RT}{b_T}\ln(C_e)$	q_e vs $\ln(C_e)$
Harkin-Jura [31]	-	$\dfrac{1}{q_e^2} = \left(\dfrac{B_{HJ}}{A_{HJ}}\right) - \left(\dfrac{1}{A_{HJ}}\right)\log(C_e)$	$\dfrac{1}{q_e^2}$ vs $\log(C_e)$
Dubinin-Radushjevich [32]	$q_e = q_{DR}\exp\left(-B_{DR}\left[RT\ln\left(1 + \dfrac{1}{C_e}\right)\right]^2\right)$	$ln(q_e) = \ln(q_{DR}) - 2B_{DR}RT\ln\left(1 + \dfrac{1}{C_e}\right)$	$ln(q_e)$ vs $RT\ln\left(1 + \dfrac{1}{C_e}\right)$
Halsey [33]	$q_e = \left(\dfrac{K_H}{C_e}\right)^{\frac{1}{n_H}}$	$\ln(q_e) = \left(\dfrac{1}{n_H}\ln(K_H)\right) - \dfrac{1}{n_H}\ln(C_e)$	$\ln(q_e)$ vs $\ln(C_e)$
Florry-Huggins [34]	$\dfrac{\theta}{C_o} = K_{FH}(1 - \theta)^{n_{FH}}$	$\log\left(\dfrac{\theta}{C_o}\right) = \log(K_{FH}) + n_{FH}\log(1 - \theta)$	$\log\left(\dfrac{\theta}{C_o}\right)$ vs $\log(1 - \theta)$
Frumpkin [35]	-	$\log\left(\dfrac{\theta}{C_o(1 - \theta)}\right) = \log(K_{Fn}) + \dfrac{2\alpha_{Fn}\theta}{2.303}$	$\log\left(\dfrac{\theta}{C_o(1 - \theta)}\right)$ vs θ

TABLE IV.
SORPTION THERMODYNAMICS AND ENERGY

Models	Non-Linear Form	Linear Form	Plot
Entropy & Enthalpy Change [19]	-	$\ln(k_d) = \ln\left(\dfrac{q_e}{C_e}\right) = \dfrac{\Delta S}{R} - \dfrac{\Delta H}{R\,T}$	$\ln(k_d)$ vs $\dfrac{1}{T}$
Gibb's Free Energy [20]	-	$\Delta G = \Delta H - T\,\Delta S$	ΔG vs T
Arrhenius Energy [18]	$k = k_o e^{(-E_a/RT)}$	$\ln(k) = \ln(k_o) - \dfrac{E_a}{RT}$	$\ln(k)$ vs $\dfrac{1}{T}$

B. Column Adsorption Studies

In column studies, breakthrough curve studies and column parameter studies are carried out. The column sorption models involved in these studies are illustrated in Table V and Table VI.

Breakthrough curves represent the adsorbent bed exhaustion time with a solution of adsorbate at fixed concentration at constant temperature and flow rate. The breakthrough curve is used to find out adsorbent efficiency for the required separation process, predict column exhaustion time and to optimize a column for given specific operating conditions [36]. So far, various breakthrough curves models have been formed and mostly used models are illustrated in Table V.

Column parameters, which are involved in analysis of column studies, are shown in Table VI.

TABLE V.
NON-LINEAR AND LINEAR BREAKTHROUGH CURVE MODELS

Breakthrough Curve Models	Non-Linear Form	Linear Form	Plot
Bohart-Adams [37]	$\dfrac{C_t}{C_o} = \dfrac{1}{1 + e^{(k_{AB}q_oZ/U - k_{AB}C_ot)}}$	$\ln\left(\dfrac{C_o}{C_t} - 1\right) = \dfrac{k_{AB}q_oZ}{U} - k_{AB}C_ot$	$\ln\left(\dfrac{C_o}{C_t} - 1\right)$ vs t
Thomas [38, 39]	$\dfrac{C_t}{C_o} = \dfrac{1}{1 + e^{((k_{th}/Q)(q_oM - C_oQt))}}$	$\ln\left[\dfrac{C_o}{C_t} - 1\right] = \dfrac{k_{th}q_oM}{Q} - k_{th}C_ot$	$\ln\left[\dfrac{C_o}{C_t} - 1\right]$ vs t
Yoon-Nelson [38, 40]	$\dfrac{C_t}{C_o} = \dfrac{1}{1 + e^{k_{YN}(\tau - t)}}$	$\ln\left(\dfrac{C_t}{C_o - C_t}\right) = k_{YN}t - \tau k_{YN}$	$\ln\left(\dfrac{C_t}{C_o - C_t}\right)$ vs t

TABLE VI.
COLUMN PARAMETERS

Column Parameters	Equation
Empty Bed Contact Time (EBCT) [41]	$EBCT = \dfrac{Bed\ Volume}{Volumetric\ Flow\ Rate}$
Bed Depth Service Time (BDST) [42]	$t = \dfrac{N_o Z}{C_o V} - \dfrac{1}{C_o k_a} \ln\left[\dfrac{C_o}{C_t} - 1\right]$
Overall Adsorption Zone [43]	$\Delta t = t_e - t_b$
Length of Adsorption Zone [43]	$Z_m = Z\left(1 - \dfrac{t_b}{t_e}\right)$
Minimum Length of Bed [43]	$Z_{min} = \dfrac{V}{k_a N_o} \ln\left(\dfrac{C_o}{C_t} - 1\right)$
Volume of Effluent [43]	$V_{eff} = Q t_e$
Adsorbate Amount [43]	$m_{total} = \dfrac{C_o Q t_e}{1000}$
Adsorbate Removal [43]	$Adsorbate\ Removal\ (\%) = \dfrac{m_{ad}}{m_{total}} \times 100$
Elution Efficiency [43]	$\eta(\%) = \dfrac{m_d}{m_{ad}} \times 100$

III. SORPS

A computer tool SORPS[1] (SORption Process Simulation) has been developed using MATLAB[2] 7.11. This tool divides sorption process in two categories i.e. batch and column studies. In batch studies; sorption process kinetics, intra-particle diffusion models, equilibrium isotherm studies, sorption thermodynamics and sorption energy can be analysed. In column studies; breakthrough curve and column parameters can be studied.

SORPS is a very helpful tool for comparing experimental results with various predefined models and finally finds the best fit model among them. SORPS displays results in both tabular and graphical forms.

A. GUI and Algorithm

At the start of SORPS, a start-up screen will open. At start-up screen, sorption process selection is to be done, among following;

- Batch studies
- Column studies
- Batch and column studies

Fig. 1 presents a screenshot of the SORPS that is compatible with Windows[3] (64-bit) and Mac-OX-S[4] (64-bit). The MATLAB programming language has made it possible to develop a clear and flexible code that is portable on any computer system running MATLAB Compiler Runtime (MCR) version 7.14 or higher.

A user friendly interface with self-explanatory steps and built-in help makes it easy to use, even for new computer users. The built-in dialog boxes that prompt error(s), warning(s) and question(s) direct a user to the right path. Selection of multiple models at a time supports comparative study and finds the best model. Further, sensitivity analysis can also be done.
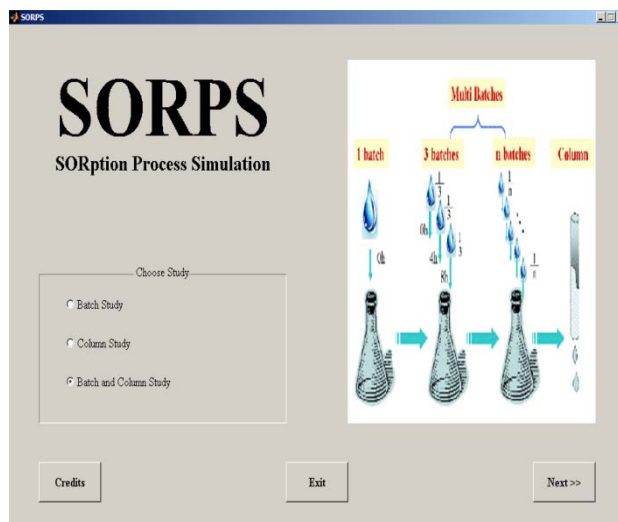

Figure 1. Start-up Screen of SORPS

The batch study is done in four different ways that's for variable sorbate, sorbent, pH and temperature. For all these ways, different models and parameters (Table I–IV) can be studied. The results of all these ways can be seen in the form of tables and graphs. The thermodynamics and energy studies are done only when experimentation is done at different temperature conditions. Kinetics, intra-particle diffusion and isotherm studies can be done for all

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1 SORPS is freeware and can be downloaded from http://www.uet.edu.pk
2 MATLAB is a register trademark of MathWorks, Incorporate http://www.mathworks.com
3 Windows is a register trademark of Microsoft Incorporate http://www.microsoft.com
4 Mac-OX-S is a register trademark of Apple Incorporate http://www.apple.com

ways. The algorithm of batch studies is shown in Fig. 2.
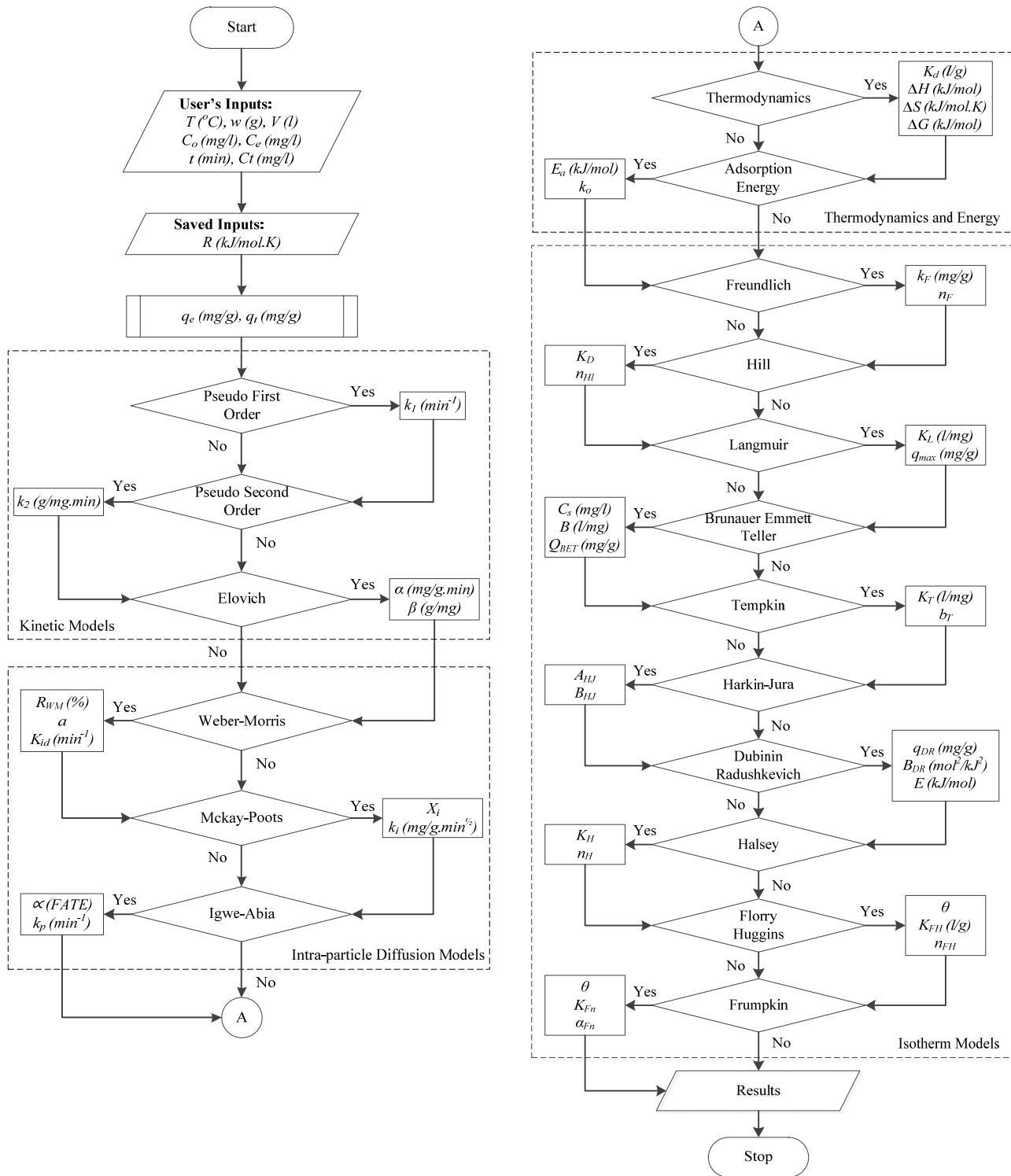
Figure 2. Batch Studies Algorithm

The column study is done in nine different ways that's for variable sorbate, sorbent, pH and temperature, bed height, sorbent mass, concentration, flow rate and column diameter. For all these ways, different models and parameters can be studied. The results of all these ways can be seen in the form of tables and graphs. The Bed Depth Service Time (BDST) activates only when breakthrough curve is to be studied at various bed depths. The algorithm of column studies is shown in Fig. 3.
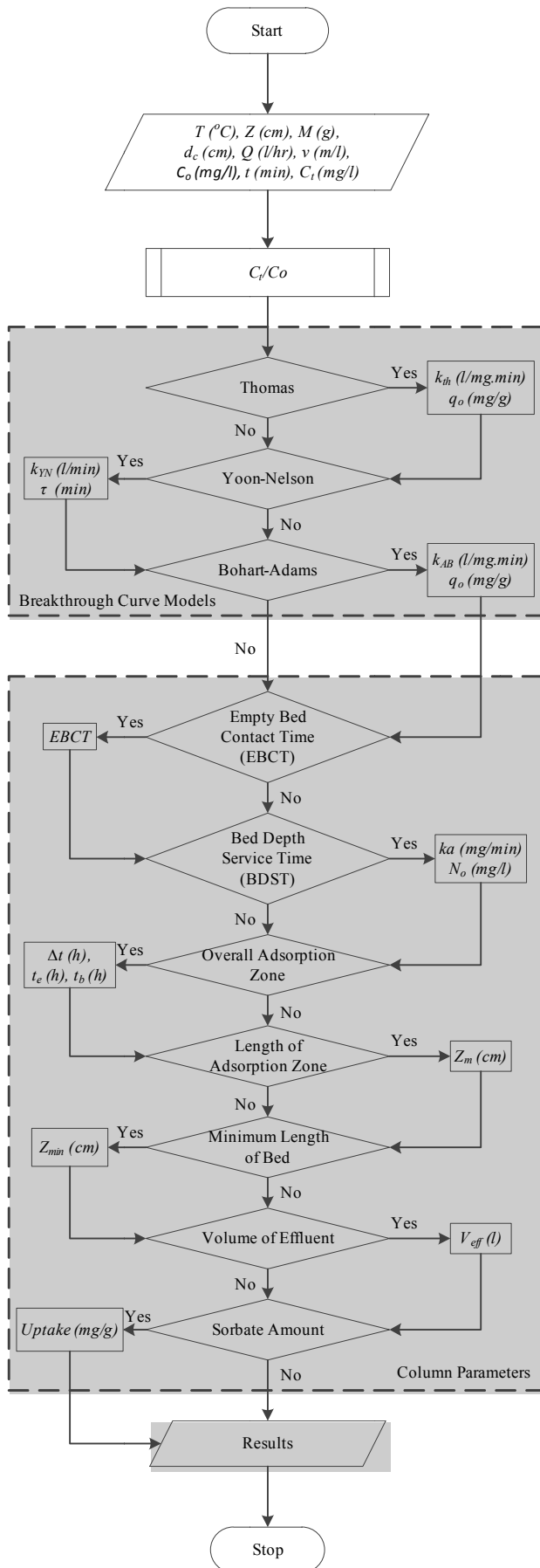
Figure 3. Column Studies Algorithm

B. Graphical Capabilities

Besides comparing results in table, SORPS has the capability to produce multiple graphs in the same window. The multiple graphs in a same window make comparison studies easier. Features like zoom in, zoom out, pan, rotation and data cursor for graphs make the critical analysis possible. The above mentioned salient features are shown in Fig. 4.
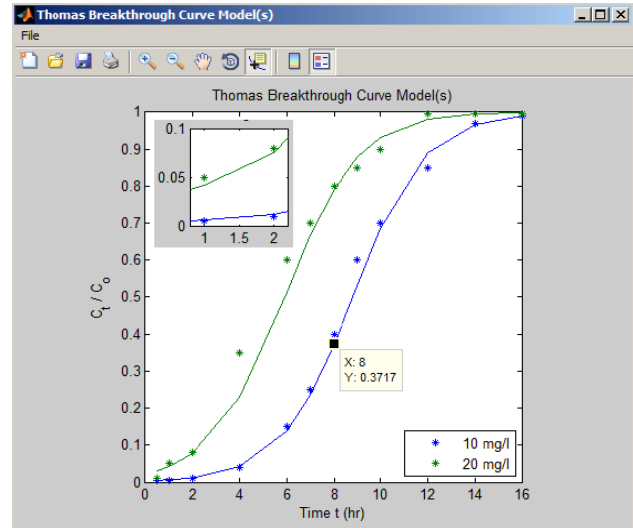

Figure 4. Thomas breakthrough cure models generated by SORPS for concentration 10 mg/l and 20 mg/l, inset plot focusing from 1 to 2 hr and where black spot telling about X-Y coordinates

IV. CASE STUDIES

Two case studies i.e. batch and column are presented for demonstrating the working of software. In batch studies, comparison of Cu(II) and Zn(II) sorbate for kinetic studies, intra-particle diffusion studies and isotherm studies is done. In column studies, the effect of operational variable (initial concentration of sorbate) on breakthrough curves is studied for Cd(II) and column parameters are also studied.

A. Batch Adsorption Studies

The batch adsorption experimentations for removal of Cu(II) and Zn(II) from water by means of rice husk ash have already been carried out [44]. In this study, the best fit models were found by comparing experimental results with theoretical models by using computer software SORPS. Only the best fit models are presented.

For comparative study of metals, initial concentration and time interval were taken similar. In this study for batch experimentation, one kinetic model, one intra-particle diffusion model and one isotherm model are studied.

Kinetic studies: The steps that manage the overall rate of removal are essential to identify. Only the pseudo-second order is studied. The pseudo-first order and Elovich models can also be studied by using SORPS. The comparison of experimental and pseudo-second order model for Cu(II) and Zn(II) are shown in Fig. 5.
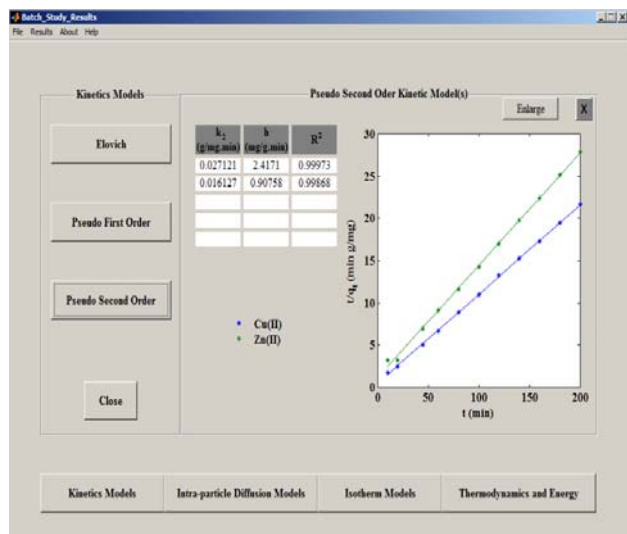
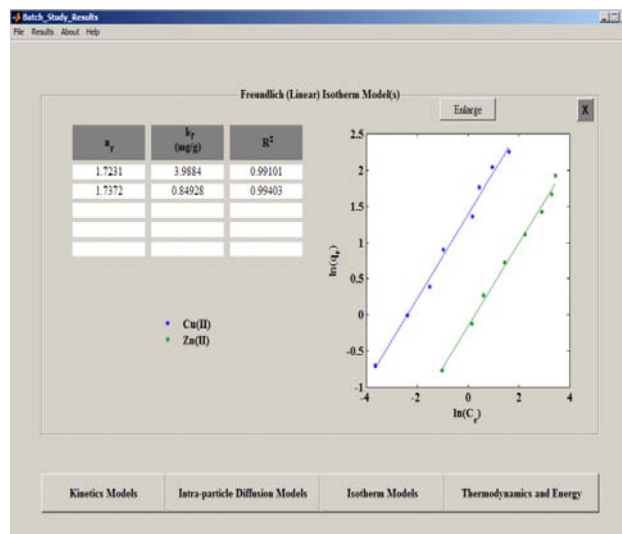Figure 5. Kinetic studies: Pseudo-first order model

Intra-particle diffusion studies: The overall rate sorption is also controlled by diffusion within particles. The Mckay-Poots and Igwe-Abia models can also be studied by using SORPS. The comparison of experimental and Weber-Morris model for Cu(II) and Zn(II) are shown in Fig. 6.
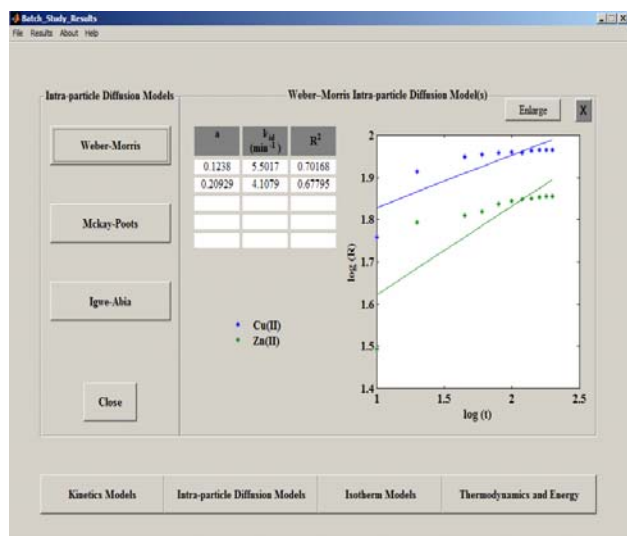

Figure 6. Intra-particle diffusion studies: Weber-Morris

Isotherm studies: The sorption isotherms are equilibrium relationships. The Freundlich and Langmuir are the most common isotherm models. Only the Freundlich model is studied. The models mentioned in Table III can also be studied. The comparison of experimental and Freundlich for Cu(II) and Zn(II) is shown in Fig. 7.

Figure 7. Isotherm studies: Freundlich model

Other than the above evaluated models, SORPS can evaluate thermodynamics parameters as well as sorption energy. Other than sorbate comparative study, SORPS can also be used for sorbent, pH and temperature comparative studies.

B. Column Adsorption Studies

The column adsorption experimentations for removal of Cd(II) have already been carried out [45]. In this study, the best fit models were found by comparing experimental results with theoretical models by using computer software SORPS.

For comparative study, only the initial concentration is varied. All other parameters are kept constant. In this study for column experimentation one breakthrough curve mode and column parameters are studied.

Breakthrough curve studies: The Bohart-Adams model is studied for variable concentrations. The comparison of experimental and Bohart-Adams are shown in Fig. 8.
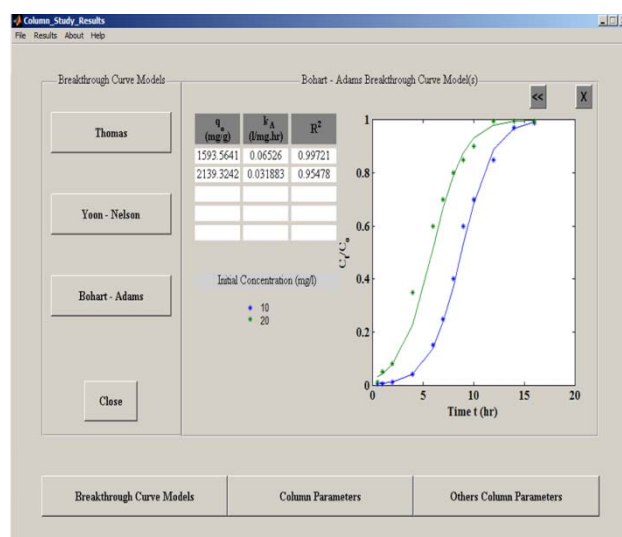

Figure 8. Breakthrough curve studies: Bohart-Adams

Column Parameters: The uptake, overall adsorption zone, length of adsorption zone, minimum length of adsorption zone and volume of effluent for variable concentrations are studied too and are shown in Fig. 9.
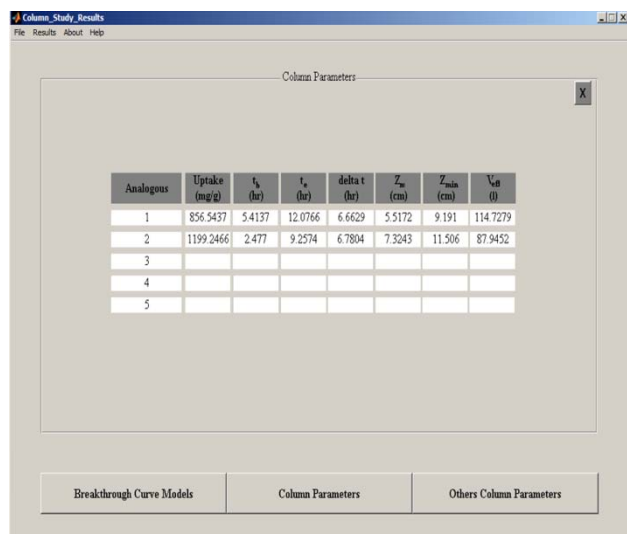

Figure 9. Column parameter studies

SORPS can also evaluate empty bed contact time (EBCT) and bed depth service time (BDST). Other than the above mentioned studies, SORPS can also be used for sorbate, sorbent, flow rate, pH, temperature, bed height, sorbent mass and column diameter comparative studies.

V. CONCLUSIONS

SORPS is a simulation tool developed for sorption process. It can be efficiently utilized for evaluating various modulated parameters involved in sorption process, such as; mechanism (kinetics and intra-particle diffusion), equilibrium isotherms, thermodynamics parameters, energy, breakthrough curves, column parameters and comparison of experimental results with theoretical models.

This software is expected to be important for industry as well as education sector. Further, graphical capabilities of software help in better understanding of sorption process. The modular approach behind SORPS has flexibility and versatility to add more features such as interface with hardware (atomic absorption spectrometer and uv-vis spectrophotometer), binary or higher order studies, non-linear fit method and multiple error analysis.

NOMELCLATURE

a	Webber-Morris: Gradient depicts adsorption mechanism	
A_{HJ}	Harkin-Jura: Constant	
B	BET: Constant relating to energy of surface interaction	l/mg
B_{DR}	Dubinin-Radushkevich: Adsorption energy constant	mol^2/kJ^2
B_{HJ}	Harkin-Jura: Constant	
b_T	Tempkin: Constant	
C_e	Adsorbate concentration at equilibrium	mg/l
C_o	Initial concentration of adsorbate	mg/l
C_s	Saturation concentration of adsorbate	mg/l
C_t	Concentration of adsorbate at time 't'	mg/l
E_a	Activation energy	kJ/mol
ΔG	Gibb's free energy	kJ/mol
h	Second order: Initial adsorption rate	$mg/g.min$
ΔH	Enthalpy change	kJ/mol
k_1	First order: Rate constant	min^{-1}
k_2	Second order: Rate constant	$g/mg.min$
k_a	BDST: Adsorption rate constant	mg/min
k_{AB}	Bohart-Adams: Mass transfer coefficient	$l/mg.min$
K_D	Hill: Constant	
k_d	Distribution coefficient	l/g
K_F	Freundlich: Adsorption capacity constant	mg/g
K_{FH}	Flory-Huggins: Constant of adsorption	l/g
K_{Fn}	Frumkin: Constant	
K_H	Halsey: Constant	
k_i	Mckay-Poots:Intraparticle diffusion	$mg/g.min^{1/2}$
k_{id}	Webber-Morris: Intraparticle diffusion rate	min^{-1}
K_L	Langmuir: Constant for affinity and energy binding sites	l/mg
k_o	Frequency factor	
k_p	Igwe-Abia: Intra-partcle diffusion constant	min^{-1}
K_T	Tempkin: Equilibrium binding constant	l/mg
k_{th}	Thomas: Rate constant	$l/mg.min$
k_{YN}	Yoon-Nelson: Rate constant	l/min
M	Mass of adsorbent bed	g
$[M]$	Igwe-Abia: Concentration of adsorbate ion	
m_{ad}	Amount of adsorbate adsorbed in column	g
m_d	Amount of adsorbate desorbed	g
m_{total}	Total amount of adsorbate send to column	g
n_F	Freundlich: Adsorption intensity constant	
n_{FH}	Flory-Huggins: No. of adsorbate occupying adsorption sites	

Symbol	Description	Units
n_H	Halsey: Constant	
n_{Hl}	Hill: Binding interaction cooperative coefficient	
N_o	Adsorption capacity of bed	mg/l
Q_{BET}	BET: Adsorption theoretical saturation capacity	mg/g
Q	Volumetric flow rate of solution in column	l/min
q_{DR}	Dubinin-Radushkevich: Adsorption saturation capacity	mg/g
q_e	Adsorption capacity at equilibrium	mg/g
q_{max}	Langmuir: Maximum adsorption capacity	mg/g
q_o	Maximum column adsorption capacity	mg/g
q_s	Hill: Maximum uptake saturation	mg/l
q_t	Adsorption capacity at time "t"	mg/g
R	Universal Gas constant (8.314 x 10^{-3})	$kJ/mol\ K$
R_L	Langmuir: Separation Factor	
R_{WM}	Webber-Morris: Percentage of adsorbate adsorb	$\%$
ΔS	Entropy Change	$kJ/mol.K$
T	Time	H
T	Temperature	K
t_b	Breakthrough time of column	H
t_e	Exhaustion time of column	H
Δt	Overall adsorption zone in column	H
U	Velocity of solution in column	cm/min
V	Volume of solution	L
V_{eff}	Volume of effluent from column	L
W	Mass of adsorbent	G
X_i	Mckay-Poots: Boundary layer thickness constant	
Z	Adsorption bed length	Cm
Z_m	Length of adsorption zone	Cm
Z_{min}	Minimum adsorption bed length	Cm

Greek Letters

Symbol	Description	Units
A	Elovich: Initial adsorption rate	$mg/g.min$
α_{Fn}	Frumkin: Constant	
B	Elovich: desorption constant	g/mg
H	Elution efficiency	$\%$
Θ	Degree of surface coverage	
T	50% adsorbate breakthrough time of column	min
$\propto$	Igwe-Abia: Fractional attainment to equilibrium (FATE)	
∞	Infinity	

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