UNIVERSITI PUTRA MALAYSIA

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By

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Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirements for the degree of Doctor of Philosophy.

SIMULATION OF SINGLE AND DUAL LAYERED RAPID PRESSURE SWING ADSORPTION

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May 2013

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Rapid Pressure Swing Adsorption (RPSA) is a cyclic process where the bed is repeatedly being subjected to rapid adsorption and desorption. The process is inherently dynamic and exhibits cyclic steady state (CSS) after sufficient number of cycles. In this thesis, two novel methods of successive substitution (MSS) accelerators are developed. The novel MSS accelerators possess three important features (i) speeding the convergence to CSS, (ii) determining the CSS unambiguously, and (iii) preserving the process variable profiles at CSS. The MSS accelerators incorporate a hybrid algorithm which combines the MSS and (i) Aitken and (ii) Muller updating scheme, and a stopping criterion. Both hybrid algorithms are tested on a cyclic process, controlled-cycle stirred tank reactor (CCSTR) described by a non-linear algebraic equation. The Muller hybrid algorithm is found to achieve CSS faster and is then adopted for the simulation of RPSA for air separation. It is found that the Muller hybrid algorithm is able to reduce the number of cycles required to reach CSS by 50%. The process variable profiles at CSS obtained from the algorithm are also found to be in excellent agreement with the MSS simulation.

A dual layered RPSA model is then developed. Verification of the applied numerical methods and computer programs are carried out successfully that the simulated results agree well with the analytical solutions and experimental data. The optimum pressurization to depressurization time ratio for the dual layered RPSA is first determined. Effects of particle sizes (300:100 μm to 300:500 μm), types of adsorbents (Zeolites 5A and AgLiX), and having non-adsorptive particles in oxygen product purity and recovery are then studied. Depending on the ratio of the length of the first layer to the length of the bed, ω, the dual layered RPSA is found to improve the oxygen product purity by 16% - 20% for particle size of 300:100 μm. It is also found that the oxygen product purity increases by almost 20% when the first layer is packed with Zeolite AgLiX and Zeolite 5A in the second layer. Higher pressure drop across the bed is induced when particles of smaller pressure drop are used in the first layer and particles of larger pressure drop are used in the second layer, hence leading to better separation. Nevertheless, the oxygen product recovery is found to be insensitive to these new configurations. The dual layered RPSA packed with non-adsorptive particles is found to have reduced the oxygen product purity. Hence, replacing the adsorbent at the product end will not help in reducing the amount of adsorbent needed for the operation.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

SIMULASI UNTUK PENJERAPAN BUAIAN TEKANAN PESAT TUNGGAL DAN DUA LAPISAN

Oleh

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Penjerapan buaian tekanan pesat (RPSA) adalah satu proses kitaran di mana katil penjerapan adalah berkali-kali tertakluk kepada penjerapan dan nyahjerapan yang pesat. Proses ini bersifat dinamik dan mempamerkan keadaan stabil kitaran (CSS) selepas beberapa kitaran yang mencukupi. Dalam tesis ini, dua novel kaedah penggantian berturut-turut (MSS) pemecut dibangunkan. MSS novel pemecut memiliki tiga ciri-ciri penting (i) mempercepatkan penumpuan kepada CSS, (ii) menentukan CSS jelas, dan (iii) memelihara profil pembolehubah proses di CSS. Pemecut MSS menggabungkan algoritma hibrid yang menggabungkan MSS dan (i) Aitken dan (ii) Muller skim mengemaskini, dan kriteria berhenti. Kedua-dua algoritma hibrid diuji dengan satu proses kitaran bernama kawalan kitaran dikacau tangki reaktor (CCSTR) yang digambarkan oleh persamaan bukan linear algebra. Algoritma Muller hibrid didapati mencapai CSS lebih cepat dan ia kemudian digunakan dalam simulasi RPSA untuk pemisahan udara. Ia mendapati bahawa algoritma Muller hibrid mampu untuk mengurangkan bilangan kitaran yang diperlukan untuk mencapai CSS sebanyak 50%. Profil pembolehubah proses di CSS diperolehi daripada algoritma juga didapati berada dalam perjanjian yang baik dengan simulasi MSS.

Satu model RPSA dua lapisan kemudian dibangunkan. Pengesahan kaedah yang digunakan berangka dan program komputer dijalankan dengan jayanya bahawa keputusan simulasi bersetuju dengan baik dengan penyelesaian analitikal dan data uji kaji. Nisbah masa tekanan kepada nyahtekanan optimum untuk berlapis dua RPSA mula-mula ditentukan. Kesan saiz zarah (300:100 μm hingga 300:500 μm), jenis adsorben (Zeolit 5A dan AgLiX), dan zarah bukan serapan dalam ketulenan produk oksigen dan pemulihan kemudiannya dikaji. RPSA dua lapisan didapati dapat meningkatkan ketulenan produk oksigen sebanyak 16% - 20% bagi saiz zarah 300:100 μm. Bergantung pada nisbah panjang lapisan pertama kepada panjang katil, ω, ia juga mendapati bahawa ketulenan produk oksigen meningkat sebanyak hampir 20% apabila lapisan pertama dipenuhi dengan zeolit AgLiX dan zeolit 5A dalam lapisan kedua. Kejatuhan tekanan yang lebih tinggi di seluruh katil adalah disebabkan apabila zarah kejatuhan tekanan yang lebih kecil digunakan dalam lapisan pertama dan zarah kejatuhan tekanan yang lebih besar digunakan pada lapisan kedua, justeru membawa kepada pemisahan yang lebih baik. Walau bagaimanapun, pemulihan oksigen produk didapati tidak sensitif kepada konfigurasi baru ini. RPSA dua lapisan yang diisi dengan zarah bukan serapan didapati telah mengurangkan ketulenan produk oksigen. Oleh itu, menggantikan adsorben pada lapisan kedua tidak akan membantu dalam pengurangan jumlah adsorben yang diperlukan untuk operasi ini.

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I certify that a Thesis Examination Committee has met on 21 May 2013 to conduct the final examination of Lai Yin Ling on her thesis entitled "**Simulation of Single and Dual Layered Rapid Pressure Swing Adsorption**" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the Doctor of Philosophy.

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DECLARATION

I hereby declare that the thesis is my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously, and is not concurrently, submitted for any other degree at Universiti Putra Malaysia or other institutions.

LAI YIN LING

Date: 21 May 2013

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NOMENCLATURE

Abbreviations

ADPF	axially dispersed plug flow
CCSTR	controlled-cycle stirred tank reactor
CSS	cyclic steady state
LDF	linear driving force
MSS	method of successive substitution
OC	orthogonal collocation
OCFE	orthogonal collocation on finite element
ODE	ordinary differential equation
PDE	partial differential equation
PSA	pressure swing adsorption
RPSA	rapid pressure swing adsorption

Symbols

A	cross section area	m^2
$A_{j,m}$	first derivative of the Lagrange interpolation polynomial	~
$B_{j,m}$	second derivative of the Lagrange interpolation polynomial	~
Bi_m	Biot number for mass transfer	~
C_F	concentration of feed reactant	~
c	gas phase concentration	mol m^{-3}
D	effective axial dispersion coefficient	$m^2\ s^{-1}$
D_{ax}	axial dispersion coefficient	$m^2\ s^{-1}$
D_c	micropore diffusion coefficient	$m^2\ s^{-1}$
D_e	effective diffusion coefficient	$m^2\ s^{-1}$
D_e^*	modified effective diffusion coefficient	$m^2\ s^{-1}$
D_f	diffusion coefficient across the external fluid film	$m^2\ s^{-1}$
D_k	Knudsen diffusion coefficient	$m^2\ s^{-1}$

D_m	molecular diffusion coefficient	$m^2\ s^{-1}$
D_p	pore diffusion coefficient	$m^2\ s^{-1}$
Da	Damkohler number	~
d_c	column inner diameter	cm
d_p	particle size	cm
d_{pore}	macropore diameter	m
Err	relative material balance error	%
f	fraction of reacting mixture removed at the end of a cycle	~
H	Henry's law constant	$m^3\ kg^{-1}$
h_k	width of element k	~
i	an index	~
j	an index	~
J	order of polynomial in the method of OC	~
JK	number of internal collocation point	~
J_v	bed permeability	$N\ s\ m^{-4}$
J_k	coefficient in the Ergun equation	$N\ s^2\ m^{-5}$
K^*	Equilibrium constant of reaction	~
K_{LDF}	dimensionless LDF mass transfer coefficient	$m\ s^{-1}$
k	slope of the semilog plot of advance *vs*. n	~
k_f	external fluid film mass transfer coefficient	s^{-1}
k_{LDF}	LDF mass transfer coefficient	s^{-1}
k_s	magnitude of the slope of ϕ vs η	~
ℓ_m	a Lagrange interpolation polynomial	~
L	length of the column	m
$\hat{M}$	cumulative molar amount at any time during a step	~
$\overline{M}$	dimensionless cumulative molar amount	~
M_w	molecular weight	g
m	an index	~
n	number of cycles or number of iterations	~
P	total pressure	bar

Pe_{∞}	limiting value of the Peclet number	~
$PROD$	adsorbent productivity	mol kg^{-1} s^{-1}
$\overline{Q}_f$	cycle-averaged feed gas rate	m^{3} s^{-1}
$\overline{Q}_p$	product delivery rate	m^{3} s^{-1}
q	adsorbed phase concentration	mol kg^{-1}
q^{*}	equilibrium adsorbed phase concentration	mol kg^{-1}
q_s	Langmuir saturation constant	mol kg^{-1}
$\bar{q}$	average adsorbed phase concentration	mol kg^{-1}
R	ideal gas constant	J mol^{-1} K^{-1}
REC	oxygen product recovery	~
r_p	radius of an adsorbent particle	m
S	dependent variable	~
u	superficial gas velocity	m s^{-1}
$\bar{u}$	dimensionless superficial gas velocity	~
T	temperature	K
t	time	s
t_c	cycle time	s
t_c^{*}	cycle half time	s
t_{cr}	characteristic time constant for micropore diffusion	s
t_f	duration of pressurization	s
t_m	characteristic time constant for macropore diffusion	s
t_w	duration of depressurization	s
V_F	volume of feed reactant	~
V_T	Total volume of reactant	~
X	conversion of reaction	~
$\overline{X}$	process state variables	~
$\overline{Y}$	convergent series	~
y	gas phase mole fraction	~
y_p	oxygen product purity	~

z	axial co-ordinate	m

Greek letters

ϕ	dimensionless pressure	~
η	similarity variable	~
φ	dimensionless adsorbed phase concentration	~
$\overline{\varphi}$	dimensionless average adsorbed phase concentration	~
φ^*	dimensionless equilibrium adsorbed phase concentration	~
Δ	absolute difference between two values	~
β_{ax}	radial dispersion factor	~
ε_b	bed porosity	~
ε_p	particle porosity	~
ε_t	total bed porosity	~
ρ_b	bed bulk density	kg m^{-3}
ρ_g	gas density	kg m^{-3}
τ	dimensionless time	~
τ_{ax}	axial tortuosity factor	~
τ_p	pore tortuosity factor	~
θ_c	dimensionless cycle half time	~
μ	gas viscosity	N s m^{-2}
ω	ratio of the length of first layer to the total length of the bed	~
ξ	dimensionless axial co-ordinate	~

Subscripts

A	oxygen
am	ambient conditions
$accum$	accumulation in the bed
B	nitrogen
e	final state
f	feed end of bed or feed condition

i	component oxygen or nitrogen
p	product end of bed
ref	reference condition
O_2	oxygen
N_2	nitrogen
n	n^{th} cycle
ss	steady state
w	waste condition
0	initial state
1	first layer
2	second layer

Superscript

acc	significant figures specified in the oxygen

CHAPTER 1

INTRODUCTION

1.1 Background

Cyclic process is a class of advanced chemical engineering unit operations. A process is known as a cyclic process the process state variables are cyclically varying with time. Examples of cyclic process are pressure swing adsorption, vacuum swing adsorption, temperature swing adsorption, pressure-vacuum swing adsorption, reverse flow reactor and simulated moving bed. Pressure swing adsorption (PSA) is now an established gas separation technology, with advantages over other separation options for middle-scale processes (Fiandaca *et al.*, 2009). It is a cyclic process, where the beds are repeatedly being subjected to adsorption and desorption. PSA processes have found many important applications such as air separation, recovery of ammonia from ammonia synthesis, ethanol dehydration, carbon dioxide recovery from combustion process, trace volatile organic component removal, hydrogen recovery from refinery gases, air drying, separations of olefins and paraffins (Skarstrom, 1960; Mikkinnen *et al.* (1993); Suzuki *et al.*, 1996; Silva and Rodrigues, 1998; Choong *et al.*, 20004; Kim *et al.*, 2006; Rao *et al.*, 2010; Chai *et al.*, 2011, 2012).

1.2 Cyclic Steady State

The transient cyclic PSA process can be modelled by using partial differential equations (PDEs) for mass conservation in the fluid phase, ordinary differential equations (ODEs) for the sorption rate in the stationary phase, and algebraic equations for the adsorption equilibrium between phases. The cyclic adsorption process has no steady state like general continuous process as it is inherently dynamic. Once the cyclic process is initiated, the process undergoes a transient stage prior to reach cyclic steady state (CSS.) At CSS, the process state variables at some instant within a cycle have the same value at the corresponding instant within each subsequent cycle (Choong, 2000). In the numerical simulation of cyclic process, the most commonly used method is the method of successive substitution (MSS). For PSA, the simulation starts with initiating the pressurisation step and followed by the depressurisation step. Once the cycle is completed, the cycle results will then be used as the initial conditions for the next cycle. Many cycles may be required for the process to reach CSS (Choong, 2000). This can be computationally demanding.

There are two types of acceleration methods in speeding up the convergence of CSS, i.e. (i) direct determination and (ii) accelerated MSS. In the direct determination method, the bed condition is solved directly with the inclusion of CSS conditions imposed as a constraint (Nilchan and Panthelides, 1998; Ko and Moon, 2002; Ding *et al.*, 2002; Jiang *et al.*, 2003; Biegler *et al.*, 2004; Cruz *et al.*, 2005; Fiandaca *et al*., 2009; Agarwal *et al*. 2009). The direct determination methods were reported to be efficient. However, they are mathematically demanding, and sometimes convergence can be an issue. The accelerated MSS is mathematically simpler. Kvamsdal and Hertberg (1997) presented the use of two updating schemes, i.e. the Aitken and the Muller methods for the convergence study. However, their study suffered from the lack of a rational stopping criterion. The error tolerance to determine the CSS needed to be tuned in order to get the same profile as obtained in the MSS. The accelerator developed by Choong *et al*. (2002), based on the concept of paired-extrapolator, was able to reduce the number of cycles required to reach CSS and bracket the CSS. However, the extrapolators suffered from rounding error, and the state variable profiles at CSS were not preserved.

1.3 Rapid Pressure Swing Adsorption

Rapid pressure swing adsorption (RPSA), an intensified PSA process, uses a single packed bed that produces continuous flow of product stream instead of multiple adsorption beds. The concept of RPSA was originally proposed by Turnock and Kadlec (1971) to reduce the complexity of multi-bed PSA. Compared to PSA, RPSA operates on shorter cycle time and smaller adsorbent bed. The radial flow RPSA, delivered enriched product gas stream in radial direction instead of the usual axial direction, was studied by Chiang and Hong (1995), and Huang and Chou (2003). Motivated by the scaling rules of Rota and Wankat (1991), Suzuki *et al*. (1996) and Murray (1996) studied the ultra-rapid pressure swing adsorption (URPSA) which utilises very short cycle time (in the order of 1s or sub-second) to enhance the productivity of RPSA. Recently, Rao (2010) studied a two-step pulsed pressure swing adsorption (PPSA) with the objective of designing a portable medical grade oxygen concentrator. His model suggested that using rapid cycling (~ 1 s) and small adsorbent (< 100 µm), it was possible to obtain very high oxygen productivity per unit mass of adsorbent. However, small particle size of less than 100 µm was found to induce much higher axial dispersion than that was predicted. The higher axial dispersion and high bed resistance due to particle clustering was experienced in his experimental work. Low oxygen purity of less than 38.5% was obtained in his experiment. The low velocity across the bed caused by high bed resistance also led to low oxygen recovery and productivity.

1.4 This research

This research consists of two parts. The objectives of both parts are summarised as below:

Part I:

1. To devise an accelerated MSS method for cyclic processes that exhibits three salient features, i.e. accelerate the convergence to CSS, (ii) determine CSS unambiguously, and (iii) preserve the process variable profiles at CSS.
2. To achieve the above objective, two hybrid algorithms combining the MSS with (i) Aitken or (ii) Muller updating scheme, with the rational stopping criterion incorporated are developed. The two algorithms are first tested on a cyclic reactor model involving non-linear algebraic equations. The more efficient hybrid algorithm will then be adopted for the RPSA model.

Part II:

3. To develop a modified configuration for RPSA, namely dual layered RPSA.
4. To study the effect of different particle size, different type of adsorbents, and non-adsorptive particles on oxygen product purity and recovery for the dual layered RPSA.

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