Lecture 9. Continuous Adsorption Systems

- McCabe-Thiele Method for Purification
- Kremser Method
- McCabe-Thiele Method for Bulk Separation
- Simulated-Moving-Bed Systems
- Models for SMB Systems
	- TMB equilibrium-stage model using a McCabe-Thieletype analysis
	- Steady-state local-adsorption-equilibrium TMB model
	- Steady-state TMB model
	- Dynamic SMB model

Continuous, Countercurrent **Operation**

- Advantage of continuous, countercurrent operation
	- : countercurrent flow maximizes the average driving force for transport \rightarrow increases adsorbent use efficiency

• McCabe-Thiele and Kremser methods for purification

- If the system is dilute in solute, and solute adsorption isotherms for feed solvent and $\qquad \qquad$ purge fluid are identical
- The operating and equilibrium lines are straight because of the dilute condition

Concentration in bulk fluid, c

McCabe-Thiele Method for Purification **ICCabe – Thiele Method**
 Purification

of operating lines based on direction for mas

on operating line lies below the equilibrium line

ion operating line
 $(c - c_F) + q_F$
 F. S. and D are solute-

free mass flow rates
 McCabe – Thiele Method for Purification

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dsorption operating line lies below the equilibrium line

scorption operating line
 $q = \frac{F}{S}(c - c_F) + q_F$

F. S. and D ar **McCabe – Thiele Method f**
 Purification

ion of operating lines based on direction for mass

corption operating line lies below the equilibrium line

rption operating line
 $=\frac{F}{S}(c-c_F)+q_F$

F. S. and D are solute–

rpt

F, S, and D are solute-

All solute concentrations

free mass flow rates

are per solute-free

carrier

- Position of operating lines based on direction for mass transfer
	- Adsorption operating line lies below the equilibrium line
	- Desorption operating line lies above the equilibrium line
- Adsorption operating line

$$
q = \frac{F}{S}(c - c_F) + q_F
$$

• Desorption operating line

$$
q = \frac{D}{S}(c - c_p) + q_R
$$
 carrier

• Equilibrium line

esorption operating line lies above the equilibr

orption operating line
 $q = \frac{F}{S}(c-c_F) + q_F$
 $\frac{F}{I}$, S, and D are solute

orption operating line
 $q = \frac{D}{S}(c-c_D) + q_R$

ilibrium line
 $q = Kc$

en c_D and c_R approach ze • When c_D and c_R approach zero, in order $\qquad \qquad \frac{F}{S} < K < \frac{D}{S}$ to avoid a large number of stages:

McCabe-Thiele Method for Desorption at Elevated Temperature

- If the temperature or pressure for the two sections can be altered to place the sections can be altered to place the
equilibrium line for desorption below that for
adsorption \rightarrow it becomes possible to use a
portion of the raffinate for desorption adsorption \rightarrow it becomes possible to use a portion of the raffinate for desorption
	- $-F/S$ can be greater than D/S
	- With a portion of raffinate used in Bed 2 (DES), the net raffinate product $is F-D$
	- $-$ The two operating lines must intersect at the point (q_R , c_R)
	- Finersect at the point \mathbf{u}_R , \mathbf{v}_R ,
- By adjusting D/F, intersect point can be moved closer to the origin to increase raffinate purity, c_R , but at the $\qquad \qquad _{q_R}$ expense of more stages and deeper beds

Kremser Method **1 1**

• When the equilibrium and operating lines are straight

Kremser Method
\nIn the equilibrium and operating lines are straight
\n
$$
N_t = \frac{\ln \left[\frac{c_1 - q_1/K}{c_2 - q_2/K} \right]}{\ln \left[\frac{c_1 - c_2}{q_1/K - q_2/K} \right]}
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A = \frac{1}{\ln \left[\frac{1}{q_1/K - q_2/K} \right]}
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A = \frac{1}{\ln \left[\frac{1}{q_1/K - q_2/K} \right]}
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A =
$$

1 and 2 refer to opposite ends which are chosen so $q_1 > q_2$

q K q K **Kremser Method**

quilibrium and operating lines are straight
 $\begin{array}{c}\n\sqrt{\frac{c_1-q_1/K}{c_2-q_2/K}}\n\end{array}\n\begin{array}{c}\n\sqrt{\frac{1}{2} \text{ and } 2 \text{ refer to opposite ends} \\
\sqrt{\frac{1}{2} \text{ which are chosen so } q_1 > q_2}\n\end{array}$

Ner of theoretical stages, N_t, in the adsorption or • For a number of theoretical stages, N_t , in the adsorption or desorption sections

- The equilibrium and operating lines are straight
 $\mathbf{V}_t = \frac{\ln\left[\frac{c_1 q_1/K}{c_2 q_2/K}\right]}{\ln\left[\frac{c_1 c_2}{q_1/K q_2/K}\right]}$
 1 and 2 refer to opposite ends
 1 and 2 refer to opposite ends
 1 and 2 refer to opposite ends
 - Values of HETP, which depend on mass-transfer resistances and axial dispersion, must be established from experimental measurements
- $-$ For large-diameter beds, values of HETP are in the range of 0.5–1.5 ft

McCabe-Thiele Method for Bulk Separation

• Continuous, countercurrent bulk separation for binary mixture

- $-$ To provide flexibility, a thermal swing is used, with Sections II and III operating at low or ambient temperature, while Sections I and IV operate at elevated temperature
- $-$ The top two sections (III and IV) provide a stripping action to produce a product rich in the less strongly adsorbed component B
- The two bottom sections (I and II) provide an enriching action to produce a product rich in component A

Simulated-Moving-Bed Systems (1)

• True-moving bed

Simulated-Moving-Bed Systems (2)

- Difficulties in operating continuous, countercurrent moving-bed (true-moving-bed, TMB) systems: adsorbent abrasion, failure to achieve particle plug flow, fluid channeling
- Continuous, countercurrent operation can be simulated by using a column containing a series of fixed beds and periodically moving the locations at which streams enter and leave the column
	- : simulated moving-bed (SMB) systems
	- Widespread commercial application for liquid separations in the petrochemical, food, biochemical, pharmaceutical, and fine chemical industries
	- An SMB can be treated as a countercurrent cascade of sections (or zones) rather than stages, where stream entry or withdrawal points bound the sections
	- As each section is divided into more subsections, the SMB system more closely approaches the separation achieved in a corresponding TMB

Simulated-Moving-Bed Systems (3)

- By periodically shifting feed and product positions by one port position in the direction of fluid flow, movement of solid adsorbent in the opposite direction is simulated
- Flow rates in the four sections are different

Models for SMB Systems

- Models for designing and analyzing SMBs
	- Models assuming steady-state conditions with continuous, countercurrent flows of fluid and solid adsorbent, approximating SMB operation with a TMB
		- § TMB equilibrium-stage models using a McCabe-Thiele-type analysis : simplest, but difficult to apply to systems with nonlinear adsorptionequilibrium isotherms
		- TMB local-adsorption-equilibrium models
			- : ignoring effects of axial dispersion and fluid-particle mass transfer; useful for establishing reasonable operating flow rates in multiple sections of an SMB (∵ for many applications, behavior of an SMB is determined largely by adsorption equilibria)
		- § TMB rate-based models
			- : account for axial dispersion in the bed, particle-fluid mass-transfer resistances, and nonlinear adsorption isotherms; preferred for a final design
	- SMB rate-based models: apply to transient operation for startup, approach to cyclic steady state, and shutdown

Steady-State Local-Adsorption-Equilibrium TMB Model (1)

• TMB local-adsorption-equilibrium model for a single section

- Assumptions
	- One-dimensional plug flow of both phases with no channeling
	- Constant volumetric flow rates (Q for liquid and Q_s for solid)
	- Constant external void fraction, $\varepsilon_{\rm b}$, of solids bed
	- Negligible axial dispersion and particle-fluid masstransfer resistances
- Local adsorption equilibrium between solute concentrations, c_i , in the bulk liquid and adsorption loading, q_i , on the solid - Constant volumetric flow rates (Q for liquid and

for solid)

- Constant external void fraction, ε_b , of solids bec

- Negligible axial dispersion and particle-fluid ma

transfer resistances

- Local adsorption equil for solid)

- Constant external void fraction, ε_b , of solids bed

- Negligible axial dispersion and particle-fluid mas

transfer resistances

- Local adsorption equilibrium between solute

concentrations, c_i , in the bookstand volumetric flow rates (Q for liquid and Q_s

c solid)

bookstand external void fraction, ε_b , of solids bed

egligible axial dispersion and particle-fluid mass-

msfer resistances

bocal adsorption equilibri μ ic flow rates (Q for liquid and Q_s
void fraction, ε_b , of solids bed
spersion and particle-fluid mass-
s
equilibrium between solute
in the bulk liquid and adsorption
solid
choric conditions
Boundary conditions
	- Isothermal and isochoric conditions

• Mass balance

$$
Q\frac{dc_i}{dz} - S\frac{dq_i}{dz} = 0
$$

$$
0 \t z = 0, c_i = c_{i, in} \text{ and } z = Z, q_i = q_{i, in}
$$

Steady-State Local-Adsorption-Equilibrium TMB Model (2)

• Usefulness of local-equilibrium theory

: approximate determinations of the amount of solid adsorbent and fluid flow rates, in each TMB section, to achieve a perfect separation of two solutes **ibrium TMB Model (2)**
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 erminations of the amount of solid adsorbent
 s, in each TMB section, to achieve a perfect

solutes
 **ion equilibrium is linear for a dilute feed, with

r** each section **volumerally are all the collect of the amount of solid adsorbent**
rates, in each TMB section, to achieve a perfect
wo solutes
orption equilibrium is linear for a dilute feed, with
s for each section j
volumetric fluid pha **Equilibrium TMB Model**
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ximate determinations of the amount of solid flow rates, in each TMB section, to achie
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ing adsorption equilibrium is linear for a dilu
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- Assuming adsorption equilibrium is linear for a dilute feed, with $K_A > K_B$
- Flow rate ratios for each section j

j j^{\prime} Ω s voidul Q_i volumetric fluid ph: $m_i = \frac{2i}{2} = \frac{1}{2}$ Q_s volumetric solid particle

• For local adsorption equilibrium, the necessary and sufficient conditions at each section for complete separation

Steady-State Local-Adsorption-Equilibrium TMB Model (3) **Equilibrium TMB Model (
** $K_{\rm B} < m_{\rm II} < K_{\rm A}$ **Ensure sharpness of the separation by
** $K_{\rm B} < m_{\rm II} < K_{\rm A}$ **Ensure sharpness of the separation by
** $K_{\rm B} < m_{\rm III} < K_{\rm A}$ **and positive (upward), respectively, in central Equilibrium TMB Model (**
 $K_{\rm B} < m_{\rm II} < K_{\rm A}$ **Ensure sharpness of the separation by**
 $K_{\rm B} < m_{\rm II} < K_{\rm A}$ **Ensure sharpness of the separation by**
 $K_{\rm B} < m_{\rm III} < K_{\rm A}$ and positive (upward), respectively, in

qu

$$
K_{\rm B} < m_{\rm II} < K_{\rm A}
$$

Ensure sharpness of the separation by causing net flow rates of A and B to be negative (downward) and positive (upward), respectively, in the two central Sections II and III

• Inequality constraints can be converted to equality constraints using the safety margin, β

Steady—**State Local**—**Adsorption**—
\n**Equilibrium TMB Model (3)**
\n
$$
K_B < m_H < K_A
$$

$$
Q_{\rm I} = Q_{\rm C} + Q_{\rm D} = Q_{\rm S} K_{\rm A} \beta \qquad Q_{\rm C} = Q_{\rm S} K_{\rm A} \beta - Q_{\rm D}
$$

 Q_c : fluid recirculation rate before adding makeup desorbent

Steady-State Local-Adsorption-Equilibrium TMB Model (4)

• Triangle method

- If values m_{II} and m_{III} within the triangular region are selected, a perfect separation is possible
- If $m_{\rm II} < K_{\rm B}$, some B appears in extract
- If $m_{III} > K_A$, some A appears in raffinate
- If $m_{\rm II} < K_{\rm B}$ and $m_{\rm III} > K_{\rm A}$, extract contains some B and raffinate contains some A
- - $-$ Above a maximum β , some sections will encounter negative fluid flow rates, and when β < 1, perfect separation will not be achieved
	- $-$ As the value of β increases from minimum to maximum, fluid flow rates in the sections increase, often exponentially
	- As separation factor K_A/K_B \rightarrow 1, permission range of β becomes smaller

Steady-State TMB Model (1)

- Unlike the local-adsorption-equilibrium model, axial dispersion **afe TMB Model (1)**

n-equilibrium model, axial dispersion

nsfer are considered

r the bulk fluid phase, f
 $\frac{(1-\varepsilon_b)}{\varepsilon_b} J_{i,j} = 0$

ween the bulk fluid phase and the sorbate in the pores
 $\frac{u_{f_i} = Q_i/\varepsilon_b A_b}$ \bullet **i** \bullet he local-adsorption-equilibrium model, axial dispe
d-particle mass transfer are considered
alance equation for the bulk fluid phase, f
 $L_j \frac{d^2 c_{i,j}}{dz^2} + u_{f_j} \frac{dc_{i,j}}{dz} + \frac{(1 - \varepsilon_b)}{\varepsilon_b} J_{i,j} = 0$ **eady-State TMB Model (1)**
 a local-adsorption-equilibrium model, axial disperparticle mass transfer are considered

ance equation for the bulk fluid phase, f
 $\frac{d^2c_{i,j}}{dz^2} + u_{f_j} \frac{dc_{i,j}}{dz} + \frac{(1 - \varepsilon_b)}{\varepsilon_b} J_{i,j} =$ **Steady-State TMB Model (1)**
the local-adsorption-equilibrium model, axial dispersion
uid-particle mass transfer are considered
balance equation for the bulk fluid phase, f
 $D_{L_j} \frac{d^2 c_{i,j}}{dz^2} + u_{f_j} \frac{dc_{i,j}}{dz} + \frac{(1 - \vare$ **Example 14**
 Example 14
 Docal-adsorption-equilibrium model, axial disper
 Docal-adsorption-equilibrium model, axial disper
 Docal-adsorption-equilibrium model, axial disper
 Docal-drop and the bulk fluid phase, Steady-State TMB Model (1)

(a) the the local-adsorption-equilibrium model, axial dispersion

fluid-particle mass transfer are considered
 $-D_{L_j} \frac{d^2 c_{i,j}}{dz^2} + u_{f_j} \frac{dc_{i,j}}{dz} + \frac{(1-\varepsilon_b)}{\varepsilon_b} J_{i,j} = 0$
 $J_i: \frac{\text{mass-transfer flux between$ **jean the TMB Model (1)**
 jean interpretence and the bulk fluid phase, f
 $\frac{-\varepsilon_b}{\varepsilon_b} J_{i,j} = 0$
 g an the bulk fluid phase and the sorbate in the pores
 if $\frac{1}{\mu_{f_i} = Q_j/\varepsilon_b A_s}$
 i, on the solid phase
 ue $\text{local}-$ adsorption-equilibrium model, axial dispersion
article mass transfer are considered
ce equation for the bulk fluid phase, f
 $\frac{c_{i,j}}{z^2} + u_{f_j} \frac{dc_{i,j}}{dz} + \frac{(1 - \varepsilon_b)}{\varepsilon_b} J_{i,j} = 0$
ss-transfer flux between the bu
- Mass-balance equation for the bulk fluid phase, f

Unlike the local–adsorption–equilibrium model, axial dispe
and fluid–particle mass transfer are considered
Mass–balance equation for the bulk fluid phase, f

$$
-D_{L_j} \frac{d^2 c_{i,j}}{dz^2} + u_{f_j} \frac{dc_{i,j}}{dz} + \frac{(1 - \varepsilon_b)}{\varepsilon_b} J_{i,j} = 0
$$

 u_f : interstitial fluid velocity $u_{f_i} = Q_i / \varepsilon_b A_b$ *he* sorbate in the pores
 $s = \frac{Q_s}{(1 - \varepsilon_b)A_b}$

• Mass-balance for sorbate, s, on the solid phase

the local–adsorption–equilibrium model, axial dispersion fluid–particle mass transfer are considered

\ns–balance equation for the bulk fluid phase, f

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-D_{L_j} \frac{d^2 c_{i,j}}{dz^2} + u_{f_j} \frac{dc_{i,j}}{dz} + \frac{(1 - \varepsilon_b)}{\varepsilon_b} J_{i,j} = 0
$$

\nJ,
$$
I_{i, j}
$$
 mass–transfer flux between the bulk fluid phase and the solate in the pores u_j : interstittal fluid velocity $u_{i,j} = Q_j/\varepsilon_i A_k$

\ns–balance for sorbate, s, on the solid phase

\n
$$
u_s \frac{d\overline{q}_{i,j}}{dz} - J_{i,j} = 0
$$

\n
$$
u_s : true \text{ moving–solid velocity}
$$

\n
$$
u_s = \frac{Q_s}{(1 - \varepsilon_b) A_s}
$$

\nl–to–solid mass transfer

\nJ, j = k_{i,j} (q_{i,j}^* - \overline{q}_{i,j})

\nprotion isotherm

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$$
q_{i,j}^* = f \{all c_{i,j}\}
$$

• Fluid-to-solid mass transfer

$$
\boldsymbol{J}_{i,j} = \boldsymbol{k}_{i,j} \left(\boldsymbol{q}_{i,j}^* - \overline{\boldsymbol{q}}_{i,j} \right)
$$

• Adsorption isotherm $\quad \bm{q}_{i,j}^* = f\{\textbf{all}\ \bm{c}_{i,j}\}$

Steady-State TMB Model (2) **Steady-State TMB Model (**
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ary conditions
 $\frac{1}{\sqrt{2}}$, $\frac{1}{\sqrt{2}}$, $\frac{1}{\sqrt{2}}$, $\frac{1}{\sqrt{2}}$, $\frac{1}{\sqrt{2}}$, $\frac{1}{\sqrt{2}}$, $\frac{1}{\sqrt{2}}$, ctions I and II where extract is withdrawn
 $\frac{1}{\sqrt{2}}$, $\frac{1}{\sqrt{$ **e TMB Model**
accounting for axial dispe
z
cet is withdrawn **Steady-State TMB Mo**
 f f $c_{i,j,0} - c_{i,j} = -\varepsilon_b D_{L_j} \frac{dc_{i,j}}{dz}$
 f f_i ($c_{i,j,0} - c_{i,j} = -\varepsilon_b D_{L_j} \frac{dc_{i,j}}{dz}$

ections I and II where extract is withdrawn **Steady-State TMB Model (2)**
 u dary conditions

the section entrance, $z=0$ (accounting for axial dispersion)
 $u_{f_j}(c_{i,j,0} - c_{i,j}) = -\varepsilon_b D_{L_j} \frac{dc_{i,j}}{dz}$

Sections 1 and II where extract is withdrawn
 $c_{i,1,z=L_j} = c_{i$ ady – State TMB Model (2)

unditions

on entrance, z=0 (accounting for axial dispersion)
 $-c_{i,j}$) = $-\varepsilon_b D_{L_j} \frac{dc_{i,j}}{dz}$

l and II where extract is withdrawn
 $c_{i,\text{II},z=0}$ $q_{i,\text{I},z=L_j} = q_{i,\text{II},z=0}$ **Steady-State TMB Model (2)**

Indary conditions

the section entrance, $z=0$ (accounting for axial dispersion)
 $u_{f_j}(c_{i,j,0}-c_{i,j})=-\varepsilon_b D_{L_j} \frac{dc_{i,j}}{dz}$

Sections 1 and 11 where extract is withdrawn
 $c_{i,1,z=t_j}=c_{i,11,z=0}$

- Boundary conditions
	- $-$ At the section entrance, $z=0$ (accounting for axial dispersion)

$$
u_{f_j}(c_{i,j,0} - c_{i,j}) = -\varepsilon_b D_{L_j} \frac{dc_{i,j}}{dz}
$$

- At Sections I and II where extract is withdrawn

$$
c_{i,I,z=L_j} = c_{i,\mathrm{II},z=0} \qquad \qquad q_{i,I,z=L_j} = q_{i,\mathrm{II},z=0}
$$

- At Sections III and IV where raffinate is withdrawn

- At Sections II and III where feed enters

ndary conditions
\nthe section entrance, z=0 (according for axial dispersion)
\n
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u_{f_j}(c_{i,j,0} - c_{i,j}) = -\varepsilon_b D_{L_j} \frac{dc_{i,j}}{dz}
$$

\nSections I and II where extract is withdrawn
\n $c_{i,1,z=L_j} = c_{i,11,z=0}$ $q_{i,1,z=L_j} = q_{i,11,z=0}$
\nSections III and IV where radiinate is withdrawn
\n $c_{i,111,z=L_j} = c_{i,111,z=0}$ $q_{i,111,z=L_j} = q_{i,111,z=0}$
\nSections II and III where feed enters
\n $c_{i,111,z=0} = (Q_{11}/Q_{11})c_{i,11,z=L_j} + (Q_{F}/Q_{11})c_{i,F}$ $q_{i,11,z=L_j} = q_{i,111,z=0}$
\nSections IV and I where make-up desorbent enters
\n $c_{i,11,z=0} = (Q_{11}/Q_{11})c_{i,111,z=L_j} + (Q_{11}/Q_{11})c_{i,10}$ $q_{i,111,z=L_j} = q_{i,11,z=0}$

- At Sections IV and I where make-up desorbent enters

$$
c_{i,I,z=0} = (Q_{\text{IV}}/Q_{\text{I}}) c_{i,\text{IV},z=L_j} + (Q_{\text{D}}/Q_{\text{I}}) c_{i,D} \qquad q_{i,\text{IV},z=L_j} = q_{i,I,z=0}
$$

Steady-State TMB Model (3)

• Volumetric fluid flow rates

$$
Q_{\text{I}} = Q_{\text{IV}} + Q_{D}
$$

\n
$$
Q_{\text{II}} = Q_{\text{I}} - Q_{E}
$$

\n
$$
Q_{\text{III}} = Q_{\text{II}} + Q_{F}
$$

\n
$$
Q_{\text{IV}} = Q_{\text{III}} - Q_{R}
$$

• To obtain the same true velocity difference between fluid and solid particles, upward fluid velocity in the SMB must be the sum of the absolute true velocities in the upward-moving fluid and the downward-moving

Dynamic SMB Model

- Equations take into account time of operation, t, use a fluid velocity relative to the stationary solid particles, and must be ms take into account time of operation, t, u
relative to the stationary solid particles, and
for each bed subsection, k, between adjace
alance equation for the bulk fluid phase, f
 $\frac{k}{\epsilon} - D_{L_j} \frac{\partial^2 c_{i,k}}{\partial z^2} + u_{f_k} \frac{\partial$ **SMB Model**

be of operation, t, use a fluid

solid particles, and must be

k, between adjacent ports

bulk fluid phase, f
 $\frac{(1-\varepsilon_b)}{\varepsilon_b}J_{i,k}=0$

be solid phase *i* is take into account time of operation, t, us
 i relative to the stationary solid particles, and

for each bed subsection, k, between adjace

balance equation for the bulk fluid phase, f
 $\frac{i}{t} - D_{L_j} \frac{\partial^2 c_{i,k}}{\partial z$ *Le* into account time of operation, t, use a fluid
ve to the stationary solid particles, and must be
ch bed subsection, k, between adjacent ports
e equation for the bulk fluid phase, f
 $\frac{\partial^2 c_{i,k}}{\partial z^2} + u_{f_k} \frac{\partial c_{i,k}}{\partial$ **Dynamic SMB Model**

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for each bed subsection, k, between adjacent ports

balance equation for the bulk f **Dynamic SMB Model**
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tive to the stationary solid particles, and must be
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nce equation for the bulk fluid phase, f
 $D_{L_j} \frac{\$ **Dynamic SMB Model**
 t relative to the stationary solid particles, and must be

for each bed subsection, k, between adjacent ports

balance equation for the bulk fluid phase, f
 $\frac{i\kappa}{t} - D_{L_j} \frac{\partial^2 c_{i,k}}{\partial z^2} + u_{f_k} \frac$ **Dynamic SMB Model**

tions take into account time of operation, t, use a fluid

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ty relative to the stationary solid particles, and must be
i for each bed subsection, k, between adjacent ports
balance equation for the bulk flu ons take into account time of operation, t, use

by relative to the stationary solid particles, and r

i for each bed subsection, k, between adjacent

balance equation for the bulk fluid phase, f
 $\frac{c_{i,k}}{\partial t} - D_{L_j} \frac{\partial^$ Exercise that the discussion and the stationary solid particles, and must be
written for each bed subsection, k, between adjacent ports
Mass-balance equation for the bulk fluid phase, f
 $\frac{\partial c_{i,k}}{\partial t} - D_{L_i} \frac{\partial^2 c_{i,k}}{\partial z^$
- Mass-balance equation for the bulk fluid phase, f

written for each bed subsection, k, between adjacent ports
\nMass–balance equation for the bulk fluid phase, f
\n
$$
\frac{\partial c_{i,k}}{\partial t} - D_{L_j} \frac{\partial^2 c_{i,k}}{\partial z^2} + u_{f_k} \frac{\partial c_{i,k}}{\partial z} + \frac{(1 - \varepsilon_b)}{\varepsilon_b} J_{i,k} = 0
$$
\nMass–balance for sorbate on the solid phase
\n
$$
\frac{\partial \overline{q}_{i,k}}{\partial t} - J_{i,k} = 0
$$
\nInterstital fluid velocity $(u_f)_{\text{SMB}} = (u_f)_{\text{TMB}} + |(u_s)|_{\text{TMB}}$
\n $u_s = L_k/t^*$ L_k : bed height between adjacent ports
\nBoundary conditions for TMB models apply to SMB models.
\nIn addition, initial conditions are needed for $c_{i,j}$ and $\overline{q}_{i,j}$

• Mass-balance for sorbate on the solid phase

$$
\frac{\partial \overline{q}_{i,k}}{\partial t} - J_{i,k} = 0
$$

$$
u_s = L_k / t^*
$$
 L_k : bed height between adjacent ports
 t^* : port-switching time

• Boundary conditions for TMB models apply to SMB models. Interstitial fluid velocity $(u_f)_{\text{SMB}} = (u_f)_{\text{TMB}} + (u_s)_{\text{TMB}}$
 $u_s = L_k/t^*$ $\frac{L_k \text{ is odd height between adjacent ports}}{t^* \text{ : port-switching time}}$

Boundary conditions for TMB models apply to SMB models.

In addition, initial conditions are needed for $c_{i,j}$ an