Development of a PSA Cycle for Producing High Purity CO_2 from Dilute Feed Streams. Part I: Feasibility Study

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Supplemental Information

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Table S1. Initial and boundary conditions for the first five steps of the 3-bed 9-step PSA cycle schedule; the cycle step sequence is F-Idle-HR-EqD-CoD-CnD-LR-EqU-LPP.

Condition	Step I, F	Step II, Idle	Step III, HR	Step IV, EqD	Step V, CoD
t = 0[b]	$y_i = y_{i,LPP,f}$ $v = v_{LPP,f}$ $q_i = q_{i,LPP,f}$ $T = T_{LPP,f}$ $P = P_{LPP,f}$	$y_i = y_{i,F,f}$ $v = v_{F,f}$ $q_i = q_{i,F,f}$ $T = T_{F,f}$ $P = P_{F,f}$	$y_i = y_{i,Idle,f}$ $v = v_{Idle,f}$ $q_i = q_{i,Idle,f}$ $T = T_{Idle,f}$ $P = P_{Idle,f}$	$y_i = y_{i,HR,f}$ $v = v_{HR,f}$ $q_i = q_{i,HR,f}$ $T = T_{HR,f}$ $P = P_{HR,f}$	$y_i = y_{i,E,f}$ $v = v_{E,f}$ $q_i = q_{i,E,f}$ $T = T_{E,f}$ $P = P_{E,f}$
z/L = 0[c]	$y_i = y_{i,F}$ $F = F_F$ LDFE $T = T_F$ MB	CMB VE ($P_- = P^*$, $c_v = 0$) LDFE EB MB	$y_i = y_{i,LR,z/L=0}$ $F = - F_{LR,z/L=0}$ LDFE $T = T_F$ MB	CMB VE ($P_- = P^*$, $c_v = 0$) LDFE EB MB	CMB VE ($P_- = P^*$, $c_v = 0$) LDFE EB MB
z/L = 1[c]	CMB OMB LDFE EB VE ($P_+ = P_H$, $c_v > 0$)	CMB OMB LDFE EB VE ($P_+ = P^*$, $c_v = 0$)	CMB OMB LDFE EB VE ($P_+ = P_H$, $c_v > 0$)	CMB OMB LDFE EB VE ($P_+ = P_{E*}$, $c_v > 0$)	CMB OMB LDFE EB VE ($P_+ = P_L$, $c_v > 0$)

[a] CMB: component mass balance, eq 2; OMB: overall mass balance, eq 1; LDFE: linear driving force equation, eq 5; EB: energy balance, eq 11; MB: momentum balance, eq 13; VE: valve equation, eq 14; F: molar flow rate; P_o: pressure outside the valve; P_L: low pressure; P_H: high pressure; P_{EqU}: pressure of equalization up step; P^*: any pressure, as it is irrelevant when c_v=0, $y_{i,F}$: concentration of species i in the feed, F_F: molar flow rate of the feed, T_F: temperature of the feed.

[b] The subscript f denotes the end of the cycle step.

[c] The molar flow rate F is assumed positive when gas is flowing towards z/L = 1 and negative when it is flowing oppositely.

Table S2. Initial and boundary conditions for the last four steps of the 3-bed 9-step PSA cycle schedule; the cycle step sequence is F-Idle-HR-EqD-CoD-CnD-LR-EqU-LPP.

Condition	Step VI, CnD	Step VII, LR	Step VIII, EqU	Step IX, LPP
$t = 0^b$	$y_i = y_{i,CoD,f}$ $v = v_{CoD,f}$ $q_i = q_{i,CoD,f}$ $T = T_{CoD,f}$ $P = P_{CoD,f}$	$y_i = y_{i,CnD,f}$ $v = v_{CnD,f}$ $q_i = q_{i,CnD,f}$ $T = T_{CnD,f}$ $P = P_{CnD,f}$	$y_i = y_{i,LR,f}$ $v = v_{LR,f}$ $q_i = q_{i,LR,f}$ $T = T_{LR,f}$ $P = P_{LR,f}$	$y_i = y_{i,E*,f}$ $v = v_{E*,f}$ $q_i = q_{i,E*,f}$ $T = T_{E*,f}$ $P = P_{E*,f}$
$z/L = 0^c$	CMB OMB LDFE EB VE ($P_+ = P_L$, $c_v > 0$)	CMB OMB LDFE EB VE ($P_+ = P_H$, $c_v > 0$)	CMB VE ($P_+ = P^*$, $c_v = 0$) LDFE EB MB	CMB VE ($P_+ = P^*$, $c_v = 0$) LDFE EB MB
$z/L = 1^c$	CMB VE ($P_- = P^*$, $c_v = 0$) LDFE EB MB	$y_i = y_{i,F,z/L=1}$ $F = -\ LRR*F_{F,z/L=1}$ LDFE $T = T_{F,z/L=1}$ MB	$y_i = y_{i,E,z/L=1}$ $F = -\ F_{E,z/L=1}$ LDFE $T = T_{E,z/L=1}$ MB	$y_i = y_{i,F,z/L=1}$ VE ($P_- = P_{F,z/L=1}$, $c_v > 0$) LDFE $T = T_{F,z/L=1}$ MB

[a] CMB: component mass balance, eq 2; OMB: overall mass balance, eq 1; LDFE: linear driving force equation, eq 5; EB: energy balance, eq 11; MB: momentum balance, eq 13; VE: valve equation, eq 14; F: molar flow rate; P_o: Pressure outside the valve; P_L: low pressure; P_H: high pressure; P^*: any pressure, as it is irrelevant when c_v=0.

[b] The subscript f denotes the end of the cycle step.

[c] The molar flow rate F is assumed positive when gas is flowing towards z/L = 1 and negative when it is flowing oppositely.