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Two-train elevated-temperature pressure swing adsorption for high-purity hydrogen production



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HIGHLIGHTS

- Two-train elevated temperature pressure swing adsorption for H₂ purification.
- Optimal process achieves 99.9994% hydrogen purity and 97.51% hydrogen recovery ratio.
- Total steam consumption is significantly reduced with reflux structures.

ARTICLE INFO

Keywords: Elevated-temperature pressure swing adsorption Potassium-promoted layered double oxide Hydrogen production Shifted gas

ABSTRACT

The trade-off between hydrogen recovery ratio (HRR) and hydrogen purity (HP) is one of the main drawbacks in normal temperature pressure swing adsorption (NT-PSA) for producing high-purity hydrogen from shifted gas. In this paper, a two-train elevated-temperature pressure swing adsorption (ET-PSA) process that achieved 99.999% HP and over 95% HRR is proposed, which has wide application potentials in fuel cells and chemical industries. Potassium-promoted layered double oxide (K-LDO), which shows reasonable working capacity and fast adsorption/desorption kinetics at elevated temperatures (200-450 °C), is adopted as the CO₂ adsorbent. CO in the shifted gas is co-purified by high-temperature water gas shift (WGS) catalysts added to the columns. The firsttrain ET-PSA adopted an eight-column thirteen-step configuration with shorter step time to remove most of the CO/CO2 in the shifted gas, and the second-train ET-PSA adopted a double-column seven-step configuration with longer step time to purify the residual gas impurities. The introduction of co-current high-pressure steam rinse and counter-current low-pressure steam purge is the key to achieve both high HRR and HP. The high-temperature steam is the main energy consumption of ET-PSA rather than low HRR in NT-PSA, and the total steam consumption is reduced by adopting the tail gas from second-train ET-PSA as the purge gas for first-train ET-PSA. The optimal results achieved 97.51% HRR and 99.9994% HP with only 0.188 rinse-to-feed ratio and 0.263 purge-to-feed ratio, which are the highest values reported for PSAs producing high-purity hydrogen from carbonbased fuels.

1. Introduction

With the growing demand for energy and increasing environmental pressure around the world, it has become necessary to replace the current main energy source (combustion of fossil fuels) with cleaner and more efficient energy systems. Hydrogen is expected to be a fuel of the future and has the potential to contribute to 90% energy generation in 2080 [1]. Emerging technology is expected to break the present energy systems by combining hydrogen as an energy carrier with fuel cells as an electricity generator [2]. Hydrogen is also an important raw material that is widely used in chemical industries (for instance,

ammonia synthesis) [3]. Hydrogen is conventionally produced by hydrocarbon reforming [4], biomass processes [5], and water splitting (including photocatalytic processes [6], electrolytic processes [7], and thermal processes [8]). Despite renewable sources attracting attention, steam methane reforming (SMR) and coal gasification (CG) are the most cost-effective processes for producing hydrogen, at present and for the near future [9].

In hydrogen production processes from SMR or CG, a two-stage water gas shift (WGS) reactor is adopted to remove carbon gases from reformed gas, followed by CO_2 absorption and methanation for CO purification, or alternatively, a pressure swing adsorption (PSA) unit

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A_i pre-exponential factor for reaction rate, s^{-1} or kg/mols P_{prige} purge pressure, Pa A_i pre-exponential factor for reaction $rate, s^{-1}$ or kg/mols q_i site concentration, mol/kg C_i gas molar concentration, mol/m^3 q_{outal} total CO_2 adsorption capacity, mol/kg $C_{reac,i}$ feed gas molar concentration, mol/m^3 q_{outal} total CO_2 adsorption capacity, mol/kg $C_{reme,i}$ fixe gas molar concentration, mol/m^3 Q_{heed} feed flow rate of the product column, m^3/s $C_{prige,i}$ given gas molar concentration for pressure-equalization $rate_e$ Co2 adsorption rate, $mol/kg s$ $rate_i$ CO2 adsorption rate, $mol/kg s$ $rate_e$ catalytic reaction rate, $mol/kg s$ $C_{pp,i}$ given gas molar concentration for product pressurization, mol/m^3 R ideal gas constant, $J/mol K$ C_{pris} given gas molar concentration, mol/m^3 t time, s C_{T} total gas molar concentration, mol/m^3 t time, s C_{T} total gas molar concentration, mol/m^3 t time, s C_{T} total gas molar concentration, mol/m^3 t time, s C_{T} total gas molar concentration, mol/m^3 t time, s C_{T} total gas molar concentration, mol/m^3 t time, s C_{T} total gas molar concentration, mol/m^3 t time, s C_{T} total gas molar concentration, mol/m^3 t time, s C_{T} total gas molar concen	Nomenclature		p_{dep}	given pressure for blowdown, Pa
A_1 pre-exponential factor for reaction rate, s^{-1} or kg/mol s q_1 site concentration, mol/kg c fitting parameter for pressure effect, $ q_{1,0}$ initial site concentration, mol/kg C_1 gas molar concentration, mol/m ³ $q_{0,0}$ initial site concentration, mol/kg $C_{rest,i}$ feed gas molar concentration, mol/m ³ q_{rest} initial site concentration, mol/kg $C_{purgs,i}$ purge gas molar concentration, mol/m ³ $Q_{product.out}$ outlet flow rate of the product column, m ³ /s $C_{purgs,i}$ given gas molar concentration for pressure-equalization $rate,$ CO ₂ adsorption rate, mol/kg s $rate,$ given gas molar concentration for product pressurization, ml/m^3 R ideal gas constant, J/mol K $C_{pp,i}$ given gas molar concentration, mol/m ³ R ideal gas constant, J/mol K $C_{pp,i}$ given gas molar concentration, mol/m ³ L time, s $C_{rmskr,i}$ mass transfer between bulk gas and particles, mol/m ³ L time, s $C_{rmskr,i}$ axial dispersion coefficient, π^2/s T temperature, K D_p diameter of adsorbent/catalyst particles, m v gas velocity, m/s k_i reaction rate, s^{-1} or kg/mol s v_{purgs} given velocity, m/s k_i reaction energy, J/mol v_{mass} rines velocity, m/s k_i reaction nate, s^{-1} or kg/mol s v_{purgs} given velocity for pressure, -equalization pressurization, m/s k_i valve rate for bressure, -equalization depressurization,			p_{purge}	purge pressure, Pa
cfitting parameter for pressure effect, - $q_{1,0}$ initial site concentration, mol/kg C_1 gas molar concentration, mol/m ³ q_{molal} total CO ₂ adsorption capacity, mol/kg $C_{red,i}$ rinse gas molar concentration, mol/m ³ q_{molal} sum of q_A and $q_{0,iy}$, mol/kg $C_{rinse,i}$ rinse gas molar concentration, mol/m ³ $Q_{perduct.out}$ outlet flow rate of the product column, m ³ /s $C_{perge,i}$ given gas molar concentration for pressure-equalizationrate cCO ₂ adsorption rate, mol/kg s $C_{pp,i}$ given gas molar concentration for product pressurization, mol/m ³ R ideal gas constant, J/mol K $C_{pp,i}$ given gas molar concentration, mol/m ³ I time, s C_{T} total gas molar concentration, mol/m ³ I time, s C_{T} total gas molar concentration, mol/m ³ I time, s $C_{transfer,i}$ mass transfer between bulk gas and particles, mol/m ³ I time, s $D_{ax,i}$ axial dispersion coefficient, m ² /s T temperature, K D_{p} diameter of adsorbent/catalyst particles, m v_{inse} rinse velocity, m/s k_i reaction rate, s ⁻¹ or kg/mol s v_{preg} given velocity for pressure, -equalization pressurization, m/s k_i reaction rate, s ⁻¹ or kg/mol s v_{preg} given velocity for pressure, -equalization pressurization, m/s k_i reaction rate, s ⁻¹ or kg/mol s v_{preg} given velocity for product pressurization, m/s k_i reaction rate, s ⁻¹ or kg/mol s	A_i	pre-exponential factor for reaction rate, s^{-1} or kg/mols	q_i	site concentration, mol/kg
C_i gas molar concentration, mol/m ³ q_{total} total CO2 adsorption capacity, mol/kg $C_{rest,i}$ reed gas molar concentration, mol/m ³ q_{AS} sum of q_A and $q_{0(s)}$ mol/kg $C_{ruse,i}$ rinse gas molar concentration, mol/m ³ Q_{feed} feed flow rate of the product column, m ³ /s $C_{purg,i}$ given gas molar concentration for pressure-equalization $rate_a$ $CO2$ adsorption rate, mol/kg s $r_{pp,i}$ given gas molar concentration for product pressurization, $rate_a$ $CO2$ adsorption rate, mol/kg s $rol M^3$ given gas molar concentration for product pressurization, $rate_a$ $CO2$ adsorption rate, mol/kg s $rol M^3$ given gas molar concentration, mol/m ³ t times, s C_{rotal} total gas molar concentration, mol/m ³ t times, s $C_{rotander,i}$ mol/mas transfer between bulk gas and particles, mol/m ³ s t times, s $C_{rander,i}$ axial dispersion coefficient, m^2/s T temperature, K D_{p} diameter of adsorbent/catalyst particles, m v gas velocity, m/s k_i reaction rate, s ⁻¹ or kg/mol s v_{parge} given velocity, m/s k_{pel} valve rate for pressure, -equalization depressurization, m/s v_{prodet} k_{pel} valve rate for blowdown, s ⁻¹ v_{pp} given velocity for product pressurization, m/s k_{eq} equilibrium constant for WGS reaction, - v_{parge} given velocity for product pressurization, m/s k_{eq} equilibrium constant for WGS reaction, - </td <td>с</td> <td>fitting parameter for pressure effect, –</td> <td>$q_{i,0}$</td> <td>initial site concentration, mol/kg</td>	с	fitting parameter for pressure effect, –	$q_{i,0}$	initial site concentration, mol/kg
$\begin{array}{ccc} C_{\text{texd},i} & \text{feed gas molar concentration, mol/m^3} & q_{AS} & \text{sum of } q_A \text{ and } q_{D(S)}, \text{ mol/kg} \\ C_{\text{purge},i} & \text{inse gas molar concentration, mol/m^3} & Q_{\text{reduct,out}} & \text{outlet flow rate of the product column, m^3/s} \\ C_{\text{purge},i} & \text{given gas molar concentration for pressure-equalization} \\ pressurization, mol/m^3 & Q_{\text{red}} & \text{feed flow rate of the product column, m^3/s} \\ Tate_a & CO_2 \text{ adsorption rate, mol/kg s} \\ rate_a & col_2 \text{ adsorption rate, mol/kg s} \\ rate_a & col_2 \text{ adsorption rate, mol/kg s} \\ rate_a & col_2 \text{ adsorption rate, mol/kg s} \\ rate_a & col_2 \text{ adsorption rate, mol/kg s} \\ rate_a & col_2 \text{ adsorption rate, mol/kg s} \\ rate_a & catalytic reaction rate, mol/kg s \\ reaction rate, s^{-1} \text{ or kg/mol} & v_{mise} & rinse velocity, m/s \\ k_{eq} & valve rate for pressure, -equalization depressurization, m/s \\ k_{eq} & valve rate for blowdown, s^{-1} & v_{pr} & given velocity for pressure, -equalization pressurization, m/s \\ k_{eq} & equilibrium constant for WGS reaction, - & v_{pr} & molar fraction of component i, - \\ m_{adsorbentistoal} & total adsorbent mass, kg/mol & x_{r} ratio of K-related sites to non-related sites, - \\ M_{g} & mixed gas molar mass, kg/mol & x_{r} ratio of fixed bed, - \\$	C_i	gas molar concentration, mol/m ³	$q_{ m total}$	total CO_2 adsorption capacity, mol/kg
$C_{\text{timse},i}$ rinse gas molar concentration, mol/m³ $Q_{\text{product,out}}$ outlet flow rate of the product column, m³/s $C_{\text{purge},i}$ purge gas molar concentration for pressure-equalizationfeed flow rate of the product column, m³/s C_{pprise} given gas molar concentration for pressure-equalizationrate_a CO_2 adsorption rate, mol/kg s $rate_a$ CO_2 adsorption rate, mol/kg srate_a CO_2 mol/m^3 $rate_a$ catalytic reaction rate, mol/kg s C_T total gas molar concentration, mol/m³ t time, s $C_{\text{transfer,i}}$ mass transfer between bulk gas and particles, mol/m³ s t time, s $D_{\text{ax,i}}$ axial dispersion coefficient, m²/s T temperature, K D_p diameter of adsorbent/catalyst particles, m v gas velocity, m/s k_i reaction rate, s^{-1} or kg/mol s v_{frase} feed velocity, m/s k_i reaction rate, s^{-1} or kg/mol s v_{product} v_{produc} k_{eeq} valve rate for bressure, -equalization depressurization, s^{-1} v_{pp} given velocity for pressure, -equalization pressurization, m/s K_{eeq} equilibrium constant for WGS reaction, - v_{pp} given velocity for product pressurization, m/s K_{eeq} colum length, m x_k ratio of K-related sites to non-related sites, - $m_{\text{adsorbents,total}}$ total adsorbents mass, kg/mol α fitting parameter for E_{ir} , J/mol p_0 standard atmospheric pressure, Pa β_s fitting parameter for $E_{$	$C_{\text{feed},i}$	feed gas molar concentration, mol/m ³	$q_{ m AS}$	sum of q_A and $q_{O(s)}$, mol/kg
$\begin{array}{cccc} C_{parge,i} & purge gas molar concentration, mol/m^3 & Q_{leed} & feed flow rate of the product column, m^3/s \\ C_{pe,i} & given gas molar concentration for pressure-equalization pressurization, mol/m^3 & Tate_C catalytic reaction rate, mol/kg s \\ P_{p,i} & given gas molar concentration for product pressurization, mol/m^3 & T & ideal gas constant, J/mol K \\ C_{p,i} & given gas molar concentration mol/m^3 & T & time, s \\ C_{ransfer,i} & mass transfer between bulk gas and particles, mol/m^3 & T & temperature, K \\ D_{p,i} & diameter of adsorbent/catalyst particles, m & \nu & gas velocity, m/s \\ E_i & activation energy, J/mol & \nu_{feed} & feed velocity, m/s \\ R_i & reaction rate, s^{-1} or kg/mol s & \nu_{parge} & purge velocity, m/s \\ k_{req} & equilibrium constant for WGS reaction, - & vol_ration of component i, - \\ m_{adsorbents,total} & total adsorbent mass, kg/mol & x_{trait} & molar fraction of component i, n \\ m_{adsorbents,total} & total adsorbent mass, kg/mol & x_{trait} & molar fraction of component i, P \\ m_{gas} & mixed gas molar mass, kg/mol & x_{trait} & molar fraction of component i, - \\ M_{gas} & mixed gas molar mass, kg/mol & x_{trait} & molar fraction of component i, n \\ P_{p} & given relaction for Component i, P \\ P_{p} & given traiter for E_{1t}, J/mol \\ P_{p} & pressure, Pa \\ P_{p} & pressure, Pa \\ P_{p} & rise pressure, Pa \\ P_{p} & rise pressure, for pressure, -equalization depressurization \\ P_{p} & rise pressure, Pa \\ P_{p} & rise pres$	$C_{\text{rinse},i}$	rinse gas molar concentration, mol/m ³	$Q_{\text{product,out}}$	outlet flow rate of the product column, m ³ /s
$\begin{array}{cccc} C_{pp,l} & given gas molar concentration for pressure-equalization pressurization, mol/m3 pressurization, mol/m3 pressurization, mol/m3 pressurization, mol/m3 pressurization, mol/m3 pressurization, mol/m3 pressure for pressure pa pressure pa pressure, Pa pressure for pressure pa pressure, Pa pressure pa pressure, Pa pressure for pressure, Pa pressure for pressure, Pa pressure for pressure, Pa pressure pressure, Pa pressure pa pressure, Pa pressure pa pressure, Pa pressure pa pressure, Pa pressure pa pressure, Pa pressure for pressure, Pa pressure pa pa paper paper$	$C_{\text{purge},i}$	purge gas molar concentration, mol/m ³	Q_{feed}	feed flow rate of the product column, m ³ /s
$C_{pp,i}$ pressurization, mol/m³ $rate_c$ catalytic reaction rate, mol/kg s $C_{pp,i}$ given gas molar concentration for product pressurization, mol/m³ R ideal gas constant, J/mol K C_T total gas molar concentration, mol/m³ t time, s $\dot{C}_{transfer,i}$ mass transfer between bulk gas and particles, mol/m³ s t_{otal} total operating time, s $D_{ax,i}$ axial dispersion coefficient, m^2/s T temperature, K D_p diameter of adsorbent/catalyst particles, m ν gas velocity, m/s E_i^0 initial activation energy, J/mol ν_{rinse} rinse velocity, m/s E_i^0 initial activation energy, J/mol ν_{rinse} rinse velocity, m/s k_i reaction rate, s^{-1} or kg/mol s ν_{purge} purge velocity for pressure, -equalization pressurization, m/s k_{eq} valve rate for blowdown, s^{-1} ν_{pp} given velocity for product pressurization, m/s K_{eq} equilibrium constant for WGS reaction, - L_b ν_{l} ratio of f-related sites to non-related sites, - m_s M_{g} mixed gas molar mass, kg/mol α fitting parameter for E_{1b} , J/mol p pressure, Pa β fitting parameter for E_{1b} , J/mol p_{l} partial pressure of component <i>i</i> , Pa ρ_a $Adsorbents.totaltata dasorbent is pressure, Pa\beta_bp_0standard atmospheric pressure, Pa\beta_bvoid ratio of fixed bed, -\rho_ap_{leed}feed pressure, Pa\rho_ccatalyst density, kg/m$	$C_{\text{pep},i}$	given gas molar concentration for pressure-equalization	rate _a	CO ₂ adsorption rate, mol/kg s
$\begin{array}{ccc} C_{\rm pp,i} & {\rm given gas molar concentration for product pressurization,} & R & {\rm ideal gas constant, J/mol K} \\ {\rm mol/m^3} & SA & {\rm specific surface area, m^2/kg} \\ C_{\rm T} & {\rm total gas molar concentration, mol/m^3} & t & {\rm time, s} \\ C_{\rm transfer,i} & {\rm mass transfer between bulk gas and particles, mol/m^3 s} & t_{\rm otal} & {\rm total operating time, s} \\ D_{\rm ax,i} & {\rm axial dispersion coefficient, m^2/s} & T & {\rm temperature, K} \\ D_{\rm p} & {\rm diameter of adsorbent/catalyst particles, m} & \nu & {\rm gas velocity, m/s} \\ E_i & {\rm activation energy, J/mol} & \nu_{\rm feed} & {\rm feed velocity, m/s} \\ E_i^0 & {\rm initial activation energy, J/mol} & \nu_{\rm frime} & {\rm rinse velocity, m/s} \\ k_i & {\rm reaction rate, s^{-1} or kg/mol s} & \nu_{\rm purge} & {\rm purge velocity for pressure, -equalization pressurization, s^{-1}} & \nu_{\rm perg} & {\rm given velocity for pressure, -equalization m/s} \\ k_{\rm eq} & {\rm valve rate for pressure, -equalization depressurization, s^{-1}} & v_{\rm pp} & {\rm given velocity for product pressurization, m/s} \\ k_{\rm eq} & {\rm column length, m} & n & nolar fraction of component i, - \\ m_{\rm adsorbents, total} & {\rm total adsorbents mass, kg/mol} & x_{\rm t} & {\rm ratio of K-related sites to non-related sites, - } \\ M_{\rm g} & {\rm mixed gas molar mass, kg/mol} & \alpha & {\rm fitting parameter for E_{16}, J/mol} \\ p_{\rm o} & {\rm standard atmospheric pressure, Pa} & \beta & {\rm fitting parameter for E_{16}, J/mol} \\ p_{\rm o} & {\rm standard atmospheric pressure, Pa} & \beta_{\rm c} & {\rm catalyst density, kg/m^3} \\ p_{\rm feed} & {\rm feed pressure, Pa} & \rho_{\rm c} & {\rm catalyst density, kg/m^3} \\ p_{\rm feed} & {\rm feed pressure, Pa} & \rho_{\rm c} & {\rm catalyst density, kg/m^3} \\ p_{\rm fitting} & {\rm pressure, Pa} & \rho_{\rm c} & {\rm catalyst density, kg/m^3} \\ p_{\rm nuse} & {\rm rinse pressure, Pa} & \rho_{\rm c} & {\rm catalyst density, kg/m^3} \\ p_{\rm rinse} & {\rm rinse pressure, Pa} & \rho_{\rm c} & {\rm catalyst density, kg/m^3} \\ p_{\rm rinse} & {\rm rinse pressure, Pa} & \rho_{\rm c} & {\rm catalyst density, kg/m^3} \\ p_{\rm rinse} & {\rm rinse pressure, Pa} & \rho_{\rm c} $		pressurization, mol/m ³	<i>rate</i> _c	catalytic reaction rate, mol/kgs
mol/m³SAspecific surface area, m²/kg $C_{\rm T}$ total gas molar concentration, mol/m³ttime, s $\dot{C}_{\rm transfer,i}$ mass transfer between bulk gas and particles, mol/m³ stotal operating time, s $D_{ax,i}$ axial dispersion coefficient, m²/sTtemperature, K D_{p} diameter of adsorbent/catalyst particles, mvgas velocity, m/s E_i activation energy, J/mol $\nu_{\rm feed}$ feed velocity, m/s E_i^0 initial activation energy, J/mol s $\nu_{\rm purge}$ given velocity for pressure, -equalization pressurization, s ⁻¹ or kg/mol s k_{ped} valve rate for pressure, -equalization depressurization, s ⁻¹ ν_{pp} given velocity for product pressurization, m/s k_{eq} valve rate for blowdown, s ⁻¹ ν_{pp} given velocity for product pressurization, m/s K_{eq} equilibrium constant for WGS reaction, - v_{l} molar fraction of component i , - M_{co_2} CO ₂ molar mass, kg/mol α fitting parameter for E_{1f} , J/mol p pressure, Pa β fitting parameter for E_{1f} , J/mol p_0 standard atmospheric pressure, Pa ρ_a adsorbent density, kg/m³ p_{feed} feed pressure, Pa ρ_c catalyst density, kg/m³ p_{read} feed pressure, Pa ρ_c gas valco fitting parameter for E_{1b} , J/mol p_{read} feed pressure, Pa ρ_c catalyst density, kg/m³ p_{read} feed pressure, Pa ρ_c catalyst density, kg/m³ P_{read} feed pressure	$C_{\mathrm{pp},i}$	given gas molar concentration for product pressurization,	R	ideal gas constant, J/mol K
$C_{\rm T}$ total gas molar concentration, mol/m³ttime, s $C_{\rm transfer,i}$ mass transfer between bulk gas and particles, mol/m³ s $t_{\rm total}$ total operating time, s $D_{\rm ax,i}$ axial dispersion coefficient, m²/sTtemperature, K $D_{\rm p}$ diameter of adsorbent/catalyst particles, m ν gas velocity, m/s E_i activation energy, J/mol $\nu_{\rm feed}$ feed velocity, m/s E_i^0 initial activation energy, J/mol $\nu_{\rm finse}$ rinse velocity, m/s k_i reaction rate, s ⁻¹ or kg/mol s $\nu_{\rm purge}$ purge velocity, m/s $k_{\rm pel}$ valve rate for pressure, -equalization depressurization, s m/s $k_{\rm dep}$ valve rate for blowdown, s ⁻¹ $\nu_{\rm pp}$ given velocity for product pressurization, m/s $K_{\rm eq}$ equilibrium constant for WGS reaction, - $vol_ratio_{a/c}$ packing volume ratio of adsorbent and catalyst, - L_b column length, m x_i molar fraction of component i , - $m_{\rm adsorbents, totaltotal adsorbents mass, kgx_{\rm rotout, i}molar fraction of component i, -M_{\rm g}mixed gas molar mass, kg/mol\alphafitting parameter for E_{\rm 1f}, J/molppressure, Pa\betafitting parameter for E_{\rm 1f}, J/molp_{\rm ressure}feed pressure, of component i, Pa\rho_{\rm a}Adsorbent density, kg/m³\rho_{\rm g}gas density, kg/m³p_{\rm ressure}feed gressure, Pa\rho_{\rm g}gas density, kg/m³p_{\rm ressure}feed pressure, Pa\rho$		mol/m ³	SA	specific surface area, m ² /kg
$ \begin{array}{ccc} \dot{C}_{transfer,i} & mass transfer between bulk gas and particles, mol/m3 s \\ \dot{C}_{transfer,i} & axial dispersion coefficient, m2/s \\ D_{p} & diameter of adsorbent/catalyst particles, m \\ D_{p} & diameter of adsorbent/catalyst particles, m \\ F_{i} & activation energy, J/mol \\ F_{i}^{0} & initial activation energy, J/mol \\ F_{i} & reaction rate, s-1 or kg/mol s \\ k_{i} & reaction rate, s-1 or kg/mol s \\ k_{eq} & valve rate for pressure, -equalization depressurization, s-1 \\ F_{eq} & valve rate for blowdown, s-1 \\ T_{insec} & rinse velocity for pressure, -equalization pressurization, m/s \\ K_{eq} & equilibrium constant for WGS reaction, - \\ T_{b} & column length, m \\ M_{CO_2} & CO_2 molar mass, kg/mol \\ M_{g} & mixed gas molar mass, kg/mol \\ P_{p} & pressure, Pa \\ P_{0} & standard atmospheric pressure, Pa \\ P_{0} & standard atmospheric pressure, Pa \\ P_{rinse} & feed pressure, Pa \\ P_{rinse} & rinse pressure, Pa \\ P_{rinse}$	C_{T}	total gas molar concentration, mol/m ³	t	time, s
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\dot{C}_{ ext{transfer},i}$	mass transfer between bulk gas and particles, mol/m ³ s	$t_{\rm total}$	total operating time, s
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$D_{\mathrm{ax},i}$	axial dispersion coefficient, m ² /s	Т	temperature, K
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	D_{p}	diameter of adsorbent/catalyst particles, m	ν	gas velocity, m/s
E_i^0 initial activation energy, J/mol v_{rinse} rinse velocity, m/s k_i reaction rate, s^{-1} or kg/mol s v_{purge} purge velocity, m/s k_{ped} valve rate for pressure, -equalization depressurization, s^{-1} v_{pep} given velocity for pressure, -equalization pressurization, m/s k_{dep} valve rate for blowdown, s^{-1} v_{pp} given velocity for product pressurization, m/s k_{dep} valve rate for blowdown, s^{-1} v_{pp} given velocity for product pressurization, m/s k_{dep} column length, m v_{i} molar fraction of component $i, m_{adsorbents, total}$ total adsorbents mass, kg $x_{roduct,i}$ molar fraction of component i in the product column, - M_{CO_2} CO ₂ molar mass, kg/mol α fitting parameter for E_{1f} , J/mol p pressure, Pa β fitting parameter for E_{1b} , J/mol p_i partial pressure of component i , Pa ρ_a adsorbent density, kg/m ³ p_{finse} rinse pressure, Pa ρ_c catalyst density, kg/m ³ p_{rinse} rinse pressure, for pressure, -equalization depressurization ρ_g $gas viscosity, Pa s$ ρ_g gas density, kg/m ³	E_i	activation energy, J/mol	v_{feed}	feed velocity, m/s
k_i reaction rate, s ⁻¹ or kg/mol s v_{purge} purge velocity, m/s k_{ped} valve rate for pressure, -equalization depressurization, s ⁻¹ v_{pep} given velocity for pressure, -equalization pressurization, m/s k_{dep} valve rate for blowdown, s ⁻¹ v_{pp} given velocity for product pressurization, m/s k_{eq} equilibrium constant for WGS reaction, - v_{pp} given velocity for product pressurization, m/s L_b column length, m x_i molar fraction of component $i, m_{adsorbents,total}$ total adsorbents mass, kg $x_{product,i}$ molar fraction of component i in the product column, - M_{CO_2} CO_2 molar mass, kg/mol α fitting parameter for E_{1f} , J/mol p pressure, Pa β fitting parameter for E_{1b} , J/mol p_0 standard atmospheric pressure, Pa ρ_a adsorbent density, kg/m ³ p_{freed} feed pressure, Pa ρ_c catalyst density, kg/m ³ p_{rinse} rinse pressure, Pa ρ_g gas density, kg/m ³ p_r size or pressure for pressure, Pa ρ_g gas viscosity, Pa s	E_i^0	initial activation energy, J/mol	v_{rinse}	rinse velocity, m/s
k_{ped} valve rate for pressure, -equalization depressurization, s^{-1} v_{pep} given velocity for pressure, -equalization pressurization, m/s k_{dep} valve rate for blowdown, s^{-1} v_{pp} given velocity for product pressurization, m/s k_{eq} equilibrium constant for WGS reaction, - L_b $v_{ol}_ratio_{a/c}$ packing volume ratio of adsorbent and catalyst, - x_i $M_{adsorbents,total}$ total adsorbents mass, kg x_i molar fraction of component i , - x_k ratio of K-related sites to non-related sites, - $mixed gas molar mass, kg/mol$ p pressure, Pa β fitting parameter for E_{1f} , J/mol p_0 standard atmospheric pressure, Pa ρ_a adsorbent density, kg/m³ p_{freed} feed pressure, Pa ρ_c catalyst density, kg/m³ p_{rinse} rinse pressure, Pa ρ_c gas viscosity, Pa s	k_i	reaction rate, s^{-1} or kg/mol s	v_{purge}	purge velocity, m/s
k_{dep} valve rate for blowdown, s ⁻¹ v_{pp} given velocity for product pressurization, m/s k_{eq} equilibrium constant for WGS reaction, – $vol_ratio_{a/c}$ packing volume ratio of adsorbent and catalyst, – L_b column length, m x_i molar fraction of component <i>i</i> , – $m_{adsorbents,total}$ total adsorbents mass, kg $X_{product,i}$ molar fraction of component <i>i</i> in the product column, – M_{CO_2} CO ₂ molar mass, kg/mol x_k ratio of K-related sites to non-related sites, – M_g mixed gas molar mass, kg/mol α fitting parameter for E_{1f} , J/mol p pressure, Pa β fitting parameter for E_{1b} , J/mol p_i partial pressure of component <i>i</i> , Pa ρ_a adsorbent density, kg/m ³ p_{freed} feed pressure, Pa ρ_c catalyst density, kg/m ³ p_r inse pressure, Pa ρ_g gas density, kg/m ³	$k_{\rm ped}$	valve rate for pressure, –equalization depressurization, e^{-1}	$v_{\rm pep}$	given velocity for pressure, –equalization pressurization, m/s
K_{eq} equilibrium constant for WGS reaction, - V_{pp} $green vertex (vertex) for product pressumation, in/sK_{eq}equilibrium constant for WGS reaction, -vol_ratio_{a/c}packing volume ratio of adsorbent and catalyst, -L_bcolumn length, mx_imolar fraction of component i, -m_{adsorbents,total}total adsorbents mass, kgx_{product,i}molar fraction of component i in the product column, -M_{CO_2}CO_2 molar mass, kg/molx_Kratio of K-related sites to non-related sites, -M_gmixed gas molar mass, kg/mol\alphafitting parameter for E_{1f}, J/molppressure, Pa\betafitting parameter for E_{1b}, J/molp_0standard atmospheric pressure, Pa\rho_aadsorbent density, kg/m3p_{feed}feed pressure, Pa\rho_ccatalyst density, kg/m3p_{rinse}rinse pressure, Pa\rho_ggas density, kg/m3p_{rinse}rinse pressure for pressure, equalization depressuriza-\mu$	k.	s	ν	given velocity for product pressurization m/s
K_{eq} equilibrium constant for WGS feaction, μ V_{C_2} V_{C_2} intraj ℓ product, intro of component i , $ M_{adsorbents,total}$ total adsorbents mass, kg x_i molar fraction of component i , $ M_{CO_2}$ CO_2 molar mass, kg/mol x_K ratio of K-related sites to non-related sites, $ M_g$ mixed gas molar mass, kg/mol α fitting parameter for E_{1f} , J/mol p pressure, Pa β fitting parameter for E_{1b} , J/mol p_0 standard atmospheric pressure, Pa ε_b void ratio of fixed bed, $ p_i$ partial pressure of component i , Pa ρ_a adsorbent density, kg/m ³ p_{frinse} rinse pressure, Pa ρ_c catalyst density, kg/m ³ p_{rinse} rinse pressure for pressure, equalization depressuriza- μ	κ _{dep} ν	equilibrium constant for WCS reaction	vol ratio.	packing volume ratio of adsorbent and catalyst. –
$m_{adsorbents,total}$ total adsorbents mass, kg $x_{product,i}$ molar fraction of component i in the product column, – M_{CO_2} CO_2 molar mass, kg/mol x_K ratio of K-related sites to non-related sites, – M_g mixed gas molar mass, kg/mol α fitting parameter for E_{1f} , J/mol p pressure, Pa β fitting parameter for E_{1b} , J/mol p_0 standard atmospheric pressure, Pa β_b void ratio of fixed bed, – p_i partial pressure of component i, Pa ρ_a adsorbent density, kg/m ³ p_{freed} feed pressure, Pa ρ_c catalyst density, kg/m ³ p_{rinse} rinse pressure for pressure, pa ρ_g gas density, kg/m ³ p_a system pressure for pressure for pressure for pressure, pa ρ_g gas viscosity, Pa s	Leq	column length m	χ;	molar fraction of component <i>i</i> . –
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	m _{e dense} te en te	total adsorbents mass, kg	Xproduct i	molar fraction of component i in the product column, –
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	McOa	CO_2 molar mass, kg/mol	XK	ratio of K-related sites to non-related sites, –
p pressure, Pa β fitting parameter for E_{1b} , J/mol p_0 standard atmospheric pressure, Pa ε_b void ratio of fixed bed, - p_i partial pressure of component i , Pa ρ_a adsorbent density, kg/m ³ p_{feed} feed pressure, Pa ρ_c catalyst density, kg/m ³ p_{rinse} rinse pressure, Pa ρ_g gas density, kg/m ³ p_{r} given pressure for pressure for pressure $-equalization$ depressuriza- μ gas viscosity, Pa s	M_{σ}	mixed gas molar mass, kg/mol	α	fitting parameter for E_{1f} , J/mol
p_0 standard atmospheric pressure, Pa ε_b void ratio of fixed bed, - p_i partial pressure of component <i>i</i> , Pa ρ_a adsorbent density, kg/m³ p_{feed} feed pressure, Pa ρ_c catalyst density, kg/m³ p_{rinse} rinse pressure, Pa ρ_g gas density, kg/m³ p_r given pressure for pressure or pressure for pressure $-equalization$ depressuriza- μ gas viscosity, Pa s	p	pressure, Pa	β	fitting parameter for E_{1b} , J/mol
p_i partial pressure of component i , Pa ρ_a adsorbent density, kg/m³ p_{feed} feed pressure, Pa ρ_c catalyst density, kg/m³ p_{rinse} rinse pressure, Pa ρ_g gas density, kg/m³ p_r gas density, kg/m³ ρ_g gas viscosity, Pa s	p_0	standard atmospheric pressure, Pa	$\varepsilon_{\rm b}$	void ratio of fixed bed, -
p_{feed} feed pressure, Pa ρ_c catalyst density, kg/m ³ p_{rinse} rinse pressure, Pa ρ_g gas density, kg/m ³ p_{sinse} gas density, kg/m ³ p_g gas viscosity, Pa s	p_i	partial pressure of component <i>i</i> , Pa	ρ_{a}	adsorbent density, kg/m ³
p_{rinse} rinse pressure, Pa ρ_{g} gas density, kg/m ³ p_{rinse} gas viscosity, Pa s	p_{feed}	feed pressure, Pa	$ ho_{\rm c}$	catalyst density, kg/m ³
μ , given pressure for pressure –equalization depressuriza- μ gas viscosity, Pa s	p_{rinse}	rinse pressure, Pa	$ ho_{ m g}$	gas density, kg/m ³
tion, Pa	$P_{\rm ped}$	given pressure for pressure, –equalization depressuriza- tion, Pa	μ	gas viscosity, Pa s

[4]. From the perspective of exergetic evaluation, PSA is a desirable hydrogen purification technology achieving above 99.9% hydrogen purity (HP) [5]. Common PSA systems work at normal temperature ranges (NT-PSA) by adopting physical adsorbents such as activated carbon, zeolite, and silica gel [10]. NT-PSA is a cyclic process where the gas impurities are first adsorbed on the surfaces of adsorbents and then desorbed by reducing the pressure [11]. Thermal energy duty for regeneration is avoided during NT-PSA operation. However, for achieving high HP, NT-PSA faces limitations such as low hydrogen recovery ratio (HRR) and high system complexity [12]. For hydrogen production from typical steam methane reformed gas (70–80% H₂, 15–25% CO₂, 3–6% CH₄, 1–3% CO, and trace N₂), a typical NT-PSA achieves 98–99.999% HP and 70–90% HRR [10].

When fixing the column number of NT-PSA, there is a trade-off between HRR and HP. Ribeiro et al. [13] demonstrated that shortening the adsorption time from 160 s to 120 s increased HP of a four-column eight-step NT-PSA from 99.8193% to 99.9992% while decreasing HRR from 71.8% to 62.7%. A similar phenomenon was found when countercurrent purge rate was increased when hydrogen was commonly adopted as purge gas [14]. When the column number was increased, both HRR and HP increased due to increase in pressure-equalization steps. Moon et al. [15] indicated that a two-column NT-PSA achieved 99.77-99.95% HP with 73.30-77.64% HRR, and a four-column NT-PSA could achieve above 99.97% HP with 79% HRR. Lopes et al. [16] proposed a ten-step NT-PSA with three pressure-equalizations, which achieved 99.981% HP and 81.6% HRR from a five-component gas (79% H₂, 17% CO₂, 1.2% CO, 2.1% CH₄, and 0.7% N₂). HRR could be further increased to 92.7% with 99.993% HP for a twelve-column thirteen-step NT-PSA to purify raw hydrogen fuel gas in IGCC power plants [17].

However, the large column number decreased productivity and increased the operating complexity and capital cost (CAPEX) [18].

Alternatively, the concept of elevated-temperature pressure swing adsorption (ET-PSA) has been proposed for producing hydrogen from shifted gas [19]. ET-PSA works at elevated temperatures (200-450 °C), thus allowing the shifted gas to directly enter the purification unit without pre-cooling. Chemisorbents like potassium-promoted layered double oxides (K-LDOs) [20] and molten salt-promoted MgO [21], which show high CO2 working capacity and fast adsorption/desorption kinetics at elevated temperatures, are adopted as CO₂ adsorbents in ET-PSA system. ET-PSA allows the use of steam as rinse and purge gas, where the co-current steam rinse squeezes residual hydrogen out of the column after the adsorption step and counter-current steam purge is adopted to replace hydrogen purge in the NT-PSA process [22]. The high temperature steam, which could be produced in a heat recovery boiler with waste heats from the gasifier, the exhaust gas from gas turbine or other subsystems, was the main energy consumption of ET-PSA [23]. The ET-PSA process can be applied in sorption-enhanced water gas shift (SEWGS), where WGS catalysts are mixed into CO2 adsorption columns to transform the residual CO in the shifted gas to produce extra H_2 [24].

A series of ET-PSA processes including four-column eight-step cycle [25], six-column eight-step cycle [26], seven-column ten-step cycle [27], eight-column eleven-step cycle [28], and nine-column eleven-step cycle [29] has been proposed. One of the optimization objectives for ET-PSA is to reduce the steam amount for rinse and purge, as it is the main energy consumer in ET-PSA [23]. For SEWGS process, Reijer et al. [26] showed that the rinse mainly affected CO_2 purity and the purge mainly affected CO_2 capture ratio. The rinse-to-carbon and purge-to-

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