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Optimal synthesis of periodic sorption enhanced reaction processes with application to hydrogen production

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ABSTRACT

A systematic design and synthesis framework for multi-step, multi-mode and periodic sorption-enhanced reaction processes (SERP) is presented. The formulated nonlinear algebraic and partial differential equation (NAPDE)-based model simultaneously identifies optimal SERP cycle configurations, design specifications and operating conditions. Key modeling contributions include a generalized boundary-condition formulation and a representation that enables the selection of discrete operation modes and flow directions using continuous pressure variables. A simulation-based constrained grey-box optimization strategy is employed to obtain optimal cycles and design parameters. The framework has been used for designing two SERP systems, namely sorption-enhanced steam methane reforming (SE-SMR) and sorption-enhanced water gas shift reaction (SE-WGSR), for maximizing hydrogen productivity and minimizing hydrogen-production cost. Specifically, a cyclic SE-SMR process is designed that obtains 95% pure hydrogen from natural gas with 35% higher productivity and 10.86% lower cost compared to existing small-scale, distributed systems. The developed synthesis framework can also be applied for other applications.

1. Introduction

There is an ever-increasing demand of hydrogen in several industries such as petrochemicals manufacturing, electronics, metallurgy, oil hydrogenation, as a product upgrader in petroleum refining, as a fuel for automotive and aerospace industry (Ramachandran and Menon, 1998), as a raw material for ammonia and methanol production (Harrison, 2008), and as an energy carrier in fuel cells and other applications. Hydrogen is predominantly produced via steam methane reforming (SMR) that accounts for approximately 95% of total hydrogen production in the United States (Energy, 2002). The production process combines mature technologies such as those of SMR and pressure swing adsorption (PSA), which are currently being operated at near-theoretical limits. This conventional hydrogen production process has high capital costs and utility consumption due to large numbers of unit operations, high reactor temperature and need for hydrogen product purification (Carvill et al., 1996). Due to the ubiquity of the hydrogen product in industrial and commercial uses, any improvements in hydrogen production will positively affect these sectors (McAuliffe, 1980).

Process improvements can be realized by improving the system fundamentally using multi-functional reactors, which carry out multiple synergistic phenomena in a single, intensified column. Integrating the two critical phenomena, namely reaction and separation, forms the basis of multi-functional reactors (Stankiewicz, 2003). Sorption Enhanced Reaction Process (SERP) is one of such applications leveraging multi-functional reactors for simultaneously carrying out reaction and separation. The SERP concept has been successfully demonstrated on several reactions for hydrogen production such as steam methane reforming (Lopez Ortiz and Harrison, 2001; Ochoa-Fernandez et al., 2005), water gas shift reaction (WGSR) (Allam et al., 2005; Jang et al., 2012), and steam reforming of glycerol (He et al., 2010). In SERP operation, the column is packed with both sorbent and catalyst to simultaneously remove reaction byproduct(s) and promote desired reactions. The SERP concept is based on the Le Chatelier's principle which states that forward reactions are favored by selective removal of reaction byproduct(s) (Hufton et al., 1999). The SERP technology has received considerable attention due to the potential advantages it offers over traditional processes (Radfarnia and Iliuta, 2014). Due to simultaneous reaction, byproduct removal and heat integration, SERP occurs at lower temperatures, requires less equipment and less utilities, and is modular thereby offering more flexibility in deployment and operation. The reaction products obtained via SERP have higher purity, selectivity and productivity along with higher reactant conversions (Han and Harrison, 1994).

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Nomenclature

Abbreviations

CSS cyclic steady state
GRAMS generalized reaction adsorption modeling and simulation
HTC hydrotalcite
PSA pressure swing adsorption
SE-SMR sorption enhanced steam methane reforming
SE-WGSR sorption enhanced water gas shift reaction
SERP sorption enhanced reaction process
SMR steam methane reforming
WGSR water gas shift reaction

Dimensionless symbols

α dimensionless LDF mass transfer coefficient
Ω dimensionless groups in column energy balance
$\bar{P}$ dimensionless pressure
$\bar{T}$ dimensionless temperature
$\bar{T}_a$ dimensionless ambient temperature
$\bar{T}_w$ dimensionless wall temperature
$\bar{v}$ dimensionless interstitial velocity
π dimensionless groups in wall energy balance
ψ dimensionless adsorption parameter
ψ_r dimensionless reaction parameter
σ dimensionless groups in column energy balance
τ dimensionless time
x_i^* dimensionless equilibrium solid loading capacity of gas species i
x_i dimensionless solid loading capacity of gas species i
Z dimensionless length
$\bar{R}_k$ dimensionless rate of reaction k

Greek symbols

α_c adsorbent-to-catalyst ratio decision variable
α_j adsorbent to catalyst density ratio at node j
α_{lb} lower bound on sorbent-to-catalyst mass ratio
α_{ub} upper bound on sorbent-to-catalyst mass ratio
Δ_r trust region
ϵ Allowable constraint violation
η_c compressor efficiency
η_h furnace efficiency
η_k effectiveness factor of reaction k
η_m motor efficiency
γ heat capacity ratio
Λ State variable
μ viscosity of the gas phase mixture
ν_{ik} stoichiometric coefficient of species i in reaction k
ω_l cubic basis radial function parameter
ϕ capital recovery factor
$\rho_{b,\,ads}$ bulk density value of adsorbent
$\rho_{b,\,cat}$ bulk density value of catalyst
ρ_{refr} density of refractory material
ρ_{steel} density of steel
$\theta(x^l)$ smooth constraint violation function
$\theta^r(x)$ approximated constraint violation function
ε_b bed porosity
ε_p particle porosity
ε_t total bed porosity
$\zeta_{p,\,q}$ exponent

Other symbols

$\bar{x}_d^l$ scaled component d of sample l
$\bar{x}_r$ trust region center with scaled variables
ΔH_{vap} heat of vaporization of steam
ΔP_{tol} pressure tolerance value between consecutive steps
$\dot{V}_{0,\,flow}$ reference volumetric flow rate to SE-SMR reactor
$\dot{V}_{flow}$ volumetric flow rate to SE-SMR reactor
ads adsorbent index
AIC annualized investment cost for hydrogen production
AMC annual maintenance cost
B set containing boundary conditions of velocity, pressure, mole fraction, gas phase temperature and wall temperature
b_i cubic basis radial function parameter
BPC balance plant cost
C_0 reference cost of high temperature valve and piping
C_{comp} purchase cost of compressor
C_{cool} purchase cost of cooler
C_{furn} purchase cost of furnace
c_{HTC} specific cost of HTC sorbent
c_{Ni} specific cost of SMR catalyst
$C_{p,\,ads}$ specific heat capacity of adsorbent
$C_{p,\,a}$ specific heat capacity of adsorbate
$C_{p,\,cat}$ specific heat capacity of catalyst
$C_{p,\,CW}$ specific heat capacity of cold water
$C_{p,\,i}$ specific heat capacity of species i
C_{pb} cost of packed bed
C_{pg} gas specific heat capacity
C_{ps} solid specific heat capacity
C_{pw} wall specific heat capacity
C_{reac} purchase cost of SE-SMR reactor
c_{refr} specific cost of refractory
C_{sol} cost of solid material
c_{steel} specific cost of steel
c_s piecewise constant parameter
C_v cost of high temperature valve and piping
d_a SE-SMR reactor and refractory diameter
D_L axial dispersion coefficient
d_{in} bed diameter
E_{com} electricity consumed by compressor
$f(x)$ black-box objective function in generalized optimization formulation
$f^r(x)$ approximated objective function
f_{ds} carbon steel design stress pressure
$F_{i,\,in}$ incoming flow rate of species i
$F_{i,\,out}$ outgoing flow rate of species i
fs feed stream fs index
$g_u(x)$ black-box constraints in generalized optimization formulation
$g_u^r(x)$ approximated black-box constraints
$g_v(x)$ known constraints in generalized optimization formulation
I_0 reference CE index
I_{2017} CE index for September 2017
IDC indirect cost
j cell j index
k reaction k index
K_z axial gas heat conductivity
L bed length
M big number = 10^{10}
m operation stage m index
m_i solid phase saturation capacity for single site Langmuir model
$m_{i,\,1}$ solid phase saturation capacity for site 1 of dual site Langmuir model
$m_{i,\,2}$ solid phase saturation capacity for site 2 of dual site Langmuir model