



# Modelling of sorption-enhanced steam methane reforming in a fixed bed reactor network integrated with fuel cell

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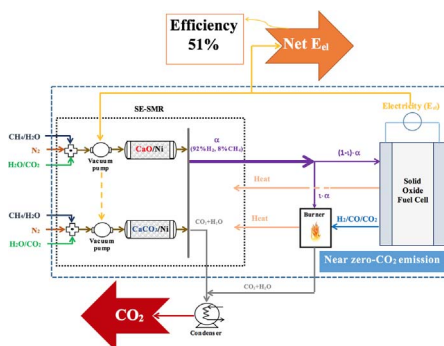
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## HIGHLIGHTS

- A fixed bed reactor network was evaluated for sorption-enhanced steam methane reforming.
- A high-purity H<sub>2</sub> stream (92%) and a concentrated CO<sub>2</sub> stream were obtained.
- The system is energy-self-sufficient with near-zero-CO<sub>2</sub> emissions.
- Integration of the system with a fuel cell led to a 51% net global efficiency.

## GRAPHICAL ABSTRACT



## ARTICLE INFO

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## ABSTRACT

In this study sorption-enhanced steam methane reforming (SE-SMR) in fixed beds is investigated by means of 1D numerical modelling, and the model is validated with the data reported in the literature. Isothermal conditions (973 K) are considered, and the equilibrium between the carbonation and calcination stages is shifted by a pressure swing:  $3.5 \cdot 10^6$  Pa and 1013 Pa, respectively. The results showed that under these operating conditions at least 8 reactors in parallel are required to continuously produce a high-purity stream of H<sub>2</sub>, and a separated stream of concentrated CO<sub>2</sub>. The average H<sub>2</sub> purity is 0.92, whilst the average H<sub>2</sub> yield and selectivity are  $2.9 \text{ mol}_{\text{H}_2} \text{ mol}_{\text{CH}_4}^{-1}$  and 90%, respectively. A thermodynamic analysis was performed, which highlighted that, by using a portion of the produced H<sub>2</sub> (about  $0.4 \text{ mol}_{\text{H}_2} \text{ mol}_{\text{CH}_4}^{-1}$ ), it is possible to fully cover heat and power demands of the process, making it completely energy self-sufficient. In the case when the proposed SE-SMR is integrated with a solid oxide fuel cell, net power generation at the scale of  $\sim 950 \text{ kW}_{\text{el}}$  can be achieved with a net efficiency of the entire system of 51%, with the important feature that CO<sub>2</sub> is concentrated.

## 1. Introduction

Currently, the interest in hydrogen production technologies is on the increase, since H<sub>2</sub> is considered as an environmentally friendly

alternative for various industrial processes. The current literature reports that H<sub>2</sub> can be used as fuel for power generation [1], as chemical raw material for the synthesis of ammonia or the refining of crude oil [1], as well as for fuel cell applications [2]. However, H<sub>2</sub> is just an

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**Nomenclature**

$A_a$	aspect ratio of the external surface area to the volume of the reactor wall, $m^{-1}$	$u$	gas superficial velocity, $m s^{-1}$
$A_{EH}$	heat surface area required by CAS, $m^2$	$T$	temperature, K
$A_r$	surface of reactor vessel, $m^2$	$T_w$	temperature of the reactor wall, K
$A_w$	aspect ratio of the internal surface area to the volume of the reactor wall, $m^{-1}$	$t$	time, s
$C_i$	concentration of species $i$ , $mol m^{-3}$	$t_{calc}$	period of calcination stage, s
$c_p$	heat capacity, $J kg^{-1} K^{-1}$	$t_{carb}$	period of carbonation stage, s
$D_{ax}$	axial dispersion coefficient, $m^2 s^{-1}$	$X_{sorb}$	sorbent conversion degree, %
$d$	diameter, m	$X_{max}$	maximum sorbent conversion, %
$E_{a,j}$	activation energy of reaction $j$ , $J mol^{-1}$	$X_{CH_4}$	methane conversion, %
$E_D$	electric power demand of vacuum pump, $W_{el}$	$V_r$	reactor volume, $m^3$
$E_{net}$	net alternate current power production, $W_{el}$	$V_{loss}$	fuel cell voltage loss, V
$E_{SOFC}$	SOFC alternate current power, $W_{el}$	$V_{SOFC}$	SOFC voltage, V
$F$	Faraday constant, $A s mol^{-1}$	$y_i$	molar fraction of gas species $i$ , –
$f_u$	SOFC fuel utilisation	$z$	axial spatial variable, m
$G$	mass flux of the gas phase, $kg m^{-2} s^{-1}$	<i>Greek letters</i>	
$g$	acceleration due to gravity, $m s^{-2}$	$\alpha_a$	thermal diffusivity at the film temperature, $m^2 s^{-1}$
$H_{ext}$	external heating and power, $J mol_{CH_4}^{-1}$	$\beta_b$	thermal expansion coefficient, $K^{-1}$
$h_f$	gas-solid heat transfer coefficient, $W m^{-2} K^{-1}$	$\gamma_{el,SOFC}$	SOFC electrical efficiency, %
$h_i$	enthalpy of gas species $i$ , $J mol^{-1}$	$\gamma_{inv}$	inverter efficiency, %
$h_{ext}$	external convective heat transfer coefficient, $W m^{-2} K^{-1}$	$\gamma_{ref}$	reforming process efficiency, %
$h_m$	gas-solid mass transfer coefficient, $m s^{-1}$	$\Delta G_f^0$	change in molar Gibbs free energy of formation, $J mol^{-1}$
$h_w$	internal convective heat transfer coefficient, $W m^{-2} K^{-1}$	$\Delta H^0$	standard enthalpy of reaction, $J mol^{-1}$
$i$	gas species ( $CH_4$ , $H_2O$ , $H_2$ , $CO$ , $CO_2$ )	$\Delta H_{Rj}$	enthalpy of reaction $j$ , $J mol^{-1}$
$j$	reaction (SMR, WGS, OSMR, CR, CAR)	$\Delta P$	maximum pressure drop, Pa
$K_i$	adsorption coefficient of species $i$	$\varepsilon_g$	bed void fraction, –
$K_j$	equilibrium constant of reaction $j$	$\zeta$	dimensionless axial spatial coordinate, –
$k_j$	rate constant of reaction $j$	$\eta_{H_2}$	$H_2$ yield, $mol_{H_2} mol_{CH_4}^{-1}$
$L$	reactor length, m	$\eta_{H_2, equivalent}$	$H_2$ -equivalent yield, $mol_{H_2} mol_{CH_4}^{-1}$
$LHV$	lower heating value, $J mol^{-1}$	$\theta$	steam-to-methane feed ratio during carbonation stage, –
$M$	molecular weight, $kg mol^{-1}$	$\iota$	partition ratio, –
$\dot{m}$	gas mass flow rate, $kg s^{-1}$	$\lambda_{amb}$	external air thermal conductivity, $W m^{-1} K^{-1}$
$m_s$	mass of solid in the reactor, kg	$\lambda_{ax}$	axial heat dispersion coefficient, $W m^{-1} K^{-1}$
$N_{Me}$	Mears number, –	$\lambda_w$	reactor wall thermal conductivity, $W m^{-1} K^{-1}$
$N_R$	number of reactors, –	$\mu_g$	gas viscosity, Pa s
$\dot{n}_{CH_4, in}$	inlet $CH_4$ molar flow rate, $mol s^{-1}$	$\nu_v$	kinematic viscosity at the film temperature, $m^2 s^{-1}$
$\dot{n}_{H_2, SE-SMR}$	$H_2$ molar flow rate at the outlet of SE-SMR process, $mol s^{-1}$	$\rho$	density, $kg m^{-3}$
$\dot{n}_{CH_4, SE-SMR}$	$CH_4$ molar flow rate at the outlet of SE-SMR process, $mol s^{-1}$	$\sigma$	internal diffusion effectiveness factor, –
$P$	pressure, Pa	$\tau_{car/cal}$	period of the carbonation/reforming and calcination cycle, s
$P_i$	partial pressure of gas species $i$ , bar	$\tau_{SE-SMR}$	total period of the SE-SMR process, s
$P_0$	standard pressure, Pa	$\phi$	portion of reactors operating in the considered stage
$Pr$	Prandtl number, –	$\varphi$	heat transfer effectiveness factor, –
$Q$	volumetric flow rate, $m^3 s^{-1}$	$\psi$	steam-to- $CO_2$ feed ratio during calcination stage, –
$\dot{Q}$	thermal power, $W_{th}$	$\omega_y$	mass fraction of component $y$ (sorbent or catalyst), –
$\dot{Q}_{burner}$	thermal power generated by external burner, $W_{th}$	<i>Subscripts</i>	
$\dot{Q}_f$	thermal power required to warm up feed gas streams, $W_{th}$	amb	ambient
$\dot{Q}_{SE-SMR}$	thermal power required by SE-SMR process, $W_{th}$	cat	catalyst
$\dot{Q}_{SOFC}$	thermal power generated by SOFC, $W_{th}$	eq	equilibrium
$\dot{Q}_{ref}$	thermal power required by SOFC internal reforming process, $W_{th}$	g	gas
$Ra$	Rayleigh number, –	in	inlet
$Re$	Reynolds number, –	obs	observed
$R_g$	ideal gas constant, $J mol^{-1} K^{-1}$	p	particle
$R_j$	reaction rate of reaction $j$ , $mol kg^{-1} s^{-1}$	r	reactor
$r_i$	rate of formation or consumption of species $i$ , $mol m^{-3} s^{-1}$	s	solid
$Sc$	Schmidt number, –	sorb	sorbent
$S_{H_2}$	$H_2$ selectivity, %	out	outlet
$s_s$	reactor wall thickness, m	w	reactor wall
$U$	external overall heat transfer coefficient from the wall to the ambient air, $W m^{-2} K^{-1}$	<i>Acronyms</i>	
		CALCR	CALCination Reaction

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