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Millisecond methane steam reforming for hydrogen production: A computational fluid dynamics study

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ABSTRACT

The potential of methane steam reforming to produce hydrogen in thermally integrated micro-chemical systems at short contact times was theoretically explored. Methane steam reforming coupled with methane catalytic combustion in microchannel reactors for hydrogen production was studied numerically. A two-dimensional computational fluid dynamics model with detailed chemistry and transport was developed. To provide guidelines for optimal design, reactor behavior was studied, and the effect of design parameters such as catalyst loading, channel height, and flow arrangement was evaluated. To understand how steam reforming can happen at millisecond contact times, the relevant process time scales were analyzed, and a heat and mass transfer analysis was performed. The importance of energy management was also discussed in order to obtain a better understanding of the mechanism responsible for efficient heat exchange between highly exothermic and endothermic reactions. The results demonstrated the feasibility of the design of millisecond reforming systems, but only under certain conditions. To achieve this goal, process intensification through miniaturization and the improvement in catalyst performance is very important, but not sufficient; very careful design and implementation of the system is also necessary to enable high thermal integration. The channel height plays an important role in determining the efficiency of heat exchange. A proper balance of the flow rates of the combustible and reforming streams is an important design criterion. Reactor performance is significantly affected by flow arrangement, and co-current operation is recommended to achieve a good energy balance within the system. The catalyst loading must be carefully designed to avoid insufficient reactant conversion or hot spots. Finally, operating windows were identified, and engineering maps for designing devices with desired power were constructed.

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Introduction

The production of synthesis gas, primarily a mixture of hydrogen and carbon monoxide, from hydrocarbons has received a great deal of interest in recent years due to the need to produce high-content hydrogen streams for fuel cell applications and internal combustion engines [1–4]. Industrially, syngas is produced by steam reforming of natural gas

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Nomenclature

$A_{catalyst}$ catalytically active surface area, m^2, Eq. (12)
$A_{geometric}$ geometric surface area, m^2, Eq. (12)
$C_{fuel,in}$ feed concentration of the fuel, mol/m^3, Eq. (25)
$C_{i,interface}$ concentration of the i-th species at the gas-washcoat interface, mol/m^2, Eq. (14)
c_p specific heat capacity at constant pressure, $J/(kg \cdot K)$, Eq. (8)
d gap distance between the plates, i.e., channel height, m, Fig. 1 and Eq. (26)
d_{pore} mean pore diameter of the catalyst, m, Eq. (17)
D diffusion coefficient, m^2/s, Eq. (6)
D^T thermal diffusion coefficient, m^2/s, Eq. (6)
$D_{i,eff}$ effective diffusion coefficient of the i-th species inside the washcoat, m^2/s, Eq. (14), as defined by Eq. (16)
$D_{i,Knudsen}$ Knudsen diffusion coefficient of the i-th species inside the washcoat, m^2/s, Eq. (16), as defined by Eq. (17)
$D_{i,molecular}$ molecular diffusion coefficient of the i-th species inside the washcoat, m^2/s, Eq. (16)
$D_{k,m}$ mixture-averaged diffusion coefficient of the k-th gaseous species, m^2/s, Eq. (6)
D_k^T thermal diffusion coefficient of the k-th gaseous species, m^2/s, Eq. (6)
Da_y transverse Damköhler number, dimensionless, as defined by Eq. (30)
$F_{cat/geo}$ catalyst/geometric surface area, m^2/m^2, as defined by Eq. (12)
Fo Fourier number, dimensionless, as defined by Eq. (32)
$F_{s\text{-}\infty}$ view factor for solid-ambient, unity, Eq. (19)
h total specific enthalpy, J/kg, Eq. (8)
h_k^o specific enthalpy of the k-th gaseous species at reference temperature, J/kg, Eq. (8)
h_o external heat loss coefficient, $W/(m^2 \cdot K)$, Eq. (19)
$\Delta_r H_m^\Theta$ standard molar enthalpy of reaction, kJ/mol, Eq. (20)
$k_{ad,k}$ adsorption rate constant of the k-th gaseous species, Eq. (24)
K ratio of catalyst loadings, Fig. 6, as defined by Eq. (29)
K_g number of the species in the gas phase, Eq. (4)
K_s number of the species on the surface of the catalyst, Eq. (9)
l reactor length, i.e., channel length, Fig. 1 and Eq. (28)
m total number of gaseous and surface species, Eq. (9)
p pressure, Pa, Eq. (2)
Pe Péclet number, dimensionless, as defined by Eq. (31)
q heat flux, W/m^2, Fig. 1 and Eq. (18)
R ideal gas constant, $J/(mol \cdot K)$, Eq. (7)
$\dot{s}_{i,eff}$ effectiveness surface molar production rate of the i-th species inside the washcoat, $mol/(m^2 \cdot s)$, Eq. (13)
$\dot{s}_m$ surface molar production rate of the m-th surface species, $mol/(m^2 \cdot s)$, Eq. (9)
S/V surface-to-volume ratio, i.e., catalytically active surface area per unit volume, m^2/m^3, Eq. (25)
T absolute temperature, K, Eq. (4)
T_{amb} ambient temperature, K, Eq. (19)
T_o reference temperature, K, Eq. (8)
$T_{w,o}$ temperature at the external surface of the solid wall, K, Eq. (19)
u streamwise velocity component, m/s, Eq. (1)
$\bar{u}$ average flow velocity, m/s, Eq. (28)
u_{in} inlet velocity, m/s, Fig. 4
v transverse velocity component, m/s, Eq. (1)
V_k diffusion velocity of the k-th gaseous species, m/s, Eq. (5)
$\vec{V}_k$ diffusion velocity vector of the k-th gaseous species, m/s, Eq. (6)
W_k relative molecular mass of the k-th gaseous species, dimensionless, Eq. (5)
$\overline{W}$ relative molecular mass of the gas mixture, dimensionless, Eq. (6)
x streamwise reactor coordinate, Fig. 1 and Eq. (1)
y transverse reactor coordinate, Fig. 1 and Eq. (1)
Y_k mass fraction of the k-th gaseous species, Eq. (4)

Greek variables

Γ site density for surface phase, mol/m^2, Eq. (9)
γ catalytically active surface area per washcoat volume, m^2/m^3, Eq. (14), as defined by Eq. (15)
γ_k sticking coefficient of the k-th gaseous species, Eq. (24)
δ wall thickness, m, Fig. 1
$\delta_{catalyst}$ thickness of the washcoat, m, Eq. (14)
ε emissivity, Eq. (19)
ε_p catalyst porosity, dimensionless, Eq. (16)
$\varepsilon_{s\text{-}\infty}$ effective emissivity for solid-ambient, Eq. (19)
η effectiveness factor, Eq. (11), as defined by Eq. (13)
θ_{free} surface coverage of free sites, Eq. (24)
λ thermal conductivity, $W/(m \cdot K)$, Eq. (4)
λ_g gas thermal conductivity, $W/(m \cdot K)$, Eq. (4)
λ_s thermal conductivity of the solid wall, $W/(m \cdot K)$, Eq. (10)
μ dynamic viscosity, $kg/(m \cdot s)$, Eq. (2)
ρ density of the gas mixture, kg/m^3, Eq. (1)
σ Stefan-Boltzmann constant, $W/(m^2 \cdot K^4)$, Eq. (19)
σ_m site occupancy of the m-th surface species, Eq. (9)
τ time scale, s, Eq. (25)
τ_p catalyst tortuosity factor, dimensionless, Eq. (16)
$\tau_{reaction}$ intrinsic reaction time scale, as defined by Eq. (25)
τ_x axial transfer time scale, as defined by Eq. (28)
τ_y transverse transfer time scale, as defined by Eqs. (26) and (27)
Φ Thiele modulus, dimensionless, Eq. (13), as defined by Eq. (14)
$\dot{\omega}_k$ gas-phase molar production rate of the k-th gaseous species, $mol/(m^3 \cdot s)$, Eq. (5)

Subscripts

amb ambient, Eq. (19)
g gas, Eq. (4)
i species index, Eq. (13)

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