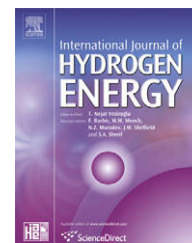


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Numerical modeling of high-temperature shell-and-tube heat exchanger and chemical decomposer for hydrogen production

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ABSTRACT

Numerical simulations of shell-and-tube heat exchanger and chemical decomposer with straight tube configuration and porous media were performed using FLUENT6.2.16 to examine the percentage decomposition of sulfur trioxide. The decomposition process can be a part of sulfur–iodine (S–I) thermochemical water splitting cycle, which is one of the most studied cycles for hydrogen production. A steady-state, laminar, two-dimensional axisymmetric shell-and-tube model with counter flow and parallel flow arrangements and simple uniform cubical packing was developed using porous medium approach to investigate the fluid flow, heat transfer and chemical reactions in the decomposer. As per the investigation, the decomposition percentage of sulfur trioxide for counter flow arrangement was found to be 93% and that of parallel flow was 92%. Also, a high pressure drop was observed in counter flow arrangement compared to parallel flow. The effects of inlet velocity, temperature and the porous medium properties on the pressure drop across the porous medium were studied. The influence of geometric parameters mainly the diameter of the tube, diameter of the shell and the length of the porous zone on the percentage decomposition of sulfur trioxide in the tube was investigated as well. A preliminary parametric study of the mentioned configuration is conducted to explore effects of varying parameters on the decomposition of sulfur trioxide. From the performed calculations, it was found that the Reynolds number played a significant role in affecting the sulfur trioxide decomposition. The percentage decomposition decreases with an increase in Reynolds number. Surface-to-volume area ratio and activation energy were also the important parameters that influenced the decomposition percentage.

A high surface-to-volume area ratio enhances the rate of the chemical reaction and high activation energy decreases the decomposition percentage. The decomposition of sulfur trioxide is calculated and compared for both counter and parallel flow arrangements.

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Nomenclature

A	pre-exponential factor (s^{-1})
C_p	specific heat at constant pressure ($J/kg/K$)
C_2	inertial resistance factor
$D_{i,m}$	diffusion co-efficient for species i in the mixture (m^2/s^{-1})
d_h	hydraulic diameter (m)
E_a	activation energy (kJ/mol)
K	reaction rate (s^{-1})
k	kinetic energy of turbulence (m^2/s^2)
k_B	Boltzmann constant ($1.38 \cdot 10^{-23} J/K^{-1}$)
L	length of tube (mm)
m	mass (kg)
\dot{m}	mass flow rate (kg/s)
p	static pressure (Pa)
Re	Reynolds number
R_{rxni}	net rate of production of species i by chemical reaction ($kg/m^3/s$)
S_i	rat of reaction of species i by addition from dispersed phase ($kg/m^3/s$)
t	time (s)
T	temperature (K)
T_{inhot}	inlet temperature of helium (K)
T_{incold}	inlet temperature of reacting flow (K)
T_{cold}	outlet temperature of reacting flow (K)
U	velocity magnitude
u_i	mean velocity component ($i = 1,2,3$) (m/s)
u_j	mean velocity component ($j = 1,2,3$) (m/s)
u_k	mean velocity component ($k = 1,2,3$) (m/s)
u'_i	fluctuating velocity components ($i = 1,2,3$) (m/s)
u'_j	fluctuating velocity components ($j = 1,2,3$) (m/s $^{-1}$)
u'_k	fluctuating velocity components ($k = 1,2,3$) (m/s $^{-1}$)
X_i	mass concentration of species i
w_i	length coordinate i (x, y, z) (m)
w_j	length coordinate j (x, y, z) (m)
w_k	length coordinate k (x, y, z) (m)
ϵ	Lennard–Jones energy parameter ($J/molecule$)
ϵ_p	porosity
ϵ_t	thermal effectiveness
λ	thermal conductivity ($W/m K^{-1}$)
μ	dynamic viscosity ($kg/m s^{-1}$)
μ_t	turbulent viscosity ($kg/m s^{-1}$)
ν	kinematic viscosity (m^2/s^{-1})
ρ	density (kg/m^{-3})
σ	Lennard–Jones characteristic length (Å)
φ_i	mole fraction of species i
ω	specific dissipation rate (s^{-1})
δ_{ij}	Kronecker delta
ΩD	diffusion collision integral

1. Introduction

One of the global concerns is that fossil fuel recourses will be diminished in the near future. The constantly growing demand for energy, combined with the realization that fossil

fuel resources are finite and diminishing, has made it critical to utilize alternate sources of energy, as well as discover methods to prolong the lifetime of our remaining fossil fuels. In addition, the green house effect due to the accumulation of carbon dioxide in the atmosphere by the large-scale burning of the fossil fuel is causing various environmental problems. Hydrogen is an important industrial chemical, particularly when used in systems for converting coal into synthetic gas and oil, and is projected to be used as a fuel in the future. Hydrogen produced by using nuclear or solar heat is more easily stored and transported than thermal energy. In addition, it is a clean fuel. If hydrogen can be obtained from other than conventional fossil-based processes, our ultimate reserves of fossil fuels can be prolonged [1].

A hydrogen economy will need significant new sources of hydrogen. Hydrogen can be an attractive energy carrier if it can be produced cleanly and in a cost-effective manner. Hydrogen can be derived from a variety of domestically available primary sources, including fossil fuels, renewable sources, etc.

One of the promising approaches to produce large quantities of hydrogen from nuclear energy is the thermochemical water splitting cycle. Unlike electrolysis, thermochemical cycles can directly convert low-level thermal energy into chemical energy by forming hydrogen and oxygen, and with overall first-law efficiencies exceeding 50%. These cycles were identified as most suitable ones that have potential advantages in efficiency, cost or reduced complexity. Although hundreds of cycles have been identified, only a few have been developed sufficiently to establish technical feasibility. The U.S. Department of Energy (DOE) Nuclear Hydrogen Initiative (NHI) is investigating thermochemical cycles for hydrogen production using high-temperature heat from advanced nuclear reactors [2]. Thermochemical cycles produce hydrogen through a series of chemical reactions resulting in the production of hydrogen and oxygen from water at much lower temperatures than direct thermal decomposition.

Since the conception of the first thermochemical cycle in 1960s, a large number of water splitting cycles have been conceptualized and a few of those are extensively investigated. The sulfur–iodine cycle (S–I) proposed by the General Atomics (GA) Company is one such cycle developed for the large-scale hydrogen production. The practicability of any thermochemical water splitting cycle (TWSC) depends mainly on two factors: high overall thermal efficiency and operational feasibility. The overall thermal efficiency of a TWSC determines the effectiveness of the cycle in receiving energy from a heat source and converting that into chemical energy. For that, a highly endothermic reaction is a prerequisite. Analysis of this cycle in the past 30 years has been focused mostly on the utilization of nuclear power as the high-temperature heat source for performing the decomposition of sulfuric acid. Thermodynamic and kinetic considerations indicate that both the extent and the rate of sulfuric acid decomposition can be improved at very high temperatures (in excess of 1000 °C) available only from solar concentrators.

The S–I cycle is one of the baseline cycle for thermochemical process for the large-scale hydrogen production. It

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