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CFD modeling and simulation of sulfur trioxide decomposition in ceramic plate-fin high temperature heat exchanger and decomposer

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ABSTRACT

In this study numerical analysis was carried out for four different types of fins namely rectangular, triangular, inverted bolt fins and ripsaw fins and three different types of arrangements namely straight, staggered and top and bottom arrangement. The obtained results were compared with each other and the design with the highest decomposition percentage of sulfur trioxide was selected. The working fluids used in the model were sulfur trioxide, sulfur dioxide, oxygen and water vapor. The operating pressure was 1.5 MPa and the operating temperature ranges from 973 K to 1223 K. From the results it was found that the ripsaw fin design with thickness of 0.05 mm gives the highest decomposition percentage of sulfur trioxide. The inverted bolt fins gives a good heat transfer rate but due to the fin arrangement and the flow disturbances caused by the arrangement the pressure drop was the highest compared to the other fins. The pressure drop and heat transfer obtained for the rectangular and triangular fins were similar to each other. The obtained decomposition percentage of sulfur trioxide for straight, staggered and top and bottom arrangement were 17.60%, 16.74% and 20.55%. The obtained decomposition percentage increased from 16.74% to 85.15% when the channel length of the heat exchanger was increased ten times.

1. Introduction

Hydrogen is widely seen as the future energy carrier due to the growth of the global energy demand and the necessity to reduce greenhouse gas emissions. Hydrogen is one of the two natural elements that combine to produce water. Though they are renewable and have less environmental impacts, non-renewable sources like coal, oil and natural gases are still needed to separate it from oxygen. The primary challenge to the increased use of hydrogen is the cost associated with its production, storage and delivery. There are two main categories of hydrogen production technologies using high temperature gas reactors (HTGRs) namely thermochemical water splitting cycles and high temperature water electrolysis.

In the thermochemical water splitting cycle hydrogen is separated from water into hydrogen and oxygen through chemical reactions at high temperatures (450 °C to 1000 °C). In this cycle all the reactants and the products are regenerated and recycled. Energy as heat is given as an input to the thermochemical cycle via one or more endothermic chemical reactions. Heat is rejected via one or more exothermic low temperature chemical reactions. Among the available thermochemical cycles, the sulfur family consisting of sulfur-iodine cycle (S-I) cycle and hybrid sulfur (H-S) cycle are found to be the most promising candidates for hydrogen production. The sulfur-iodine water splitting cycle proposed by General Atomics (GA) is a promising candidate for thermochemical hydrogen production [1]. It consists of three chemical reactions that sum to the dissociation of water:

$$I_2 + SO_2 + 2H_2O \rightarrow 2HI + H_2SO_4 \ (120\,^{\circ}C) \ \text{(Exothermic)} \quad (1)$$

$$H_2SO_4 \rightarrow H_2O + SO_2 + 1/2O_2 \ (850\,^{\circ}C) \ \text{(Endothermic)} \quad (2)$$

$$2HI \rightarrow I_2 + H_2 \ (450\,^{\circ}C) \ \text{(Endothermic)} \quad (3)$$

The net reaction is the decomposition of water to hydrogen and oxygen. The sulfur-iodine thermochemical water splitting cycle is shown in Fig. 1 [2].

Many works have been conducted for the sulfuric acid decomposition process using high temperature heat exchangers and chemical decomposers. The Bunsen reaction for the production of hydriodic and sulfuric acids from water, iodine and sulfur dioxide was studied by Giaconia et al. [3]. A study on sulfur-iodine cycle for hydrogen production by a water splitting reaction was done by Barbarossa et al. [4]. Experiments have been done in a homogenous gas phase in the presence of solid catalysts Ag–Pd intermetallic alloy and Fe_2O_3 supported on SiO_2 in the temperature range

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Nomenclature

A_s	cross-sectional area, m^2
C_p	specific heat constant pressure, J kg^{-1} K^{-1}
D_h	hydraulic diameter, m
D_{AB}	mass diffusivity of the binary mixture, m^2 s^{-1}
f	friction factor
k	thermal conductivity of the fluid, W m^{-1} k^{-1}
$\dot{m}$	mass flow rate, kg s^{-1}
P	static pressure, Pa
q''	heat flux, W m^{-2}
R	gas constant, J K^{-1} mol^{-1}
Re	Reynolds number
Sc	Schmidt number
T	temperature, K
$\overline{Nu}$	average Nusselt number
U	mean velocity component (i = 1,2,3), m s^{-1}

Greek

v	volumetric flow rate, ml min^{-1}
μ	dynamic viscosity, kg m^{-1} s^{-1}
ρ	density, kg m^{-3}
Δp	pressure drop, Pa

Subscripts

b	average value
w	wall
i	inlet
o	outlet

of 773 K to 1373 K. From the results it was observed that the thermal dissociation of sulfuric acid was strongly affected by temperature and hence a suitable catalytic material must be selected to decrease decomposition temperature. The results showed that the operative temperatures have a minor effect on the phase behavior.

Compact heat exchangers (CHE) play an important role in the field of aerospace, transportation, nuclear and other industries. The need for lightweight, space saving and economical heat exchanger has driven to the development of compact heat exchangers. Surface area density greater than 700 m^2/m^3 is achieved by incorporating fins ribs, etc. CHEs are widely in demand due to their improved effectiveness, smaller volume, higher surface area density and power savings. A plate-fin heat exchanger is a form of compact heat exchanger made of block of alternating layers of corrugated fins separated by parting sheets. Surface interruption prevents the continuous growth of the thermal boundary layer by periodically interrupting it. Thus the thicker thermal boundary layer which offers high thermal resistance to heat transfer are maintained thin and their resistance to heat transfer is reduced. In a plate-fin heat exchanger, fins are easily rearranged in cross-flow, counter flow, or parallel flow arrangements. The cost of plate-fin heat exchanger is slightly higher compared to conventional heat exchangers due to higher level of detail required during manufacture. However the cost can be outweighed by the added heat transfer enhancement. The widely used plate fin heat exchanger has a variety of augmented surfaces such as plain fins, wavy fins, offset strip fins, perforated fins, pin fins and louvered fins.

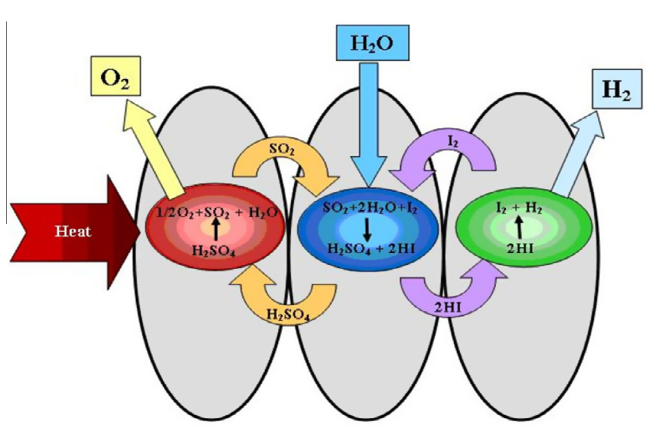

Fig. 1. Sulfur-iodine thermochemical water splitting cycle [2].

Ranganayakulu and Seetharamu [5] carried out an analysis of a cross-flow compact plate-fin heat exchanger for the combined effects of two-dimensional longitudinal heat conduction through the exchanger wall, flow non-uniformity and temperature distribution was carried out using the finite element method. The exchanger effectiveness and thermal deterioration due to these effects were studied for various design and operating conditions.

Research has been carried out by Ma et al. [6] to find heat transfer and pressure drop performances of ribbed channels in the high temperature heat exchanger. The effects of inlet temperature and rib height on the ribbed channel have been studied. From the results it was found that the Nusselt number and the friction factor were unsuitable to compare heat transfer and pressure drop performances at different temperature conditions. Schulte-Fischedick et al. [7] proposed a ceramic high temperature plate-fin heat exchanger for externally fired combustion process. Thermal performance and pressure drop in ceramic heat exchanger was evaluated using CFD simulations by Monteiro et al. [8]. Correlations for the Colburn and the friction factors for the Reynolds number ranging from 500 to 1500 were evaluated. Simulations with conjugate heat transfer were conducted and the results showed the influence of mass flow rate on pressure drop and effectiveness of the heat exchanger.

Due to the high heat transfer effectiveness the compact heat exchangers are widely used in the nuclear industry for the production of hydrogen. Ponyavin et al. [9] carried out a numerical analysis on the three-dimensional computational model of the ceramic high temperature heat exchanger to investigate fluid flow, heat transfer, chemical reaction and stress analysis within the decomposer. A decomposition rate of 0.515% was achieved for SO_3 using this design. Numerical simulation of shell-and-tube heat exchanger and chemical decomposer with straight tube configuration and porous media was studied to find the decomposition percentage of sulfur trioxide by Kuchi et al. [10]. From the results it was found that the decomposition percentage of SO_3 was 93% for counterflow arrangement and 92% for parallel flow arrangement.

In the research done by Subramanian et al. [11] ceramic high temperature heat exchanger was used as a sulfuric acid decomposer for hydrogen production within the sulfur-iodine thermochemical cycle. The activity and stability of several metal oxide supported platinum catalysts were explored for sulfuric acid decomposition reaction. In the study by Ginosar [12] reactions were carried out using a feed of concentrated sulfuric acid (96 wt%) at atmospheric pressure and temperatures between 800 and 850 °C. The results showed that the higher surface area catalysts namely Pt/Al_2O_3 and Pt/ZrO_2 had the highest activity but deactivated rapidly. Sandia