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PUMP DESIGN AND COMPUTATIONAL FLUID DYNAMIC ANALYSIS FOR HIGH TEMPERATURE SULFURIC ACID TRANSFER SYSTEM

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In this study, we proposed a newly designed sulfuric acid transfer system for the sulfur-iodine (SI) thermochemical cycle. The proposed sulfuric acid transfer system was evaluated using a computational fluid dynamics (CFD) analysis for investigating thermodynamic/hydrodynamic characteristics and material properties. This analysis was conducted to obtain reliable continuous operation parameters; in particular, a thermal analysis was performed on the bellows box and bellows at amplitudes and various frequencies (0.1, 0.5, and 1.0 Hz). However, the high temperatures and strongly corrosive operating conditions of the current sulfuric acid system present challenges with respect to the structural materials of the transfer system. To resolve this issue, we designed a novel transfer system using polytetrafluoroethylene (PTFE, Teflon®) as a bellows material for the transfer of sulfuric acid. We also carried out a CFD analysis of the design. The CFD results indicated that the maximum applicable temperature of PTFE is about 533 K (260 °C), even though its melting point is around 600 K. This result implies that the PTFE is a potential material for the sulfuric acid transfer system. The CFD simulations also confirmed that the sulfuric acid transfer system was designed properly for this particular investigation.

KEYWORDS : High Temperature Sulfuric Acid Transfer System, Sulfur-Iodine (SI) Cycle, Sulfuric Acid Decomposition, Hydrogen Production, Computational Fluid Dynamics (CFD)

1. INTRODUCTION

Among various hydrogen production technologies, steam reforming technology is responsible for producing ~90 % of the hydrogen used in recent years [1]. This method is the most common process for producing commercial bulk hydrogen at high temperatures (700-1100 °C) under various conditions. However, the steam reforming technology utilizes fossil fuels and therefore does not prevent carbon dioxide from being released into the atmosphere. Among various hydrogen production technologies that do not utilize fossil fuels, nuclear hydrogen is the most likely candidate for commercialization.

There are currently over 400 nuclear hydrogen production cycles proposed. Nuclear hydrogen production cycles, and the sulfur-iodine (SI) thermochemical cycle have attracted much attention recently because its theoretical heat transfer efficiency for hydrogen is above 50 % [2]. The Japan Atomic Energy Research Institute (JAERI) has been involved in the study of the SI thermochemical hydrogen production cycle [3-5], which was originally proposed by General Atomics [6].

The SI thermochemical cycle consists of three chemical reactions that result in dissociation of water into hydrogen and oxygen;

(a) Bunsen reaction :
$I_2 + SO_2 + 2H_2O \rightarrow 2HI + H_2SO_4$ (T ~ 120 °C)
(b) Sulfuric acid decomposition :
$H_2SO_4 \rightarrow SO_2 + H_2O + 1/2O_2$ (T > 800 °C)
(c) Hydriodic acid decomposition :
$2HI \rightarrow I_2 + H_2$ (T > 350 °C)

Net $H_2O \rightarrow H_2 + 1/2O_2$

As shown above, the chemical reaction can be represented as the Bunsen reaction (a), the sulfuric acid decomposition reaction (b), and the hydriodic acid decomposition reaction (c).

Extensive experimental and theoretical research has been carried out worldwide over the last decade to investigate the potential of these hydrogen production processes [7-9]. However, much of the research has focused on the development of supplementations to address specific problems associated with this process [10-17]. For the sulfuric acid concentration/decomposition reaction, challenges involving material corrosion in the presence of a high temperature energy source emerged and investigations on catalyst activity and stability were subsequently carried out [10-14]. Onuki *et al*. [14] determined that material resistance was crucial for the development of the hydriodic acid concentration/decomposition reaction. The sulfuric acid decomposition reaction takes place at high temperatures and is catalyzed by an expensive metal catalyst. This reaction requires the highest temperature during the thermochemical hydrogen production process and therefore dictates the temperature requirement of the primary energy source [15]. To improve these problems, Giaconia *et al*. [16] investigated the bunsen reaction and evaluated the effects of various operation parameters on the product phase behavior. Goldstein *et al*. [17] identified an upper limit and estimated the ideal efficiency of the thermochemical SI process when used in conjunction with a high temperature reactor.

A device that can be used to transfer sulfuric acid at high temperatures during the SI process is shown in Fig. 1. The pump used to carry sulfuric acid during the SI process is a very important piece of equipment. According to the SI process flow sheet [18], to transfer sulfuric acid to a vaporizer of a sulfuric acid decomposer at a gauge pressure of 0.1 atm, the sulfuric acid should be cooled to 177 °C or instead of the vaporizer of a multistage distillation column. Some of the disadvantages associated with the sulfuric acid transfer system include the risk of handling and the reduced efficiency which is caused by the transfer, re-heating, and pressurization of the sulfuric acid. The thermal stability of the materials used in the sulfuric acid decomposition reaction is also an important consideration because the hot sulfuric acid produces harsh chemical environments during the reaction.

Generally, a ceramic piston pump is used to transfer sulfuric acid. The ceramic is used as a piston material and its fluid limitation temperature is less than 115 °C [19]. Therefore, it is necessary to improve the inner material used for transferring hot sulfuric acid within the pump. However, research regarding the use of proper materials in this pump for transferring sulfuric acid has been very limited thus far.

In this study, we proposed a novel sulfuric acid transfer system for the SI thermochemical cycle. Polytetrafluoroethylene (PTFE, Teflon®) [20] exhibits a coefficient of friction against polished steel in the range of 0.05 to 0.13, which is one of the lowest measured values for a solid. PTFE is a crystalline polymer, which is usable for a part working under a temperature lower than 533 K (260 °C), with a melting point of ~ 600 K (327 °C) [20]. This feature makes it suitable for applications that require reduced friction between two solid components, such as gears or moving parts. We proposed that PTFE could be used as the inner material of the sulfuric acid transfer system. The proposed sulfuric acid transfer system was evaluated using a computational fluid dynamics (CFD) analysis. To determine the thermodynamic/hydrodynamic characteristics and material properties [21], the CFD analysis was performed under similar conditions as those of actual driving processes by utilizing user-defined functions (UDFs) [22] with varying frequencies and amplitudes. In particular, by performing a thermal analysis on the bellows and bellows end-plate, the durability characteristics of the PTFE used on the moving parts during the continuous operation of the transfer system were evaluated.

2. MODELING AND CFD METHOD OF THE SULFURIC ACID TRANSER SYSTEM

2.1 Design Modeling

Fig. 1 (a) is shown as the concentration and decomposition steps of sulfuric acid in SI process [23]. In the dotted(······) section, the process is illustrated to show that sulfuric acid is transferred from the multistage distillation column to a vaporizer using the sulfuric acid transportation system. The sulfuric acid transfer system previously suggested was presented in Fig. 1 (b). Due to the operation temperature limit of ceramic piston pumps, forced cooling was needed so the thermal efficiency was lowered in this system. In Fig. 1 (c), the process for sulfuric acid transportation was illustrated. The thermal efficiency is larger than in the previous system (Fig. 1 (b)) because the forced cooling was not required in our system.

Fig. 2 shows a schematic of our newly designed sulfuric acid transfer system and CFD analysis region. The pump parts and check valve in the sulfuric acid transfer system is presented in Fig. 2 (a), and the dimensions of the pump section and the calculated segments (bellows box, bellows, and bellows end-plate) of the system is shown in Fig. 2 (b). The pumping segment shown in Fig. 2 (a) consisted of a check valve (60), a bellows box (21, which is connected to the check valve), and a driving unit (23, which contracts /expands the bellows inside the bellows box). After a flow path with connecting the bellows box (21) and check valve (60) was established, the sulfuric acid solution from check valve introduced to bellows box (21) before being pumped to outside. The cooling water cooled the introducing inlet (42) of bellows (22) and discharging to outlet (44). For the expansion and contraction of the bellows (22), the piston (26) located in the actuator (23), moved the round trip in the cylinder (25) and provided the driving force. At this time, the reciprocating cycle of the piston was the frequency and the forward / backward amplitude of piston (26) was controlled by micrometer head (36).

When the bellows (22) was contracted by lowering the upper check ball, the check valve (60) closed the outlet flow, and the sulfuric acid was introduced to the bellows box (21) when the inlet flow path was opened with raising a lower check ball. When the bellows (22) was expanded, the flow path was opened by raising the