581f Simulation of Decomposition of Sulfur Trioxide Gas on Self-Catalytic Metallic Material

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The development of a three-dimensional numerical model is discussed in this paper which predicts the homogeneous decomposition of sulfur trioxide gas into sulfur dioxide and oxygen on a catalytic surface for hydrogen production by the sulfur-iodine thermochemical water splitting cycle. This cycle is one of the concepts under development by the U.S. Department of Energy, Nuclear Hydrogen Initiative.

The effects of catalyst surface temperature and operating pressure on the decomposition of sulfur trioxide was studied on a three-dimensional model using Computational Fluid Dynamics (CFD) Techniques. A three-dimensional computational mesh was created using the preprocessor GAMBIT 2.1, the simulation was done with a CFD software package FLUENT 6.2, and Tec plot was used for post processing the problem.

Research has been performed on the decomposition of sulfur trioxide in the past three decades however in most of the cases the shell and tube configuration with a packed catalyst bed either on the shell side or on the tube side was considered for the experiments. In the present problem, the catalyst is part of the decomposer structure and assumed to effectively coat the inner walls of the channels of the decomposer and the reactions involved are one forward wall surface reaction and another reverse volumetric reaction as shown below.

$SO_3 \rightarrow SO_2 + \frac{1}{2} O_2$ (wall surface reaction in the presence of catalyst)

$SO_2 + \frac{1}{2} O_2 \rightarrow SO_3$ (volumetric reaction)

As a part of initial work, the performance of the catalyst was studied on a two-dimensional numerical model where the decomposition of sulfur trioxide is analyzed in a circular reactor tube whose surface is coated with the catalyst ALFA-4. Decomposition of sulfur trioxide was analyzed for different wall surface temperatures for a reactor tube of 4 mm diameter and having a length of 500 mm and the results are plotted in Figure 1 and the values are tabulated in Table 1.

The results of this study indicate that a high percentage of decomposition is expected to occur at reasonably high temperatures that are well within the limits of a high temperature nuclear reactor. This study is occurring in collaboration with the development of self-catalytic metallic materials at the Massachusetts Institute of Technology that will serve as the decomposer. Experimental prototypes of the decomposer channels will be used in the future to validate CFD design computations. This research is funded under the auspices of the U.S. Department of Energy Office of Nuclear Energy, Science & Technology (grant #DE-FG-04-01AL677358).

Table1: Percentage decomposition of sulfur trioxide in a reactor tube of diameter 4 mm and length 500 mm for different wall surface temperatures.

Tube Wall Surface Temperature		Percentage Decomposition of SO_3
C	K	
400	673	0.171
450	723	2.046
500	773	13.535

550	823	46.534
600	873	74.767
650	923	83.893
700	973	86.600
750	1023	87.776
800	1073	88.535
850	1123	89.147
900	1173	89.699
950	1223	90.213
1000	1273	90.703

Figure1: Percentage decomposition of sulfur trioxide in a reactor tube of diameter 4 mm and length 500 mm for different wall surface temperatures.