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Application of Conjugate Heat Transfer and Flow Analyses for Design Optimization of the SI Decomposer

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Abstract

This paper deals with the development of a three-dimensional conjugate heat transfer and fluid flow numerical model to perform the design optimization of a SI (sulfuric acid) decomposer. The SI decomposer is used as part of the plant for hydrogen production.

Hydrogen can prove to be an attractive energy carrier if it can be demonstrated that it can be produced cleanly and in a cost-effective manner. Nuclear energy can be used as an abundant source of energy for high temperature processes (up to 1000°C) for production of hydrogen. The Sulfur Iodine Cycle, a baseline candidate thermo-chemical process consists of three chemical reactions that result in the dissociation of water. These reactions are as follows:

$I_2 + SO_2 + 2H_2O \rightarrow 2HI + H_2SO_4$ (120°C min.)

$H_2SO_4 \rightarrow H_2O + SO_2 + ½\ O_2$ (850°C min.)

$2HI \rightarrow H_2 + I_2$ (450°C min.)

$H_2O \rightarrow H_2 + ½\ O_2$

Theoretically, only water and heat need to be added to the cycle (Fig.1).

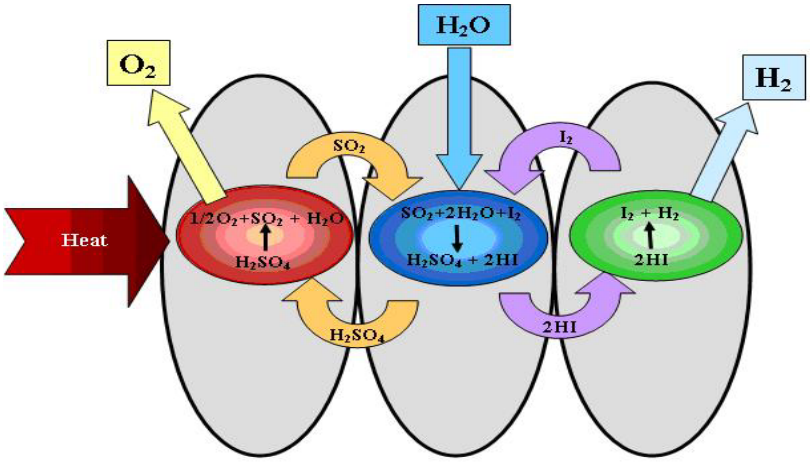

Fig.1 Involved In Sulfur-Iodine Thermo Chemical Water Splitting Cycle

All of the reactants, other than water, are regenerated and recycled.

The very important and critical part of the plant is the high temperature heat exchanger for SI Processes - Preheater & Decomposer.

The real design of the shell and plate heat exchanger is shown on Fig. 2.

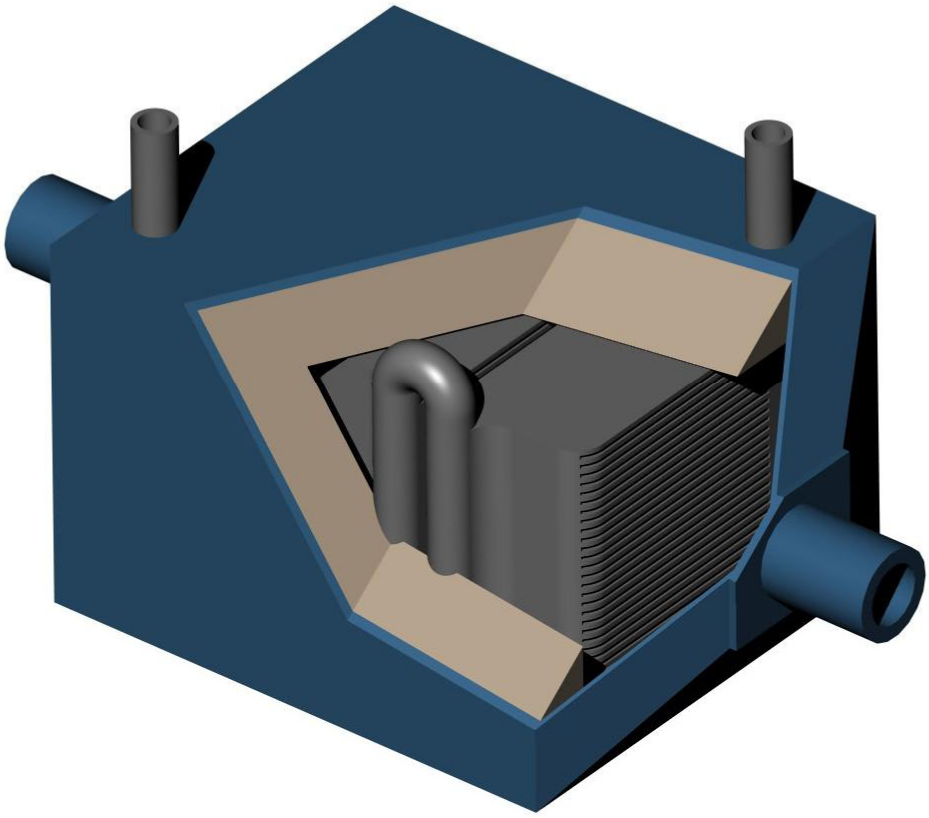

Fig.2 Shell and plate heat exchanger.

The main purpose of the article is to perform the design optimization of a SI (sulfuric acid) decomposer based on maximum performance and minimum pressure drop.

For parametric optimization of the decomposer the single channel model was developed. The geometry and mesh files were created using mesh generator Gambit version 2.0.4. For optimization of the calculated geometry the Gambit journal file was used. With the help of the journal file is possible to change any geometrical parameter of the investigated section.

All of calculation process was performed using Fluent software version 6.2.16. The solution of the velocity field was accomplished using the SIMPLE algorithm that resulted in a faster convergence of the iterations. Conjugate heat transfer (which includes conduction through the material and convection through the fluids) was used in order to solve the energy equation. No other thermal boundary conditions were required for the problem since the solver will calculate heat transfer directly from the solution in the adjacent cells. In the present study, a general curvilinear coordinate grid generation system is used to discretize the computational domain into a finite number of control volumes. With proper control of the grid density, the computational domain can be considered for four main regions (hydrogen region, silicon carbide region, chemical reactions region, products of the chemical reactions

region). The first order upwind numerical scheme is used to discretize the governing equations. For the preliminary calculations the chemical reaction model didn't used. All of liquids properties were calculated using mix option in Fluent for the middle temperature of each channel. The silicon carbide properties were constant except thermal conductivity, which was calculated using polynomial approximation.

A plan of numerical experiments for the design optimization of the SI decomposer was developed.

The model calculations were performed according the presented plan of numerical experiments for the design optimization of the SI decomposer.

Based on results of the calculation the optimized geometry and operation conditions are obtained.