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NUMERICAL MODELING OF HIGH TEMPERATURE SHELL AND TUBE HEAT EXCHANGER AND CHEMICAL DECOMPOSER FOR

HYDROGEN PRODUCTION

by

Gayatri Kuchi

Bachelor of Technology in Mechanical Engineering Jawaharalal Nehru Technological University, India May 2003

> A thesis submitted in partial fulfillment of the requirements for the

Master of Science Degree in Mechanical Engineering Department of Mechanical Engineering Howard R. Hughes College of Engineering

Graduate College University of Nevada, Las Vegas May 2008

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Thesis Approval

The Graduate College University of Nevada, Las Vegas

March 25,20 08

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Numerical Modeling of High Temperature Shell and Tube Heat Exchanger

and Chemical Decomposer

is approved in partial fulfillment of the requirements for the degree of

Master of Science in Mechanical Engineering

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1017-53

ABSTRACT

Numerical Modeling of High Temperature Shell and Tube Heat Exchanger and Chemical Decomposer for Hydrogen Production

by

Gayatri Kuchi

Dr. Yitung.Chen, Examination Committee Chair Associate Professor of Mechanical Engineering, University of Nevada, Las Vegas

This thesis deals with the development of a three-dimensional numerical model of high temperature shell and tube heat exchanger and chemical decomposer to examine the percentage decomposition of a sulfur trioxide gaseous mixture for the production of hydrogen by the sulfur-iodine thermochemical water splitting cycle, a candidate cycle in the U.S.Department of Energy Nuclear Hydrogen Initiative. A counter flow type straight tube shell and heat exchanger concept is chosen for the analysis. The reacting fluid is a mixture of sulfur trioxide gas and water vapor inside the tubes of the heat exchanger and high temperature helium is the gas which flows through the shell. Proceeding with the simple, basic two-dimensional tube model, the percentage decomposition of sulfur trioxide gaseous mixture was investigated. 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 a porous medium approach to investigate the fluid flow, heat transfer and chemical reactions in the decomposer. 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 percentage decomposition of sulfur trioxide in the tube was investigated as well. 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.

Flow rate uniformity in the heat exchanger tubes was also investigated. Simulations of the three dimensional straight tube configuration, tube configuration with baffle plate arrangement and with pebble bed region inside the tubes were performed to examine the flow distribution on tube side. It was found the flow maldistribution along the tube direction is very serious with the simple tube configuration. An improvement of the header configuration has been done by introducing a baffle plate into the header section. With the introduction of the baffle plate, there was a noticeable decrease in the flow maldistribution in the tubes. Uniformity of flow was also investigated with catalytic bed inside the tubes. A significant decrease in flow maldistribution was observed with this arrangement. Simulations were performed on three dimensional numerical model of the shell and tube heat exchanger with and without baffles to evaluate the percentage decomposition of sulfur trioxide where it was found that the baffles play an important role in increasing the percentage decomposition of sulfur trioxide.

TABLE OF CONTENTS

ABSTRACTiii	
LIST OF FIGURES	
NOMENCLATURE	
ACKNOWLEDGEMENTS xii	
CHAPTER 1 INTRODUCTION11.1 Introduction11.2 Research objective41.3 Literature review51.4 Outline of Thesis14	
CHAPTER 2 DESCRIPTION OF THE PROBLEM, GOVERNING EQUATIONS AND	ı
BOUNDARY CONDITIONS 15	
2.1 Description of the problem	
2.2 Equations of fluid flow, heat and species transfer	
2.3 Chemical reactions and kinetics	
2.4 Numerical method and algorithm	
2.4.1 The finite volume method	
2.4.2 Solution method	
2.4.3 Segregated solution algorithm	
2.5 Boundary conditions	
2.5.1 Velocity inlet boundary conditions	
2.5.2 Pressure outlet boundary conditions	
2.5.3 Thermal boundary conditions	
2.5.4 Wall boundary conditions	
2 5 5 Fluid boundary conditions	
2.5.6 Solid boundary conditions	,
2.5.7 Axis boundary conditions	,
2.6 Physical properties model	
CHAPTER 3 VALIDATION	,
3.1 Chemical reaction model	
CHAPTER 4 CFD SIMULATION OF FLUID FLOW DISTRIBUTION AND INSIDE THE TUBE OF THE HEAT EXCHANGER AND DECOMPSER	
4.1 Baseline design investigations	

v

4.1.1 Parametric studies	. 34
4.2 Two dimensional shell and tube model	. 37
4.2.1 Investigation on counter flow arrangements	. 37
4.2.2 Investigations on parallel arrangements	. 38
4.3 Material properties	. 39
4.4 Numerical results	. 40
CHAPTER 5 3D FLOW DISTRIBUTION ON THE TUBE SIDE OF HI	GH
TEMPERATURE SHELL AND TUBE HEAT EXCHANGER AND CHEMIC	AL
DECOMPOSER	. 44
5.1 Investigations on 3D tube configuration	. 44
5.2 Boundary conditions	. 48
5.3 Computational mesh	. 48
5.4 Numerical results	. 49
CHAPTER 6 3D NUMERICAL CALCULATIONS OF SHELL AND TUBE HE	AT
EXCHANGER AND CHEMICAL DECOMPOSER	. 54
6.1 Investigations on 3D shell and tube model	. 54
6.2 Boundary conditions	. 55
6.3 Numerical results	. 59
6.4 Parametric study	. 60
6.5 Numerical analysis of shell and tube heat exchanger with baffles	. 63
6.6 Numerical results	. 65
6.7 Numerical analysis of shell and tube heat exchanger with 9 baffles	. 69
6.8 Numerical results	. 69
6.9 Parametric study	. 73
CHAPTER 7 RESULTS AND DISCUSSIONS	. 79
7.1 Results and discussions for two and three-dimensional models	. 79
CHAPTER 8 CONCLUSIONS AND FUTURE WORK	. 84
8.1 Conclusions based on 2d results	. 84
8.1.2 Conclusions based on 3d results	. 85
8.2 Future work recommendations	. 87
ADDENDRY LOUENICAL DEACTION MODELL DIG DUDEDDUE DED ZONE	00
APPENDIX I CHEMICAL REACTION MODELLING IN PEBBLE BED ZONE	. 89
ADDENIDIV IL EFFECTIVENESS CALCULATION	02
AFFENDIA II EFFEU II VEINESS CALCULATION	.92
REFERENCES	06
	. 70
VITA	103
T 1 1 1 x	105

LIST OF FIGURES

Figure 1.1	S-I thermochemical cycle	4
Figure 1.2	Effect of temperature on H ₂ SO ₄ decomposition yield	7
Figure 1.3	Effect of catalyst on H ₂ SO ₄ decomposition yield	8
Figure 1.4	Percentage decomposition of SO ₃ at 20 atm. Vs. feed decomposition	8
Figure 2.1	Shell and tube heat exchanger and decomposer	. 16
Figure 2.2	Two dimensional tube geometry	. 17
Figure 2.3	Two dimensional shell and tube geometry	. 18
Figure 2.4	Iterative solution method for the segregate solver	. 24
Figure 3.1	Experimental setup	. 29
Figure 3.2	Sulfur trioxide decomposition for 1 wt % Pt/ TiO ₂ catalyst	. 30
Figure 4.1	Computational mesh	. 32
Figure 4.2	Grid independent study	. 33
Figure 4.3	Pressure distribution	. 33
Figure 4.4	Temperature distribution	. 34
Figure 4.5	Percentage decomposition of SO ₃ vs. Reynolds number	. 35
Figure 4.6	Percentage decomposition of SO ₃ vs. surface to volume ratio	. 35
Figure 4.7	Percentage decomposition of SO ₃ vs. diameter of the tube	. 36
Figure 4.8	Percentage decomposition of SO ₃ vs. length of the porous zone	. 36
Figure 4.9	Tube model of shell and tube heat exchanger (counter flow)	. 37
Figure 4.10	Tube model of shell and tube heat exchanger (parallel flow)	. 38
Figure 4.11	Computational mesh	. 39
Figure 4.12	Pressure distribution (counter flow)	. 40
Figure 4.13	Temperature distribution (counter flow)	. 40
Figure 4.14	Pressure distribution (parallel flow)	. 41
Figure 4.15	Temperature distribution (parallel flow)	. 41 [.]
Figure 4.16	Percentage decomposition of SO ₃ vs. mass flow rate of helium	. 42
Figure 4.17	Percentage decomposition of SO ₃ vs. diameter of the shell	. 42
Figure 4.18	Percentage decomposition of SO ₃ vs. activation energy	. 43
Figure 5.1	Tube configuration (baseline case)	. 45
Figure 5.2	Baffle plate	. 46
Figure 5.3	Dimensions of baffle plate	. 46
Figure 5.4	Location of baffle plate	. 46
Figure 5.5	Tube configuration with pebbles	. 47
Figure 5.6	Computational mesh	. 48

Figure 5.7	Grid independent study	. 49
Figure 5.8	Y velocity distributions	. 50
Figure 5.9	Pressure distributions for base case	. 50
Figure 5.10	Slice plane for the tube configuration	. 51
Figure 5.11	Y velocity distributions with baffle plate	. 51
Figure 5.12	Pressure distribution with baffle plate	. 52
Figure 5.13	Y velocity distributions	. 53
Figure 5.14	Pressure distributions with porous medium	. 53
Figure 6.1	Three dimensional shell and tube heat exchanger	. 54
Figure 6.2	Modified heat exchanger	. 56
Figure 6.3	Computational mesh	. 57
Figure 6.4	Grid independent study	. 58
Figure 6.5	Temperature distribution	. 59
Figure 6.6	Pressure distribution	. 60
Figure 6.7	Mass flow rate of He vs. decomposition percentage	. 62
Figure 6.8	Temperature distributions along the tubes for low mass flow rate of He	. 62
Figure 6.9	Temperature distributions along the tubes for high mass flow rate of He.	. 62
Figure 6.10	Mass flow rate of SO ₃ vs. decomposition percentage	. 63
Figure 6.11	Shell and tube heat exchanger with baffles	. 64
Figure 6.12	Computational grid	. 65
Figure 6.13	Stream lines inside heat exchanger with five baffles	. 66
Figure 6.14	Temperature distribution of the heat exchanger with five baffles	. 67
Figure 6.15	Temperature distribution along slices with five baffles	. 67
Figure 6.16	Average mass fraction of SO ₃	. 68
Figure 6.17	Average mass fraction of SO ₂	. 68
Figure 6.18	Stream lines inside heat exchanger with nine baffles	. 70
Figure 6.19	Temperature distribution of the heat exchanger with nine baffles	. 71
Figure 6.20	Temperature distribution along slices with nine baffles	. 71
Figure 6.21	Average mass fraction of SO ₃	. 72
Figure 6.22	Average mass fraction of SO ₂	. 73
Figure 6.23	Operating pressure vs. decomposition percentage	. 73
Figure 6.24	Temperature distribution along slices with five baffles	. 75
Figure 6.25	Temperature distribution along slices with nine baffles	. 75
Figure 6.26	Average mass fraction of SO ₃ along slices with five baffles	. 76
Figure 6.27	Average mass fraction of SO ₃ along slices with nine baffles	. 76
Figure 6.28	Average mass fraction of SO ₂ along slices with five baffles	. 77
Figure 6.29	Average mass fraction of SO ₂ along slices with nine baffles	. 77

NOMENCLATURE

A	pre-exponential factor, s ⁻¹			
C_p	specific heat at constant pressure, J·kg ⁻¹ ·K ⁻¹			
C_2	inertial resistance factor			
$D_{i,m}$	diffusion coefficient for species <i>i</i> in the mixture, $m^2 \cdot s^{-1}$			
d_h	hydraulic diameter, m			
E_a	activation energy, kJ/mol			
K	reaction rate, s^{-1}			
k	kinetic energy of turbulence, $m^2 \cdot s^{-2}$			
k_B	Boltzmann constant $(1.38 \cdot 10^{-23} \text{ J} \cdot \text{K}^{-1})$			
L	length of tube, mm			
m	mass, kg			
ṁ	mass flow rate, $kg \cdot s^{-1}$			
р	static pressure, Pa			
Re	Reynolds number			
R _{rxni}	net rate of production of species <i>i</i> by chemical reaction, $kg \cdot m^{-3} \cdot s^{-1}$			
S_i	rate of reaction of species <i>i</i> by addition from dispersed phase, kg·m ⁻³ ·s ⁻¹			
t	time, s			
Т	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), $m \cdot s^{-1}$	

 u_j mean velocity component (j=1,2,3), m·s⁻¹

 u_k mean velocity component (k=1,2,3), m·s⁻¹

 u'_i fluctuating velocity components (i = 1; 2; 3), m·s⁻¹

 u'_i 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

Lennard-Jones energy parameter, J/molecule

 ε_p porosity

Е

 ε_l thermal effectiveness

 λ thermal conductivity, W·m⁻¹·K⁻¹

 μ dynamic viscosity, kg·m⁻¹·s⁻¹

 μ_t turbulent viscosity, kg·m⁻¹·s⁻¹

 ν kinematic viscosity, m²·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

 Ω_D diffusion collision integral

ACKNOWLEDGMENTS

I am extremely happy to take this opportunity to acknowledge my debts and gratitude to those who were associated with the preparation of this thesis. Words fail to express my profound regards from the inmost recess of my heart to my advisor Dr. Yitung Chen for the invaluable help, constant guidance and wide counseling extended to me right from the selection of the research topic to the successful completion of this thesis.

I am extending my sincere thanks to Dr.Robert F.Boehm, Dr.Anthony E. Hechanova, and Dr. Rama Venkat, for their direct and indirect contribution throughout this investigation. I want to thank Dr.Ponyavin, Dr. Nie and Dr. Hsuan-Tsung (Sean) Hsieh for their help, support, interest and valuable suggestions. Finally I would like to acknowledge the financial support of the United States Department of Energy (USDOE).

CHAPTER 1

INTRODUCTION

1.1. 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 convert low level thermal energy directly in to chemical energy by forming hydrogen and oxygen, and with overall first-law efficiencies exceeding 50%. These cycles were identified as most suitable ones which 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 few of those 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 thirty 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 as well as kinetic considerations indicate that both the extent and 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 largescale hydrogen production. It consists of the following three chemical reactions which yield the dissociation of water:

$I_2 + SO_2 + 2H_2O \rightarrow 2HI + H_2SO_4$	(120°C)	(1)
$2\text{HI} \rightarrow \text{H}_2 + \text{I}_2$	(450°C)	(2)

 $H_2SO_4 \rightarrow H_2O + SO_2 + 1/2O_2$ (850°C) (3)

The whole process takes in water and high-temperature heat and releases hydrogen and oxygen. All reagents are recycled and also there are no effluents. Reaction 3 is the most thoroughly investigated part of the S–I cycle, since it constitutes the heart of the cycle, and it is generally accepted that the efficiency of the whole process depends on the efficiency of H_2SO_4 decomposition. Sulfuric acid decomposition is carried out at 850°C in two steps. In the first step, sulfuric acid is assumed to decompose into water and sulfur trioxide. In the second step, sulfur trioxide decomposes to produce oxygen and sulfur dioxide according to the following reactions:

$$H_2SO_4 = H_2O + SO_3 \tag{4}$$

 $SO_3(g) = SO_2(g) + 0.5O_2(g)$ (5)

3

The produced sulfur dioxide is recycled. The hydrogen iodide can be decomposed at about 450°C, releasing hydrogen and recycling the iodine (eq. 2). The net reaction is the decomposition of water in to hydrogen and oxygen. In the S-I cycle most of the input heat goes in to the dissociation of sulfuric acid (eq. 4). The whole process takes in only water and high temperature heat and releases only hydrogen, oxygen and low temperature heat. Figure 1.1 represents the schematic diagram of how different chemicals are involved in different reactions in the S-I cycle [3].



Figure 1.1: Recycling of different chemicals involved in different reactions in S-I thermochemical cycle [3]

1.2. Research objective

The U.S.Department of Energy (DOE) gave the motivation for this work in support of the Next Generation Nuclear Plant (NGNP) program that deals with the production of hydrogen. Some of the research objectives that have been outlined are

4

- Development of a three-dimensional numerical model of high temperature shell and tube heat exchanger and decomposer with catalytic bed inside the tubes for decomposition of sulfur trioxide as a part of hydrogen production process based on the sulfur-iodine thermochemical water splitting cycle.
- Investigation of fluid flow uniformity in the tube configuration of the heat exchanger.
- Investigation of fluid flow, heat transfer, pressure drop and the decomposition percentage of sulfur trioxide on the three-dimensional numerical model of the heat exchanger and decomposer with segmental baffles.

1.3. Literature review

The sulfur-iodine (S-I) cycle is a baseline candidate among the variety of the thermochemical processes. The cycle consists of several chemical reactions that result in the dissociation of water. One of the most critical components of the process is the high temperature heat exchanger for sulfuric trioxide decomposition process. The process design of the heat exchanger was developed by General Atomics [3]. Huang et al. [4] made a detailed analysis of the sulfur-iodine thermochemical cycle for hydrogen production.

They used Aspen Technologies HYSYS chemical process simulator (CSP) to develop flowsheets for sulfuric acid decomposition that include all mass and heat balances. Based on the HYSYS analyses, two new process flowsheets have been developed. These new sulfuric acid decomposition processes are simpler and more sable than previous processes and yield higher conversion efficiencies for sulfuric acid decomposition and sulfur dioxide and oxygen formation.

Many kinds of decomposers like micro-channel heat exchangers etc. have been proposed for sulfuric acid decomposition. A detailed study of high temperature heat exchangers has been done by Bengt et al. [5]. A ceramic high temperature heat exchanger has been proposed to use as a sulfuric acid decomposer for hydrogen production by Ponyavin et al. [6]. A two-dimensional numerical model has been developed by Muramalla et al. [7] that predicted the wall catalyzed homogenous decomposition of sulfur trioxide. Ishikawa et al. [8] studied the decomposition of sulfuric acid and production of HBr as a part of research and development of thermochemical hydrogen production from water. A detailed study by Ozturk et al. [9] presents a new design and thermodynamic and engineering analysis of the sulfuric acid decomposition reaction of sulfur-iodine thermochemical cycle for hydrogen production.

1.3.1. Numerical studies of the function of catalyst inside the heat exchanger and decomposer

Catalyst plays a very important role in the decomposition of sulfuric acid. Sulfuric acid is decomposed on a catalyst at high temperatures according to the reactions (4) and (5). Sulfuric acid dissociates nearly completely into water and sulfur trioxide at the vapor phase according to reactions (4) above 450° C, reaction (5) proceeds by use of a catalyst at higher temperatures. Thus, the so-called decomposition of sulfuric acid is reduced to the decomposition of SO₃. Two different sets of experiments were done for two different catalysts, platinum and iron oxide for the decomposer model according to the description in the General Atomics report [10]. GA conducted the experiments for the temperature range from 700°C to 900°C at different pressure conditions and for different mole flow

range from 700°C to 900°C at different pressure conditions and for different mole flow rates. They concluded that the performance of iron oxide is good at higher temperatures but it is very poor at lower temperatures where as there is not much variation in the platinum catalyst over the same temperature range. Percentage decomposition of sulfuric acid in the presence of platinum catalyst is around 35% even at temperatures closer to 700°C where as for the catalyst iron oxide there is no decomposition observed at that temperature.

The catalytic activity of metal oxides was studied by Tagawa et al. [11] in an attempt to find some suitable catalysts for the decomposition of sulfuric acid in thermochemical water splitting process. Barbarossa et al. [12] studied the catalytic thermal decomposition of sulfuric acid in sulfur-iodine cycle for hydrogen production. Figures 1.2 and 1.3 show the effect of temperature and catalyst on H_2SO_4 decomposition yield [12].



Figure 1.2: Effect of temperature on H_2SO_4 decomposition yield [12]

7



Figure 1.3: Effect of catalyst on H₂SO₄ decomposition yield [12]

Seo et al. [13] numerically investigated the characteristics of a catalytic heat exchanger which can integrate heat generation and heat exchange. Lin et al. [14] studied the design aspects of sulfur trioxide decomposition reactor encompassing the reaction kinetics, heat transfer and mechanical considerations, which adopt a shell and tube heat exchanger with catalyst placed on the shell side of the reaction.



Figure: 1.4: Percentage decomposition of SO₃ at

20 atm vs. feed decomposition [14]

The decomposition of SO_3 at 20 atm and various temperatures vs. feed composition is shown in Figure 1.4. The percentage decomposition of SO_3 was very low at lower temperatures below 1000K. However satisfactory conversions were obtained at temperatures greater than 1073K.

However, no investigations were done for sulfur trioxide decomposition using a shell and tube heat exchanger with catalytic bed which acts like a porous medium placed inside the tube.

The transport of gases in porous materials is a crucial component of many important processes in science and technology. Flow and diffusion through porous media represent a vast field of study with many scientific and engineering applications, including catalysis. A detailed understanding of the complexities of flow and diffusion in porous materials is essential for the design, development, and optimization of catalysis and adsorption. Evans et al. [15] gave a detailed analysis regarding the gaseous diffusion in porous media and the effect of pressure gradients. The effect of pressure gradients is to introduce in to the fundamental kinetic theory equations both a pressure diffusion term and an external force term, which is needed to keep the porous medium from being pushed along by the pressure gradient. Teruel et al. [16] developed an alternative model to address the turbulent flows in porous media. A new set of k- ε equations for rigid and isotropic porous media were developed in this study treating spatial and time fluctuations as a unique identity. Turbulent flow in porous medium was numerically investigated by Kuwahara et al. [17] exploiting the periodic boundary conditions. Only one structural unit

was taken as a calculation domain to simulate a porous medium of regular arrangement in an infinite space.

In the current research, the mixture of gases is made to pass through the tubes of the shell and tube heat exchanger which contains catalytic bed which behaves like a porous medium where, it is assumed to contain fixed uniform spherical packing of pellets.

1.3.2. Numerical and experimental studies of the shell and tube heat exchanger

Shell and tube heat exchangers are commonly used as oil coolers, power condensers, preheaters and steam generators in both fossil fuel and nuclear-based energy production applications. They are also widely used in process applications and in the air conditioning and refrigeration industry. Although they are not specially compact, their robustness and shape make them well suited for high pressure operations. Many important concepts about heat exchanger performance were discussed by Clayton [18]. Stehlik et al. [19] showed desirable features of heat exchangers and then concentrated on shell and tube heat exchangers both as individual units and as the items of heat exchanger networks. Kim et al. [20] analyzed the influences on the shell side heat transfer in shell and tube heat exchangers using 32 different test heat exchangers. Results show that the heat transfer coefficient in the nozzle region is 40% greater than in the parallel region if the length of the apparatuses is 30 times the hydraulic diameter. A new correlation suitable for predicting the heat transfer coefficient was presented, which consists of a superposition of Nusselt number for the flow in the nozzle region and that for the longitudinal flow.

Crudely designed heat exchangers often have lower performance and higher operating costs than more accurate designs. For many years, various types of baffles have been

10

used in shell-and-tube heat exchangers to improve heat transfer while maintaining a reasonable pressure drop across the exchanger. The most commonly used baffle, the segmental baffle, causes the shell side fluid to flow across the tube bundle. This improves heat transfer by enhancing turbulence or local mixing on the shell side of the exchanger, but at the cost of a high pressure drop. This is caused by flow separation at the edge of the baffles with subsequent flow contraction and expansion. Due to its broad application, many research results have been reported in this field [21-32]. Compared to segmental baffles, disc and doughnut baffles have not achieved similar popularity mainly because of manufacturing difficulties. They have higher effectiveness to heat transfer pressure drop then segmental baffles [21][33][34][35], which is due to the radial flow between centre and the periphery, which eliminates bundle bypass and uses much lower cross flow velocity than segmental baffles [33]. Local heat transfer and pressure drop on the shell side of shell and tube heat exchangers with segmental baffles were investigated by Li et al. [36] for different baffle spacing and showed that the pressure drop and the average heat transfer are increased by an increased baffle spacing due to a reduced leakage through the baffle-shell clearance.

1.3.3. Numerical and experimental studies of flow distribution inside the heat exchanger and decomposer manifolds

One of the most important factors influence on the performance is uniformity of the flow rate distribution inside the heat exchanger. The uniformity of flow distribution depends on inlet manifold geometry, internal channels configuration and flow regimes.

The problem of flow maldistribution in heat exchangers has been recognized for a long time. A number of experimental investigations of the problem are possible to find in

11

literature [37-41]. Flow characteristics of flow field in the entrance of plate-fin heat exchanger have been investigated by means of particle image velocimetry (PIV) [37]. The experimental results indicate that performance of fluid maldistribution in conventional entrance configuration is very serious, while the improved entrance configuration can effectively improve the performance of fluid flow distribution in the entrance. The flow inside a heat exchanger, which is a component developed for cooling a high-current protons linear accelerator has been investigated experimentally by Faure et al. [38]. The study focused on velocity distribution between the heat exchanger tubes. It is found that for the range of investigated inlet Reynolds numbers, velocity distribution among the tubes does not depend on the flow rate. Shell side cross-flow velocity measurements have been made within the horizontal pass partition lane of an E-type cylindrical shell and tube heat exchanger using a particle tracking technique [39]. It was found that the cross-flow velocity variation in a baffle space within a shell and tube heat exchanger increases with increasing distance between the upstream and downstream baffles. Jiao et al. [40] obtained a correlation of the dimensionless flow maldistribution parameter and the Reynolds number under different distributor configuration parameters. The experimental studies prove that the performance of flow distribution in heat exchangers can be effectively improved by the optimum design of the distributor's configuration parameter. The flow maldistribution due to port to channel flow has a severe effect on the heat exchanger thermal performance which has been investigated experimentally by Rao et al. [41]. The authors have conducted an experimental study on the port to channel flow maldistribution in a small package of a 37 channel plate heat exchanger by creating the flow maldistribution while inserting a reduced cross-sectional area of a wooden mandrel in both inlet and outlet ports of the heat exchanger.

Computation studies of fluid flow distributions in inlet manifolds of heat exchangers have been performed in [42-45]. Zhang et al. [42] proposed a structure of two-stagedistribution and the numerical investigation shows the flow distribution in plate-fin heat exchanger is more uniform if the ratios of outlet and inlet equivalent diameters for both headers are equal. In this paper, a simple way is put forward to homogenize the flow distribution. A baffle with small size holes is installed in the traditional header to optimize the header configuration. Dynamic behavior of plate heat exchangers with flow maldistribution from the port to channel was reported by Srihari et al. [43]. Fluid axial dispersion characterizes back mixing and other notable deviations from plug flow through the heat exchanger. Variations of the heat transfer coefficient, due to nonuniform distribution of fluid velocity throughout the channels, were also reported. Solutions were obtained with Laplace transforms and numerical inversion from the frequency domain. Predicted results show that the dynamic response and thermal performance deteriorates with flow maldistribution. Lalot et al. [44] studied the gross flow maldistribution in an electrical heater and found that the perforated grid can improve the fluid flow distribution. Wen et al. [45] employed CFD technique to simulate and analyze the performance of fluid flow distribution and pressure drop in the header of plate-fin heat exchanger. A baffle with small-size holes is recommended to install in the header in order to improve the performance of flow distribution. Research work has been done to analyze the performance of flow distribution in a single tube of the high temperature shell and tube heat exchanger considering porous media inside the tube by Kuchi et al. [46].

1.4. Outline of thesis

This thesis research focuses on designing and simulating a three-dimensional shell and tube heat exchanger and chemical decomposer for decomposition of sulfur trioxide into sulfur dioxide, as a part of hydrogen production using computational fluid dynamics (CFD) analysis. Chapter 2 explains the description of the problem, geometry of the numerical model, calculation inputs, boundary conditions, associated governing equations and methodology of solution. Validation of the chemical reaction model is shown in Chapter 3. Chapter 4 discusses the two-dimensional numerical model, results, calculations, and parametric of fluid flow distributions and pressure drops inside the tube of the high temperature heat exchanger and decomposer. Chapter 5 deals with the work that examines the uniformity in the flow distribution in cross-section of the threedimensional tubes of high temperature shell and tube heat exchanger and decomposer. This chapter also includes the grid independent study that was performed, the numerical approach, and the numerical results. Chapter 6 describes the fluid and thermal analysis including chemical reaction modeling, which was performed on the three-dimensional shell and tube heat exchanger with baffles to investigate the percentage decomposition of sulfur trioxide. The grid independent study, numerical approach and numerical results were also discussed in Chapter 6. Conclusions based on both 2D and 3D modeling and some suggestions for future work are discussed in Chapter 7.

14

CHAPTER 2

DESCRIPTION OF THE PROBLEM, GOVERNING EQUATIONS AND BOUNDARY CONDITIONS

2.1. Description of the problem

The sulfur trioxide (SO_3) decomposition is a very important reaction which has an effect on hydrogen production. So SO₃ decomposer should be designed with care to attain highest possible decompositions for given operation conditions. There is no specific design that has been proposed for the sulfur trioxide decomposer. It can be a counter flow or a parallel flow or cross flow type heat exchanger. However a shell and tube heat exchanger design is adopted as the decomposer in this study.

Although today a set of common types of heat exchangers (double-pipe, spiral, plateand-frame, plate-fin, compact heat exchangers) are used in heat transfer applications, the shell-and-tube heat exchangers are still the most common type in use. They have larger heat transfer surface area-to-volume ratios than the most of common types of heat exchangers, and they are manufactured easily for a large variety of sizes and flow configurations. They offer great flexibility to meet almost any service requirement. The reliable design methods and shop facilitates are available for their successful design and construction. They can be designed for high pressures relative to the environment and high pressure differences between the fluid streams. They are the cost effective heat exchangers which can operate at high pressures, and their construction facilitates disassembly for periodic maintenance and cleaning. A shell and tube heat exchanger with straight tubes offers few advantages compared to other types. There is no leakage problem of one fluid stream in to the other. Cleaning of the tube is mechanically easy and also the individual tubes are replaceable. They are economically cheap and affordable and offer leakage proof design with small capital investment and affordability

The geometry of the shell and tube heat exchanger and decomposer considered is shown in Figure 2.1.



Figure 2.1: Shell and tube heat exchanger and decomposer (All dimensions are in mm)

The shell-and-tube heat exchanger consisting of 24 tubes enclosed within a cylindrical shell is taken for study purpose. Dimensions of the heat exchanger are shown in Figure 2.1. One fluid flows through the tubes and a second fluid flows within the space between the tubes and the shell. The design of a heat exchanger and decomposer requires a balanced approach among the thermal design, pressure drop and chemical reactions. SO₃ mixture enters the reactor tubes at around 973 K. The shell side fluid is helium which enters the heat exchanger at around 1223 K. The tube side fluid i.e., the reacting

mixture acts as a cold fluid where as shell side fluid acts as a hot fluid which provides the thermal energy required for SO₃ decomposition. According to GA flow sheet [3], the mass flow rate of the helium is 71 kg/hr, the mass flow rate of the mixture is 158.66 kg/hr, and the operation pressure for all of the flows is 1.5 MPa. Catalytic bed is designed inside the tubes which acts like a porous zone through which the mixture of sulfur trioxide and water vapor (acid vapor mixture) passes and gets decomposed into sulfur dioxide and oxygen.

Assuming uniform flow at the inlet and outlet of the heat exchanger, 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 for preliminary analysis using porous medium approach to investigate the fluid flow, heat transfer and chemical reactions in the decomposer.



Figure 2.2: Two-dimensional tube geometry



Figure 2.3: Two-dimensional shell and tube geometry

As shown in Figure 2.2, the tube model is 4.5 m in length and 0.04 m in diameter with an entrance length of 1.5 m. The shell dimensions are shown in Figure 2.3. The shell is 0.08 m in diameter. The length of the catalytic bed which acts as a porous zone is 1.5 m.

2.2. Equations of fluid flow, heat and species transfer

The preliminary analysis shows that the Reynolds number for the flow in the tube side as well as in the shell side of the heat exchanger and decomposer is less than 1000; therefore the laminar flow model was used for the calculations.

The governing equations for continuity, momentum and energy for the twodimensional laminar flow can be expressed as follows:

$$\frac{\partial}{\partial w_i} (\rho \, u_i) = 0 \tag{2.1}$$

$$\frac{\partial}{\partial w_{i}} \left(\rho u_{i} u_{k} \right) = \frac{\partial}{\partial w_{i}} \left(\mu \frac{\partial u_{k}}{\partial w_{i}} \right) - \frac{\partial p}{\partial w_{k}}$$
(2.2)

$$\frac{\partial}{\partial w_i} \left(\rho u_i T \right) = \frac{\partial}{\partial w_i} \left(\frac{\lambda}{Cp} \frac{\partial T}{\partial w_i} \right) + S_h$$
(2.3)

The governing equation for different species involved in the reaction modeling can be written as:

$$\frac{\partial}{\partial w_{j}} \left(\rho D_{i,m} \frac{\partial X_{i}}{\partial w_{j}} - \rho u_{j} X_{i} \right) + R_{rxni} + S_{i} = 0$$
(2.4)

However, when the three-dimensional heat exchanger with 24 tubes was considered, the Reynolds number at the shell entrance and also inside the tubes was higher than 2300 therefore a turbulence model should be applied for the flow calculations in the regions. The shear-stress transport (SST) k- ω model has been chosen to calculate the flows. The model is so named because the definition of the turbulent viscosity is modified to account for the transport of the principal turbulent shear stress (Menter et al. [47]). It is the feature that gives (SST) k- ω model an advantage in terms of performance over both the standard k- ε and k- ω models especially for the flows with recirculation regions. Momentum conservation for the turbulence model is:

$$\frac{\partial}{\partial w_{i}}(\rho u_{i}u_{k}) = \frac{\partial}{\partial w_{i}}\left(\mu\frac{\partial u_{k}}{\partial w_{i}} - \rho u_{i}'u_{j}'\right) - \frac{\partial p}{\partial w_{k}}$$
(2.5)

where

$$-\rho u_i' u_j' = \mu_i \left(\left(\frac{\partial u_i}{\partial w_j} + \frac{\partial u_j}{\partial w_i} \right) \right) - \frac{2}{3} \rho k \delta_{ij}$$
(2.6)

Transport equations for the SST k- ω model:

$$\frac{\partial}{\partial w_{i}}(\rho k u_{i}) = \frac{\partial}{\partial w_{j}} \left(\Gamma_{k} \frac{\partial k}{\partial w_{j}} \right) + \widetilde{G}_{k} - Y_{k}$$
(2.7)

$$\frac{\partial}{\partial w_i} (\rho \omega u_i) = \frac{\partial}{\partial w_j} \left(\Gamma_{\omega} \frac{\partial \omega}{\partial w_j} \right) + G_{\omega} - Y_{\omega} + D_{\omega}$$
(2.8)

In these equations, \tilde{G}_k represents the generation of turbulence kinetic energy due to mean velocity gradients. G_{ω} represents the generation of ω . Γ_k and Γ_{ω} represent the effective diffusivity of k and ω , respectively. Y_k and Y_{ω} represent the dissipation of k and ω due to turbulence. D_{ω} represents the cross-diffusion term

$$\Gamma_{k} = \mu + \frac{\mu_{i}}{\sigma_{k}}$$

$$\Gamma_{\omega} = \mu + \frac{\mu_{i}}{\sigma_{\omega}}$$
(2.9)
(2.10)

Where, σ_k and σ_{ω} are the turbulent Prandtl numbers for k and ω , respectively.

2.3. Chemical reactions and kinetics

The catalytic surface reaction model is implemented to determine the mole fractions of SO₃, SO₂, and O₂, as results of the sulfur trioxide decomposition: SO₃ \rightarrow SO₂+0.5O₂. The chemical reaction is highly temperature and pressure dependent.

Assuming that the reaction is the first order homogeneous reaction (Spewock et al. [48]), the rate equation for the reaction is written as:

$$R_{rxn} = -KC_{SO_3} \tag{2.11}$$

The reaction rate constant (K) is obtained by using the Arrhenius equation (Scott [49]):

$$K = A e^{\left(\frac{-E_a}{RT}\right)}$$
(2.12)

Platinum catalyst is used to enhance the decomposition. The activation energy (E_a) and pre-exponential factor (A) for the chemical reaction are obtained by using the experimental data of Ginosar [50]. For the 1 wt % Pt catalyst pre-exponential factor A = 0.16 1/s; E_a =32.67 kJ/mol. For the 0.1 wt % Pt catalyst pre-exponential factor A = 1.14 1/s; E_a =46.24 kJ/mol. Calculations for the catalytic data are shown in APPENDIX I. The obtained values for the activation energy agree with experimental data of Tagawa et al. [11] and Ishikawa et al. [8].

To investigate the fluid flow, heat transfer and chemical reactions in the catalytic bed region, porous medium approach has been used. Since the obtained Reynolds number for the two-dimensional model is 678, a laminar flow is employed and Darcy's law is applied for the porous media model. For two-dimensional as well as for three-dimensional models in this study, simple uniform spherical packing of pellet diameter (Dp) 5.0 mm was applied. The porosity has been found out and the value obtained was 0.476. The inertial and viscous resistance co-efficient are found out from [51] equations 2.17 and 2.18.

$$\alpha = (D_p^2 / 150)^* (\varepsilon^3 / (1 - \varepsilon)^2)$$
(2.13)

where α is the permeability of the material.

Viscous resistance = $1/\alpha = 1.6 \times 10^5 \text{ m}^{-2}$.

The inertial resistance is calculated by:

$$C_2 = (3.5/D_p)^*((1-\epsilon)/\epsilon^3)$$
 (2.14)

Calculated value, $C_2 = 3401 \text{m}^{-1}$

The surface area to volume ratio of the porous zone is also calculated, which is defined as the surface area of the pore wall per unit volume (A/V) and can be assumed as a measure of catalyst loading.

Calculated A/V value is 628.

2.4. Numerical method and algorithm

A mixture of chemical species undergoing chemical reactions while flowing through the heat exchanger tubes placed with catalytic bed, make the flow complex. In this case the actual physical device is replaced by a discrete number of points that represent the entire geometry of the cell where, not only the production and destruction of species are found but also the pressure, temperature, etc. are also found. These equations will be solved only at the discrete points representing the geometry of the cell where the distributions of pressure, temperature, etc are found. The approach requires defining the mathematical equations that govern the physical process. These equations will be solved only at the discrete points representing the geometry. FLUENT, a commercial computer program, based on finite-volume method is among the most powerful packages of existing commercial software for solving fluid flow, heat transfer and chemical reaction problems [52]. The purpose of this research study is to determine the percentage decomposition of SO₃ in a shell and tube heat exchanger and chemical decomposer and the effect of different parameters on sulfur trioxide decomposition is numerically studied using FLUENT.
2.4.1. The finite volume method

The finite volume methods (FVM), often called control volume methods, are formulated from the inner product of the governing partial differential equations with a unit function. This process results in the spatial integration of the governing equations. The integrated terms are approximated by either finite differences or finite elements, discretely summed over the entire domain. Physically, the conservation of mass, momentum and energy are assured in the formulation of FVM via the finite difference method (FDM) itself. The finite volume scheme approximation is done for the program used in this study.

2.4.2. Solution method

The segregated solver was used to solve the governing integral equations for the conservation of mass, momentum, energy and species equations. The solution is obtained by using a control-volume based technique which consists of:

- Division of the domain on to discrete volumes using a computational grid.
- Integration of governing equations on the individual control volumes to construct algebraic equations for the discrete dependent variables ("unknowns"), such as velocity, pressure, temperature, species mass fractions, reaction rates and conserved scalars.
- Linearization of discretized equations and solutions of the resultant linear equation system to yield updated values of the dependent variables.

2.4.3. Segregated solution algorithm

The numerical scheme used in this study is a first order upwind differencing scheme, and the solver used is a segregated solver (Figure 2.4). SIMPLE (semi-implicit method for pressure-linked equations) algorithm is used to resolve the coupling between pressure and velocity. The governing equations, which are discrete and nonlinear, are linearized using an implicit technique with respect to a set of dependent variables in every computational cell. The governing equations were linearized by the "implicit" method with respect to the set of dependent variables.

The resulting algebraic equations are solved iteratively using an additive correction multigrid method with a Gauss-Seidel relaxation procedure.



Figure 2.4: Iterative solution method for the segregate solver

The grid independence studies for 2-D and 3-D are performed for the each investigated geometry to check the dependence of the calculated parameters (pressure,

temperature, velocities, decomposition percentage) on mesh size. The grids systems are refined until the calculated parameters became independent from the grid size.

2.5. Boundary conditions

2.5.1. Velocity inlet boundary conditions

Velocity inlet boundary conditions are used to define the flow velocity, along with all other relevant scalar properties of the flow, at the flow inlets. This type of boundary condition at the inlet is intended to be used in incompressible flow. It requires the specification of velocity magnitude and direction, the velocity components, or the velocity magnitude normal to the boundary. In this case, the velocity normal to boundary specification method was used.

2.5.2. Pressure outlet boundary conditions

The pressure outlet boundary condition requires the specification of gauge pressure at the outlet. Flow quantities are extrapolated from the interior. A set of the "backflow" conditions are also specified, and specifying realistic values of backflow quantities reduced convergence difficulties. To set the static pressure the appropriate gauge pressure should be entered. Backflow temperature and turbulence parameters were set normal to the boundary with a realistic value. At the pressure outlets FLUENT uses the boundary condition pressure input as the static pressure of the fluid at the outer plane, and extrapolates all other conditions from interior of the domain.

2.5.3. Thermal boundary conditions

When choosing to solve an energy equation, it is required to define the thermal boundary condition at the walls. Since the wall zone in three dimensional modeling is a fluid/solid interface) a conjugate heat transfer problem is encountered. The code allows user to choose whether or not the two sides of the wall are "coupled". When the "coupled" option is chosen no other additional thermal boundary conditions are required, because the solver will calculate heat transfer directly from the solution in the adjacent cells.

2.5.4. Wall boundary conditions

Wall boundary conditions are used to bound fluid and solid regions. Since the flow is modeled as viscous flow, the no-slip boundary condition is enforced at wall. The catalytic surface reaction is enabled at the wall which allows fluid to react when it comes in contact with the wall.

2.5.5. Fluid boundary conditions

A fluid zone is a group of cells for which all active equations are solved. The only required input for a fluid zone is the type of fluid material. In the present case the fluid is a mixture of four different species. The type of fluid is specified in the material panel and the fluid properties of the all individual fluids as well as the mixture properties are first defined in the material properties panel of FLUENT.

2.5.6. Solid boundary conditions

A "solid" zone is a group of cells for which the heat conduction problem is solved; no equations are solved. The only required input for the solid zone is the material of solid which is input in to the material conditions panel of the FLUENT code.

2.5.7. Axis boundary conditions

The axis boundary condition is specified as axi-symmetric which allows the user not to have to specify any other boundary condition at the axis. FLUENT uses the adjacent cell values to determine the appropriate physical values for a particular variable at any point on the axis.

2.6. Physical properties model

An important step in the set up of the numerical model is the definition of the physical properties. For the fluid materials the values of density, thermal conductivity, viscosity, specific heat capacity for the individual species and also for the mixture are independent of temperature required for the calculation purposes. The physical properties may be dependent or independent of temperature depending upon the type of approach chosen.

When there is large temperature difference between the fluid and the surface the assumption of constant fluid transport properties may cause some errors, because the transport properties of most fluids vary with temperature. In the present case the properties of the mixture depend not only on the temperature at that location but also on the individual species concentration at that location.

The properties for all individual species (H_2O , SO_3 , SO_2 . and O_2) are dependent on temperature and are calculated by FLUENT material panel using the kinetic theory. Material properties such as thermal conductivity, viscosity and specific heat are dependent on both temperature and the individual species concentrations and so they are calculated using mass weighted mixing law. Density of the mixture is calculated using incompressible-ideal gas relationship.

27

CHAPTER 3

VALIDATION

3.1. Chemical reaction model

To validate the used chemical reaction model, the comparison of the calculations with experiments completed by Ginosar [50] has been performed. For the experiments, a hightemperature continuous flow catalyst test system, established in Idaho National Laboratory (INL), was used to examine the catalytic reaction in flowing, concentrated sulfuric acid at atmospheric pressure (Figure 3.1). Concentrated sulfuric is pumped into a heated zone where the acid vaporizes and decomposes to SO₃ and steam. Generated vapors flow over a bed of catalyst for the reduction of SO_3 to produce SO_2 and oxygen. The inlet section, where preheat, vaporization, and SO_3 generation takes place, has an inside diameter of 4 mm, an outside diameter of 6 mm, and had approximately 30 cm of tube in the heated furnace. The SO₃ decomposition section, with approximately 30 cm in the heated zone, had an inside diameter of 10 mm and an outside diameter of 12 mm. The initial 10 to 12 cm of the decomposition section was packed with den stones which aided temperature stabilization. The catalyst sample was packed inside the decomposition section starting at about 15 cm downstream of the inlet section and was held in place with plugs of quartz wool. Gas temperatures exiting the catalyst bed were measured using a type K thermocouple that was sheathed inside a quartz tube that was sealed from the reaction

environment. The tests were performed using a feed of concentrated sulfuric acid (95 to 96 wt %) at a flow rate of approximately 50 grams per hour.



Figure 3.1: Experimental setup (Ginosar [50])

Results of comparisons of the sulfuric trioxide decomposition obtained experimentally with calculated results are shown in Figure 3.2. The maximal difference between experimental and calculated results is 25%. From Figure 3.2 it can be observed that we are over estimating the decomposition percentage. The possible reason for the difference between the experimental and calculated results is that the uniform catalytic pebbles sizes distribution was used in the calculation whereas in the experiment the size of the pebbles was non-uniform. In this current research, 1 wt % Pt/TiO₂ catalyst was used for enhancing the chemical reaction for two and three-dimensional models.



Figure 3.2: Sulfur trioxide decomposition for 1 wt % Pt/TiO₂ catalyst

CHAPTER 4

CFD SIMULATION OF FLUID FLOW DISTRIBUTION INSIDE THE TUBE OF THE HEAT EXCHANGER AND DECOMPOSER

4.1. Baseline design investigations

The purpose of the calculation is to check the percentage decomposition of SO₃ inside the tubes of the heat exchanger and decomposer. A single tube of the heat exchanger has been modeled (Figure 2.2) for calculation of percentage decomposition of SO₃. The used models includes fluid flow model with heat transfer and chemical reaction calculations. Because of symmetry, only half of the geometry has been modeled. Sulfur trioxide and water vapor mixture enters the tube at a temperature of 973K shown in Figure 2.2. The boundary conditions used are:

Tube side inlet temperature = 973 K

Tube wall temperature = 1173 K

Tube side mass flow rate = 0.0018 kg/s

Operating pressure = 1.5 atm

Center line= axisymmetric boundary condition.

Preliminary analysis shows that the Reynolds number of the flow in the tube of the heat exchanger and decomposer is less than 1000; therefore the laminar flow model was used for the calculations. The entered mixture passes through the catalytic bed where, the

decomposition of sulfur trioxide into sulfur dioxide and oxygen takes place. Gambit 2.2.30 is used for creating the computational mesh. Optimum computational mesh (Figure 4.1) was created for the tube model with 9,909 nodes and 8,800 elements.



Figure.4.1: Computational mesh

Mesh independent study was performed on the tube geometry. The main objectives of the mesh independence investigation are:

- Examination of the solution sensitivity and computational time from the mesh changes (refinement and coarsening)
- Selection of the optimal mesh for analyzing the problem using CFD techniques.

Investigation of decomposition of sulfur trioxide in the tube using numerical models requires an appropriate mesh density. To find out the type of mesh, which provides stable and accurate results, analysis was carried out with different mesh densities varying from course to fine and the results are compared with the base mesh. Nine different types of meshes with variation in mesh densities at the center as well as at the walls are considered for the investigation. Since in the present problem the decomposition of sulfur trioxide reaction is a wall surface reaction, all the nine different grids were created with

fine mesh close to walls as well as in the catalytic bed zone. Figure 4.2 shows the variation of pressure drop in the tube for different kinds of meshes. Since the difference in pressure drops for the base case and further cases with finer mesh is less than 5%, the mesh with 9,909 nodes was chose for study purpose



Figure 4.2: Grid independent study



Figure 4.3: Pressure distribution



Figure 4.4: Temperature distribution

Pressure distribution is shown in Figure 4.3. The pressure drop in the tube with catalytic bed was found to be 623 Pa. Because of the catalytic bed which is placed inside the tube, we can find an increase in the pressure drop. From Figure 4.4 it is shown that the temperature is almost constant along the tube top wall because of constant wall temperature boundary condition.

The decomposition percentage of sulfur trioxide in the tube model of the shell and tube heat exchanger is found to be 95%. The inlet velocity is very small which increases the residence time of the mixture. As the residence time increases the reaction takes place for a longer time which further increases the decomposition percentage of SO₃.

4.1.1. Parametric studies

Parametric studies were performed on the tube configuration for different Reynolds numbers, different surface to volume ratios. Figure 4.5 shows the parametric study that was performed on different Reynolds numbers where, we can observe that as we increase the Reynolds number the decomposition percentage of SO_3 decreases because of less residence time.



Figure 4.5: Percentage decomposition of SO₃ vs. Reynolds number



Figure 4.6: Percentage decomposition of SO₃ vs. surface to volume ratio

Figure 4.6 shows the parametric study that was performed on different surface to volume ratios where, we can observe that as we increase the surface to volume ratio the decomposition percentage of SO_3 increases because of an increase in the surface area for collision of molecules. Parametric studies were also performed for different lengths of the

catalytic bed zone and for different diameters of the tube. Figures 4.7 and 4.8 show the parametric study for different diameters of the tube and for different lengths of the porous zone where, we can observe that as the diameter increases, the velocity decreases, which increases the residence time thereby increasing the percentage decomposition of SO₃. And for increased lengths of the catalytic bed zones, the reaction takes place for longer time which enhances the decomposition percentage of SO₃.



Figure 4.7: Percentage decomposition of SO₃ vs. diameter of the tube



Figure 4.8: Percentage decomposition of SO₃ vs. length of the porous zone

4.2. Two-dimensional shell and tube model

Shell has been incorporated in to the existing tube geometry. A two-dimensional axisymmetric model of the shell and tube model has been investigated numerically for percentage decomposition of sulfur trioxide.

4.2.1. Investigations of counter flow arrangement

Both parallel and counter flow arrangements were numerically investigated to find out the percentage decomposition of SO₃. Because of symmetry, only half of the geometry has been modeled. Figure 4.9 shows the counter flow arrangement with simple uniform spherical packing with 1 wt% of platinum. The wall which divides the shell and the tube is 5 mm thick and the material considered for the wall is silicon carbide (SiC). Sulfur trioxide and water vapor mixture enters the tube at a temperature of 973 K. Helium at a very high temperature about 1223 K is made to pass through the shell from the opposite side, shown in Figure 4.9.



Figure 4.9: Tube model of shell and tube heat exchanger (counter flow)

The catalysts are located in the decomposer region and their packing is simple spherical packing. The entered mixture passes through the catalytic bed of platinum spheres, where, the decomposition of sulfur trioxide into sulfur dioxide and oxygen takes place. Gambit 2.2.30 is used for creating the computational mesh. The inlet temperature of the mixture and the inlet temperature of helium, inlet velocity of the mixture and helium, exit pressure were used as the boundary conditions.

Tube side inlet temperature = 973 K

Tube side mass flow rate = 0.0018 kg/s

Operating pressure = 1.5 atm

Shell side inlet temperature=1223 K

Shell side mass flow rate= 0.0197 kg/s

Shell wall: adiabatic

Center line= axisymmetric boundary condition

The inlet velocity is calculated using the mass flow rate, the inlet area and the density of sulfur trioxide mixture. Pressure outlet is selected for outflow boundary conditions.

4.2.2. Investigations on parallel flow arrangement

A 2D axisymmetric shell and tube model of the heat exchanger with parallel flow arrangement has also been considered to investigate the percentage decomposition of sulfur trioxide.



Figure 4.10: Tube model of shell and tube heat exchanger (Parallel flow)

Sulfur trioxide and water vapor mixture is made to pass through the tube and helium is made to pass through the shell from the same side as shown in Figure 4.10. Same operating and boundary conditions were applied to this model as for counter flow arrangement to investigate the percentage decomposition of sulfur trioxide. The entering mixture passes through the catalytic bed zone where the decomposition takes place, producing sulfur dioxide. The tube wall is 5.0 mm thick and is made of SiC.

4.3. Material properties

It was assumed that the gas properties (density and dynamic viscosity) for the flow areas do not depend on temperature significantly, therefore the properties were taken constants for the areas with pressure 1.5 atm for the average temperatures and concentrations. The mix gas properties for the reacting flow were calculated for the component mass concentrations: $\rho_{SO3} = 0.8164$; $\rho_{H2O} = 0.1836$. The calculated properties of gases for the areas are below:

Density of helium flow: 0.653 kg/m^3

Density of the reacting flow: 7.243 kg $/m^3$

Viscosity of helium flow: $1.99 \cdot 10^{-5} \text{ kg}/(\text{m}\cdot\text{s})$

Viscosity of the reacting flow: $1.5 \cdot 10^{-5} \text{ kg}/(\text{m}\cdot\text{s})$

Figure 4.11 shows the optimum computational mesh for the geometry with 19,266 nodes and 16,625 elements.



Figure 4.11: Computational mesh

4.4. Numerical results

Figure 4.12 shows the pressure distribution inside the tube for counter flow arrangement. The pressure drop in the tube is approximately 535 Pa. Figure 4.13 shows the temperature distribution inside the tube where the temperature difference for the hot fluid is 314.5 K and that of the cold fluid is 235 K.



Figure 4.12: Pressure distribution (counter flow)



Figure: 4.13: Temperature distribution (counter flow)

The decomposition percentage of sulfur trioxide is found to be 93 %. The pressure and temperature distributions for parallel flow arrangement are shown in Figures 4.14 and 4.15, respectively.



Figure: 4.14: Pressure distribution (parallel flow)



Figure 4.15: Temperature distribution (parallel flow)

The pressure drop for parallel flow arrangement is found to be 546 Pa which is less than that of the counter flow arrangement and the temperature difference for the hot side fluid is 220 K and that of the cold side fluid is 27.5 K. The decomposition percentage of sulfur trioxide was 92 % for parallel flow arrangement. Thus, counter flow arrangement works better than parallel flow arrangement.

A comparison was made to check the productivity of the two types of flow arrangements. The percentage decomposition of sulfur trioxide for both parallel and counter flow arrangements with different mass flow rates of helium passing through the shell and for different diameters of the shell has been found out. As shown in Figures 4.16 and Figure 4.17, the decomposition percentage of sulfur trioxide is more for counter flow arrangement due to more temperature difference compared to parallel flow, when the mass flow rate of helium and the diameter of the shell are increased.



Figure 4.16: Percentage decomposition of SO₃ vs. mass flow rate of helium



Figure 4.17: Percentage decomposition of SO3 vs. diameter of the shell

Because sulfur trioxide decomposition reaction is catalytic surface reaction, the choice of the catalyst is very important to get high decomposition percentage. In the used numerical model different types of the catalyst are modeled by selection of appropriate activation energy value for the Arrhenius equation. Besides, the concentration of the catalyst in the catalyst carrier influence to the activation energy significantly. For example, for the 1 wt % Pt the activation energy is $3.267 \cdot 10^7$ J/kg-mol; for the 0.1 wt % Pt the activation energy is $4.624 \cdot 10^7$ J/kg-mol. The parametric studies for different activation energies have been completed in the research. From Figure 4.18 it can be observed that, the sulfuric trioxide decomposition percentage increases with the decrease of the activation energy for the both parallel and counter flow cases



Figure 4.18: Percentage decomposition of SO₃ vs. activation energy

CHAPTER 5

3-D FLOW DISTRIBUTION ON THE TUBE SIDE OF HIGH TEMPERATURE SHELL AND TUBE HEAT EXCHANGER

AND CHEMICAL DECOMPOSER

5.1. Investigations on 3-D tube configuration

The uniformity of the flow distribution in the heat exchanger is very critical because the flow maldistribution among the tube or shell sides can result in decreasing of chemical decomposition and increasing of pumping power. In the current study the flow rate uniformity in the heat exchanger tubes has been investigated. Simulations of the straight tube configuration, tube configuration with baffle plate arrangement and with pebble bed region inside the tubes were performed to examine flow distribution on the tube side. The investigated 3-D tube configuration of the shell and tube heat exchanger is shown in Figure 5.1. Based on the literature search the dimensions for the computational domain chosen were 24 tubes of 1.5 m length and 16 mm in diameter. In the current work flow calculations were performed for the mixture of sulfur trioxide and water vapor (acid vapor mixture) passing through the tubes for the following three cases.

Case 1 (Baseline design): This case is a simple one without any catalyst placed inside the tubes. The dimensions of the tube configuration are shown in Figure 5.1.



Figure 5.1: Tube configuration (Baseline case)

In this case the acid vapor mixture passes through the tubes. Hydrodynamic analysis was performed on this simple tube configuration to analyze the fluid flow uniformity.

Case 2 (Improved inlet manifold configuration): The preliminary analysis of the baseline design showed that the flow distribution in the tubes is very non-uniform. Therefore, an improvement in the inlet manifold configuration is recommended. Based on this a baffle is designed and is installed in the inlet manifold section. A baffle plate of 5 mm thickness and 90 mm in diameter has been designed as per the model on which three different kinds of holes in diameter are punched and is installed in the traditional header to optimize the inlet manifold configuration. It has been found that the best position for the perforated grid is midway between the inlet tube and the core of the header [42]. A model of the baffle plate is shown in Figure 5.2.





Figure 5.2: Baffle plate

Figure 5.3: Dimensions of baffle plate (mm)

The holes are spotted symmetrically small, medium and big holes from the axial line to the boundary on the baffle plate as shown in Figure 5.3. Small holes are spotted in the baffle according to the velocity distribution and the punched ratio is gradually increasing in symmetry from the axial line to the boundary and its location in the header is shown in Figure 5.4.



Figure 5.4: Location of the baffle plate

To avoid flow maldistribution, this improved inlet manifold configuration with baffle plate is best suited to the applications where the catalyst is placed on the shell side in the decomposition of sulfur trioxide of the high temperature shell and tube heat exchanger. Case 3 (Tube configuration with pebble bed zone): Fluid flow calculations were performed for the tube configuration with porous media zone in the tubes to check the flow uniformity. A catalytic bed zone is created inside the tubes along the whole length and porous medium approach has been applied to this catalytic bed. Tube configuration with pebble bed is shown in Figure 5.5, where a pebble bed zone is created inside the tubes along the whole length and the catalytic zone one-third from the tubes inlet section so that, when the acid vapor mixture passes through the tube, a temperature rise is found along the tube, which further leads to an increase in the decomposition percentage of sulfur trioxide. The baffle plate has been removed in this arrangement. Spherical pellets of diameter 5.0 mm filled the space inside the tubes. A porous medium approach has been applied to this type of catalytic bed arrangement inside the tubes and flow uniformity was investigated.



Figure 5.5: Tube configuration with pebbles inside the tube

5.2. Boundary conditions

A mass flow inlet rate boundary condition was applied to the inlet of the computation domain and the pressure outlet boundary condition was used to the outlet. The non slip boundary conditions are used for all of the walls. The mass flow inlet for the baseline conditions is 0.044 kg/sec based on GA flowsheet [3].

Since the flow at the entrance region (Re=60,841) is turbulent, a turbulent model has been used to compute the flow distributions. The SST (Shear-Stress Transport) $k-\omega$ turbulence model was used with enhanced wall functions for the near wall treatment.

5.3. Computational mesh

A computational mesh has been generated using the pre-processor Hypermesh 7.0. The implemented mesh involved 783,373 cells and 505,368 nodes (Figure 5.6)



Figure 5.6: Computational mesh

Figure 5.7 shows the variation of pressure drop in the tube for three different kinds of meshes. Since the difference in pressure drops for the base case and further cases with finer mesh is less than 5%, the mesh with 505,368 nodes was chosen for study purpose.



Figure 5.7: Grid independent study

5.4. Numerical results

5.4.1. Baseline case (Case 1)

Y-velocity distributions of the fluid part excluding the tube wall at the midsection of the channel are shown in Figure 5.8, where the difference in the velocities in the tubes closer to the center is more than twice than the velocities in the tubes at the periphery. The flow maldistribution in the tubes along the y direction is very serious. The velocities of central passages straightly facing the inlet tube are higher becoming more and fainter along the y-direction. A reverse flow occurs in the inlet section and the flow branches off to the two sides



Figure 5.8: Y-velocity distributions at the mid section of the tube configuration (m/s)

The velocities in the two ends of the header are also lower for the fluid has been distributed before it reaches the end of the header. Figure 5.9 shows the pressure distribution along the slice taken in the tubes. The position of the slice is shown in Figure 5.10. Due to the obtained flow maldistribution, the improvement of the selected tube configuration has become more exigent.



Figure 5.9: Pressure distribution for baseline case (Pa)



Figure 5.10: Slice plane of the tube configuration

5.4.2. Tube configuration with baffle plate (Case 2)

Y-velocity and pressure distributions at the midsection of the channel are shown in Figures 5.11 and 5.12, respectively. Figure 5.12 shows the pressure drop in the tube configuration for Case 2 taken along the slice shown in Figure 5.10 which is less when compared to the baseline case. So baffle serves better in reducing the pressure drop.



Figure 5.11: Y velocity distributions at the mid section with baffle plate (m/s)



Figure 5.12: Pressure distribution with baffle plate (Pa)

Although a reverse flow occurs at the inlet section, there is a considerable improvement in the flow distribution. The difference in the velocities in the tubes closer to the center and that at the periphery is very small compared to the Case 1. The improved header installed with baffle can effectively enhance the flow uniformity. It is noticeable that the baffle configuration has the relationship with header configuration and fluid flow condition, which must be in consideration in the optimization of baffle configuration. It can be foreseen that the fluid flow can be distributed uniformly when the baffle is suitable in dimensions, the holes punched on it are distributed in an in-line arrangement and the punched ratio increases gradually from the axial line to the boundary. As discussed by Lin et al. [14] for a high temperature shell and tube heat exchanger, if the catalyst is placed on the shell side, this arrangement helps to reduce the flow maldistribution.

5.4.3. Tube configuration with porous medium (Case 3)

In this type of arrangement, the baffle plate has been removed. Instead of baffle plate, the whole tube has been filled with pebbles which act as a porous medium for the flow through it. From Figure 5.13, it is clear that the problem of flow maldistribution has been solved with a noticeable uniformity in the flow distribution. The difference in the velocities in the tubes closer to the center and in the tubes at the periphery is negligible. The pebble bed zone offers a very high resistance to the inlet flow, due to which the flow has been re-distributed in the header section resulting in a uniform flow in the tubes. An increase in the pressure drop can be seen from Figure 5.14 taken along the slice shown in Figure 5.10



Figure 5.13: Y velocity distributions at midsection of the tube configuration (m/s)



Figure 5.14: Pressure distribution with porous medium (Pa)

CHAPTER 6

THREE-DIMENSIONAL NUMERICAL CALCULATIONS OF SHELL AND TUBE HEAT EXCHANGER AND CHEMICAL DECOMPOSER

6.1. Investigations on 3-D shell and tube model

A sulfur trioxide decomposer needs a design that enhances chemical decomposition. A counter flow type heat exchanger with hot fluid flowing through the shell and cold fluid flowing through the tubes is considered using the three-dimensional numerical analysis. A three-dimensional numerical model of the conceptual design of sulfur trioxide is shown in Figure 6.1.



Figure 6.1: Three-dimensional shell and tube heat exchanger (mm)

Twenty four tubes of 16 mm diameter were modeled for numerical analysis. The tube is 4 mm thick with a tube pitch of 31.75 mm. The shell diameter considered is 210 mm. A dividing plate of 4 mm thickness has been used in the inlet manifold section which prevents mixing of both the fluids. The material of heat exchanger at this point is considered as silicon carbide (SiC). The decomposer essentially is a counter flow type heat exchanger with hot fluid (helium) entering the decomposer from one end (shell) and allowing the cold fluid (reacting mixture) to enter the tubes at the other end. The required thermal energy for the reaction is obtained from high temperature helium. Due to the presence of the pebble bed region inside the tubes, the flow is assumed to be uniform based on previous investigations. Preliminarily, fluid flow analysis was performed on the shell and tube heat exchanger model.

6.2. Boundary conditions

Mass flow inlet rate boundary condition was applied to the inlet of the computation domain and the pressure outlet boundary condition was used to the outlet. The non-slip boundary conditions are used for all of the walls. The reacting mixture mass flow rate is 158.66 kg/hr and the helium mass flow rate is 71 kg/hr based on the GA flowsheet [3]. The operating pressure is 1.5 atm and the shell wall is assumed to be adiabatic.

Since the flow at the tube entrance region (Re=60,841) and also at the helium entrance region (Re=12,469), is turbulent, a turbulent model has been used to compute the flow distributions. The SST (Shear-Stress Transport) k– ω turbulence model was used with enhanced wall functions for the near wall treatment.

Preliminary analysis shows that reverse flow occurred in most of the sections, due to insufficient entrance length particularly at the tube entrance, tube exit and also at the shell inlet and at the shell outlet. So the length of the shell inlet as well as at the outlet was increased by three times. The diameter of the tube at the inlet as well as at the exit sections was also increased from 40 mm to 60 mm. Figure 6.2 shows the modified design of the heat exchanger.



Figure 6.2: Modified heat exchanger

Computational mesh was generated using Hypermesh 7.0. After grid independent study the mesh with 1,046,816 elements and 1,269,192 nodes was selected for study purpose. Figure 6.3 shows the computational mesh.



(a)



Figure 6.3: Computational mesh

Figure 6.4 shows the grid independent study that was performed on the heat exchanger. The variations in the pressure drop on the tube side as well as on the shell side were the parameters which were observed during the grid independent study. The variations were less than 6 %, therefore, the geometry is independent of mesh.



Figure 6.4: Grid independent study
Numerical analysis including thermal and fluid flow analysis was carried out on the modified model of the shell and tube heat exchanger for sulfur trioxide decomposition. Analysis also includes the chemical reaction modeling inside the tubes.

6.3. Numerical results

Numerical analysis shows that the decomposition percentage of sulfur trioxide in the tubes of the heat exchanger was 17 %. Figure 6.5 shows the temperature distribution of the heat exchanger. The outlet temperature of the shell fluid is 1050 K.



Figure 6.5: Temperature distribution of the heat exchanger with baffles (K)



Figure 6.6: Pressure distribution on the shell side (Pa)

Figure 6.6 shows the pressure distribution on the shell side of the heat exchanger. Heat exchanger effectiveness was calculated based on the temperatures of the hot and cold fluids. A detailed description of the calculations is given in APPENDIX II. The effectiveness of the heat exchanger was 0.67 and the throughput of sulfur dioxide was 0.0032 kg/s.

6.4. Parametric study

Parametric study was performed on the heat exchanger in order to find the effect of variation of parameters like mass flow rate of the reacting mixture and the mass flow rate of helium on percentage decomposition of sulfur trioxide. Figure 6.7 shows the effect of variation of mass flow rate of helium. It was found that as the mass flow rate of helium was increased, there was an increase in the decomposition percentage of sulfur trioxide. This is because as more amount of helium enters the shell, more heat is getting

transferred to the tubes as a result of which there is an increase in the decomposition percentage.



Figure 6.7: Mass flow rate of He vs. decomposition percentage

Figure 6.8 shows the cross-section of tube temperature distribution along the slice shown in Figure 5.10 and when the mass flow rate of helium is lowest (decreased by 0.5 times). Figure 6.9 shows the temperature distribution in the tubes for the same slice (Figure 5.10) when the helium mass flow rate is highest (increased by 4 times). From Figures 6.8 and 6.9 we can observe that the temperature in the tubes is more when the mass flow rate of helium is increased.



Figure 6.8: Temperature(K) distribution along the tubes cross section for low m_{He}



Figure 6.9: Temperature(K) distribution along the tubes cross section for high m_{He}

Figure 6.10 shows the effect of variation of mass flow rate of the reacting mixture entering the tubes. An increase in the percentage decomposition of sulfur trioxide was observed as the mass flow rate of the reacting mixture entering the tubes decreased. This is because, as the mass flow rate of the mixture is decreased, the residence time of the mixture during chemical reaction is increased. This further enhances the chemical reaction and decomposition percentage as well.



Figure 6.10: Mass flow rate of SO₃ mixture vs. decomposition percentage

6.5. Numerical analysis of shell and tube heat exchanger with baffles

In order to increase the decomposition percentage of sulfur trioxide in the heat exchanger along with enhancement of the heat transfer, baffles were added to the heat exchanger. Five conventional segmental baffles were added to the existing design of shell and tube heat exchanger. The baffles are 5 mm thick with a cut of 20%. Baffle to baffle spacing is 245 mm. The baffle arrangement on the tubes is shown in Figure 6.11.



(b)

Figure 6.11: Shell and tube heat exchanger with five baffles

Numerical analysis was performed on the heat exchanger with baffles for finding the percentage decomposition of sulfur trioxide. The computational grid was generated with 1,744,162 nodes and 1,466,494 elements. Figure 6.12 shows the computational mesh.



Figure 6.12: Computational grid

6.6. Numerical results

The decomposition percentage of sulfur trioxide in the tubes of the heat exchanger was found to be 20 % when five baffles were considered at 1.5 atm and with the mass flow rate of helium as 71 kg/hr and that of the mixture as 158.66 kg/hr. Figure 6.13 shows the streamlines inside the heat exchanger. We can observe few circulations in the helium inlet and outlet sections.



Figure 6.13: Streamlines inside the heat exchanger with five baffles (K)

Figure 6.14 shows the temperature distribution of the heat exchanger. No significant increase in the decomposition percentage was observed in the heat exchanger because, the heat from helium was not effectively used in decomposing sulfur trioxide. The reason for this is that, there are few tubes in the periphery of the tube configuration where the temperature was very less through out the length of the tubes which reduced the rate of chemical reaction.



(a)



Figure 6.14: Temperature distribution of the heat exchanger with five baffles (K)

Figure 6.15 shows the temperature distribution along the slices which were taken on the tube configuration.



Figure 6.15: Temperature distribution along slices with five baffles (K)

Figure 6.16 shows the distribution of SO_3 in the tubes, at one slice in the x direction taken along the slice shown in Figure 5.10. From the figure it is observed that as we move from the tube inlet towards the tube outlet, the mass fraction of SO_3 decreases due to the

chemical reaction that is taking place in the tubes. Figure 6.17 shows the distribution of SO_2 in the tubes taken along the slice shown in Figure 5.10. We can find that the average mass fraction of SO_2 increases as we move towards the tube outlet. Because of the chemical reaction that is taking place, SO_3 is getting decomposed into SO_2 .



Figure 6.16: Average mass fraction of SO₃ taken along central tubes



Figure 6.17: Average mass fraction of SO₂ taken along central tubes

The heat exchanger effectiveness was calculated based on the temperatures of the hot and cold fluids. A detailed description of the calculations is given in APPENDIX II. The

effectiveness of the heat exchanger was 0.70 and the throughput of sulfur dioxide was 0.007 kg/s.

6.7. Numerical analysis of shell and tube heat exchanger with 9 baffles.

The heat exchanger design was modified in terms of number of baffles. Baffles were increased from five to nine in order to observe the variation in decomposition percentage of SO₃. The baffles are 5 mm thick with a cut of 20%. Baffle to baffle spacing is 125 mm. Numerical analysis was performed on the heat exchanger with nine baffles for finding the percentage decomposition of sulfur trioxide.

6.8 Numerical results

Decomposition percentage of sulfur trioxide in the tubes of the heat exchanger was found to be 26 % when nine baffles were considered at 1.5 atm with helium mass flow rate of 71 kg/hr and that of the mixture of 158.66 kg/hr. Figure 6.18 shows the streamlines inside the heat exchanger, where we can observe small circulations in the shell inlet as well as in the outlet region.



Figure.6.18: Streamlines inside the heat exchanger (K)

Figure 6.19 shows the temperature distribution of the heat exchanger along the tube side as well as along the shell side.



(a)



Figure.6.19: Temperature distribution of the heat exchanger with nine baffles (K)

Figure 6.20 shows the temperature distribution along the slices when nine baffles were considered.



Figure.6.20: Temperature distribution of the heat exchanger with nine baffles (K)

The distribution of SO_3 in the tubes at one slice taken along the tubes (Figure 5.10) is shown in Figure 6.21. Due to the chemical reaction that is taking place in the tubes, the mass fraction of SO_3 is getting decreased. From Figure 6.22 it can be observed that because SO_3 is getting decomposed in to SO_2 and O_2 , we can find that the mass fraction of SO_2 increases as we move towards the tube outlet.



Figure 6.21: Average mass fraction of SO3 taken along central tubes

Heat exchanger effectiveness was increased to 0.78 compared to the heat exchanger with five baffles which was 0.70. As the number of baffles is increased, the reaction proceeds for a longer time as a result of which an increase in the decomposition percentage is observed. The throughput of SO_2 was also increased to 0.0075 kg/s.



Figure 6.22: Average mass fraction of SO₂ taken along central tubes

6.9. Parametric study

Parametric study was performed to observe the effects of different operating pressures on decomposition percentage considering five and nine baffles. Figure 6.23 shows the effect of variation of operating pressure for five as well as for nine baffles.



Figure 6.23: Operating pressure vs. decomposition percentage

From the performed parametric study it was observed that there is an increase in the decomposition percentage of SO_3 with an increase in the operation pressure for the five as well as for the nine baffle arrangement. As we increase the operating pressure, the density of the fluid increases which results in a decrease of velocity of the fluid for a constant mass flow rate. So as the velocity decreases, the residence time of the mixture increases which enhances the reacting time of the mixture. This results in an increase in the decomposition percentage.

The increase in the decomposition percentage was more in the heat exchanger with nine baffles compared to the heat exchanger with five baffles.

6.10. Comparison of temperature, SO_3 , and SO_2 distributions in the tubes of the heat exchanger with five and nine baffles

A comparison of temperature distributions inside the tubes was made in the heat exchanger with five and nine baffles. Slices in y-direction were taken at three different positions. Figure 6.24 shows temperature distribution at the three slices which were taken along the y-direction of the heat exchanger considering five baffles. Figure 6.25 shows the temperature distribution along the slices for the heat exchanger when nine baffles were considered. From Figures 6.24 and 6.25 we can observe that the temperature in the tubes is high for nine baffles compared to five baffles which resulted in enhancing the decomposition percentage of SO₃.

74



Figure 6.24: Temperature distribution along slices with five baffles (K)



Figure 6.25: Temperature distribution along slices with nine baffles (K)

Comparisons were also made for observing the difference in average mass fractions of SO₃ for both the cases (five and nine baffles). Figure 6.26 shows the average mass fraction of SO₃ along the slices that were taken along the tubes considering five baffles. Figure 6.27 shows the average mass fraction of SO₃ in the tubes considering nine baffles. Comparing Figures 6.26 and 6.27 it is clear that the average mass fraction of SO₃ is less in the tubes with nine baffles compared to five baffles which implies that decomposition in the tubes with nine baffles is more than the decomposition in the tubes with five baffles.



Figure 6.26: Average mass fraction of SO₃ along slices with five baffles



Figure 6.27: Average mass fraction of SO₃ along slices with nine baffles

Figure 6.28 shows the average mass fraction SO_2 along the slices which were taken on the tube configuration of heat exchanger and decomposer with five baffles. Slices at the same locations were also taken for the heat exchanger with nine baffles (Figure 6.29).



Figure 6.28: Average mass fraction of SO₂ along slices with five baffles





77

Because the decomposition percentage of SO_3 is more in the heat exchanger with nine baffles, it can be observed from Figures 6.28 and 6.29 that the average mass fraction of SO_2 in the tubes is more in the heat exchanger with nine baffles compared to the heat exchanger with five baffles.

CHAPTER 7

RESULTS AND DISCUSSIONS

7.1. Results and discussions for two and three-dimensional models

Fluid flow, heat transfer and chemical reaction calculations were done for the tube model as well as for the two-dimensional shell and tube configuration using porous media approach, with counter and parallel flow arrangements. The pressure drop for the counter flow arrangement is found to be 546 Pa and the temperature difference for the hot fluid is 314.5 K and that of the cold fluid is 235 K. Due to the transfer of heat form helium in the shell to acid vapor mixture in the tube, we can find an increase in temperature along the tube. The percentage decomposition of sulfur trioxide is found to be 93% for counter flow arrangement. The pressure drop for this type of arrangement is found to be 568 Pa which is less compared to the counter flow arrangement and the temperature difference for the hot fluid is observed as 220 K and that of the cold fluid is 27.5 K. Since much of the heat is utilized in the decomposer region; we can find a decrease in temperature along the tube. The decomposition percentage of sulfur trioxide is found to be 92% for parallel flow arrangement. The decomposition percentage of sulfur trioxide was very high (95 %) in the tube model and shell and tube model as well. The reason is that in a single fluid two-dimensional model the thermal energy required for

sulfur trioxide decomposition reaction is supplied by the constant wall surface temperature boundary condition which provides an unlimited heat source at the desired temperature. Various factors affected the decomposition percentage of sulfur trioxide in the tube. The percentage decomposition of SO₃ decreases with increasing the Reynold number due to increase in the velocity and decrease in the residence time of the fluid. A high surface to volume area ratio enhances the rate of chemical reaction by increasing the area of collisions of molecules in the catalytic bed region. The diameter of the tube also affected the decomposition percentage. Because more area is available for the reaction to take place, the decomposition percentage increased with an increase in the diameter of the tube. In addition to this, when the diameter is increased the velocity decreases, which increases the residence time. Increasing the residence time allows the reaction to happen for longer time thereby enhancing the decomposition percentage. A preliminary parametric study of the shell and tube configuration is conducted to explore effects of varying parameters on the decomposition of sulfur trioxide. The obtained results can be used for the optimization of the shell and tube high temperature heat exchanger and decomposer design and operating conditions to increase the decomposition performance and minimize pressure drops.

. Uniformity of the flow distribution in the heat exchanger is very critical because the flow maldistribution among the tube or shell sides can result in decreasing of chemical decomposition and increasing of pumping power. Crudely designed heat exchangers often have lower performance and higher operating costs than more accurate designs. One of the most important factors influence on the performance is uniformity of the flow rate distribution inside the heat exchanger. The uniformity of flow distribution depends

80

on inlet manifold geometry, internal channels configuration and flow regimes. . In the current study the flow rate uniformity in the heat exchanger tubes has been investigated. Simulations of the straight tube configuration, tube configuration with baffle plate arrangement and with pebble bed region inside the tubes were performed to examine flow distribution on the tube side. The preliminary analysis of the baseline design showed that the flow distribution in the tubes is very non uniform. The difference in the velocities in the tubes closer to the center is more than twice than the velocities in the tubes at periphery. Due to the obtained flow maldistribution, the improvement of the selected tube configuration has become more exigent. Since the fluid velocities near the axial line are high, while they are low far away from the center, a simple improvement in the configuration is investigated to homogenize the flow distribution. A baffle plate is designed and installed. Although a reverse flow occurs at the inlet section there is a considerable improvement in the flow distribution. The difference in the velocities in the tubes closer to the center and that at the periphery is very small compared to the case 1. The improved header installed with baffle can effectively enhance the flow uniformity. It is noticeable that the baffle configuration has the relationship with header configuration and fluid flow condition, which must be in consideration in the optimization of baffle configuration. It can be foreseen that fluid flow can be distributed uniformly when the baffle is suitable in dimensions, the holes punched on it are distributed in in-line arrangement and the punched ratio increases gradually from the axial line to the boundary. For a high temperature shell and tube heat exchanger, if the catalyst is placed on the shell side, this arrangement helps to reduce the flow maldistribution. In the third case the problem of flow maldistribution has been solved with a noticeable uniformity in the flow distribution. The difference in the velocities in the tubes closer to the center and in the tubes at the periphery is negligible. The pebble bed zone offers a very high resistance to the inlet flow, due to which the flow has been re-distributed in the header section resulting in a uniform flow in the tubes.

A counter flow type heat exchanger with hot fluid flowing through the shell and cold fluid flowing through the tubes is simulated numerically to observe the variation in the decomposition percentage. For the base case the decomposition percentage of sulfur trioxide is 17 %. The pressure drop in the tube side of the heat exchanger was 0.30 Mpa. The reason for a decrease in the decomposition percentage is because the heat energy required for sulfur trioxide decomposition is supplied by the hot helium flowing through the decomposer. The thermal energy supplied by the helium is limited when compared with the constant temperature boundary condition. So the percentage decomposition values are less than the constant wall surface temperature as in two-dimensional case. Fro the performed parametric study it was found that as the mass flow rate of helium was increased, there was an increase in the decomposition percentage of sulfur trioxide. This is because as more amount of helium enters the shell, more heat is getting transferred to the tubes as a result of which there is an increase in the decomposition percentage.

The heat required for decomposing sulfur trioxide can also be enhanced by introducing baffles in to the heat exchanger. Numerical analysis performed on the heat, exchanger with baffles show that there is a slight increase in the decomposition percentage of SO₃. The decomposition percentage of sulfur trioxide in the tubes of the heat exchanger was found to be 20 % when five baffles were considered at 1.5 atm and with the mass flow rate of helium as 71 kg/hr and that of the mixture as 158.66 kg/hr. The

82

pressure drop on the tube side is found to be 0.33 Mpa. No significant increase in the decomposition percentage was observed in the heat exchanger because, the heat from helium was not effectively used in decomposing sulfur trioxide. The reason for this is that, there are few tubes in the periphery of the tube configuration where the temperature was very less through out the length of the tubes which reduced the rate of chemical reaction. The effectiveness of the heat exchanger was 0.70 and the throughput of sulfur dioxide was 0.007 kg/s. Decomposition percentage of sulfur trioxide in the tubes of the heat exchanger was found to be 26 % when nine baffles were considered at 1.5 atm with helium mass flow rate of 71 kg/hr and that of the mixture of 158.66 kg/hr. The pressure drop o the tube side is found to be 0.37 Mpa. Heat exchanger effectiveness was increased to 0.78 compared to the heat exchanger with five baffles which was 0.70. As the number of baffles is increased, the reaction proceeds for a longer time as a result of which an increase in the decomposition percentage is observed. The throughput of SO₂ was also increased to 0.0075 kg/s

CHAPTER 8

CONCLUSIONS AND FUTURE WORK RECOMMENDATIONS

8.1 Conclusions based on two-dimensional results

High temperature shell and tube heat exchanger with catalytic bed inside the tube has been used in the decomposition of sulfur trioxide as a part of hydrogen production process. Numerical methods predicted the decomposition percentage of sulfur trioxide for different operating conditions and for different designs of the heat exchanger. Some of the conclusions on both two-dimensional and three-dimensional investigations are summarized below.

8.1.1. Conclusions based on two-dimensional results

- The Reynolds number played a significant role in affecting the sulfur trioxide decomposition. The percentage decomposition of SO₃ decreases with increasing the Reynolds number due to increase in the velocity and decrease in the residence time of the fluid.
- The surface to volume area ratio was also one of the important parameter which influenced the decomposition percentage. A high surface to volume area ratio enhances the rate of chemical reaction by increasing the area of collisions of molecules in the catalytic bed region.

84

- The length of the pebble bed region also played an important role in increasing the decomposition percentage. The length of the pebble bed region provides more surface area which helps in achieving higher decompositions.
- The decomposition percentage of sulfur trioxide is more for a counter flow arrangement due to more temperature difference compared to parallel flow, when the mass flow rate of helium and the diameter of the shell are increased.
- From the parametric studies for different activation energies that have been completed in the research, it is observed that, the sulfuric trioxide decomposition percentage increases with the decrease of the activation energy for the both parallel and counter flow arrangements. The important consideration over here is to find a high efficient and low cost catalyst.

8.1.2. Conclusions based on three-dimensional results

The flow rate uniformity in the heat exchanger tubes has been investigated. Simulations of the straight tube configuration, tube configuration with baffle plate arrangement and with pebble bed region inside the tubes were performed to examine flow distribution on the tube side. The conclusions made are summarized below:

• The flow maldistribution in the tubes along the tube direction is very serious. The velocities of central passages straightly facing the inlet tube are higher becoming more and decreases along the y-direction. To avoid flow maldistribution, this improved inlet manifold configuration with baffle plate is best suited for the cases where the catalyst is placed on the shell side in the decomposition of sulfur trioxide of the high temperature shell and tube heat exchanger. The pressure drop

in the Case 2 (Design with baffle plate) is lower than the simple base line case (Simple tube configuration). So, it can be inferred that the baffle plate serves better in reducing the pressure drop along with improving the flow distribution. Although a reverse flow occurs at the inlet section, there is a considerable improvement in the flow distribution when baffle plate is considered.

- In the Case 3 type of arrangement, the problem of flow maldistribution has been solved with a noticeable uniformity in the flow distribution.
- From the performed numerical analysis on the three-dimensional shell and tube heat exchanger, it was observed that the percentage decomposition of sulfur trioxide in the presence of catalytic bed is 17 %. SO₃ decomposition can be increased by increasing the heat energy supplied to the mixture. Temperature of the helium coming from the intermediate heat exchanger (IHX) connected to nuclear reactor power plant is constant at 1143 K, which may not be increased due to the nuclear reactor safety and material issues. There are two different ways to increase the heat energy supplied to the mixture without varying the helium temperature. One way is by increasing the mass flow rate of helium side and other way is to increase the inlet temperature of the reacting mixture. The mass flow rate of the helium can be increased either by increasing the velocity of helium or by increasing the diameter of the tubes on the helium side keeping the diameter of the reacting mixture side constant. Also increasing the inlet temperature of the reacting mixture side results in higher percentage decomposition of SO₃.
- The heat required for decomposing sulfur trioxide can also be enhanced by introducing baffles in to the heat exchanger. Numerical analysis performed on the

heat exchanger with baffles show that there is a slight increase in the decomposition percentage of SO_3 .

8.2. Future work recommendations

Numerical modeling of the shell and tube heat exchanger with pebble bed region inside the tubes was modeled in both 2D and 3D. These models can further improve the decomposer performance. However there are some modifications in the numerical models which would help in predicting the SO₃ decomposition with better accuracy. Some of them are discussed below

- Sulfur trioxide decomposition reaction is modeled assuming that the mixture of sulfur trioxide and water vapor enters the decomposer tubes but in reality there is a possibility that some undecomposed sulfuric acid (H₂SO₄) may enter the decomposer. So the sulfuric acid decomposition reaction that results in sulfur trioxide and water vapor should also be included in the model along with the SO₃ decomposition reaction.
- Effects of different parameters on the decomposition of sulfur trioxide such as Reynolds number, diameter of the tube, length of the pebble bed zone, surface to volume ratio were investigated using two-dimensional model. Operating pressure and inlet temperature of the reacting mixture are two more parameters the have considerable effect on the decomposition of sulfur dioxide. So using the same two-dimensional models, investigation is to be carried out on both the parameters to find out how SO₃ decomposition can be affected.

87

- From the three-dimensional numerical modeling it is clear that the percentage decomposition of sulfur trioxide is less because of insufficient supply of heat energy to the reacting mixture. So analytical calculations need to be carried out to find out exactly how much thermal energy is required to decompose at least 50% of the sulfur trioxide. Modifications either on the helium side or on the mixture side are needed to the thermal energy requirements. The possible modifications can be
 - 1. Increasing the velocity on the helium side which allows higher mass flow rates of helium.
 - 2. Increasing the diameter of the tubes carrying the helium keeping the mass flow rate constant.
 - 3. Increasing the diameter of the tubes carrying the reacting mixture keeping the mass flow rate of the mixture constant.
 - 4. Increasing the inlet temperature of the reacting mixture entering the decomposer.
- The heat exchanger and decomposer was modeled with segmental baffles. Helical baffles can be modeled to enhance the heat transfer in the heat exchanger to find out how SO₃ decomposition can be affected.
- Different catalytic bed arrangements inside the tube can be modeled for finding out the affects on sulfur trioxide decomposition.
- Different arrangement of tubes inside the shell can be modeled. Inline arrangement of tubes was considered in this research. Staggered arrangement of tubes can be modeled to find out the variation in SO₃ decomposition.

APPENDIX I

CHEMICAL REACTION MODELING IN PEBBLE BED ZONE

A porous media approach has been used to calculate flow parameters in the pebble bed region. The calculation geometry and dimensions are shown in Figure I.1.The dimensions are the same as those in the Ginosar [50] experiments in the sulfur trioxide decomposition region. The computation mesh has refinement in the porous media zone (Figure I.2)



Figure I.1: Dimensions



Figure I.1: Boundaries and mesh (4,200 elements, 4,496 nodes)

Operational and boundary conditions:

Wall temperature = 1123.15 K;

Operating pressure 1 atm;

Re = 90.

Inlet conditions: $\dot{m} = 50$ g/hour; T=873.15 K, $x_{s0_3} = 0.8163$; $x_{s0_3} = 0$; $x_{H,0} = 0.1837$;

 $x_{o_2} = 0$.

Because of the flow Reynolds number equals 90 the fluid flow within the investigated geometry is assumed to be laminar. The flow in the region is modeled by the addition of momentum source term to the standard fluid flow equations. The governing equations for continuity, energy and species transport are the same as shown in Chapter 2.

The momentum equation is the following:

$$\frac{\partial}{\partial w_i} \left(\rho u_i u_k \right) = \frac{\partial}{\partial w_i} \left(\mu \frac{\partial u_k}{\partial w_i} \right) - \frac{\partial p}{\partial w_k} + S_i$$
(I.1)

The source term S_i has viscous loss term and inertial loss terms:

$$S_{i} = -\left(\frac{\mu}{\alpha} + C_{2} \frac{l}{2} \rho u_{mag} u_{i}\right)$$
(I.2)

where α is the permeability and C_2 is the internal resistance factor.

Darcy's law is applied for the porous media model. The inertial and viscous resistance coefficients are found out using expressions from Nield and Bejan [51].

$$C_2 = \frac{3.5}{D_p} \frac{1 - \varepsilon_p}{\varepsilon_p^3} \tag{I.3}$$

$$\alpha = \frac{D_{\rho}^2}{150} \frac{\varepsilon_{\rho}^3}{\left(1 - \varepsilon_{\rho}\right)^2} \tag{I.4}$$

Considering the assumption of the pellets uniform packing, the porosity of the chemical reaction region, ε_p , is obtained equal 0.476.

According to the equations:

 $C_2 = 3401 \text{ m}^{-1}$.

Viscous resistance = $l/\alpha = 1.5 \times 10^7 \text{ m}^{-2}$.

The surface area is 0.03 m^2 .

The surface-to-volume ratio of the porous zone is 4000 m^{-1} .

The surface-to-volume ratio is applied to the porous zone region where the chemical reaction $(SO_3 \rightarrow SO_2 + 0.5O_2)$ is tacking place.

APPENDIX II

EFFECTIVENESS CALCULATION

One way of measuring a heat exchanger's performance is to calculate its effectiveness. The heat exchanger effectiveness is defined as the ratio of the actual heat transfer to the heat transfer attainable in an infinitely long counter flow exchanger.

In the parallel flow case shown in Figure II.1, the two fluids enter the exchanger with (typically known) inlet temperatures, T_{Hin} and T_{Cin} and in the ideal case leave the exchanger at the same (unknown) temperature T_M - which is somewhere in between T_{Hin} and T_{Cin} .



Figure II.1: Temperature distributions in a parallel flow heat exchanger.

An alternative is to operate the exchanger in counter flow. In this case, again, we will assume that we know the inlet temperatures, T_{Hin} and T_{Cin} . Also, there will eventually be no driving force (in an infinitely long exchanger). There are two ways in which this can happen: the hot stream can leave at the same temperature as the cold stream inlet, or the cold stream can leave at the same temperature as the hot stream inlet.

Inside the heat exchanger the hot and cold fluid temperature distributions would have the form sketched in Figure. II.2.



Figure.II.2: Temperature distributions in a counter flow heat exchanger.

The effectiveness can be calculated as:

$$\epsilon = \frac{C_C(T_{C_{out}} - T_{C_{in}})}{C_{min}(T_{H_{in}} - T_{C_{in}})} = \frac{C_H(T_{H_{in}} - T_{H_{out}})}{C_{min}(T_{H_{in}} - T_{C_{in}})}$$

Where, C_C is the heat capacity of the cold fluid

C_H is the heat capacity of the hot fluid

C_{min} is the lower of two fluids heat capacities

II.1. Effectiveness and throughput calculations for the shell and tube heat exchanger

The inlet temperature of the hot fluid: 1223 K

The average outlet temperature of the hot fluid: 1054.7 K

Inlet temperature of the cold fluid: 973 K

Average outlet temperature of cold fluid: 1169.19 K

Substituting the values we get:

 $T_{h1} = 1223 \text{ K}, T_{h2} = 1054.7 \text{ K}, T_{c1} = 973 \text{ K}, T_{c2} = 1169.19 \text{ K},$

Calculated $\varepsilon = 0.67$

Throughput of SO₂ calculations:

Throughput is calculated as:

Mass flow rate of the reacting mixture \cdot average mass fraction of SO₂ at the tube outlet Calculated value= 0.0032 kg/s.

II.2. Effectiveness and throughput calculations for the shell and tube heat exchanger with five baffles

The inlet temperature of the hot fluid: 1223 K

The average outlet temperature of the hot fluid: 1035.6 K

Inlet temperature of the cold fluid: 973 K
Average outlet temperature of cold fluid: 1153.5 K

Substituting the values we get:

 $T_{h1} = 1223 \text{ K}, T_{h2} = 1036.6 \text{ K}, T_{c1} = 973 \text{ K}, T_{c2} = 1153.5 \text{ K},$

Calculated $\varepsilon = 0.70$

Throughput of SO₂ calculations:

Throughput is calculated as:

Mass flow rate of the reacting mixture \cdot average mass fraction of SO₂ at the tube outlet Calculated value= 0.0070 kg/s.

II.3. Effectiveness calculation for the shell and tube heat exchanger with nine baffles

The inlet temperature of the hot fluid: 1223 K

The average outlet temperature of the hot fluid: 1033 K

Inlet temperature of the cold fluid: 973 K

Average outlet temperature of cold fluid: 1145 K

Substituting the values we get:

 $T_{h1} = 1223 \text{ K}, T_{h2} = 1033 \text{ K}, T_{c1} = 973 \text{ K}, T_{c2} = 1145 \text{ K},$

Calculated $\varepsilon = 0.78$

Throughput of SO₂ calculations:

Throughput is calculated as:

Mass flow rate of the reacting mixture \cdot average mass fraction of SO₂ at the tube outlet Calculated value= 0.0075 kg/s.

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96

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