

THE CHEMICAL REACTOR FOR THE DECOMPOSITION OF SULPHURIC ACID FOR THE HYBRID SULPHUR PROCESS

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TITLE: The Chemical Reactor for the Decomposition of Sulphuric Acid for the Hybrid Sulphur Process

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ABSTRACT

The utilisation of alternate sources of energy has reached critical levels due to the constantly growing demand for energy and the diminishing of fossil fuels. The production of hydrogen through the Hybrid Sulphur process is a possible alternative that may contribute towards alleviating the pressure on the world's energy resources. The two-step thermochemical cycle for decomposing water into hydrogen and oxygen offers the potential to obtain acceptable thermal efficiencies, while still using common and inexpensive chemicals. The process mainly makes use of two unit process operations: an electrolyser and a chemical decomposition reactor. This research project focuses on the concept design of the decomposition reactor operated adiabatically as a multi-stage reactor system with inter-stage heating, in order to simplify the reactor design. This approach allows for the independent evaluation of the reaction kinetics and the heat transfer mechanism.

Keywords: Hydrogen, Hybrid Sulphur, Decomposition Reactor, NGNP, High temperature, Nuclear energy

TITEL: Die Chemiese Reaktor vir die Ontbinding van Swael Suur vir die Hibried Swael Proses

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OPSOMMING

Die gebruik van alternatiewe bronne van energie het kritiese vlakke bereik as gevolg van die aanhoudende toename in die aanvraag na energie, en die feit dat fossiel brandstof se beskikbaarheid as bron aansienlik afgeneem het. Die produksie van waterstof deur middel van die Hibried Swael (HYS) proses is 'n moontlike alternatiewe oplossing wat kan bydra om die druk op die wêreld se energiebronne te verlig. Die twee-stap termochemiese siklus vir die ontbinding van water in waterstof en suurstof bied die moontlikheid om aanvaarbare termiese doeltreffendheid te bereik deur die gebruik van algemeen beskikbare, en bekostigbare chemikalieë. Die proses maak hoofsaaklik gebruik van twee proses eenhede, naamlik 'n elektroliseerder en 'n chemiese-ontbindingsreaktor. Die navorsingsprojek fokus op die konsep ontwerp van die chemiese reaktor wat adiabaties bedryf word as 'n multi-stadium reaktor sisteem met inter-stadium verhitting, met die doel om die ontwerpvergelyking te vereenvoudig. Dit stel die navorser in staat om die reaksie kinetika onafhanklik van hitteoordrag in die reaktor te ondersoek

Sleutelterm: Waterstof, Hibried Swael, Ontbindings Reaktor, VGKA, Hoë temperatuur, Kernkrag

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LIST OF ABBREVIATIONS

This list contains the abbreviations as used in this dissertation.

<i>Abbreviation</i>	<i>Term</i>
BTU	British Thermal Units
HTGR	High Temperature Gas-Cooled Reactor
HYS	Hybrid Sulphur Cycle
MWt	Mega Watt Thermal
NGNP	Next Generation Nuclear Plant
PBMR	Pebble Bed Modular Reactor
VHTR	Very High Temperature Reactor

LIST OF SYMBOLS

This list contains the variables as used in this dissertation.

Variable	Definition	Unit
A	Preexponential Factor	[-]
A_{cs}	Reactor cross sectional area	[cm ²]
C_A	SO ₃ concentration	[mol/dm ³]
C_C	SO ₂ concentration	[mol/dm ³]
C_D	O ₂ concentration	[mol/dm ³]
C_I	H ₂ O concentration	[mol/dm ³]
C_{p_i}	Temperature dependent heat capacity	[J/mol·K]
ΔC_p	Change in heat capacity per mole reacted	[J/mol·K]
C_{SO_3}	Initial SO ₃ concentration at reactor inlet	[mol/dm ³]
E_A	Activation energy	[J/mol]
F	Volumetric flow rate	[cc/hr]
F_{A0}	Molar flow rate	[mol/s]
g	Dimensional reactor length	[m]
ΔG°_0	Standard Gibbs Energy change of reaction	[-]
ΔH_{rx}	Heat of reaction at ref. temperature	[J/mol]
k	Reaction rate constant	[hr ⁻¹]
k_1	Specific reaction rate constant	[s ⁻¹]
K_C	Equilibrium constant	[-]
R	Gas constant	[J/mol]
r_A	Reaction rate	[mol/dm ³ ·s]
r_{rxn}	Rate of reaction	[cc/hr·SO ₃ reacted/vol]
S_v	Space velocity	[hr ⁻¹]
T	Temperature	[K]
T_R	Reference temperature	[K]
T_0	Inlet temperature	[K]
V	Volume	[m ³]
X	Conversion	[-]
x	Mole fraction SO ₃	[-]
θ_i	Theta	[-]

Chapter 1

Introduction

CHAPTER 1 INTRODUCTION

1.1 Introduction

According to the Energy Information Administration of the Department of Energy of the United States, the total marketed energy consumption of the world in 2004 was estimated at 447 quadrillion BTU [1]. This is expected to grow to about 559 quadrillion BTU in 2015, and then to 702 quadrillion BTU in 2030, which will amount to a projected increase of 57% over this period. The growth is displayed in Figure 1 below.

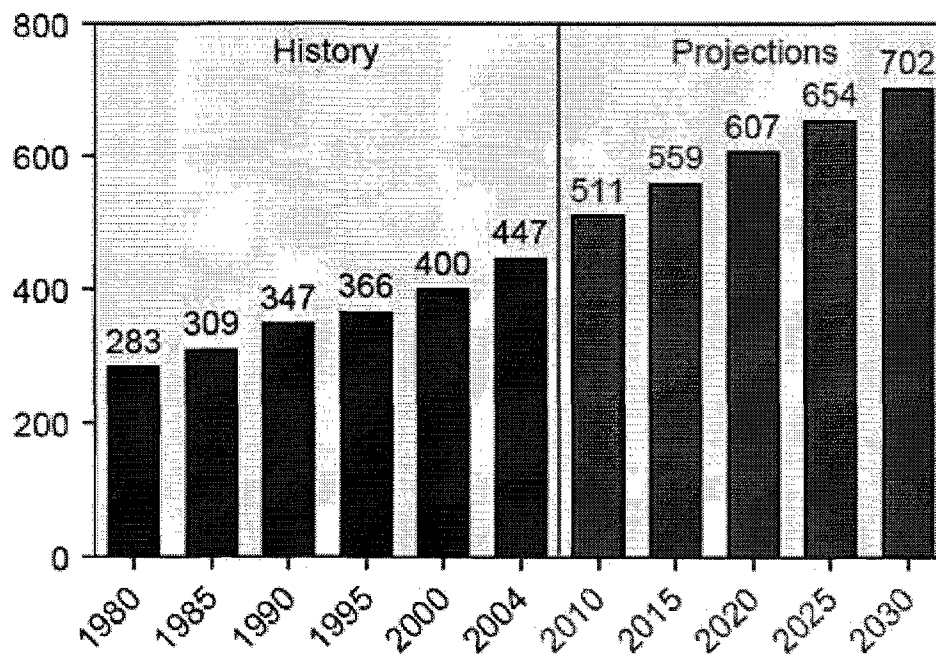


Figure 1: Projected world energy demand [2], [3]

To date the most significant part of this amount of energy, approximately 90%, was derived from the combustion of fossil fuels, of which coal (27%), oil (39.5%), and gas (23.5%) were the primary contributors. The remainder of the marketed energy consumption of the world was derived from nuclear power (7.4%) and renewable energies, such as hydroelectricity (2.6%) [4].

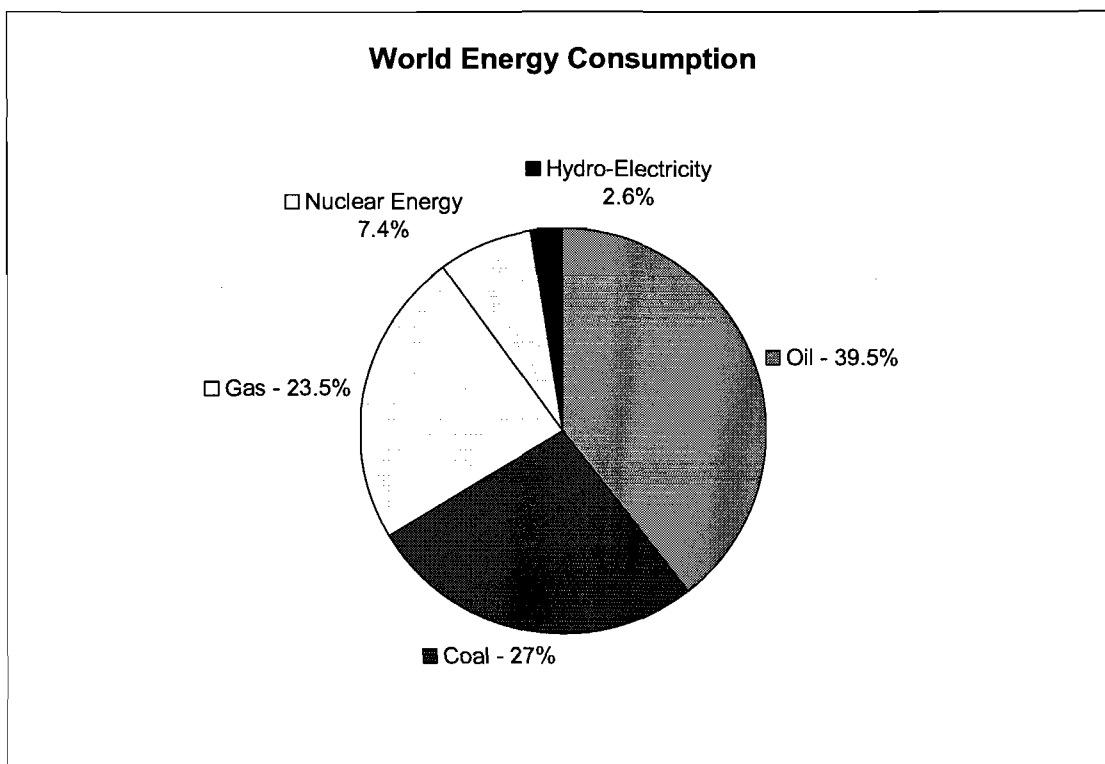


Figure 2: Total marketed world energy consumption

Approximately 30% of the primary energy that is consumed is used for the production of electricity. The only other significant non-fossil contributors to electricity production are nuclear energy and hydroelectric power supply. Comparing these two sources, hydroelectricity represents about 20% and nuclear energy about 17% of the global electricity supply [5].

Although the energy intensity of many commercial and industrial products and appliances has fallen, the rate of energy consumption has rapidly increased. This is not only because of population growth or the development of new consumer needs, but also because of a trend of developing countries that want to achieve higher economic growth and social levels by means of improving industry and infrastructure. Therefore, the growth of the energy trade is not reserved for industrialised countries only, but has become a worldwide trend [6].

Table 1: Worldwide energy consumption and carbon dioxide emissions

Region	Energy consumption (quadrillion BTU)				Carbon dioxide emissions (million metric tonnes)			
	1990	2001	2010	2025	1990	2001	2010	2025
Industrialised nations	182.8	211.5	236.3	281.4	10,462	11,634	12,938	15,643
Eastern Europe	76.3	53.3	59	75.6	4,902	3,148	3,397	4,313
Developing nations								
<i>Asia</i>	52.5	85	110.6	173.4	3,994	6,012	7,647	11,801
<i>Middle East</i>	13.1	20.8	25	34.1	846	1,299	1,566	2,110
<i>Africa</i>	9.3	12.4	14.6	21.5	656	843	971	1,413
<i>Central and South America</i>	14.4	20.9	25.4	36.9	703	964	1,194	1,845
Total developing	89.3	139.2	175.5	265.9	6,200	9,118	11,379	17,168
Total world	348.4	403.9	470.8	622.9	21,563	23,899	27,715	37,124

To respond to the high demand for energy, a balanced and stable program will be required without pursuing extreme policies. This will have the best prospect of achieving the lowest long-term social cost, and be able to address the future with a variety of options and flexible strategies [5]. It is for this reason that it is important to evaluate current energy sources, their future prospects, and the social and environmental impact they may have.

Considering the impact certain energy sources have, it is necessary to acknowledge that the usage of fossil fuels brings about several disadvantages. These include:

- its limited supply and the fact that it is not a renewable energy source;
- pollution during mining and the processing phase; and
- carbon dioxide emissions as by-product, which is believed to be responsible for global warming.

The negative impact of fossil fuels is undeniable, increasing the need to search for a less-polluting, potentially renewable primary energy source. A possible answer to the problem is the use of nuclear energy. Electricity is already generated on a large scale internationally by means of nuclear plants, curbing the emissions of greenhouse gasses emitted by coal-based electricity generation facilities. Fossil fuels are, however, firmly entrenched in the transportation sector, and are a major constituent of the above-mentioned world energy usage of fossil fuels. A viable, environmentally-attractive transportation fuel that has the potential to replace fossil fuels, is hydrogen,

which could be coupled with fuel cells to become even more efficient. The transition to hydrogen as fuel, referred to as the hydrogen economy, will mean that a factor of more than eighteen times the current hydrogen use will be needed if this fuel is to serve only as a transportation energy source [7]

1.2 Background

The worldwide consumption of hydrogen is estimated at approximately 50 million tonnes per annum. The majority of this hydrogen is used for ammonia production, which is further processed to make fertiliser. It is also used for heavy crude oil that is converted to clean liquid fuels. The decline in the availability of light crude oil that does not necessitate additional hydrogen for conversion to gasoline is another reason for the increasing demand. Coupled with this is an increased use of heavy crude oils that entails very large amounts of hydrogen for conversion to gasoline. Should the development of automotive fuel cells occur in such a manner so that the desired cost goals are reached, this could lead to the transportation sector also being fuelled by hydrogen. The effect of this could result in an increase in hydrogen consumption over a period of a number of decades of one to two orders of magnitude [8].

Contemporary production of hydrogen makes use of fossil fuels and natural gas, nullifying the environmental advantage of hydrogen. The hydrogen industry in the United States currently produces 11 million tonnes of hydrogen a year, consuming 5% of the country's natural gas usage and releasing 74 million tonnes of CO₂ into the atmosphere [9]. Hydrogen that is produced from nuclear energy could solve this problem. At present no large scale, cost-effective, environmentally-attractive hydrogen production process has been identified that can be commercialised in the short term.

A number of techniques have been proposed for utilising nuclear power for the production of hydrogen. These will be discussed in greater length in Chapter 2. One of the most promising initiatives for hydrogen production is the use of the Hybrid Sulphur Cycle or HyS, which is a two-step thermochemical cycle. The process

fundamentally concerns the decomposition of water into oxygen and hydrogen using sulphuric acid as a promoter to enhance the chemical reactions.

1.3 Problem Statement

As is the case with any large industrial process, the need to operate under process conditions that support economic viability is imperative. Combining this with the highly competitive nature of the fuel and energy industry, the necessity to maximise process efficiencies is unquestionably important for ensuring feasibility. Techno-economic studies on the Hybrid Sulphur Cycle process have shown that the performance of the decomposition reactor used in the cycle has a significant influence on the efficiency of the system. Currently, the practice is to investigate the operation of the sulphuric acid decomposition reactor operating at pressure ranges between 8 and 9 MPa. This is done in order to avoid a high-pressure differential across the intermediate heat exchanger when heat is transferred from the primary to the secondary helium circuit. Helium gas from the Pebble Bed Modular Reactor (PBMR) is provided at these high pressures. The reduction of SO_3 to SO_2 is however favoured by low pressures, while maintaining high operating temperatures. Considering this, the need to investigate the possibility of operating at lower operating pressures is important in striving for higher process efficiencies. This becomes evident when comparing the efficiencies of high and low pressure operations operating conditions.

At a pressure of 8 to 9 MPa and temperature of 900°C , for example, the maximum conversion of SO_3 to SO_2 (reversible reaction, therefore maximum conversion is equilibrium conversion) that can be achieved is about 48% [10]. If the reactor operates at 95% of the equilibrium conversion, a conversion of only 45% SO_3 to SO_2 can be achieved. The surplus SO_3 that has not been converted to SO_2 upon leaving the reactor, is cooled down downstream of the reactor and converted back to sulphuric acid. This could lead to a build-up of large quantities of sulphuric acid, which is recycled in the system. This has a negative impact on the process overall due to the magnitude of recycling of the corrosive substance throughout the system. It also consumes unnecessary energy through heating and cooling, which contributes to lower thermal efficiencies. One option of improving the conversion of SO_3 to SO_2 is

to lower the reactor operating pressure, while operating at high temperatures in the order of 900°C.

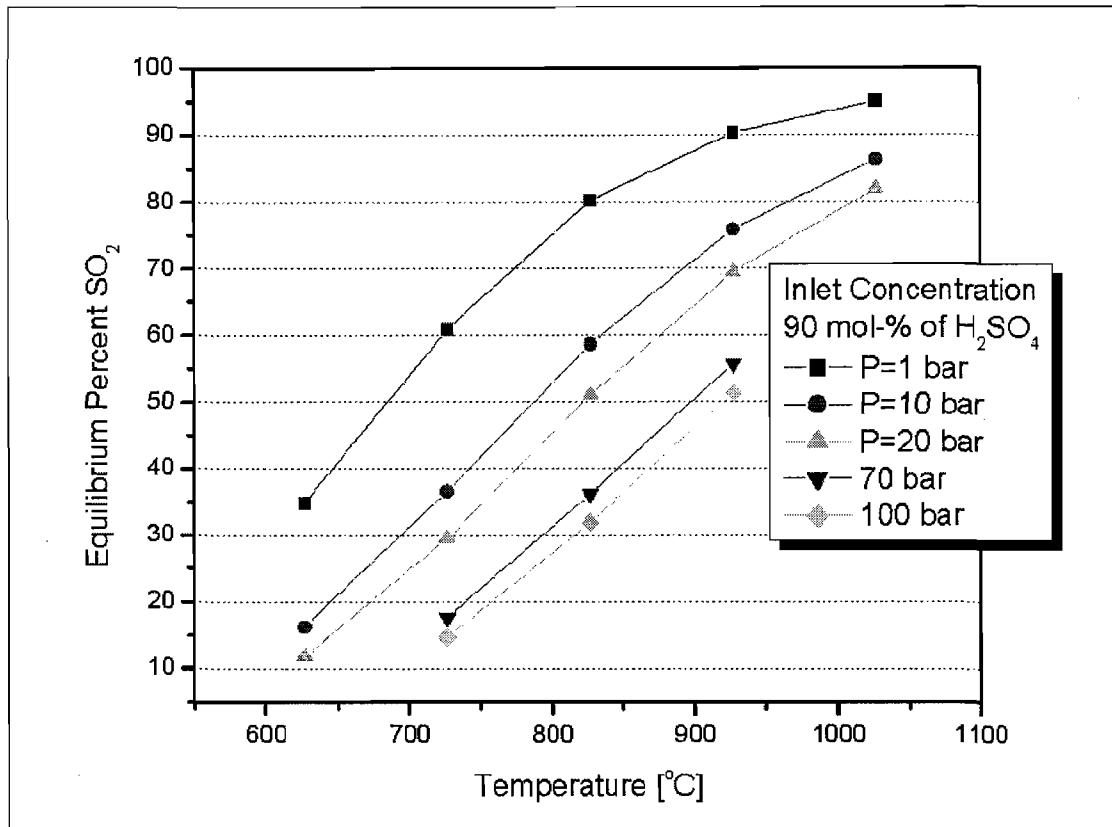


Figure 3: Effect of pressure on SO_3 decomposition

Literature indicates that operating the reactor between 1 and 5 bar will contribute to much higher conversions compared to that achieved at the proposed 8 to 9 MPa levels [10]. An illustration of this effect can be seen in Figure 3 above. Increasing conversion through higher operational temperatures above 950°C will result only in a small improvement.

1.4 Research Methodology

The design of the Hybrid Sulphur cycle decomposition reactor entailed an investigation into all possible information relevant to the primary decomposition reactions that will occur in the reactor system. This includes current available reaction kinetics, heats of formation of the elements and temperature-dependent, variable heat

capacities for the main reactions that occur. The recommended catalysts that support these reactions are also be identified.

Upon completion of the gathering of relevant data and information, basic hand calculations were carried out, to develop and formulate the net reaction rate law. Once this was done, the design equations applicable to the decomposition reactor were developed and solved by making use of the software program PolyMathTM. This tool allows for effective numerical analysis techniques to be used for solving simultaneous ordinary differential and explicit algebraic equations.

Mass, mole, and energy balances were performed across the reactor, in order to calculate the temperature change as a function of conversion. This, in conjunction with the primary design equations and variables allows for the eventual determination of the temperature profile along the length of the reactor. In turn, this contributes to the calculation of the conversion profile of SO_3 to SO_2 along the reactor length. Finally, this design data was used to determine the number of stages required by the decomposition reactor in order to produce a given amount of hydrogen, as well as the frequency and magnitude of the inter-stage heating required.

1.5 Objective of the Research Project

The decomposition reactor is modelled as a multi-stage reactor system operating under adiabatic process conditions. This was done by controlling the inlet temperature to each stage at 870°C by means of inter-stage heating. As a result of inter-stage heating, the overall conversion that was obtained in the process can be increased. Operating the reactor adiabatically also simplifies the reactor and heat exchanger design.

The objective of the research is as follows:

- the concept design of a chemical decomposition reactor capable of achieving 95% of the maximum possible equilibrium conversion at selected pressure and temperature

- design the reactor to operate adiabatically to simplify reactor and heat exchanger design.
- determine the optimum operating conditions necessary for achieving maximum reactor performance;
- establish the reactor size;
- establish reactor space velocity;
- determine species concentration profiles; and
- determine the reactor temperature profiles

1.6 Outline of the Dissertation

In Chapter 2, a literature study will be documented, which highlights the energy drive undertaken in South Africa with regard to the identification of possible alternative sources of energy and fuel. The review will also examine the means by which hydrogen can be produced on a large industrial scale. The different thermochemical process ways of hydrogen production will be listed with a detailed account on the Hybrid Sulphur cycle as well as previous studies undertaken pertaining to it. A preliminary evaluation of the possible equilibrium conversion that can be achieved for the sulphur trioxide to sulphur dioxide decomposition reaction will be investigated in Chapter 3, along with the effect that temperature and pressure have on it. This data will be used in Chapter 4 along with specific design equations to enable the sizing of the reactor system within the frame of the given design limits, to establish the SO_3 decomposition reactor performance. Chapter 5 will present the primary results in table and graph format as well as provide data specification for the most important process units of the design. Conclusions drawn from the investigation and design as well as recommendations for further studies will be addressed in Chapter 6

Chapter 2

Literature Study

CHAPTER 2 LITERATURE STUDY

2.1 Introduction

After providing a background to the study in Chapter 1, this chapter investigates the energy drive with regard to hydrogen research and development undertaken by the Department of Science and Technology of South Africa coupled with a Next Generation Nuclear Power (NGNP) reactor as process heat source. The primary process means of commercial hydrogen production are identified and evaluated with a detailed account description of the HYS process. This is done in order to establish the optimum operating conditions to enhance the overall system performance applicable to the decomposition reactor.

2.2 Drivers for Energy Research and Development in South Africa

At present, South Africa is undertaking a major drive in energy research and development. During the *South African Hydrogen Economy and Fuel Cells Indaba* held on the twenty-fourth of May 2005, the Minister of Science and Technology, Mr Mosibudi Mangena remarked on the following in his speech [11]:

“We have chosen to embark on a journey of bringing issues relating to the hydrogen economy to the forefront in our country. To this end, my department identified the Hydrogen Economy and related Fuel Cells technologies as a ‘Frontier Science and Technology’ area that could potentially change the innovation course of the country’s natural resources, and yield multiple social and economic benefits”.

“Hydrogen and fuel cells are believed to be the energy solutions for the twenty-first century, by enabling clean efficient production of power and heat from a range of primary energy sources”.

The main reasons for the current drive in energy research and development in South Africa are:

- Eskom, South Africa’s leading power supplier has reached the limits of its available electricity generation capacity.

- The environmental impact of coal-based power stations contributes to more than 75% of South Africa's greenhouse gas emissions that result from energy generation and use.
- A third of the population does not have access to a reliable source of energy.

Recently the White Paper on the Energy Policy of South Africa was delivered to address the above-mentioned factors [12]. The five main objectives are:

- increasing access to affordable energy services;
- improving energy governance;
- stimulating economic development;
- managing energy-related environmental impacts; and
- securing supply through diversification.

The security of supply through diversification has to be addressed by investigations and research into the following fields:

- clean coal technologies;
- safe and efficient cooking fuels and appliances;
- bio-fuels and alternative fuels to gasoline;
- the PBMR; and
- hydrogen and fuel cells technologies.

The need for hydrogen technologies research, to enable its harnessing as an important future supplier of energy in South Africa, is therefore undeniable.

2.3 High-Temperature Gas-Cooled Reactors

The use of nuclear technology as a driver for the process heat application of hydrogen production is important to consider because of the thermal constraints imposed with regard to the specific hydrogen production process type that is chosen. One type of the NGNP reactors that have been identified for its safe and reliable operation as well as for its efficient and economic generation of energy is the High-Temperature Gas-

Cooled (HTGR) reactor. Approximately four decades of research have contributed to the current design of HTGRs, which includes operational experience regarding six prototype reactors [13].

Some of the most important features of the concept of HTGR reactors include the following [14]:

- electricity production;
- high temperature production of heat up to 1000°C;
- high temperature production of steam of about 530°C;
- fundamental safety features; and
- prospective for economic attractiveness.

The use of a HTGR with an industrial power plant will have the option of three energy connection points:

- high-temperature heat;
- low-temperature heat; and
- electricity.

With regard to the electricity production, steam turbines can be used with efficiencies of between 40 and 43%, while the implementation of gas turbines could provide efficiencies of approximately 48%. The combination of gas and steam turbines could provide efficiencies of 50%, while cogeneration applications could supply efficiencies of between 80 and 90% [15]

The successful application of a HTGR for process heat related utilisation will require the following:

- Most of the chemical process reactions (endothermic reactions) will require a gas outlet temperature of 950 to 1100°C.
- The inlet gas temperatures should vary between 350 and 500°C, in order to use the recuperation heat of the product gas.

- The system pressure should be low enough to ensure the efficiency of the chemical process reactions are raised.
- The reduction of the risk of radioactive release should an accident occur would require a separate operation between the nuclear and the chemical system.

2.4 Hydrogen Production Methods

Small-scale production of hydrogen is generally achieved by the process of electrolysis of water, which has been well recognised [16]. In areas where low-cost electricity is offered though, this process becomes more feasible for large-scale production. The process of converting electricity to hydrogen using the process of electrolysis is quite high at approximately 80%. Unfortunately, the efficiency of converting heat to electricity, be it by means of nuclear, fossil, or geothermal process varies between 30 and 50% [8]. As a result of this, the overall conversion efficiency of the heat $\rightarrow$ electricity $\rightarrow$ hydrogen process steps drops to between 24 and 40%. Generally, the hydrogen production costs through electrolysis are quite high. Thermal energy can be used to substitute for some of the electrical energy if the electrolysis is carried out at temperatures of 700 to 900°C. Hydrogen production costs through this method could be lower than conventional electrolysis because the process heat is more economical than electricity. An additional incentive is that enhanced chemical kinetics are achieved within the electrolyser because of the higher temperatures. The improved kinetics is an important contribution that the higher temperatures make to the process because a reduction of equipment size and inefficiencies are attained.

The use of direct thermochemical processes for hydrogen production using nuclear energy can be generalised by the net reaction in which heat plus water yields hydrogen and oxygen [8, 17, 18]. If high temperatures in the range of 750°C and beyond are used, low production costs are realised, as well as high conversion efficiencies from heat to hydrogen. The rate of the chemical kinetics are increased as a result of the temperature, and for this reason, a smaller plant size will be required and thus lower capital costs.

2.5 Thermochemical Cycles

Different process routes for the production of hydrogen from other thermochemical processes exist. By far the most important question to be answered in addressing hydrogen production technologies is the production on a large scale in such a manner that satisfies safety requirements, environmental impact, and economic competitiveness compared to other hydrogen production processes. One of the promising initiatives for hydrogen production is the use of thermochemical cycles. Thermochemical cycles produce hydrogen and oxygen through a series of thermochemical reactions.



The products are derived from water at a much lower temperature than direct thermal decomposition. The energy supply is delivered in the form of heat and used to drive the endothermic reactions at a specific temperature range. The temperatures usually vary between 750°C to 1000°C. An important factor to note is that the chemicals used in the process are also recovered and recycled continuously.

The reason thermochemical cycles are considered a promising initiative for hydrogen production is because of the promise of acceptable efficiencies and the option of scaling to large capacities. Another advantage that thermochemical cycles possess is the potential for lower costs than conventional electrolysis of water. The cycles were extensively investigated between the 1960s and 1980s with over 200 cycles that have been investigated [19]. Unfortunately, a large amount of these cycles were found to be unworkable, requiring extremely high temperatures, and considered inefficient. Owing to recent advances in materials and chemical technology development over the past two decades, there is significant potential for process improvement of the cycles previously identified as promising.

Two families of thermochemical processes were identified for their potential high efficiencies and feasibilities, supporting the possibility of producing hydrogen at a

cost competitive with that of petrol. These are the sulphur-based family cycles and the calcium-bromine cycle.

2.5.1 Sulphur-based Cycles

The sulphur-iodine, sulphur-bromine hybrid and hybrid-sulphur cycles are known as the sulphur-based family of thermochemical cycles. This family of cycles has demonstrated high performance potential and is currently being investigated in South Africa, the United States, Japan, and France. The primary reason for this interest is the projected high efficiency of the cycles. The cycles are operated at high temperatures and the heat is provided by NGNPs. Efficiencies of over 40% are possible and improvements have been proposed that could improve cycle efficiency to as much as 60%. These cycles are also considered the most developed and supported, with extensive research being done, and have the potential for multi-cycle variations. The sulphur-based cycles have also been extensively demonstrated at laboratory scale to confirm their performance characteristics. Of all the sulphur-based cycles, the hybrid sulphur cycle is among the least complex of any of the thermochemical cycles that have been researched and demonstrated [19]. The two-step process involves only sulphur compounds, water, hydrogen, and oxygen.

2.5.2 Calcium-bromine Cycle

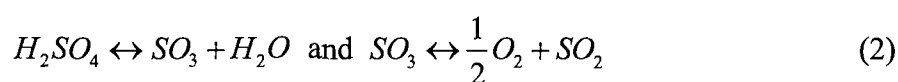
The calcium-bromine cycle's process steps have been demonstrated and involve lower peak temperatures and solid gas reactions. The cycle is considered secondary to the sulphur-based family of cycles because it is projected to have a lower overall efficiency and is technically much more complex. It also does not enjoy significant ongoing research, in contrast with the sulphur-cycles that have been selected as the preferred process route.

2.6 The Hybrid Sulphur Process Description

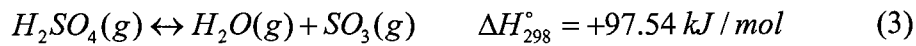
The Westinghouse Sulphur Cycle, also known as the Hybrid Sulphur Cycle or HyS, is a two-step thermochemical cycle for decomposing water into oxygen and hydrogen. This process was originally developed in the early 1970s by the Westinghouse Electric Corporation [18, 20]. In 1983, however, work on the process was terminated. This was mainly due to the rich availability of hydrogen from the steam reforming of natural gas at low prices, in conjunction with diminished interests in developing advanced nuclear reactors. A study undertaken in 2002 reviewed all known thermochemical hydrogen production processes and comparative evaluations of the leading contenders were done [17]. In total, 822 separate references were cited in the study, with 115 different unique cycles identified. The cycles were assessed according to a set of numerical criteria, which found the Hybrid Sulphur Cycle to be ranked first.

In essence, the process makes use of two major unit process operations: an electrolyser and a chemical decomposition reactor. The energy requirements of the decomposition reactor are provided by high temperature process heat generated by the PBMR. The transfer of energy is done by hot helium gas at a temperature of 900°C exiting the PBMR. The gas should reach the decomposition reactor at a temperature of 870 °C because of heat losses at a pressure between 8 and 9 MPa.

The process makes use of two general chemical reactions for the production of oxygen and hydrogen. Oxygen production occurs when sulphur trioxide is thermally reduced, which is obtained from the thermal decomposition of sulphuric acid [20]:



The reaction can be simplified even further when the decomposition of sulphuric acid is viewed in two sub-steps. In the first step, sulphuric acid decomposes into water and sulphur trioxide in the absence of a catalyst and a temperature of 400°C to 500°C, and in the second step, sulphur trioxide is reduced catalytically into oxygen and sulphur dioxide according to the following reactions [21]:



At temperatures above 730°C (roughly 1000 K), the equilibrium for reaction 1 lies to the right. Various catalysts have been investigated and can be used for accelerating the rate of sulphur trioxide reduction to sulphur dioxide and oxygen. The sulphur oxides formed during the reactions that occur in the cycle serve as recycled intermediates within the system. The cycle is completed by using the sulphur dioxide dissolved in concentrated sulphuric acid (50 to 70 wt %), to depolarise the anode of the electrolyser cell. Sulphuric acid, rather than oxygen is produced as product at the anode. Hydrogen protons migrate across the electrolyte and hydrogen gas is produced at the cathode. The overall electro-chemical reaction is:

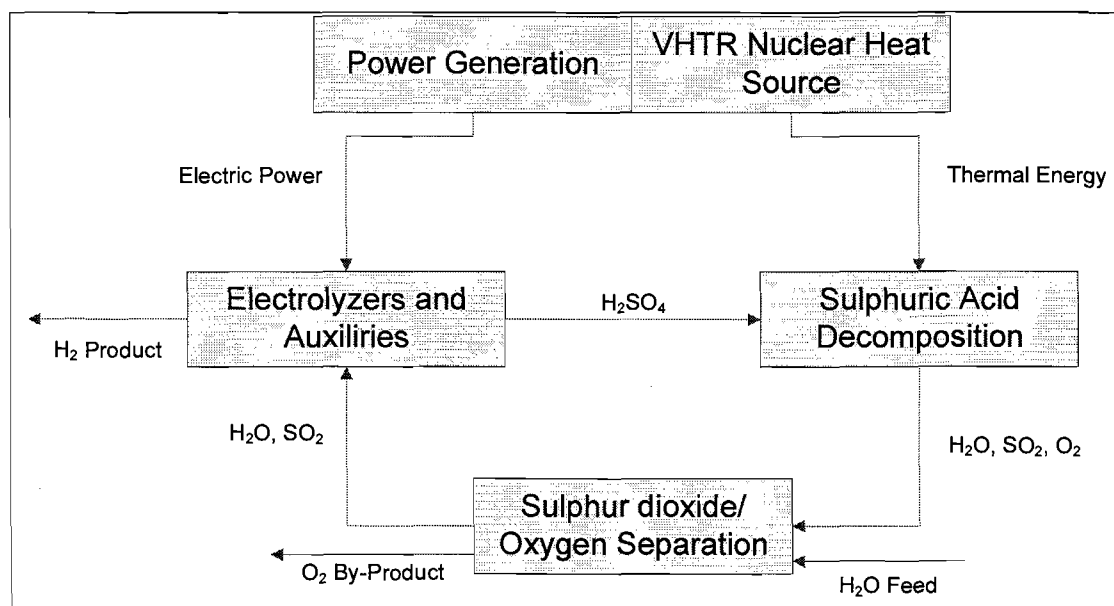
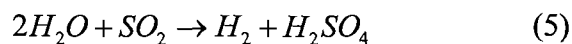
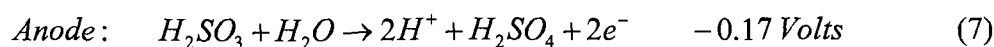


Figure 4: A simplified flow diagram of the HyS process

The individual reactions are:



Even though the electrolyser requires power, the quantity required is much less than that of conventional electrolysis (approximately 15%) [20]. Although the equilibrium voltage is low in dilute concentrations, it increases with concentration and temperature. In dilute concentrations and at 80°C the voltage required is approximately 0.2V but can be higher at higher temperatures or concentrations. The actual operating voltage is however higher, presently at levels of between 0.7V to 0.8V. A significant amount of commercial electrolyzers requires as much as 2.0 V to decompose water, compared to the theoretical voltage of 1.23 V. This is in contrast to the power requirement of reaction 4, which requires 0.7 volts at unit activity for reactants and products. High thermal efficiency can be achieved in the electrolyzer due to the reduction in heat and work required for the decomposition of water.

2.7 Previous Studies Undertaken

A study by Spewock, Brecher, and Talko investigated the thermal catalytic decomposition of sulphur trioxide to sulphur dioxide and oxygen [22]. Part of the study was done to investigate the effect of two different catalysts on the reaction rate. Owing to proprietary reasons, the catalysts were only referred to as WX-1 and WX-2. The reaction order for each catalyst was determined by testing the integral reactor data obtained in their research against integrated mass balances and reaction rate equations. Subsequent to the reaction order determination, the rate constant was expressed as a function of a reaction group, which contained a complex function of initial and final sulphur trioxide concentrations. These concentrations also varied with reaction order.

The mass balance constructed over the differential volume element of the reactor is as follows:

$$F \frac{dx}{dz} = -A_{cs} \cdot r_{rxn} \quad (8)$$

The assumption was made that the decomposition rate is first order with respect to SO_3 concentration, which gives:

$$r_{rxn} = k_t C_{\text{SO}_3} = (k_t C_{\text{SO}_3}^0) x = k \cdot x \quad (9)$$

Substituting delivers

$$\frac{dx}{dg} = -\left(\frac{k}{S_v}\right) x \quad (10)$$

Taking the boundary condition for $x=x_0$ at $g=0$ the solution to equation 9 becomes

$$\left(\frac{x}{x_0}\right) = e^{-\left(\frac{k}{S_v}\right)g} \quad (11)$$

The mole fraction of SO_3 that leaves the reactor is expressed as

$$x_L = x_0 \cdot e^{-\left(\frac{k}{S_v}\right)} \quad (12)$$

The Arrhenius equation is used to model the reaction rate constant, k , according to:

$$k = A \cdot e^{-E/RT} \quad (13)$$

A semilog plot of $\ln(x_0/x_L)$ vs $1/T$ can then be used to determine the activation energy E , and the pre-exponential factor, A . Equation 11 then becomes:

$$\ln \left[\ln \left(\frac{x_0}{x} \right) \right] = -\ln \frac{S_v}{A} - \frac{E}{R} \cdot \frac{1}{T} \quad (14)$$

Subsequent to the derivation of the modelling equations, the pre-exponential factor and activation energy were determined. This was achieved by plotting curves of $\ln(x_0/x)$ versus $1/T$ using data obtained with the catalysts. For catalyst WX-1, this plot

gave a slope of 27.49 deg^{-1} . This yielded a value of 54.5 kcal/mole for the activation energy. A value of $7.657 \times 10^{13} \text{ hr}^{-1}$ for the pre-exponential factor was obtained at the intercepts. The expected conversion that can be obtained with catalyst WX-1 at various temperatures and space velocities is illustrated in Figure 5 below.

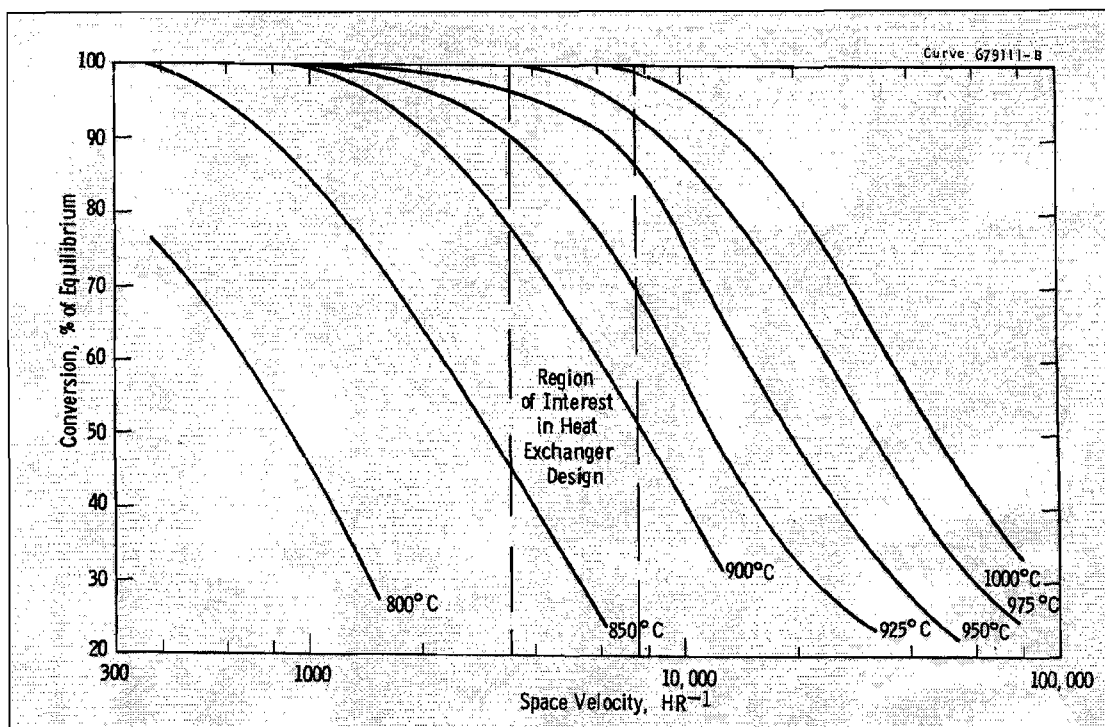


Figure 5: Predicted sulphur trioxide conversions at atmospheric pressure over WX-1 catalyst

This indicates that catalyst WX-1 is a poor catalyst at temperatures below 900°C , even at relatively high space velocities. For catalyst WX-2, the activation energy was determined as 17.46 kcal/mole and the pre-exponential factor as $2.45 \times 10^8 \text{ hr}^{-1}$ for space velocities of $30,000 \text{ hr}^{-1}$ and $60,000 \text{ hr}^{-1}$.

2.8 Catalyst Activity and Stability

As mentioned previously, the decomposition of sulphuric acid involves the non-catalytic thermal decomposition to SO_3 and H_2O at temperatures above 350°C , followed by the reduction of SO_3 to SO_2 . This reduction step will not take place in the absence of a catalyst, even if favourable operating temperatures are maintained.

The decomposition reaction environment is extremely harsh, and for this reason, catalyst stability is an important consideration. Some of the factors include exposure

to high temperatures, corrosive chemicals, high-temperature steam, oxygen, SO_3 , and SO_2 .

In a study by Ginosar et al, three catalysts were investigated by exposing them to reaction conditions similar to the design constraints of this investigation [23]. The catalysts used were 0.1-0.2 wt% Pt supported on alumina, zirconia, and titania. The results indicated that the catalysts with the higher surface area, that being Pt/ Al_2O_3 and Pt/ ZrO_2 , had the highest activities of the catalysts but deactivation occurred swiftly. The catalyst with the lower surface area, Pt/ TiO_2 , proved to have good stability in short-term tests performed, but failed to uphold activity for tests of 200h of uninterrupted operation.

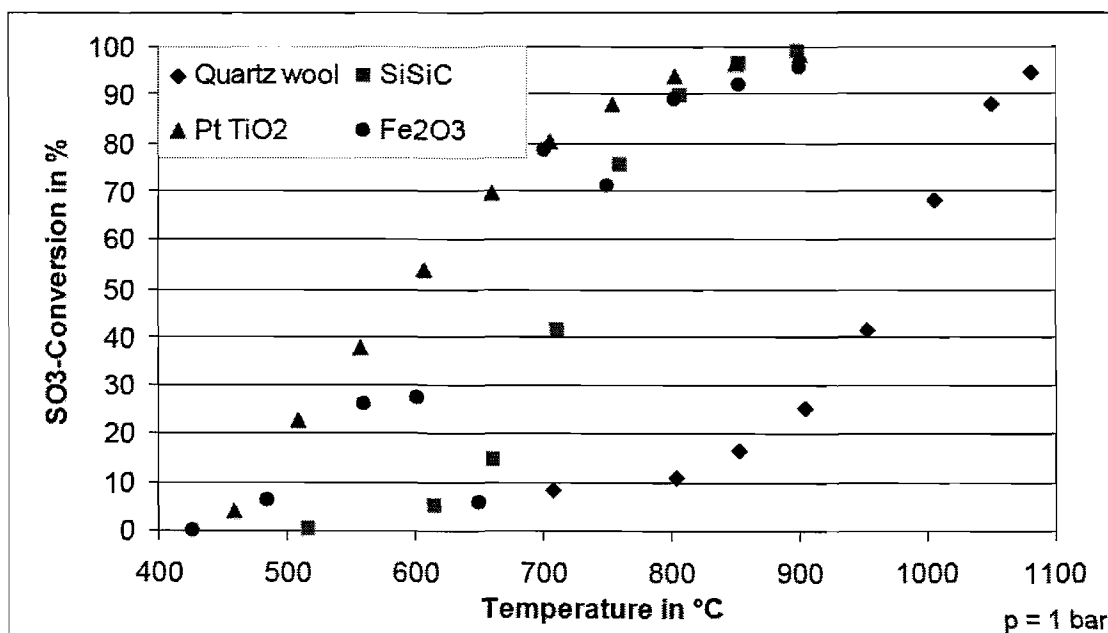


Figure 6: Comparison of catalysts

In a study by Noglik, the production of hydrogen from water using solar energy was investigated [24]. Of interest were the SO_3 conversion levels obtained using a Fe_2O_3 catalyst that gave exceptional conversions at temperatures of 900°C. This can be seen in Figure 6.

In a study by Westinghouse regarding a potential candidate catalyst, the successful candidate was required to fulfil two major criteria [25]:

- Sufficient activity to produce near-equilibrium conversions; and
- The ability to maintain near-equilibrium conversions over an extended period of time

Based on the above-mentioned criteria and experimental results obtained, catalyst ALFA-4 (iron oxide) was selected because of its satisfactory performance and low cost. Near-equilibrium conversions were obtained with the catalyst at temperatures above 1123 K, based on the extensive experimental studies executed. It was, however, noted that at temperatures below 1023 K sulphur was detected on the catalyst. It is believed that the H_2SO_4 feed reacts with the substrate or the iron oxide catalyst, and in the process, the catalyst may become poisoned, and its performance may degrade. Due to the limited application of the catalyst at temperatures below 1023 K, the heat exchanger – reactor configuration may become constrained at reduced operational temperatures of a PBMR. With an outlet temperature of $\sim 900^\circ\text{C}$ or about 850°C to the decomposer after heat exchange, the room allowed for the decomposition reaction to take place before reheating of the stream occurs become very limited. This could imply many stages of reheating, piping etc.

At temperatures above 1073 K, satisfactory conversions were achieved. For catalyst ALFA-4, the activation energy was determined as 46,924 cal/gmol and the pre-exponential factor as $3.75 \times 10^{13} \text{ hr}^{-1}$. The catalyst that has been selected for use in this research project's design is the ALFA-4 catalyst because of its stability and performance when compared to other commercial catalysts available.

Extensive research has still to be done, in order to develop a suitable catalyst. To date, test runs on catalyst lifetime of only approximately 500 hrs have been done, while 20,000 hrs are required for a commercial catalyst.

2.9 Current H_2SO_4 decomposition approaches

Although various H_2SO_4 decomposition approaches are available on laboratory scale as well as others that show potential on a larger scale, three decomposition reactor approaches can be identified for this purpose:

- Sandia Bayonet design
- Shell and Tube decomposer
- Ceramatec compact decomposer design

The Sandia Bayonet reactor consists of one closed ended SiC tube which is co-axially aligned with an open ended SiC tube [26]. This arrangement provides two concentric flow paths, as indicated in Figure 13 where its application in contrast to inter-stage heating is discussed in Section 2.9. In an effort to enhance heat transfer a baffle tube may be included, with high temperature external heat application, except near the open end. At the open end of the annulus concentrated liquid H_2SO_4 is fed, from where it is vaporized before it passes through the annular catalyst bed for the decomposition reaction to take place. The SO_2 , O_2 and H_2O vapor product returns through the center of the Bayonet reactor where it loses its heat to the feed through recuperation. A partially condensed and cooled product exits through the open end into a metal manifold at a temperature low enough to enable the use of PTFE seals.

A ceramatec compact decomposer design involves making use of a ceramic high-temperature heat exchanger as a sulphuric acid decomposer. The inner walls of the decomposition channels of the decomposer are coated by a catalyst which is used to decompose the SO_3 to SO_2 and O_2 . Both the heat exchanger and decomposer are made of silicon carbide (SiC) [27].

Another alternative is to design the SO_3 decomposer in the form of a shell and tube type heat exchanger under a countercurrent contact between the process stream and the helium flow. This ensures a large heat transfer surface is achieved and a temperature difference within the decomposer is achieved. The tube side is packed with catalysts and this is also where the decomposition of SO_3 takes place.

Chapter 3

Equilibrium Conversions

CHAPTER 3 Equilibrium Conversion Calculations

3.1 Introduction

As a first step in the design of a chemical reactor, a preliminary evaluation of the possible equilibrium conversion that can be achieved for the desired chemical reactions should be undertaken. The outcome may determine whether an experimental investigation of a new process is worthwhile. Similarly, the equilibrium conversion of a reaction provides a goal by which to measure improvements in a design process. Even though reaction rates are not susceptible to thermodynamic treatment, equilibrium conversions are [28]. It is for this reason that the aim of this chapter is to determine the effect of temperature and pressure on the equilibrium conversion of sulphur trioxide to sulphur dioxide. Once this is completed, the data will be used in Chapter 4, in order to express the rate of the reaction as a function of conversion, and subsequently solve the major design equations, to enable the sizing of the reactor system within the frame of the given design limits.

3.2 Gibbs Energy Method

Before calculating the possible equilibrium conversion that can be obtained, the equilibrium constant of the reaction needs to be determined. One way to describe the equilibrium position of a chemical reaction is to present the concentration of the reactants and products at that point. This is done by expressing it in terms of an equilibrium constant expression, which relates concentration of reactants and products at equilibrium at a given temperature to a numerical constant [29].

The equilibrium constant K can be calculated at any temperature by making use of:

- the standard heat of reaction; and
- and the standard Gibbs-energy change of reaction at a specific reference temperature.

K can be solved by the following equation:

- $-\ln K = \Delta G^\circ / RT$ (15)

where K is also represented by the equation

- $K = K_0 K_1 K_2$ (16)

The first factor (K_0) in the equation corresponds to the equilibrium constant at reference temperature T_0 :

- $K_0 \equiv \exp\left(\frac{-\Delta G_0^\circ}{RT_0}\right)$ (17)

The second factor (K_1) acts as a multiplier that compensates for the effect of temperature. The product of $K_0 \cdot K_1$ then represents the equilibrium constant at a temperature T , with the assumption that the heat of reaction is independent of temperature [28]:

- $K_1 \equiv \exp\left[\frac{\Delta H_0^\circ}{RT_0}\left(1 - \frac{T_0}{T}\right)\right]$ (18)

The third factor (K_2) is introduced to compensate for the smaller temperature influence that arises as a result of the change of ΔH° with temperature:

- $K_2 \equiv \exp\left(-\frac{1}{T} \int_{T_0}^T \frac{\Delta Cp^\circ}{R} dT + \int_{T_0}^T \frac{\Delta Cp^\circ}{R} \frac{dT}{T}\right)$ (19)

K_2 can be further reduced to:

$$\bullet \quad K_2 = \exp \left\{ \Delta A \left[\ln \tau - \left(\frac{\tau-1}{\tau} \right) \right] + \frac{1}{2} \Delta B T_0 \frac{(\tau-1)^2}{\tau} + \frac{1}{6} \Delta C T_0^2 \frac{(\tau-1)^2 (\tau+2)}{\tau} + \frac{1}{2} \frac{\Delta D}{T_0^2} \frac{(\tau-1)^2}{\tau^2} \right\} \quad (20)$$

The equilibrium constant values for the temperature interval between 300K and 1500K were calculated and displayed in Table 2, along with the various Gibbs energies for each of the components involved in the decomposition reaction.

Table 2: Equilibrium constant values for SO₃ decomposition reaction

	SO ₃	SO ₂	0.5 O ₂	Reaction		
T (K)	ΔG° (J/mol·K)	ΔG° (J/mol·K)	ΔG° (J/mol·K)	ΔG° (J/mol·K)	ln K	K
300	-472810	-371320	-61530	70725	-28.35	4.85E-13
400	-499320	-396750	-82500	61320	-18.44	9.83E-09
500	-527290	-423330	-104270	51825	-12.47	3.85E-06
600	-556470	-450820	-126640	42330	-8.49	2.06E-04
700	-586800	-479120	-149530	32915	-5.66	3.50E-03
800	-618170	-508160	-172890	23565	-3.54	0.0289
900	-650450	-537900	-196710	14195	-1.90	0.1500
1000	-683510	-568210	-220890	4855	-0.58	0.5577
1100	-717370	-599030	-245410	-4365	0.48	1.6117
1200	-751990	-630340	-270300	-13500	1.35	3.8693
1300	-787110	-662160	-295390	-22745	2.10	8.2015
1400	-822980	-694420	-320860	-31870	2.74	15.4550
1500	-859390	-727040	-346540	-40920	3.28	26.6038

Once the equilibrium constants have been obtained, the equilibrium conversion can be calculated. The first step taken to determine the equilibrium conversion of SO₃ to SO₂ as a function of temperature and pressure is to obtain the various T_c , P_c and w values of the decomposition reaction components. These values are shown in the following table.

Table 3: Thermodynamic values of SO₃, SO₂, and O₂

	SO ₃	SO ₂	O ₂
T_c (K)	490.9	430.8	154.6
P_c (bar)	82.1	78.84	50.43
w	0.424	0.245	0.022

By making use of the data in Table 3, the T_r , P_r , B^0 , B^I , and Omega values for SO₃, SO₂, and O₂ can be calculated. The following equations are used:

- $T_r = T / T_c$ (21)

- $P_r = P / P_c$ (22)

- $B^0 = 0.083 - \frac{0.422}{T_r^{1.6}}$ (23)

- $B^1 = 0.139 - \frac{0.172}{T_r^{4.2}}$ (24)

- $\phi = \exp \left[\frac{P_r}{T_r} (B^0 + \omega B^1) \right]$ (25)

The temperature interval selected was 100 K and the temperature range 300 K to 1300 K. The standard pressure was set at 1 bar while the operating pressure was set at values of 1 bar, 3 bar, 30 bar and 90 bar. The thermodynamic values of SO₃, SO₂, and O₂ are given in Table 40 to Table 51 in Appendix A.

With the omega values determined, the equilibrium conversion can be calculated by setting equation 26 equal to equation 27, and determining the mole fraction Y for each component.

- $\left(\left(\frac{P}{P_0} \right)^{-V_{tot}} \right) \cdot K \cdot \left(\frac{\phi_{SO_3}}{\phi_{SO_2} \cdot \phi_{O_2}^{0.5}} \right)$ (26)

- $\frac{Y_{SO_2} \cdot Y_{O_2}^{0.5}}{Y_{SO_3}}$ (27)

The mole fraction for each component is calculated as follows

- $Y_{SO_3} = \frac{n_{i_{SO_3}} + (V_{SO_3} \cdot \varepsilon)}{n_{i_{TOT}} + (V_{TOT} \cdot \varepsilon)}$ (28)

- $Y_{SO_2} = \frac{n_{i_{SO_2}} + (V_{SO_2} \cdot \varepsilon)}{n_{i_{TOT}} + (V_{TOT} \cdot \varepsilon)}$ (29)

- $Y_{O_2} = \frac{n_{i_{O_2}} + (V_{O_2} \cdot \varepsilon)}{n_{i_{TOT}} + (V_{TOT} \cdot \varepsilon)}$ (30)

where ε represents the extent of the reaction and it is also the variable that changes to allow the two equations (equation 26 and equation 27) to be set equal to each other. The final mole fraction values and equilibrium conversion values are then calculated, as displayed in the tables below.

Table 4: Mole fraction and equilibrium conversion values at one-bar pressure

P = 1 bar				
T (K)	Y(SO ₃)	Y(SO ₂)	Y(O ₂)	X
600	0.993414	0.00439	0.002195	0.006586
700	0.957705	0.028197	0.014098	0.042295
800	0.840858	0.106095	0.053047	0.159142
900	0.61419	0.257207	0.128603	0.38581
1000	0.356536	0.428976	0.214488	0.643464
1100	0.178032	0.547978	0.273989	0.821968
1200	0.086812	0.608792	0.304396	0.913188
1300	0.043877	0.637415	0.318708	0.956123

Table 5: Mole fraction and equilibrium conversion values at three-bar pressure

P = 3 bar				
T (K)	Y(SO ₃)	Y(SO ₂)	Y(O ₂)	X
600	0.995507	0.002996	0.001498	0.004493
700	0.970297	0.019802	0.009901	0.029703
800	0.886003	0.075998	0.037999	0.113997
900	0.706523	0.195651	0.097826	0.293477
1000	0.466255	0.35583	0.177915	0.533745
1100	0.262212	0.491858	0.245929	0.737788
1200	0.137957	0.574695	0.287348	0.862043
1300	0.072608	0.618262	0.309131	0.927392

Table 6: Mole fraction and equilibrium conversion values at thirty-bar pressure

P = 30 bar				
T (K)	Y(SO ₃)	Y(SO ₂)	Y(O ₂)	X
600	0.998051	0.001299	0.00065	0.001949
700	0.985075	0.00995	0.004975	0.014925
800	0.945508	0.036328	0.018164	0.054492
900	0.844417	0.103722	0.051861	0.155583
1000	0.681855	0.212096	0.106048	0.318145
1100	0.484472	0.343685	0.171843	0.515528
1200	0.312139	0.458574	0.229287	0.687861
1300	0.188195	0.541203	0.270602	0.811805

Table 7: Mole fraction and equilibrium conversion values at ninety-bar pressure

P =90 bar				
T(K)	Y(SO3)	Y(SO2)	Y(O2)	X
600	0.998501	0.001	0.0005	0.001499
700	0.991027	0.005982	0.002991	0.008973
800	0.961793	0.025471	0.012736	0.038207
900	0.89087	0.072754	0.036377	0.10913
1000	0.762444	0.158371	0.079185	0.237556
1100	0.592913	0.271392	0.135696	0.407087
1200	0.419452	0.387032	0.193516	0.580548
1300	0.275572	0.482952	0.241476	0.724428

A plot of the equilibrium conversion obtained for the decomposition reaction $\text{SO}_3 \rightarrow \text{SO}_2 + 0.5\text{O}_2$ with temperatures at different operating pressures is shown in Figure 7. The plot clearly indicates the tremendous impact that elevated pressures have on the equilibrium conversion that could be achieved. It is therefore clear that the lowest operating pressure will result in the highest conversion possible. Examining the equilibrium conversions achieved, an operating pressure of 3 bar has been selected as the operating pressure for the reactor. This pressure allows for a conversion of between 70 and 80%, at an operating temperature of 870°C, and sufficient pressure drop across the reactor system.

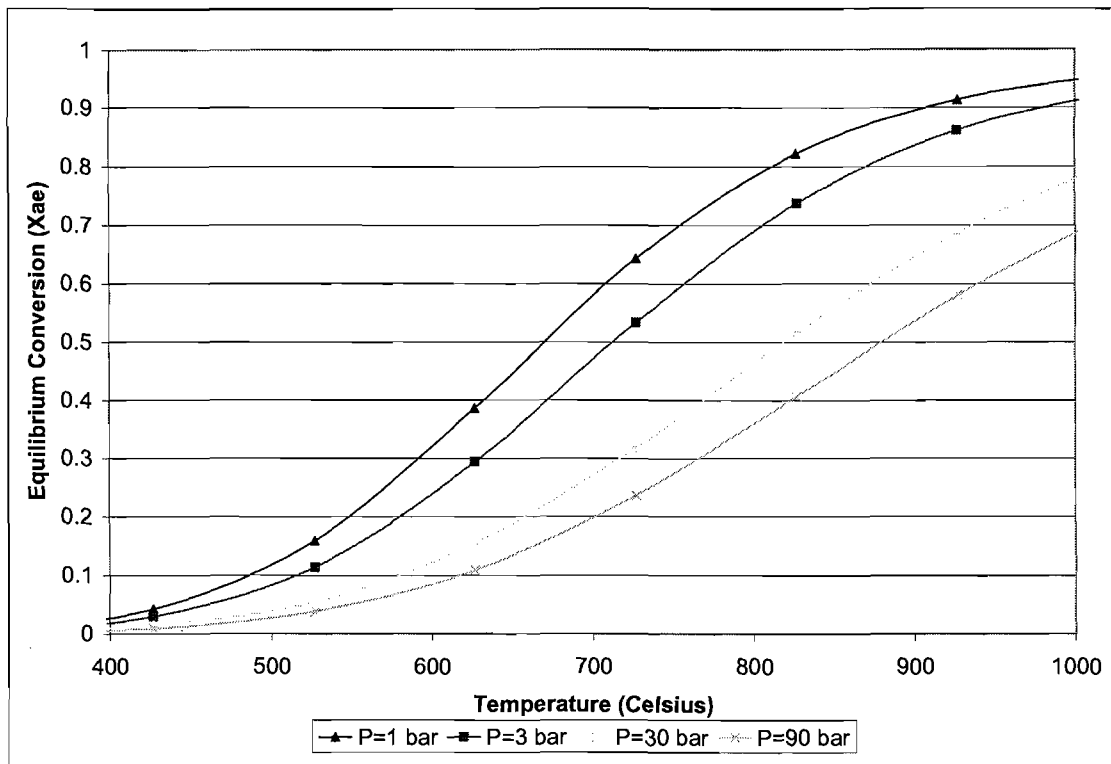


Figure 7: Equilibrium conversion of SO_3 to SO_2 as a function of temperature at various pressures

In order to validate the calculations that were done on the equilibrium conversion of the decomposition of SO_3 , a study by Parma et al. was consulted [30]. Amongst others, the equilibrium conversion for SO_3 decomposition to SO_2 was determined as a function of temperature for operating pressures of 1 bar, 3 bar, 6 bar, and 12 bar. The results that were obtained by Parma et al. for the operating pressures of 1 bar and 3 bar were compared to those achieved using the Gibbs free energy method. The results were identical, with both the 1-bar (operating temperature 700°C) and 3-bar (operating temperature 800°C) operating pressures yielding a 60% and 70% conversion respectively. The equilibrium conversions calculated by Parma et al. and confirmed by measurements at 1 and 3 bar are shown in Figure 8 below.

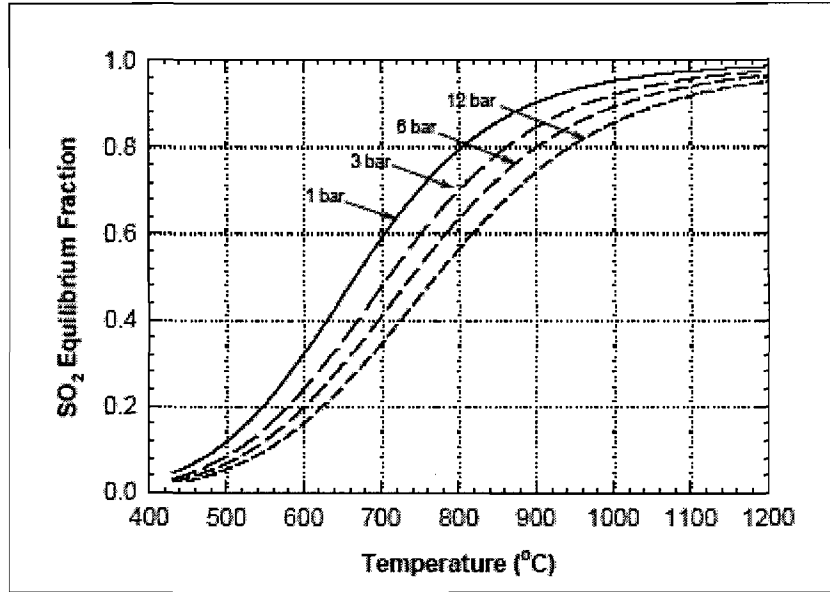


Figure 8: Equilibrium conversion as a function of temperature as performed by Parma et al.

3.3 Equilibrium Constant Method

In addition to the Gibbs energy method that was used to solve for the equilibrium conversion as a function of temperature and pressure, there is another method that can be used to validate the results obtained using the Gibbs energy method. This method entails using equilibrium constant data at a specific temperature along with a correlation that describes K_c in terms of temperature, pressure and most important of all, equilibrium conversion.

The two equations described above were then set equal to each other, to obtain the equilibrium conversion at various temperatures and pressures. The first equation that is used is shown below, using an experimentally determined K_c value of 0.041 at a temperature of 973 K (*Oakridge Laboratories*).

$$K_c = K_c(T_2) \exp \left[\frac{\Delta H_{rx}}{R} \left(\frac{1}{T_2} - \frac{1}{T} \right) \right] \quad (31)$$

The following empirical equation can be derived from the equilibrium data:

$$K_c = \frac{\left[4.86 \cdot 10^{-5} \cdot P_0 \cdot \left(\frac{X_{AE}}{1 + 0.237 \cdot X_{AE}} \right) \cdot \frac{1173}{T} \right] \cdot \left[4.86 \cdot 10^{-5} \cdot P_0 \cdot \left(\frac{0.5 X_{AE}}{1 + 0.237 \cdot X_{AE}} \right) \cdot \frac{1173}{T} \right]^{0.5}}{4.86 \cdot 10^{-5} \cdot P_0 \cdot \left(\frac{1 - X_{AE}}{1 + 0.237 \cdot X_{AE}} \right) \cdot \frac{1173}{T}} \quad (32)$$

The equilibrium conversion can be determined at different temperatures and pressures. Values for the equilibrium conversion were determined at pressures of 1 bar, 3 bar, 30 bar, and 90 bar to compare it to those determined using the Gibbs energy method. These values are shown in Table 8 to Table 11.

Table 8: Equilibrium conversion as a function of T and P using Kc method at one bar

Po	101	101	101	101	101	101	101
Xae	0.0305	0.124	0.33	0.598	0.8025	0.909	0.9559
T in K	700	800	900	1000	1100	1200	1300
T in C	426	526	626	726	826	926	1026
Kc	0.000348	0.002913	0.015207	0.057039	0.168236	0.414359	0.888403

Table 9: Equilibrium conversion as a function of T and P using Kc method at three bar

Po	303	303	303	303	303	303	303
Xae	0.0218	0.088	0.2459	0.485	0.711117	0.854267	0.926813
T in K	700	800	900	1000	1100	1200	1300
T in C	426	526	626	726	826	926	1026
Kc	0.000348	0.002913	0.015207	0.057039	0.168236	0.414359	0.888403

Table 10: Equilibrium conversion as a function of T and P using Kc method at thirty bar

Po	3003	3003	3003	3003	3003	3003	3003
Xae	0.01	0.0422	0.1256	0.279	0.481357	0.673255	0.809595
T in K	700	800	900	1000	1100	1200	1300
T in C	426	526	626	726	826	926	1026
Kc	0.000348	0.002913	0.015207	0.057039	0.168236	0.414359	0.888403

Table 11: Equilibrium conversion as a function of T and P using Kc method at ninety bar

Po	9009	9009	9009	9009	9009	9009	9009
Xae	0.0069	0.0295	0.089	0.204984	0.375406	0.562989	0.720832
T in K	700	800	900	1000	1100	1200	1300
T in C	426	526	626	726	826	926	1026
Kc	0.000348	0.002913	0.015207	0.057039	0.168236	0.414359	0.888403

The equilibrium conversion as a function of temperature and pressure using the K_c method is shown in Figure 9. When compared to the equilibrium conversion values determined using the Gibbs energy method, it was found that the values were almost the same, with differences in conversion between the two methods not exceeding 2 to 3%.

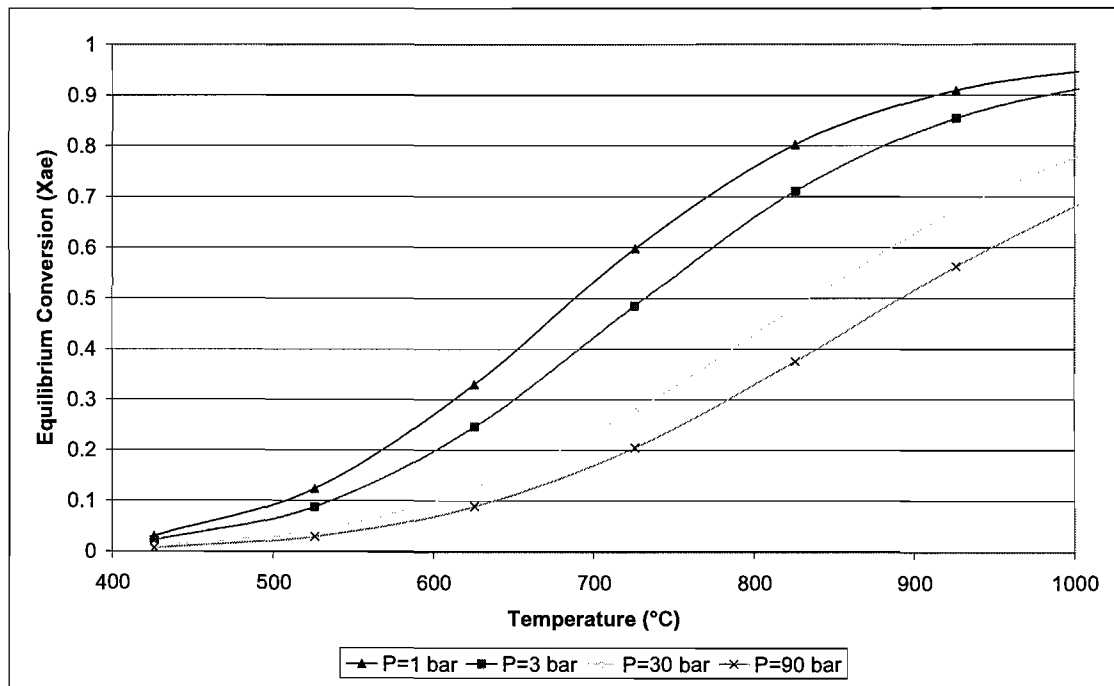


Figure 9: Equilibrium conversion as a function of T and P using K_c method

3.4 Inter-stage Heating

The concept of inter-stage heating can be used to increase the equilibrium conversion achieved for the decomposition of SO_3 to SO_2 very effectively. The reaction is endothermic and will result in the temperature of the reaction mixture dropping with an increase in conversion. Owing to the temperature drop, the rate of the reaction will also diminish and reach a point where no conversion of reactants will occur anymore. At this point, the product stream is heated in an inter-stage heat exchanger, to raise the temperature once more before the stream is sent to the next reactor stage where conversion of the reactants will occur once again. This principle is illustrated in Figure 10.

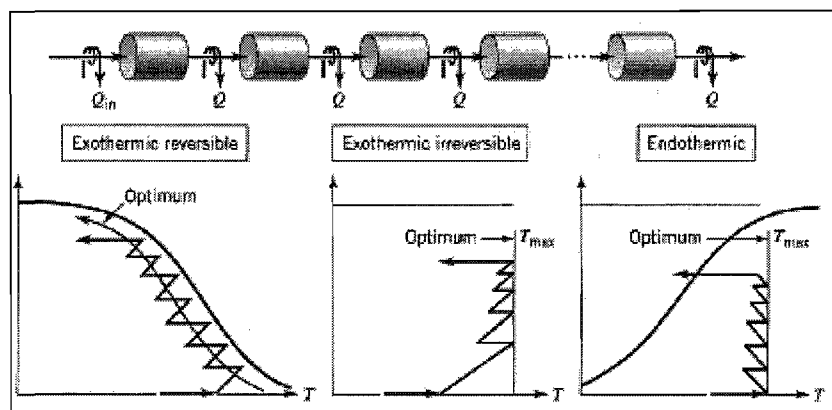


Figure 10: The principle of inter-stage heating and cooling for endothermic and exothermic reactions respectively

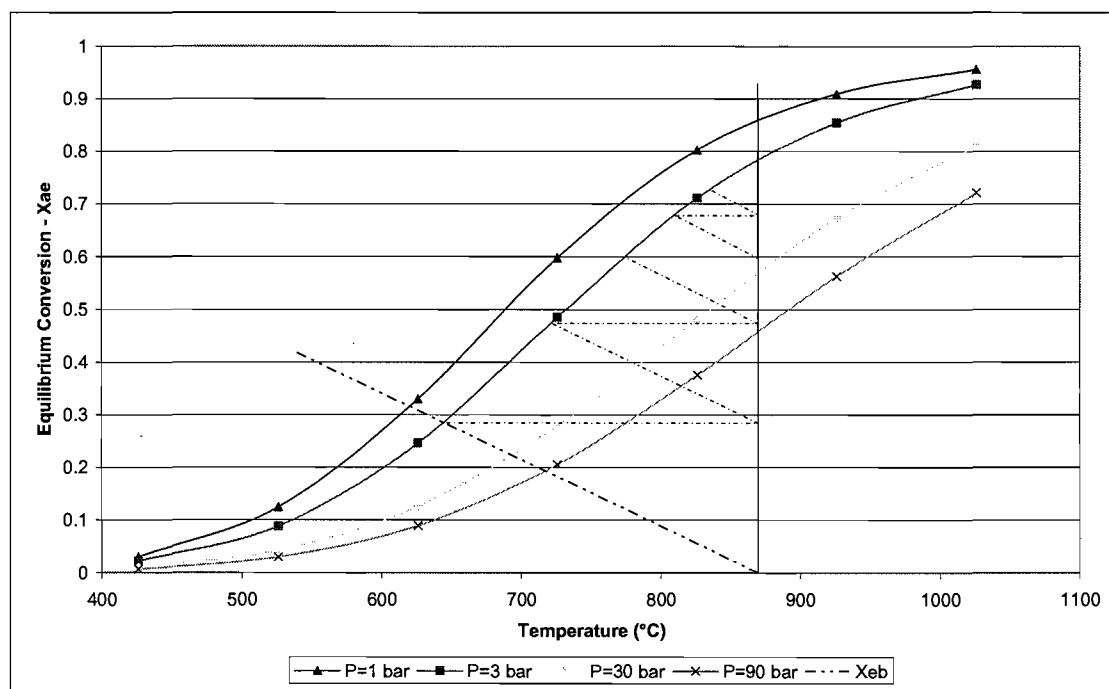


Figure 11: Equilibrium conversion achievable for three-bar operation making use of inter-stage heating

When inter-stage heating is applied to the SO_3 decomposition reaction at 3-bar operational pressure, an equilibrium conversion of 72% can be achieved (Figure 11). In contrast to this, the equilibrium conversion achieved at 90-bar operation drops to approximately 42% (Figure 12).

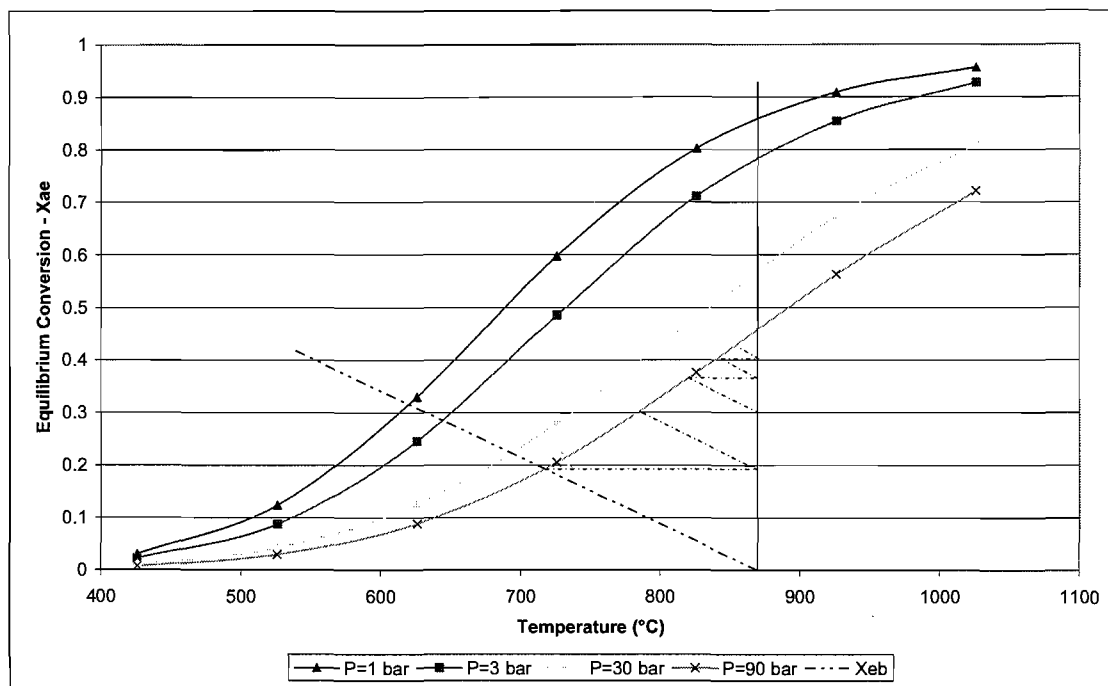


Figure 12: Equilibrium conversion achievable for 90-bar operation making use of inter-stage heating

It should be noted though that other configurations are possible and in current use with regards to the heating of the SO_3 to SO_2 product stream. An example of a more integrated configuration, where the decomposition reaction and heat transfer are done in the same unit is the Bayonet decomposition reactor developed by Sandia National Laboratories (SNL) [26]. As mentioned in Section 2.9, the reactor consists of one closed ended SiC tube co-axially aligned with an open ended SiC tube to form two concentric flow paths. In an effort to enhance heat transfer, a baffle tube is also included. High temperature heat is added to the reactor except near its open end. At the open end of the annulus concentrated liquid H_2SO_4 is fed, where it is vaporized before passing through an annular catalyst bed. Heat provided by the external heat source is then applied to the catalyst bed where the decomposition reaction takes place. A schematic diagram of the reactor is shown in Figure 13.

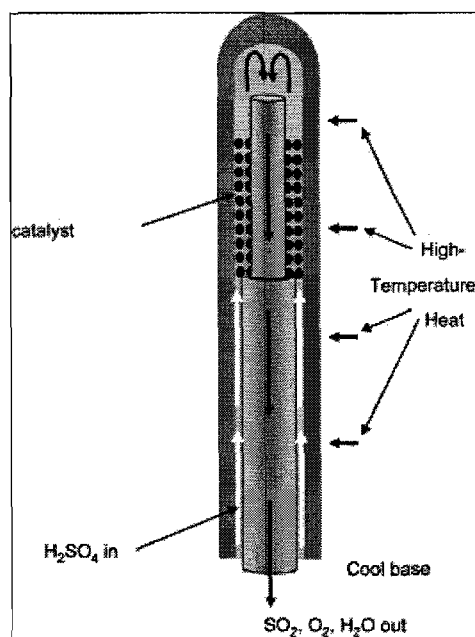


Figure 13: Schematic diagram of the SNL Bayonet decomposition reactor

Although other configurations like the SNL Bayonet decomposition reactor are available and in current use, inter-stage heating was selected in this study to investigate the reaction mechanism independently from heat application in an effort to better understand the impact heat transfer and kinetics have on the decomposition reaction and which one has a greater effect on enhancing conversions of SO_3 to SO_2 .

Chapter 4

Reactor Design

CHAPTER 4 Reactor Design

4.1 Introduction

The primary design of the reactor entails the development of design equations based on the chemical reactions that take place in the reactor system and as such allow for the selection of reactor type. The first equation is the reaction conversion that could be achieved as a function of the reactor volume. The temperature decrease along the length of the reactor is also determined because of the endothermic nature of the reaction. This is executed by performing an energy balance across the reactor. In addition to this, the rate equation for the decomposition reaction is determined and the concentration profiles of the species as a function of conversion along the reactor path established. The aim of this chapter is to study the effect of operating parameters, such as temperature and pressure, on the performance of the SO_3 decomposition reactor.

4.2 Reactor Volume as a Function of Conversion

The calculation of the reactor volume required to achieve a conversion X in a flow system necessitates the establishment of a formula that relates the reaction rate as a function of conversion. In order to achieve this functional dependence, it is necessary to convert the reaction rate law from its dependence on the concentrations of the reacting species to a dependence on conversion. The reaction system can then be designed.

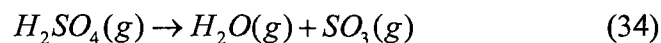
It has been calculated that a feed stream of 135 kg/s could be treated with the suitable heat supplied by a 500 MWt PBMR reactor. The feed stream was introduced to the reactor at a pressure of 300 kPa and consists of 90mol% H_2SO_4 and 10mol% H_2O

The primary design of the reactor entailed the development of certain design equations, which include the determination of the reactor volume required as well as the temperature profile across the length of the reactor.

In order to ascertain the specific volume of the reactor, the first step was to set the equation that establishes the relationship between the reaction conversion that can be achieved as a function of the reactor volume. This is very important, as the basis of the design is driven by the eventual conversion that can be achieved. The equation for the conversion as a function of reactor volume is as follows:

$$\frac{d(X)}{d(V)} = \frac{-r_A}{F_{A0}} \quad (33)$$

In order to solve it, $-r_A$ and F_{A0} needs to be determined. As a first step, solving for F_{A0} can be done based on the assumption that the decomposition of the 90mol% H_2SO_4 feed stream will virtually decompose completely to SO_3 and H_2O (based on literature). It then follows that the subsequent product stream of the decomposition reaction of:



consists of a 0.474mol% SO_3 and 0.526mol% H_2O . With this established, F_{A0} can be determined from the equation:

$$F_{A0} = (y_{A0})(F_{T0}) \quad (35)$$

where y_{A0} amounts to 0.474 and F_{T0} to 2850 mol/s. This allows for the calculation of F_{A0} .

$$F_{A0} = (0.474)(2850 \text{ mol/s}) = 1350 \text{ mol/s} \quad (36)$$

The calculation of $-r_A$ however is not as simple as that of F_{A0} . The basis of the calculation of the rate law involves one of the reactants that disappears as a result of the reaction, in this case SO_3 . The rate of the disappearance of SO_3 or $-r_A$ depends on two primary factors:

- temperature; and
- composition.

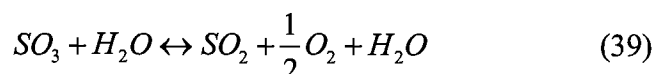
Owing to the non-isothermal nature of the design, the specific temperature profile down the length of the reactor was also addressed in the design (refer to Section 4.3) and subsequently influenced the rate law. In most reactions, the rate law is expressed as a product of the reaction rate constant k (refer to Chapter 3) and a function of the concentrations of the various species involved in the reaction to give:

$$-r_A = [k_A(T)] [\text{fn}(C_A, C_B, \dots)] \quad (37)$$

Experimental studies are used to determine the dependence of the reaction rate $-r_A$ on the concentrations of the species present $[\text{fn}(C_j)]$. The concentration of the reacting species may however also be expressed in terms of conversion X :

$$C_j = h_j(X) \quad (38)$$

With this relationship between concentration and conversion established, $-r_A$ can in fact be calculated as a function of X , and in so doing, the design equation of dX/dV can be determined. The formulation of the rate law is based on the decomposition reaction of SO_3 to give the following first-order reversible gas phase reaction:



and

$$-r_A = -k_1 \cdot \left[C_A - \frac{C_I \cdot C_C \cdot C_D^{0.5}}{K_C} \right] \quad (40)$$

It is better to include water (C_I) (which acts as a non-reacting species that affects the kinetics of the reaction) in the rate equation, for the reason that the volumetric flow rate varies with conversion. The concentration of the inert gas (C_I) is not constant and will be evident from the concentration profiles across the length of the SO_3 decomposition reactor as will be illustrated in greater detail in Chapter 5. The concentration of each of the species, expressed in moles per unit volume as a function of conversion, is shown below after first developing a stoichiometric table for the flow system.

Table 12: Stoichiometric table for the flow system [31]

Species	Symbol	Feed Rate to Reactor (mol/time)	Change within Reactor (mol/time)	Effluent Rate from Reactor (mol/time)
SO ₃	A	F _{A0}	-F _{A0} ·X	F _A = F _{A0} ·(1-X)
SO ₂	C	0	+F _{A0} ·X	F _C = F _{A0} ·X
O ₂	D	0	+0.5F _{A0} ·X	F _D = 0.5F _{A0} ·X
H ₂ O	I	F _{I0} =θ _I F _{A0}	-	F _I =θ _I ·F _{A0}
Total		F_{T0}	Total	F_T=F_{T0}+(d/a+c/a+b/a-1)·F_{A0}·X

$$\bullet \quad SO_3 \Rightarrow C_A = C_{A0} \cdot \left(\frac{1-X}{1+\varepsilon X} \right) = 0.01496 \cdot \left(\frac{1-X}{1+0.237 \cdot X} \right) \frac{\text{mol}}{\text{dm}^3} \cdot \frac{T_0}{T} \quad (41)$$

$$\bullet \quad SO_2 \Rightarrow C_C = \left(\frac{C_{A0} \cdot X}{1+\varepsilon X} \right) = \frac{0.01496 \cdot X}{1+0.237 \cdot X} \cdot \frac{\text{mol}}{\text{dm}^3} \cdot \frac{T_0}{T} \quad (42)$$

$$\bullet \quad O_2 \Rightarrow C_D = \left(\frac{C_{A0} \cdot \frac{1}{2} X}{1+\varepsilon X} \right) = \frac{0.01496 \cdot \frac{1}{2} \cdot X}{1+0.237 \cdot X} \cdot \frac{\text{mol}}{\text{dm}^3} \cdot \frac{T_0}{T} \quad (43)$$

$$= \frac{0.00748 \cdot X}{1+0.237 \cdot X} \cdot \frac{\text{mol}}{\text{dm}^3} \cdot \frac{T_0}{T}$$

$$\bullet \quad H_2O \Rightarrow C_I = \left(\frac{C_{A0} \cdot \theta_I}{1+\varepsilon X} \right) = \frac{0.01496 \cdot 1.1097}{1+0.237 \cdot X} \cdot \frac{\text{mol}}{\text{dm}^3} \cdot \frac{T_0}{T} \quad (44)$$

$$= \frac{0.01660}{1+0.237 \cdot X} \cdot \frac{\text{mol}}{\text{dm}^3} \cdot \frac{T_0}{T}$$

The successful completion of the concentration of each of the species requires solving for the variables C_{A0} , θ_I and ε . The pressure dependence of C_{A0} term can be varied according to the required operating pressure.

$$\bullet \quad C_{A0} = y_{A0} \cdot C_{T0} = y_{A0} \cdot \left(\frac{P_0}{R \cdot T_0} \right) \quad (45)$$

$$= 0.474 \cdot \left(\frac{\text{Operating pressure (kPa)}}{8.314 \cdot 1143} \right)$$

$$= 0.01496 \text{ mol/dm}^3$$

The operating pressure was varied between 300 kPa (3 bar) and 9000 kPa (90 bar). An operating pressure of 3 bar was selected for the initial calculation of C_{A0} . The variable that needs to be determined is θ_I . Making use of the feed stream composition data, θ_I is determined from the following equation:

$$\theta_I = \frac{F_{I0}}{F_{A0}} = \frac{y_{I0}}{y_{A0}} = \frac{0.526}{0.474} = 1.1097 \quad (46)$$

The last remaining variable that needs to be solved for (dX/dV) is ε . The definition for ε is:

$$\varepsilon = \frac{\text{change in total number of moles for complete conversion}}{\text{total number of moles fed to the reactor}} \quad (47)$$

In symbol form, this reduces to a formula that is more applicable for ε 's calculation because of the availability of data and information of the variables within its formula, which states:

$$\varepsilon = \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \right) \cdot \frac{F_{A0}}{F_{T0}} \quad (48)$$

and this further reduces to

$$\varepsilon = y_{A0} \cdot \delta \quad (49)$$

With y_{A0} already calculated, only δ remains. All of the species are in gas phase, and therefore, the generalised reaction becomes:

$$\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \quad (50)$$

$$\delta = \frac{1}{2} + 1 + 1 - 1 - 1 = 0.5$$

Finally, ε can be calculated with all the variable's values having been established:

$$\begin{aligned} \varepsilon &= 0.47 \times 0.5 \\ &= 0.237 \end{aligned} \quad (51)$$

Reflecting on the rate law once again, the equilibrium constant of reaction (K_C) and specific reaction rate constant (k_I) are required to complete the formula:

$$-r_A = -k_1 \cdot \left[C_A - \frac{C_I \cdot C_C \cdot C_D^{0.5}}{K_C} \right] \quad (52)$$

The specific reaction rate constant as developed from the Arrhenius equation gives:

$$k_1 = A \cdot \exp\left(\frac{-E_A}{R \cdot T}\right) \quad (53)$$

where the kinetic data of hematite as catalyst was used with a pre-exponential factor of $3.75 \times 10^{13} \text{ h}^{-1}$ and an activation energy of 196 000 J/mol [14]. The catalyst was recommended by Lin and Flaherty after it had fulfilled two important criteria:

- i. sufficient activity to produce near-equilibrium conversions; and
- ii. an ability to maintain near-equilibrium conversions over an extended period of time [25].

Apart from the above, the catalyst was selected because of its satisfactory performance based on experimental results and its low cost [14]. The equation of the equilibrium constant was determined as:

$$K_C = K(T_2) \cdot \exp\left[\left(\frac{\Delta H_{Rx}^\circ}{R}\right) \cdot \left(\frac{1}{T_2} - \frac{1}{T}\right)\right] \quad (54)$$

where the heat of reaction at temperature T is given in terms of the enthalpy of each species at temperature T that forms part of the reaction. The heat of reaction is:

$$\Delta H_{Rx}^\circ(T_R) = \frac{d}{a} H_D^\circ(T_R) + \frac{c}{a} H_C^\circ(T_R) - \frac{b}{a} H_B^\circ(T_R) - H_A^\circ(T_R) \quad (55)$$

and amounts to +98.92 kJ/mol as shown in the Table 13 below:

Table 13: Heat of reaction of species

ΔH_{298}°	SO ₃	SO ₂	O ₂
98.93	-395.77	-296.84	0
kJ/mol	kJ/mol	kJ/mol	kJ/mol

With all the variables determined within the rate law equation, the conversion as a function of reactor volume (dX/dV) can be generated.

4.3 Reactor Temperature as a Function of Reactor Volume

The temperature profile along the length of the reactor volume can be calculated by performing an energy balance across the reactor. This is solved using the following differential equation for adiabatic operation:

$$\frac{d(T)}{d(V)} = \frac{(-r_a) \cdot [-\Delta H_{Rx}(T)]}{F_{A0} \cdot (\sum \theta_i \cdot C_{p_i} + X \cdot \Delta C_p)} \quad (56)$$

In order to solve the equation certain variables contained within the formula need to be calculated, as some of the variables have already been addressed earlier in this chapter and their calculation pathways highlighted.

The first variable to be addressed is the heat of reaction at a given temperature:

$$\Delta H_{Rx}(T) = \Delta H_{Rx}^\circ(T_R) + \Delta C_p(T - T_R) \quad (57)$$

where

$$\Delta H_{Rx}^\circ(T_R) = \frac{d}{a} H_D^\circ(T_R) + \frac{c}{a} H_C^\circ(T_R) - \frac{b}{a} H_B^\circ(T_R) - H_A^\circ(T_R) \quad (58)$$

as stated previously and

$$\Delta C_p = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + \frac{E}{T^2} \quad (59)$$

The heat capacity of each of the four species as a function of temperature is given by their respective equations as follows:

- Sulphur Trioxide:

$$C_p(SO_3) = 24.02 + (119.46 \times T) + (-94.38 \times T^2) + (26.96 \times T^3) + \left(\frac{-0.117}{T^2} \right) \quad (60)$$

- Sulphur Dioxide:

$$C_p(SO_2) = 21.43 + (74.35 \times T) + (-57.75 \times T^2) + (16.35 \times T^3) + \left(\frac{0.086}{T^2} \right) \quad (61)$$

- Oxygen:

$$C_p(O_2) = 29.659 + (6.13 \times T) + (-1.18 \times T^2) + (0.0957 \times T^3) + \left(\frac{-0.219}{T^2} \right) \quad (62)$$

- Water:

$$C_p(H_2O) = 30.09 + (6.83 \times T) + (6.79 \times T^2) + (-2.53 \times T^3) + \left(\frac{0.082}{T^2} \right) \quad (63)$$

The constants used for the different species in calculating the heat capacity are summarised in Table 14. The constants were used to determine the heat capacity of the reaction at every temperature point within each stage of the reactor.

Table 14: Heat capacity constants of reacting species

Constant	SO ₃	SO ₂	O ₂	Δ
A	24.025	21.43	0.5 * 29.659	12.23
B	119.46	74.35	0.5 * 6.137	-42.04
C	-94.38	-57.75	0.5 * -1.186	36.04
D	26.96	16.35	0.5 * 0.0957	-10.55
E	-0.1175	0.0867	0.5 * -0.219	0.0944

Integration of the heat capacity equation delivers the final equation that can be used in the temperature as a function of reactor volume (dT/dV) differential equation:

$$\Delta C_p = \Delta A(T - T_R) + \frac{\Delta B}{2} \cdot (T^2 - T_R^2) + \frac{\Delta C}{3} \cdot (T^3 - T_R^3) + \frac{\Delta D}{4} \cdot (T^4 - T_R^4) - \frac{\Delta E}{(T - T_R)} \quad (64)$$

This corresponds to Fogler who states that [24]:

$$\Delta H_{Rx}(T) = \Delta H_{Rx}^\circ(T_R) + \int_{T_R}^T \Delta C_p dT \quad (65)$$

and substitution gives:

$$\Delta H_{Rx}(T) = \Delta H_{Rx}^\circ(T_R) + \int_{T_R}^T (\Delta \alpha + \Delta \beta T + \Delta \gamma T^2) dT \quad (66)$$

where

$$\Delta \alpha = \frac{d}{a} \alpha_D + \frac{c}{a} \alpha_C - \frac{b}{a} \alpha_B - \alpha_A \quad (67)$$

$$\Delta \beta = \frac{d}{a} \beta_D + \frac{c}{a} \beta_C - \frac{b}{a} \beta_B - \beta_A \quad (68)$$

$$\Delta \gamma = \frac{d}{a} \gamma_D + \frac{c}{a} \gamma_C - \frac{b}{a} \gamma_B - \gamma_A \quad (69)$$

with the final equation:

$$\Delta H_{Rx}(T) = \Delta H_{Rx}^{\circ}(T_R) + \Delta \alpha(T - T_R) + \frac{\Delta \beta}{2}(T^2 - T_R^2) + \frac{\Delta \gamma}{3}(T^3 - T_R^3) \quad (70)$$

which is in agreement with the format of the heat capacity equation stated earlier.

4.4 Reactor Temperature as a Function of Conversion

Owing to the highly endothermic nature of the reduction reaction of SO_3 to SO_2 , the temperature decreases significantly with conversion down the length of the reactor.

An energy balance performed provides the following equation:

$$\dot{Q} - \dot{W}_s - F_{A0} \sum \theta_i \cdot C_{p_i} \cdot (T - T_0) - F_{A0} X [\Delta H_{Rx}^{\circ}(T_R) + \Delta C_p(T - T_R)] = 0 \quad (71)$$

where $\dot{Q}$ and $\dot{W}_s$ are neglected due to the absence of shaft work and the fact that the reactor is operated adiabatically. Simplification then provides the following equation:

$$-X [\Delta H_{Rx}^{\circ}(T_R) + \Delta C_p(T - T_R)] = \sum \theta_i \cdot C_{p_i} \cdot (T - T_0) \quad [W_s = 0; \dot{Q} = 0] \quad (72)$$

Solving for X, gives conversion as a function of temperature:

$$X = \frac{(\sum \theta_i \cdot C_{p_i}) \cdot (T - T_0)}{-[\Delta H_{Rx}^{\circ}(T_R) + \Delta C_p(T - T_R)]} \quad (73)$$

This equation relates conversion (X) and temperature (T) through the energy balance. In order to simplify the reactor design and to focus more on the chemical reaction kinetics, it was decided to operate the reactor adiabatically with inter-stage heating (therefore $\dot{Q}=0$).

4.5 Proposed Reactor Concept Lay-out

The proposed layout for the H_2SO_4 decomposition reactor can be seen in Figure 14. The reactor system includes one H_2SO_4 decomposer, two Pre-Heaters, and one Multi-Stage SO_3 decomposition reactor with inter-stage heating.

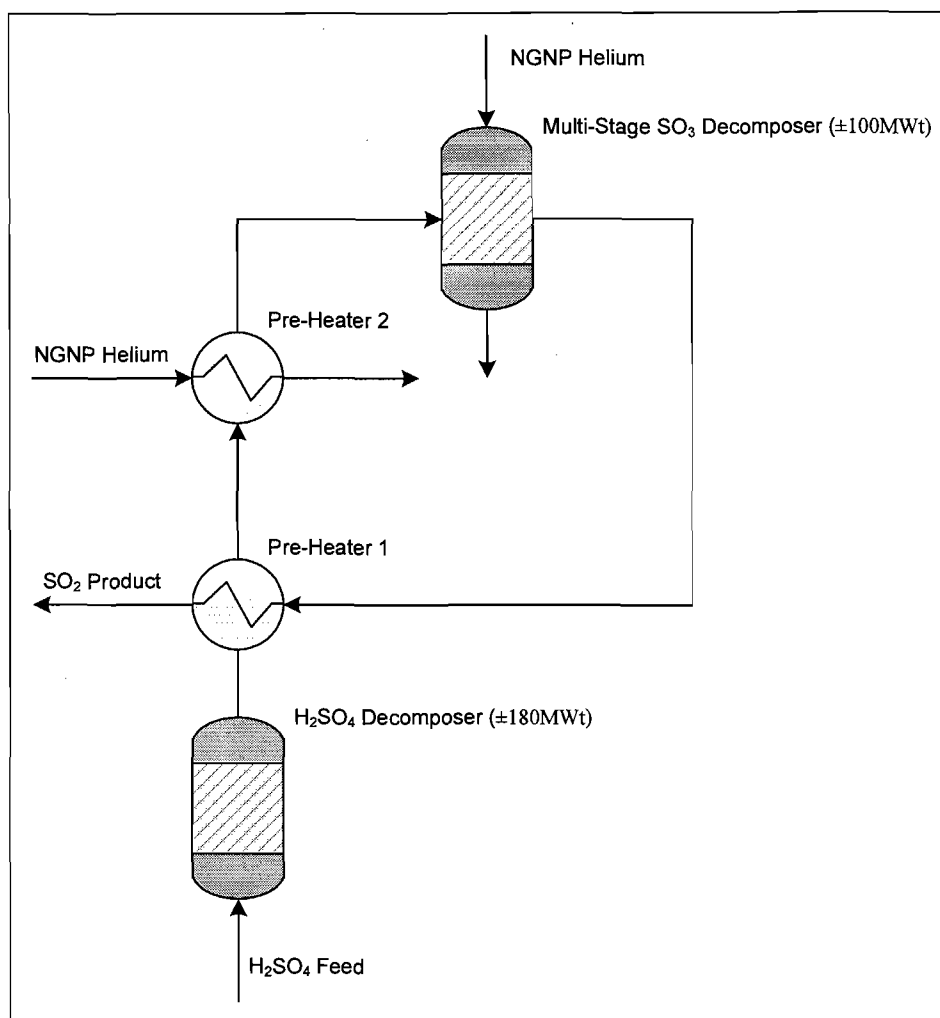


Figure 14: Proposed reactor concept

A feed consisting of 90 mol% H_2SO_4 enters the H_2SO_4 decomposer first. The reaction comprising the decomposition of H_2SO_4 to SO_3 is simplified by assuming that the two reactions can be separated, with the first decomposition reaction of H_2SO_4 to SO_3 taking place in the H_2SO_4 decomposer reactor. Further reaction could take place without the two pre-heaters. This reaction takes place in the absence of a catalyst and it can be assumed that nearly 100% decomposition could be achieved, based on equilibrium calculations when the operational temperature exceeds 700 C [21]. The total energy usage, outlet stream temperatures of the product and the helium streams, as well as the mass flow of helium consumed, to raise the product stream in the decomposer were determined, the results of which will be discussed in Chapter 5. The product stream leaving the H_2SO_4 decomposer enters Pre-Heater 1 and is heated further to 1143K in Pre-Heater 2, prior to entering the Multi-Stage SO_3 decomposition reactor. The same results as described above for the H_2SO_4 decomposer will be given

in Chapter 5 for the two pre-heaters. The feed stream leaving Pre-Heater 2 at 1143 K is introduced into the SO_3 decomposition reactor, where it is reduced to SO_2 and then proceeds on to the next process unit operation, which is the separation of SO_2 and O_2 . A schematic layout of the Multi-Stage SO_3 decomposer reactor system with inter-stage heating can be seen in Figure 15. Each of the five reactor stages were designed and data is given regarding their conversion profiles as a function of reactor volume, temperature profiles, concentration profiles of the reacting species, as well as the reaction rate profile. The volume of each of the reactor stages was calculated, to obtain 95% equilibrium conversion that can be obtained at their respective operating conditions. The mass flow of Helium required by each intermediate heat exchanger to preheat the partially converted feed stream back to 1143 K was calculated before entering the next reactor stage where subsequent conversion takes place.

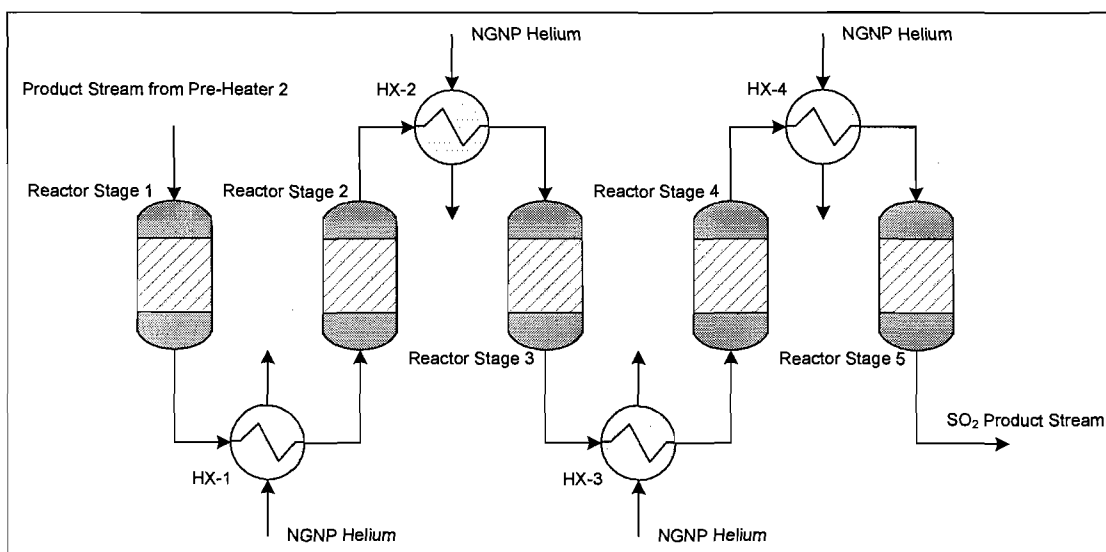


Figure 15: Multi-Stage SO_3 decomposer reactor system with intermediate heating

Chapter 5

Reactor Design Results

CHAPTER 5 Reactor Design Results

5.1 Introduction

This chapter provides the primary results of the design undertaken and displays them in table and graph format. This includes the following for each of the reactor stages:

- conversion as a function of reactor volume;
- temperature as a function of reactor volume;
- reaction rate as a function of reactor volume; and
- concentration profiles of SO_3 , SO_2 , O_2 , and H_2O as a function of reactor volume.

The data specification for the most important process units is also given, including mass and energy balances. The results obtained from Microsoft Excel and Polymath can be found in Appendix B and Appendix C.

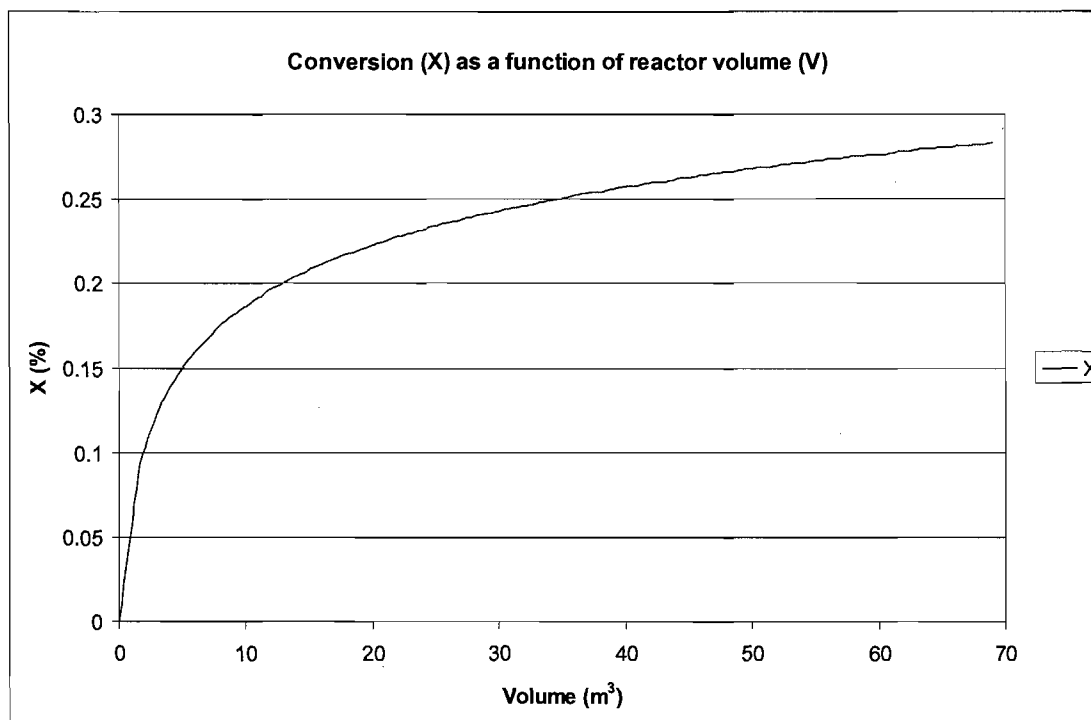
5.2 Reactor Stage Results

5.2.1 First Stage Reactor

The volumetric sizing of the first stage reactor was calculated making use of the differential equation of conversion as a function of volume as given in Chapter 4. The volumetric size was calculated by designing the reactor stage in such a manner that a 95% equilibrium conversion would be achieved corresponding to a set conversion value pre-determined from the equilibrium conversion curves of the decomposition of SO_3 to SO_2 , as shown in Chapter 3. A value of $L/D = 6$ has been assumed for reactor dimensions in Table 15.

Table 15: First stage reactor dimensions, flow rate, and space velocities, to obtain 28% conversion

Volume	69.00	m^3
Cross Sectional Area	4.701	m^2
Length	14.679	m
Diameter	2.446	m
v_0	90220	dm^3/s
Tau	0.765	s
SV	1.308	s^{-1}

**Figure 16:** Conversion as a function of reactor volume for the first stage reactor

It is evident from the equilibrium conversion curve in Figure 16 that the conversion increases sharply during the first 20m^3 of the reactor volume, where the reactant concentrations are at high temperature. From this point, the rate decreases slightly until the maximum possible conversion that could be achieved is 28.3% with a corresponding reactor stage volume of 69 m^3 .

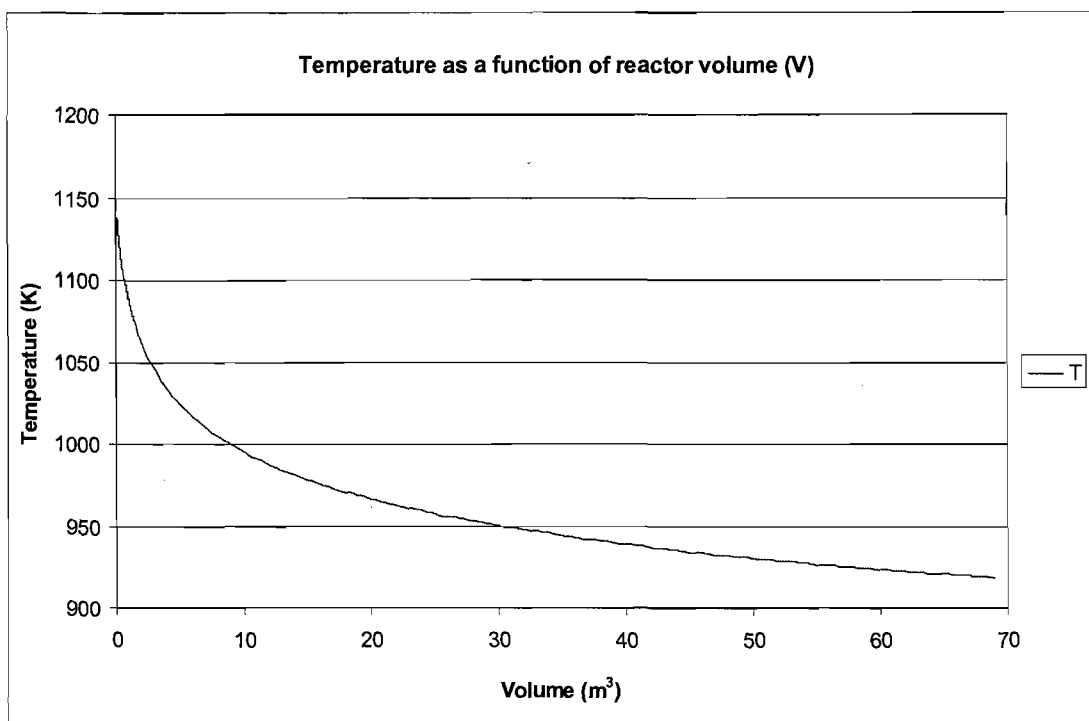


Figure 17: Temperature as a function of reactor volume for the first stage reactor

The temperature in the first stage reactor drops sharply over the first 20m³ of reactor volume because of the relatively high conversions that are achieved and the endothermic nature of the reaction as displayed in Figure 17. From this point, the temperature gradually decreases until it reaches its final stage temperature of 918 K. The total drop in temperature across the length of the first stage of the reactor is 225 K.

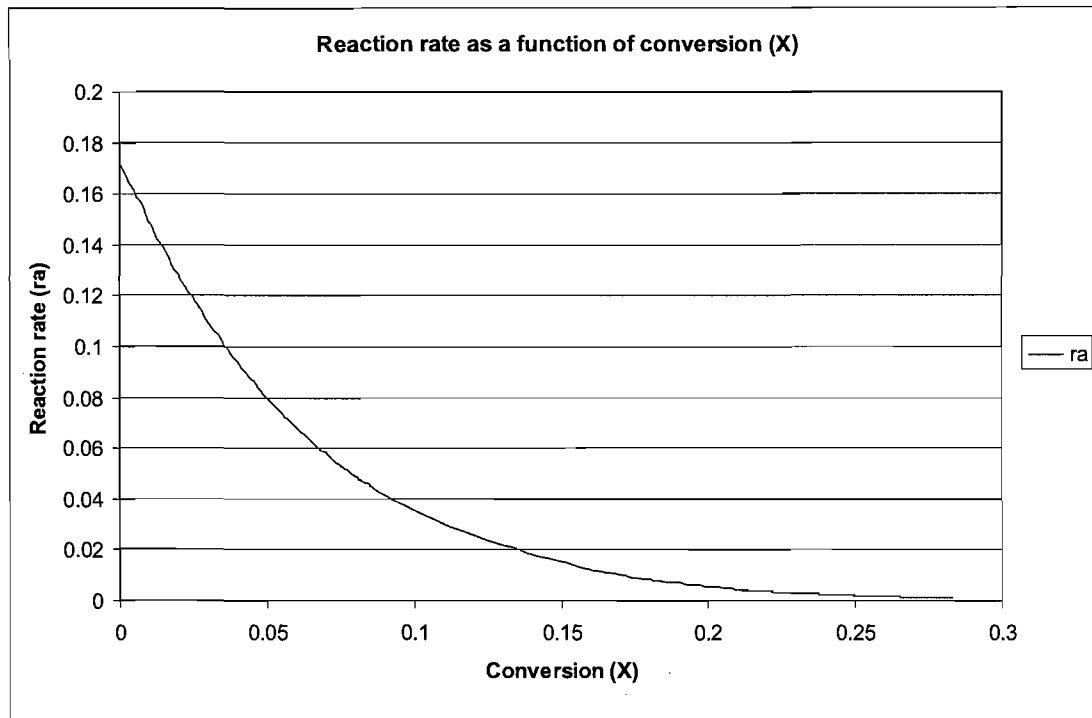


Figure 18: Reaction rate as a function of conversion for the first stage reactor

The concentration profiles of the species SO_3 , SO_2 , O_2 and H_2O can be seen in Figure 19 to Figure 22. A combined concentration profile is also included in Figure 23 to indicate how the concentration of each of the species changes with regard to each other. As can be seen, the reaction rate decreases rapidly with an increase in conversion from 0% to 15% and reaches a value of zero at an equilibrium conversion of 28.3%

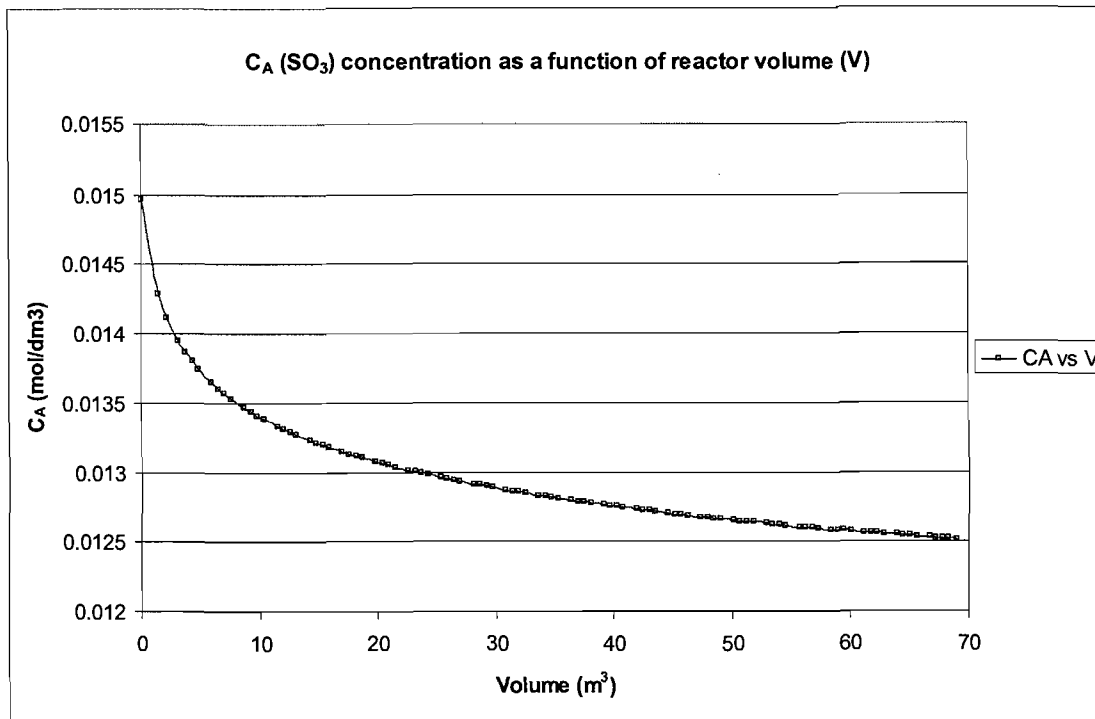


Figure 19: Concentration of SO₃ as a function of reactor volume for the first stage reactor

Decrease in SO₃ concentration with conversion of SO₃

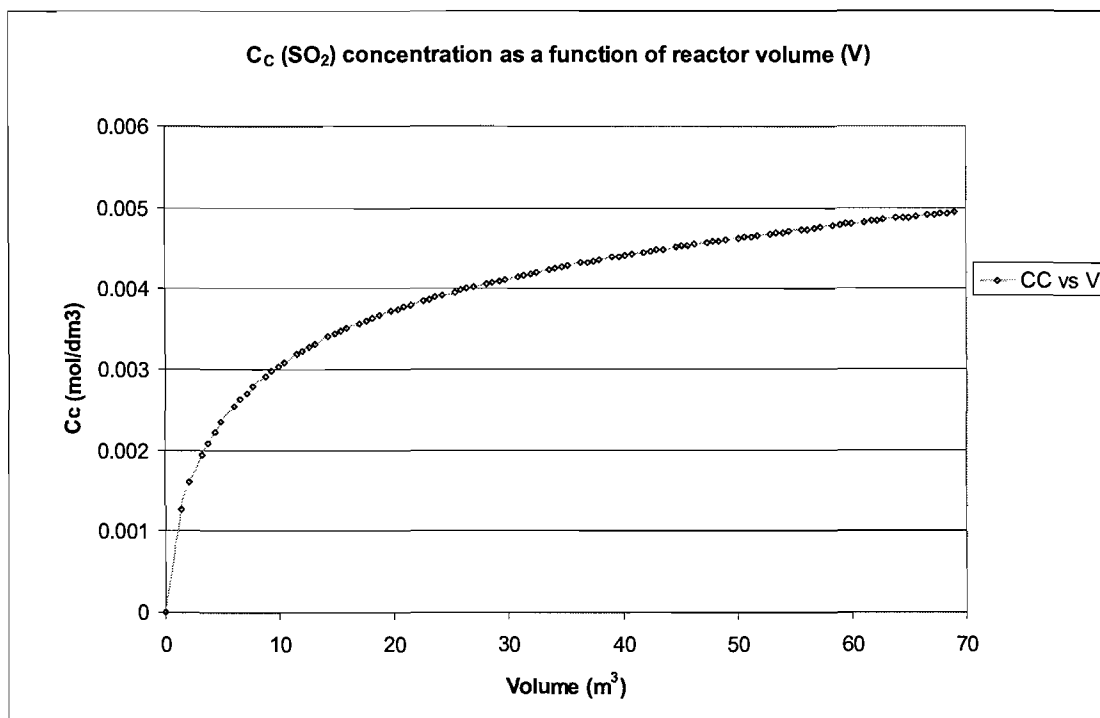


Figure 20: Concentration of SO₂ as a function of reactor volume for the first stage reactor

Increase in SO₂ concentration with conversion of SO₃

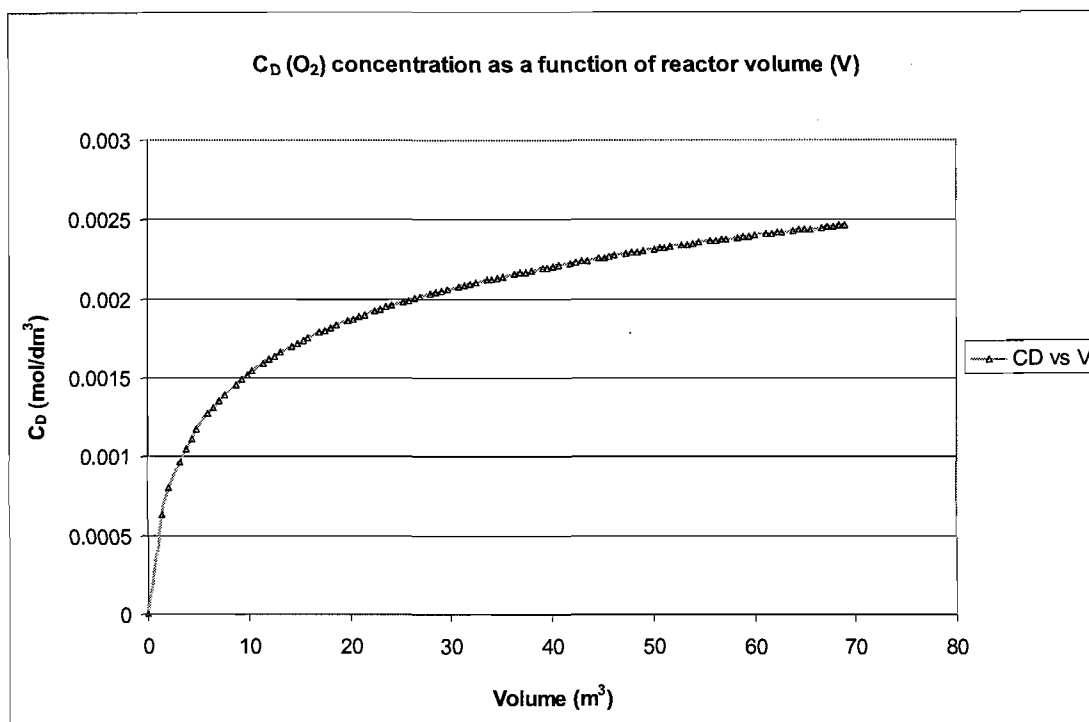


Figure 21: Concentration of O₂ as a function of reactor volume for the first stage reactor

Increase in O₂ concentration with conversion of SO₃

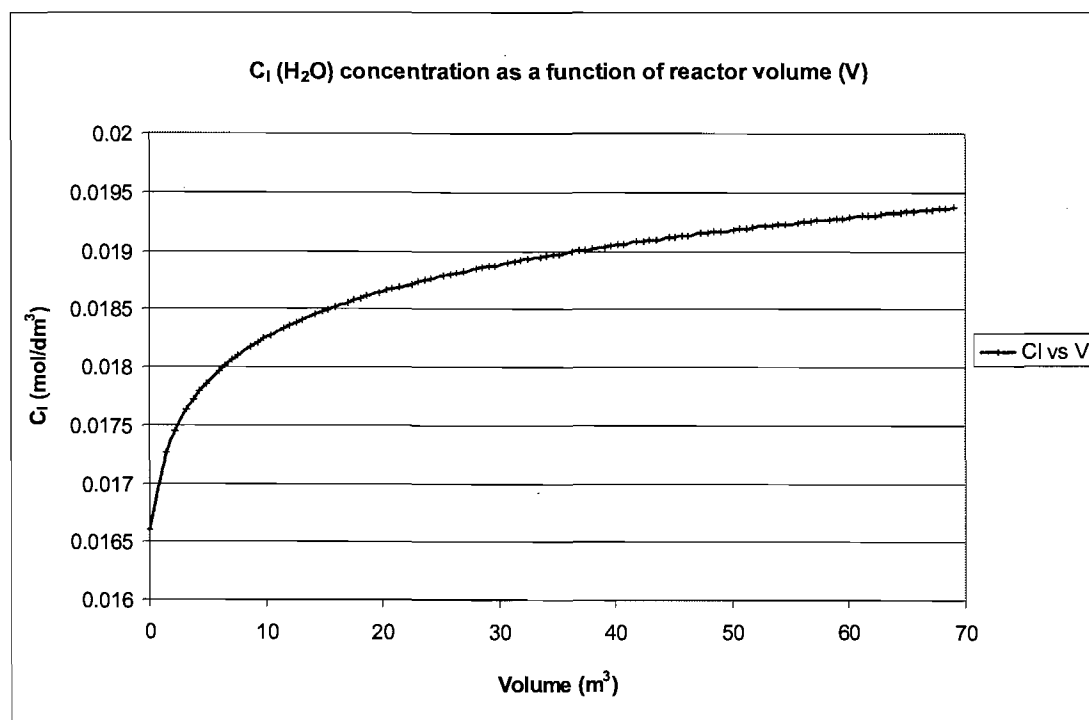


Figure 22: Concentration of H₂O as a function of reactor volume for the first stage reactor

Increase in H₂O concentration with SO₃ conversion. Although water is inert and does not partake in the reaction, its concentration increases because, although there is a

volume increase with reaction, the net result is a decrease in gas volume as a result of the drop in reaction temperature.

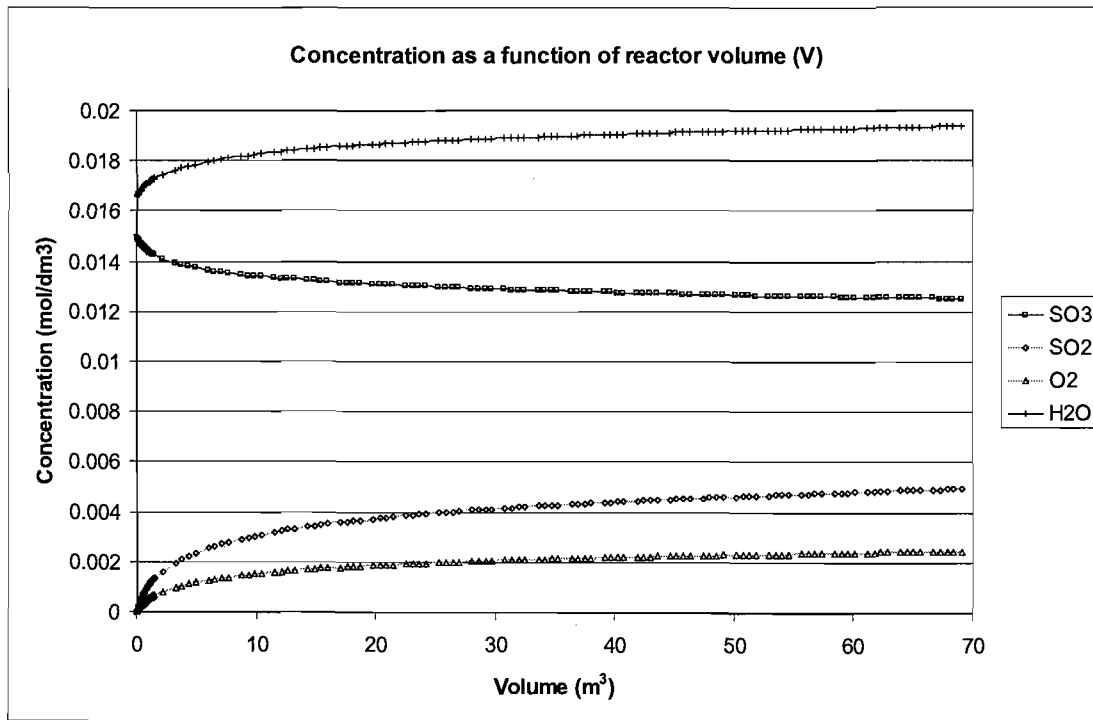


Figure 23: Concentration profile of all species as a function of reactor volume for the first stage reactor

5.2.2 Second Stage Reactor

In contrast to the first stage reactor, the second stage reactor has a significantly smaller volumetric size. The total equilibrium conversion is increased to just over 47%, which already exceeds the total equilibrium conversion that could be achieved in five reactor stages of the decomposition reactor when operating at a pressure of 90 bar. The conversion rises sharply from 28.3% to 40% at the inlet of the reactor stage and then increases gradually as it approaches equilibrium conversion at the operating temperature and pressure.

Table 16: Second stage reactor dimensions, flow rate, and space velocities

Volume	12	m ³
Cross Sectional Area	1.464592	m ²
Length	8.193409	m
Diameter	1.365568	m
v_0	96268.4	dm ³ /s
Tau	0.124652	s
SV	8.022365	s ⁻¹

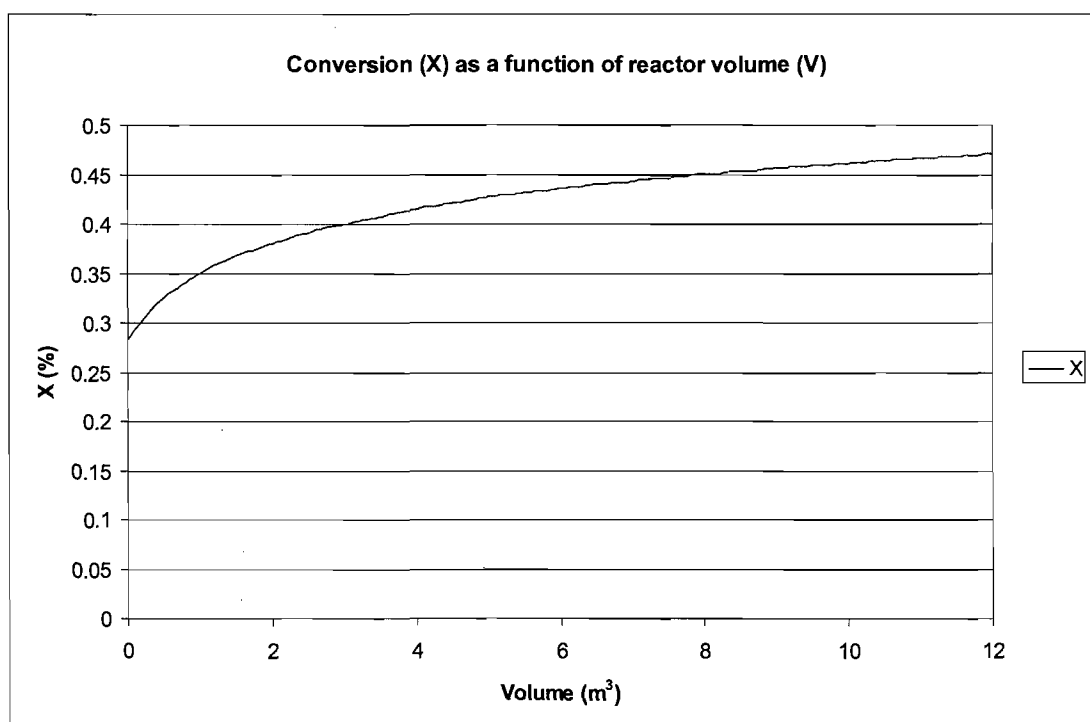


Figure 24: Conversion as a function of reactor volume of the second stage reactor

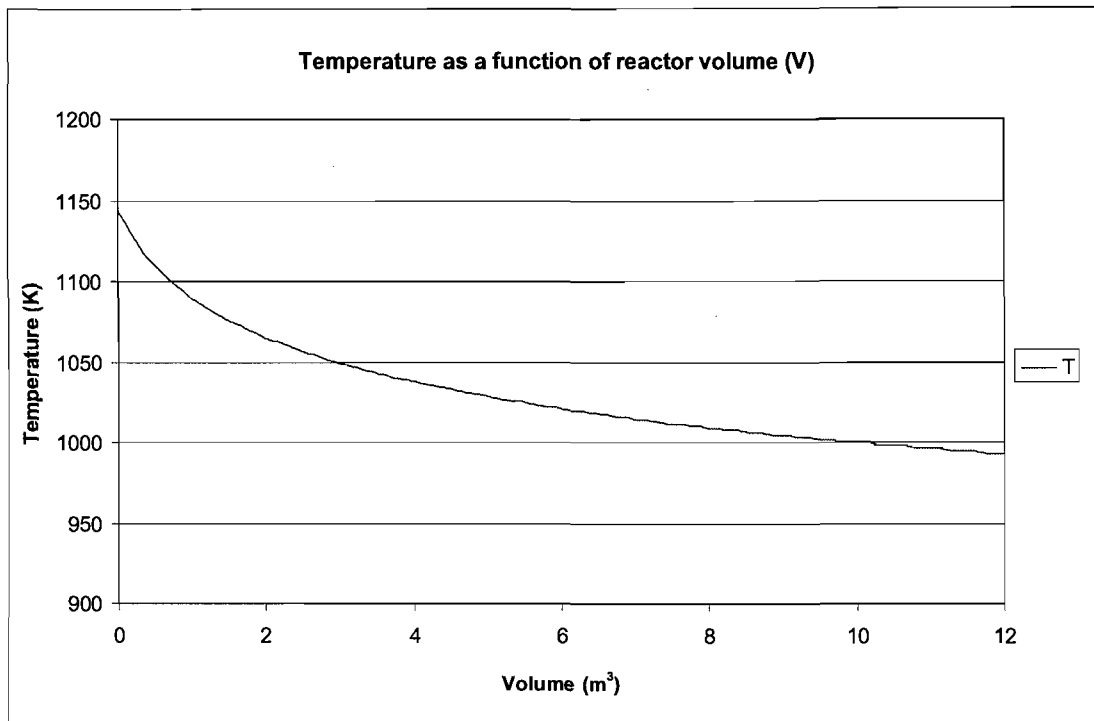


Figure 25: Temperature as a function of reactor volume for the second stage reactor

The second stage reactor experiences a more gradual decline in temperature than the first stage reactor. A total temperature drop of 151 K is achieved in comparison with the 225K in the first stage reactor. This is because of the lower conversion that has taken place compared with the first stage reactor.

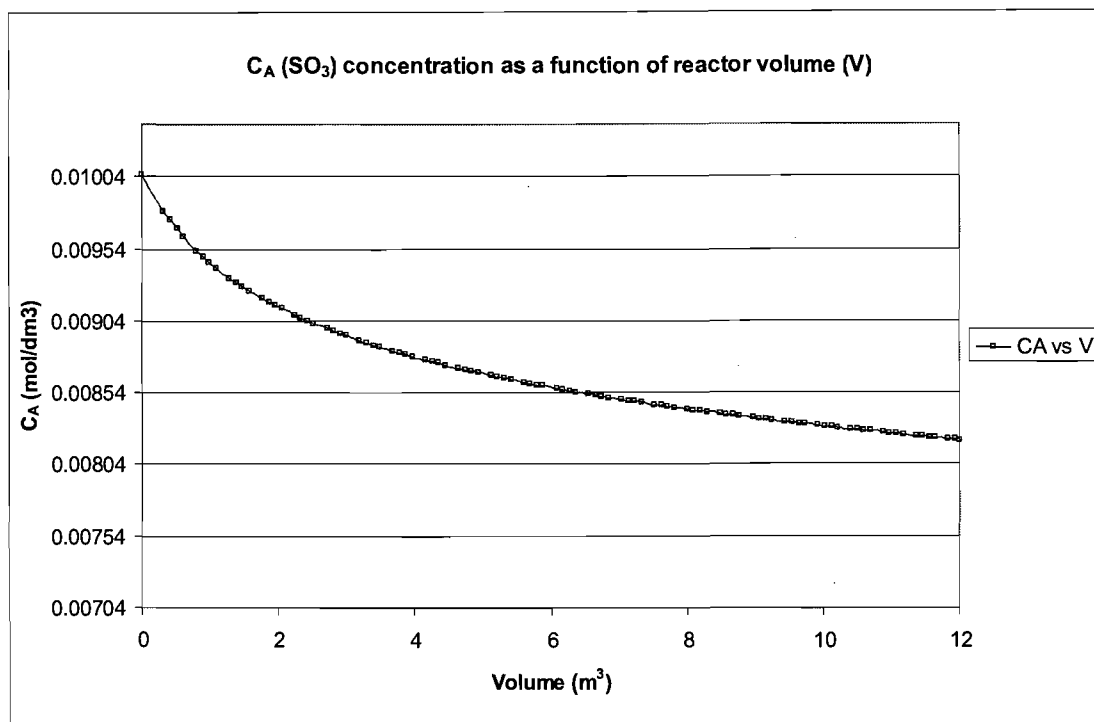


Figure 26: Concentration of SO₃ as a function of reactor volume for the second stage reactor

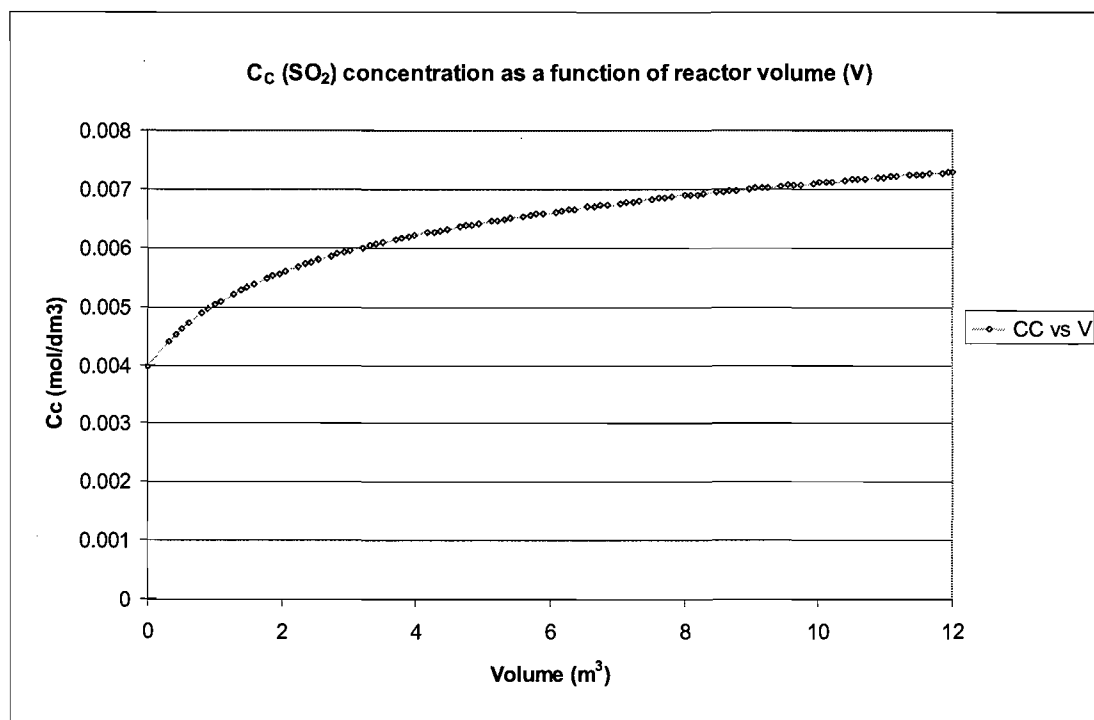


Figure 27: Concentration of SO₂ as a function of reactor volume for the second stage reactor

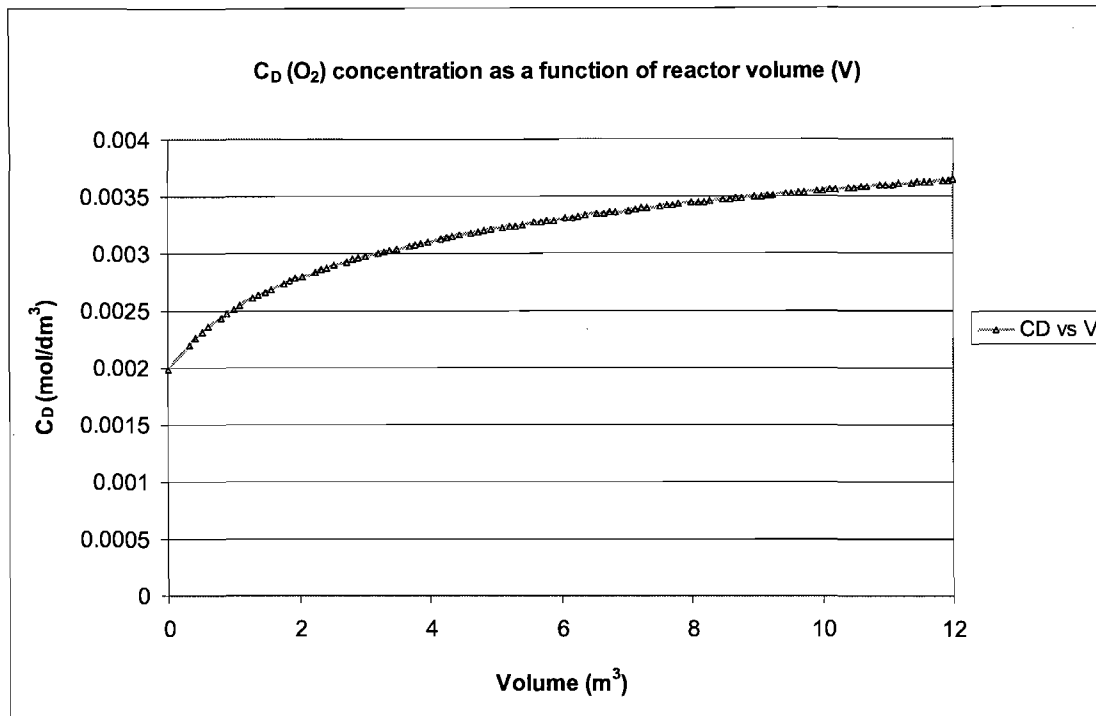


Figure 28: Concentration of O₂ as a function of reactor volume for the second stage reactor

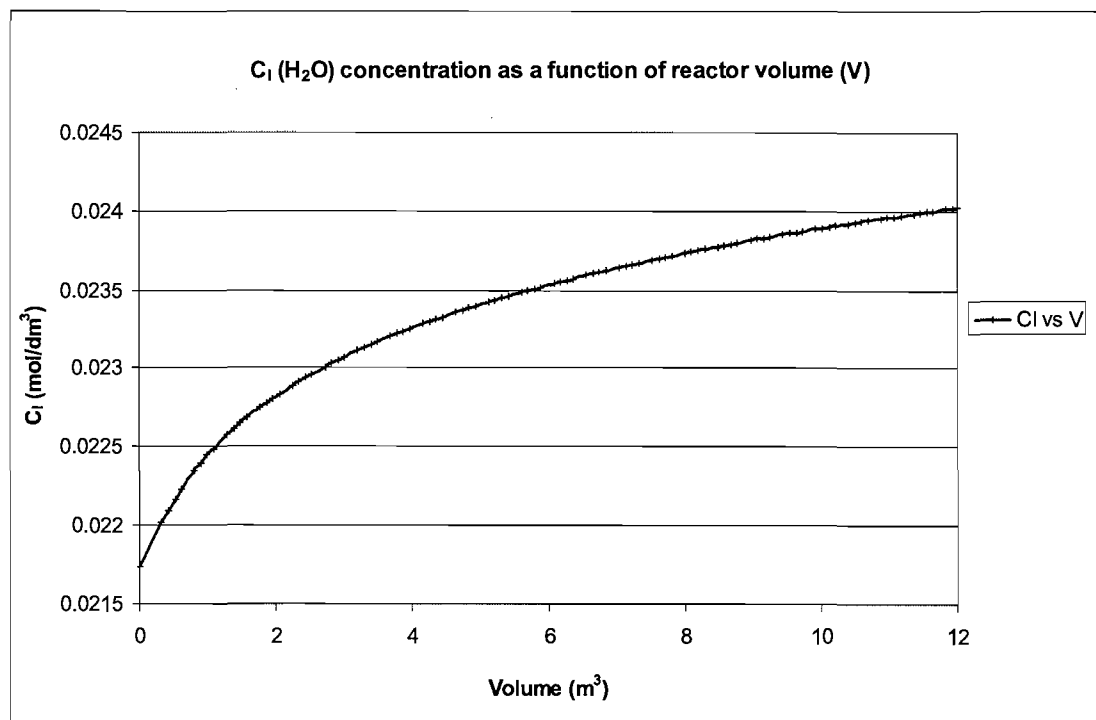


Figure 29: Concentration of H₂O as a function of reactor volume for the second stage reactor

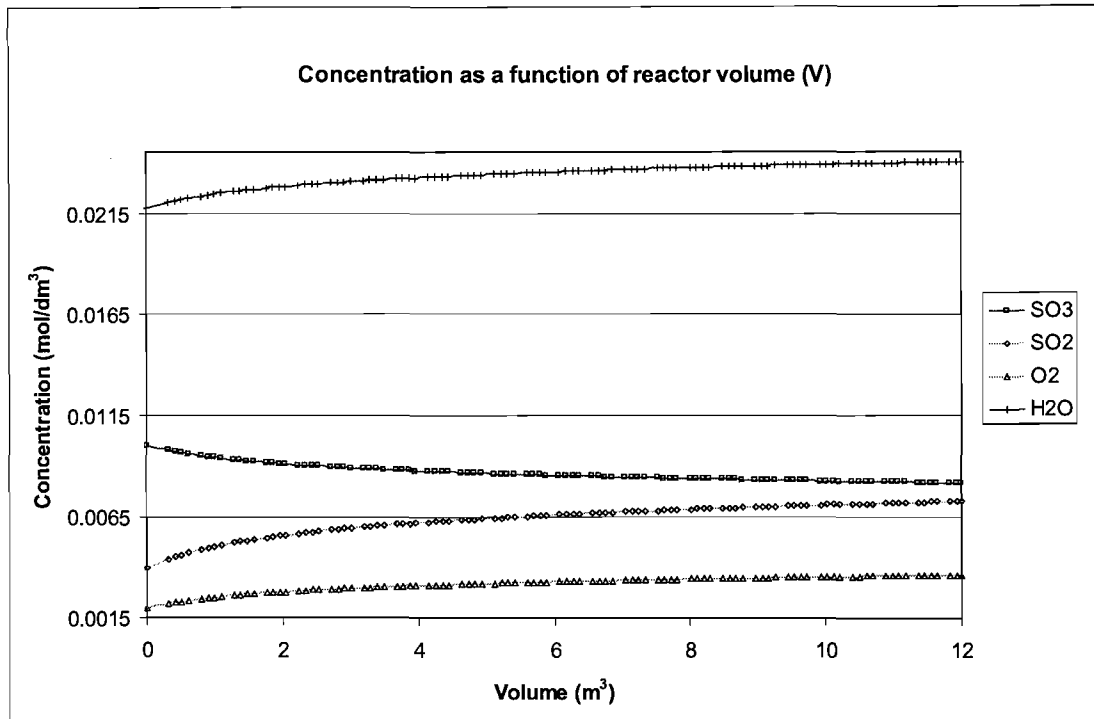


Figure 30: Concentration profile of all species as a function of reactor volume for the second stage reactor

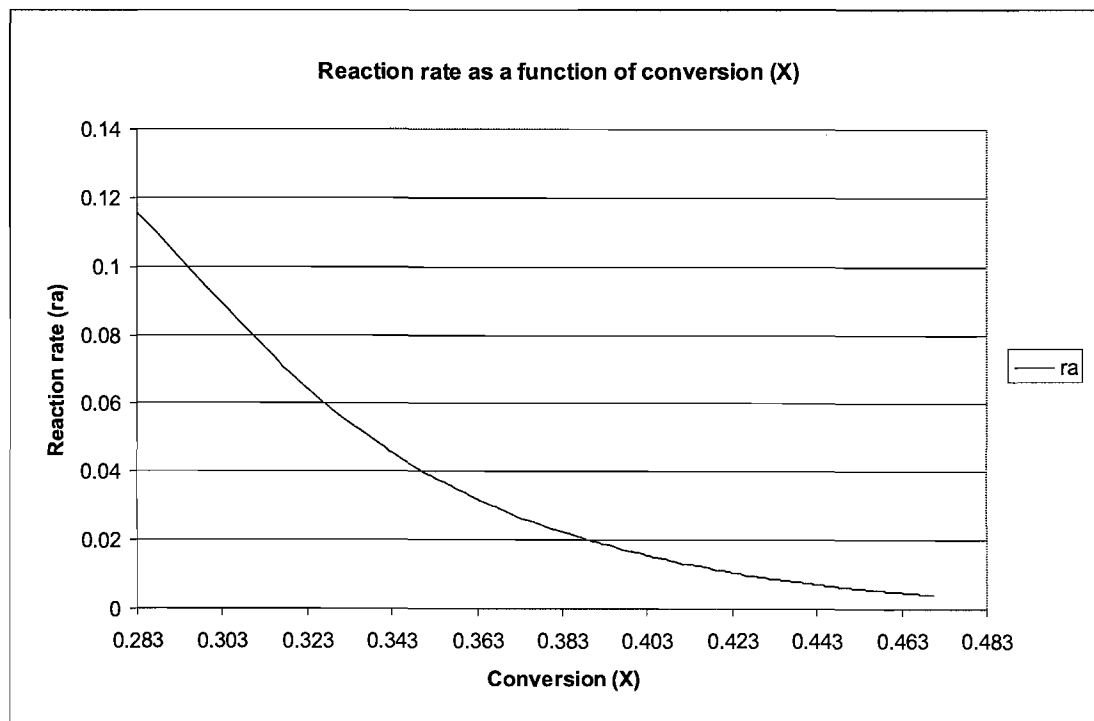


Figure 31: Reaction rate as a function of conversion for the second stage reactor

The rate of reaction decreases rapidly over the first 8% conversion taking place in the reactor and compares well with that achieved in the first stage reactor.

5.2.3 Third Stage Reactor

The third stage reactor accounts for about 12% of the total conversion achieved in the Multi-Stage reactor system and does so in a comparatively small reactor volume of only 3.66m³. This is in stark contrast to the 69m³ of the first stage reactor, which is responsible for 28.3% conversion. This is because of the higher operating temperatures in the reactor. The conversion achieved as a function of reactor volume of the third stage reactor has a very gradual slope and does not increase as sharply as across the first few m³ of reactor volume as the two previous stages.

Table 17: Third stage reactor dimensions, flow rate and space velocities

Volume	3.66	m ³
Cross Sectional Area	0.663	m ²
Length	5.51	m
Diameter	0.919	m
v₀	100266.7	dm ³ /s
Tau	0.0365	s
SV	27.393	s ⁻¹

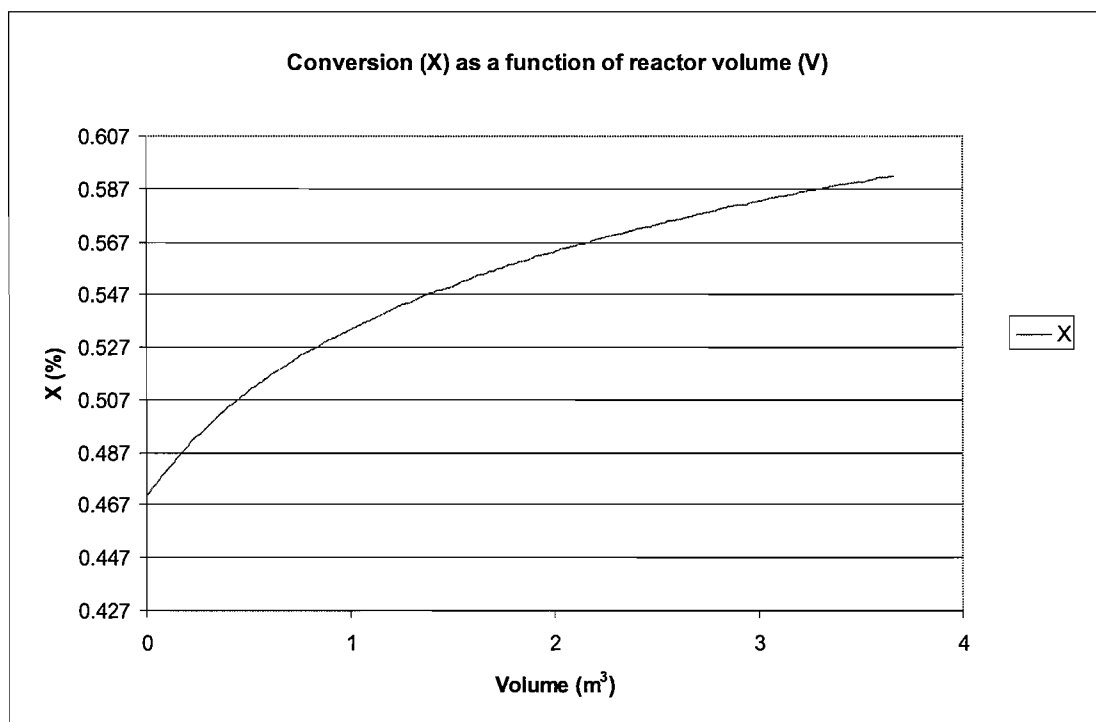


Figure 32: Conversion as a function of reactor volume of the third stage reactor

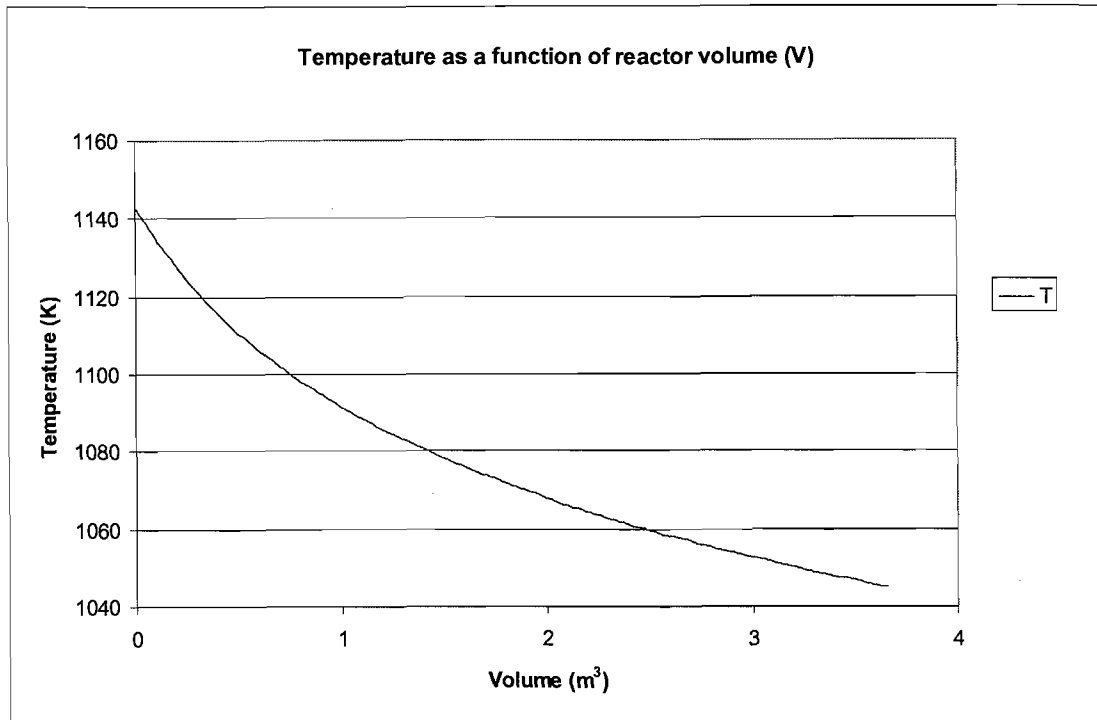


Figure 33: Temperature as a function of reactor volume for the third stage reactor

The temperature profile across the third stage reactor is also quite gradual and does not decrease dramatically. A total temperature drop of 98 K is achieved in this stage compared with the 225 K in the first stage reactor.

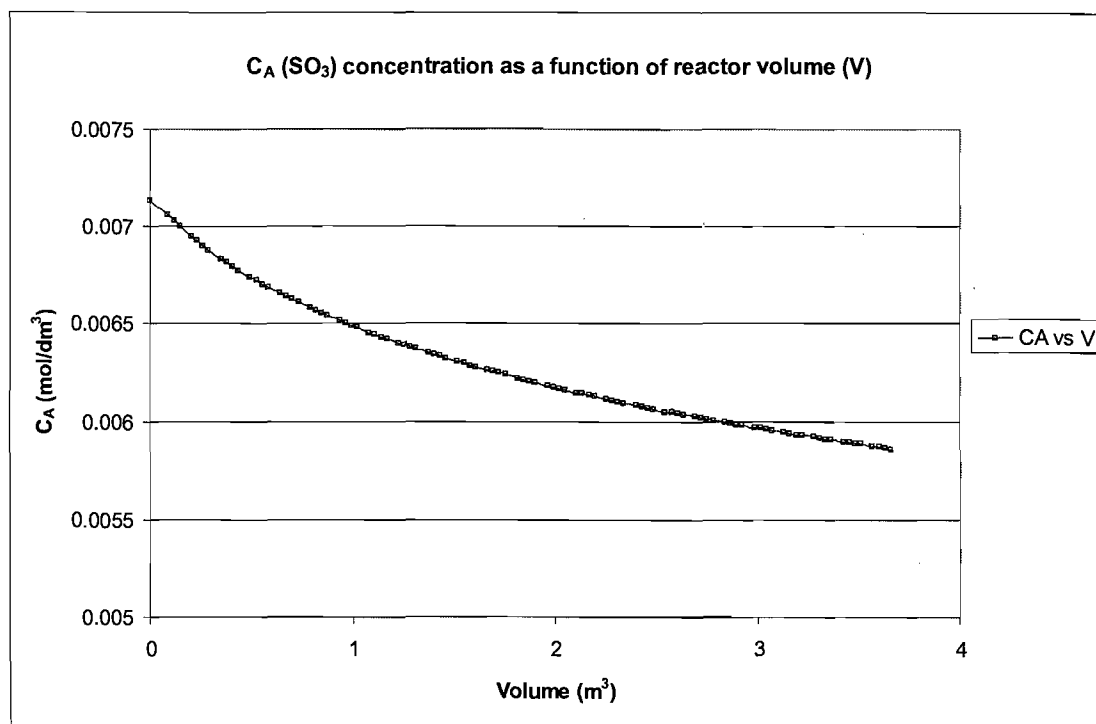


Figure 34: Concentration of SO_3 as a function of reactor volume for the third stage reactor

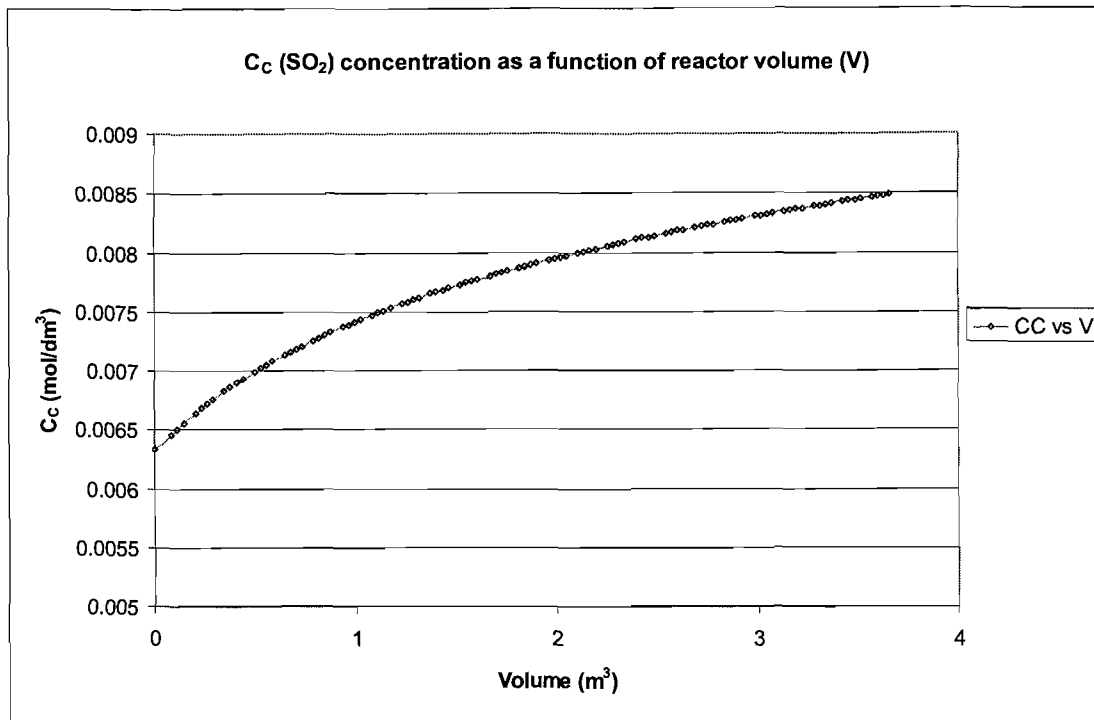


Figure 35: Concentration of SO₂ as a function of reactor volume for the third stage reactor

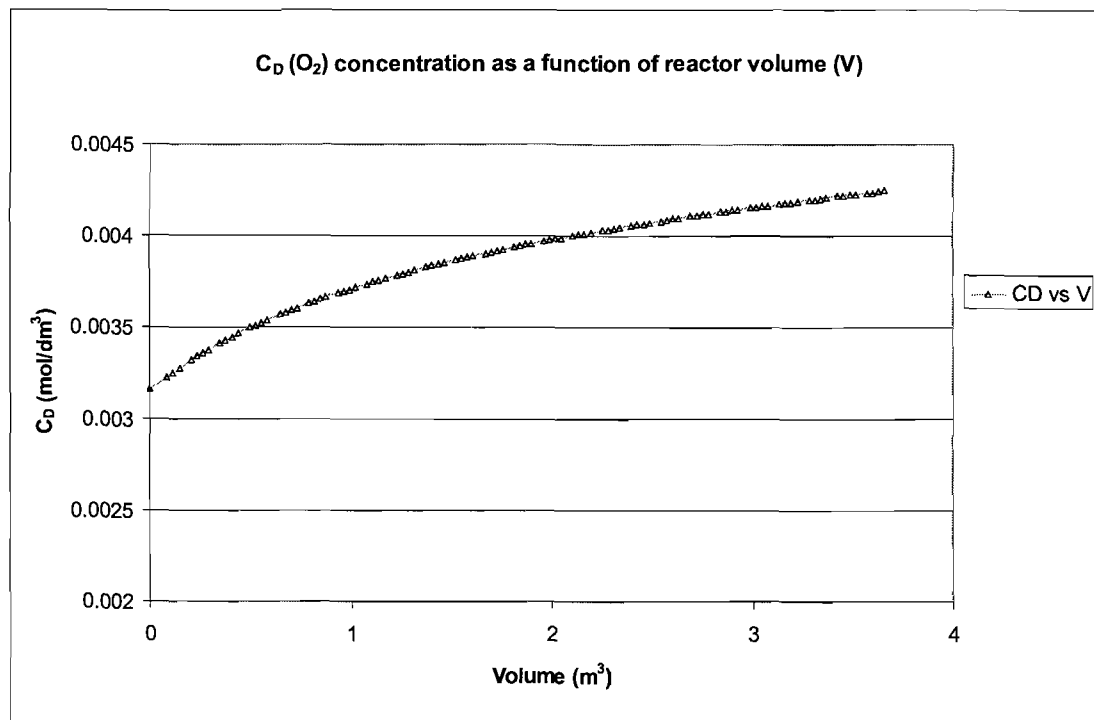


Figure 36: Concentration of O₂ as a function of reactor volume for the third stage reactor

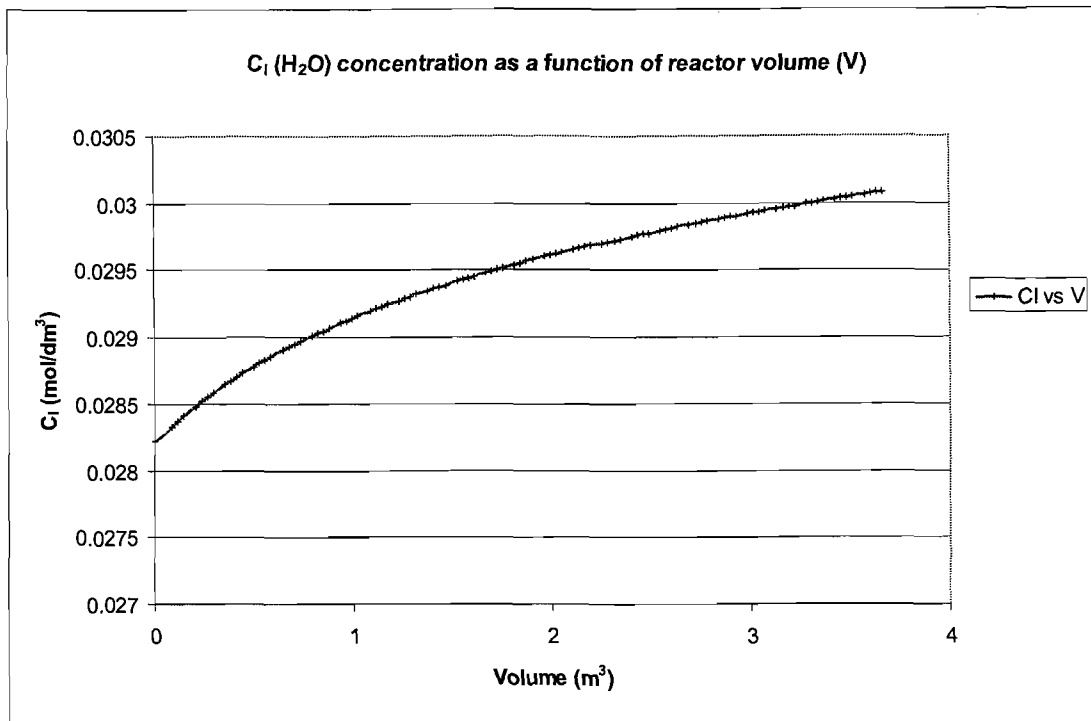


Figure 37: Concentration of H₂O as a function of reactor volume for the third stage reactor

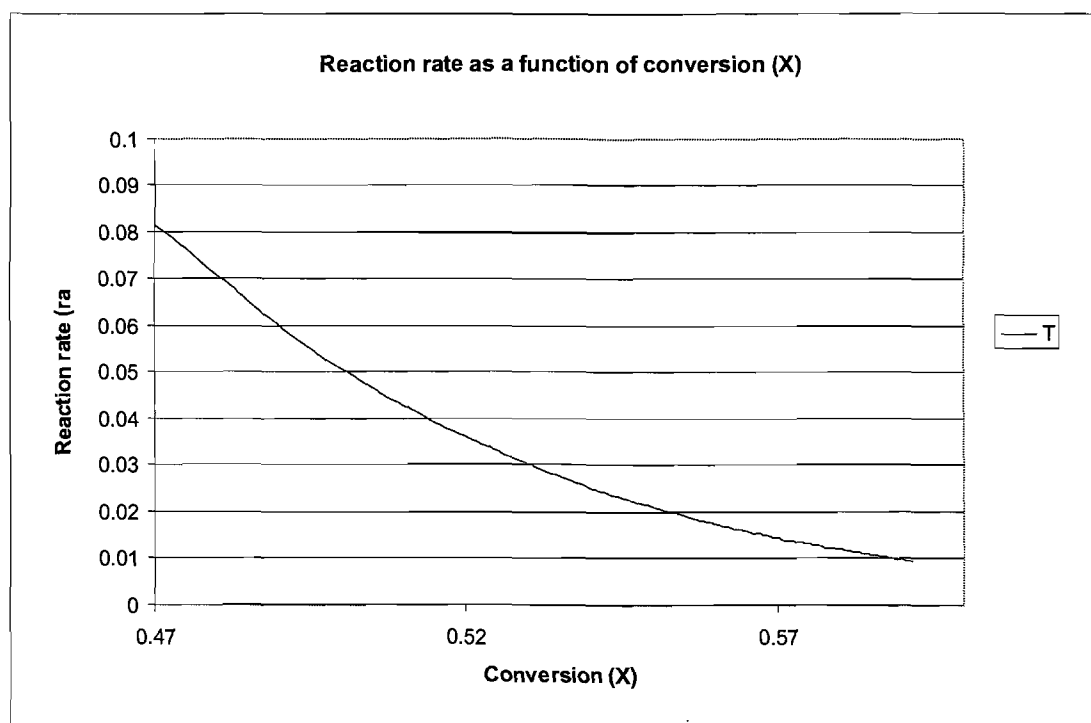


Figure 38: Reaction rate as a function of conversion for the third stage reactor

The reaction rate can also be seen to have decreased compared with the previous two stages with regard to its initial rate levels because of the decrease in the concentration of the reacting species. The decrease in the reaction rate is not as substantial compared

with that of the first stage because of the higher operating temperatures that persist in the reaction. It is evident that the reaction rate is highly dependent on the temperature within the reactor stages.

5.2.4 Fourth Stage Reactor

As expected the fourth stage reactor volume decreased even more compared with the volume of the third stage reactor. With a volume of only 1.52 m^3 , the fourth stage reactor is responsible for a total conversion of approximately 8%.

Table 18: Fourth stage reactor dimensions, flow rate and space velocities

Volume	1.525	m^3
Cross Sectional Area	0.371	m^2
Length	4.119	m
Diameter	0.686	m
v_0	102875.3	dm^3/s
Tau	0.014825	s
SV	67.451	s^{-1}

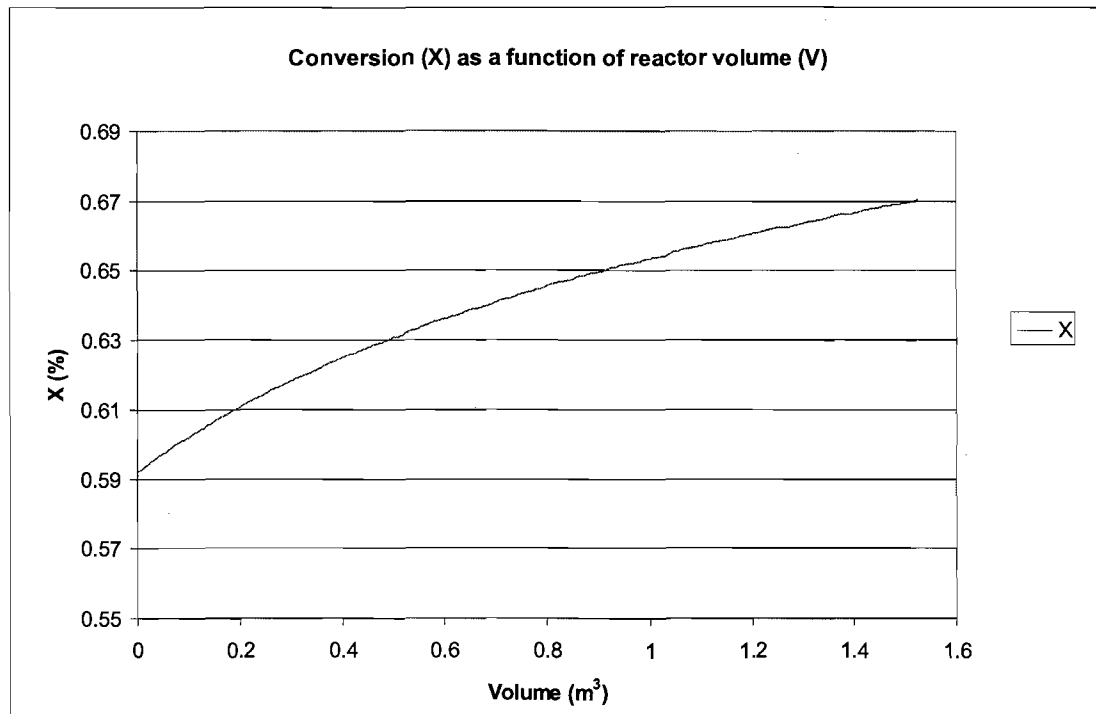


Figure 39: Conversion as a function of reactor volume of the fourth stage reactor

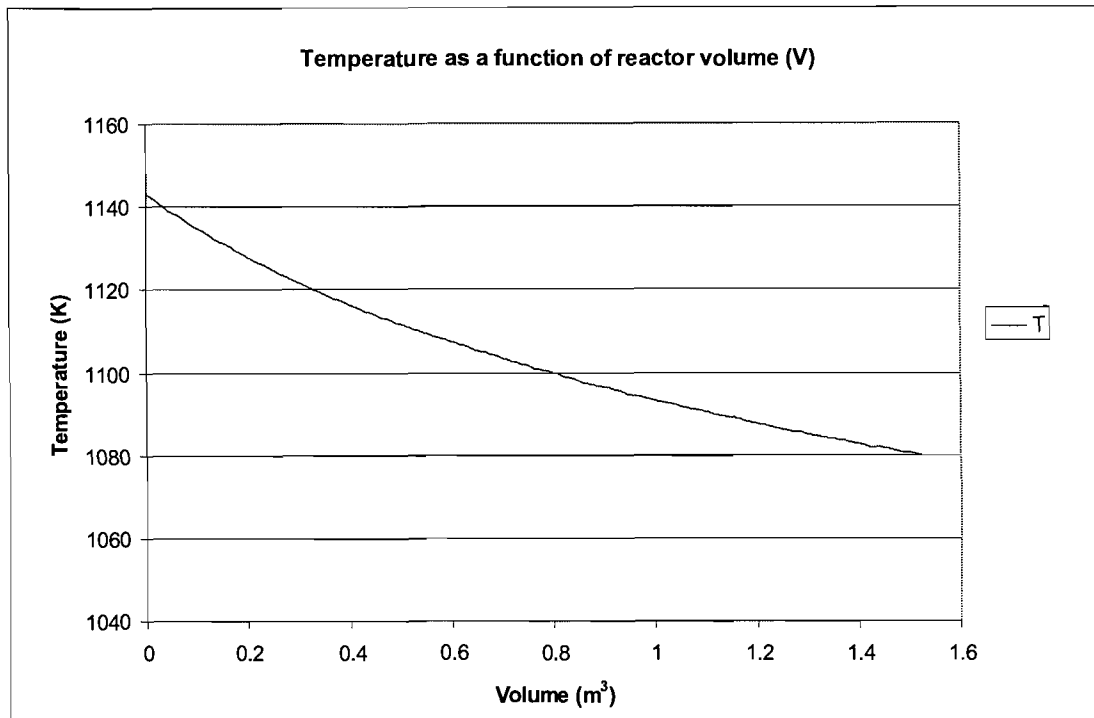


Figure 40: Temperature as a function of reactor volume for the fourth stage reactor

It is evident from Figure 40 that a temperature drop of 63 K is achieved across the fourth stage reactor. The temperature profile is very gradual, and it is expected that this tendency will increase with greater manifestation in the final reactor stage.

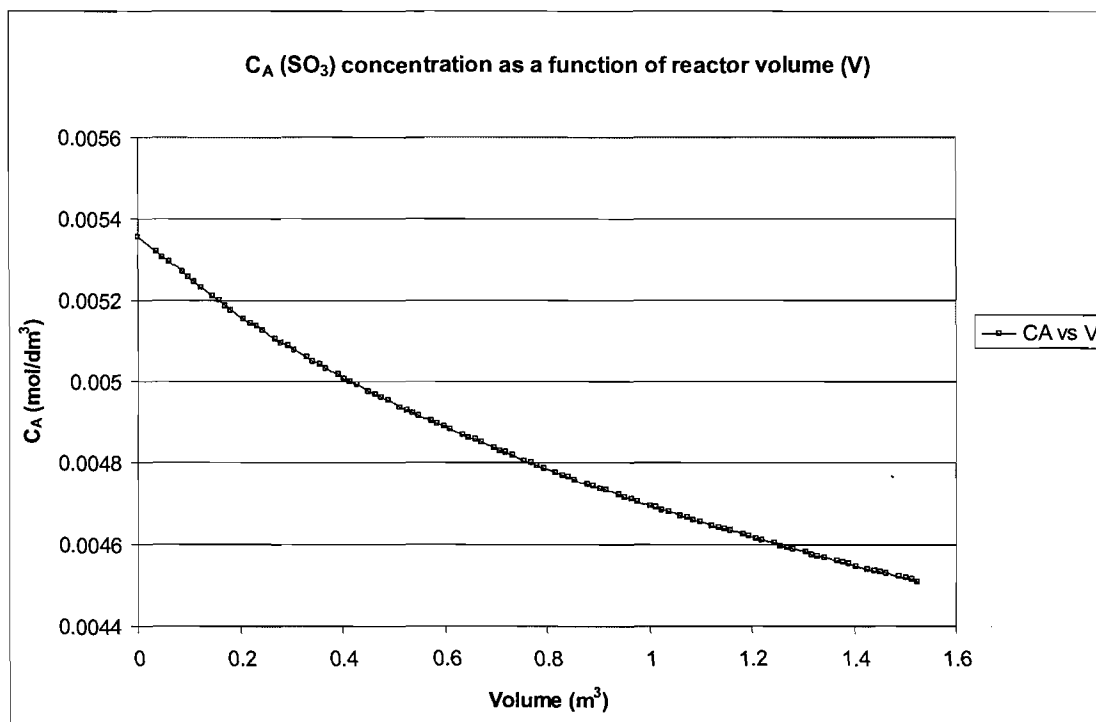


Figure 41: Concentration of SO_3 as a function of reactor volume for the fourth stage reactor

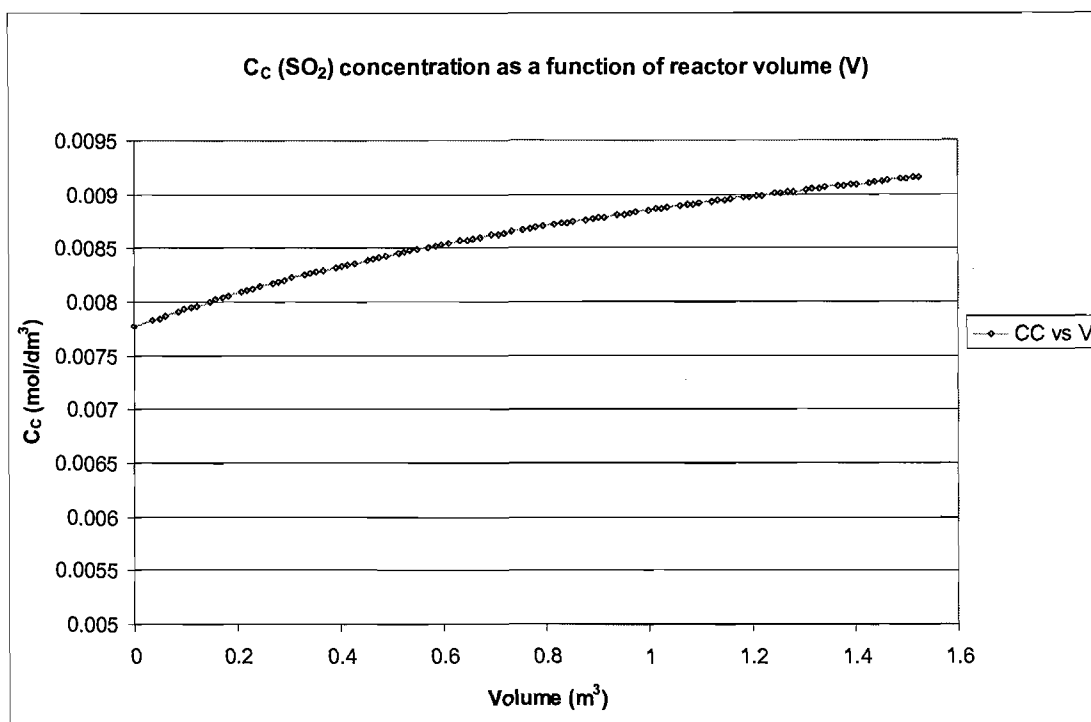


Figure 42: Concentration of SO_2 as a function of reactor volume for the fourth stage reactor

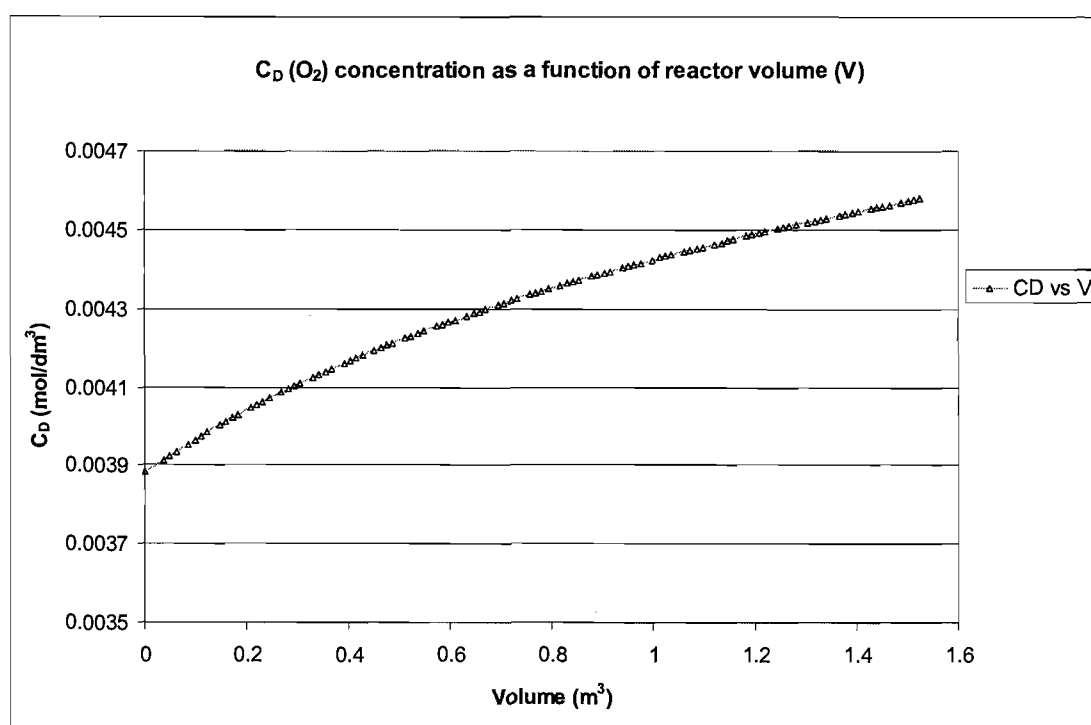


Figure 43: Concentration of O_2 as a function of reactor volume for the fourth stage reactor

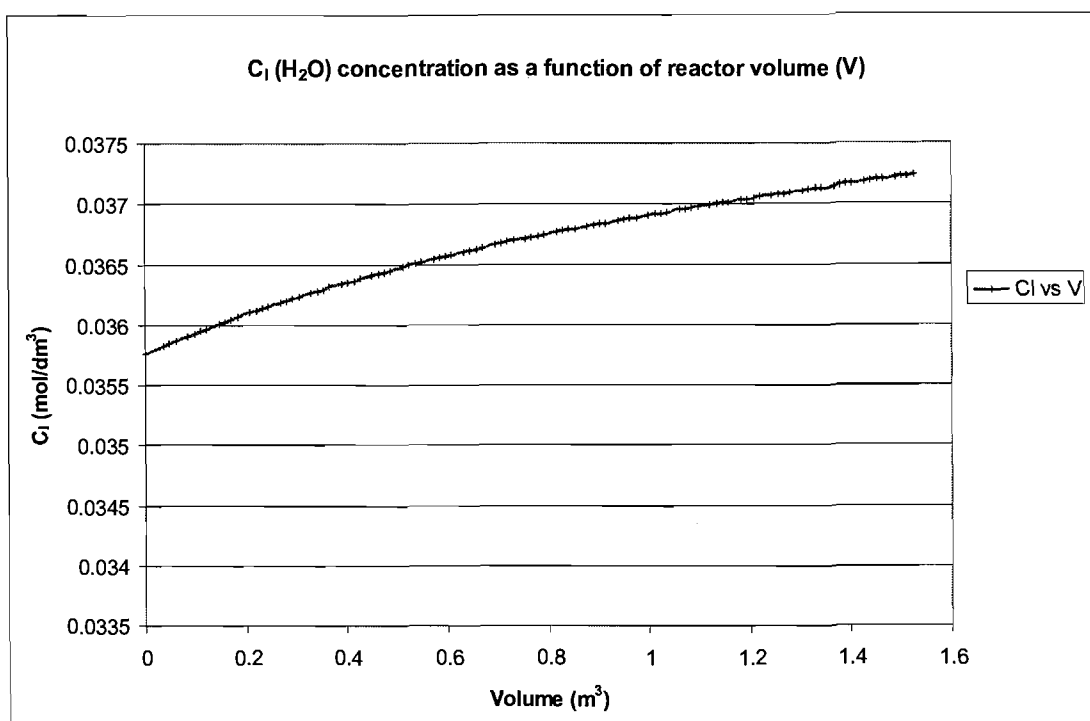


Figure 44: Concentration of H_2O as a function of reactor volume for the fourth stage reactor

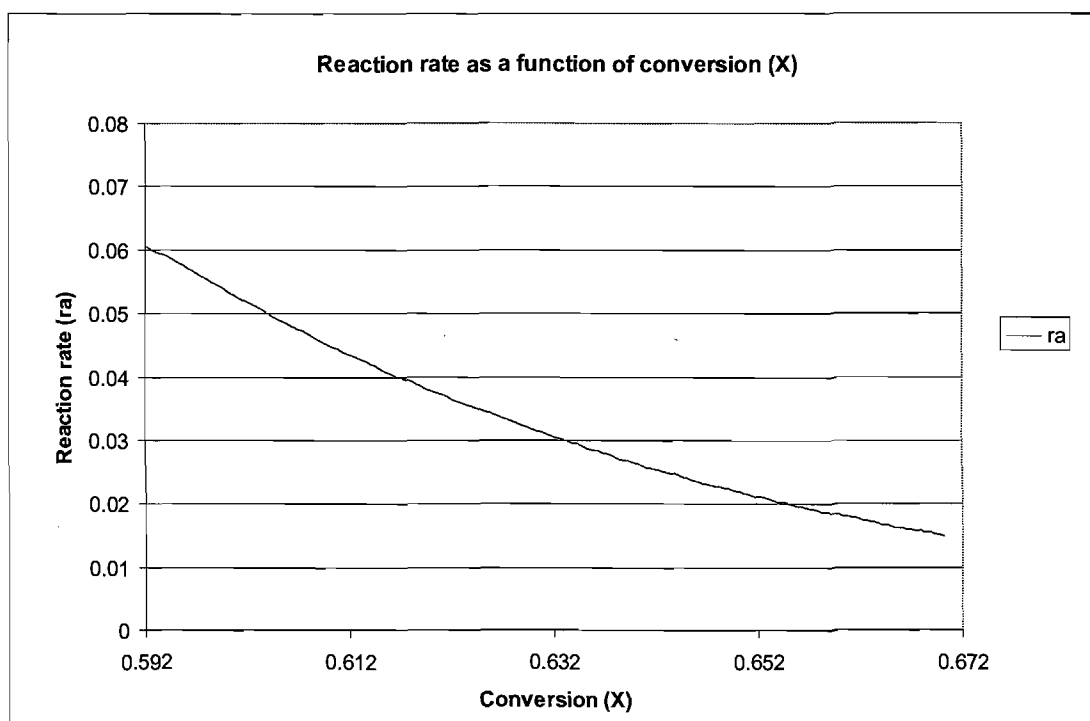


Figure 45: Reaction rate as a function of conversion for the fourth stage reactor

5.2.5 Fifth Stage Reactor

The fifth stage reactor is the smallest of the five reactor stages with regard to its volumetric size and dimensions. Even though it is responsible for contributing only 5% of the total conversion achieved in the reactor system, this percentage is critical in light of the impact it has on the overall viability of the reactor system, and can have a major influence on the general success of the operation. It can be seen from Figure 46 that the characteristic sharp increase in conversion for the initial few m^3 as displayed in Figure 16 of the first reactor stage is now completely absent. In contrast, the conversion increases at virtually a constant rate per m^3 of reactor volume.

Table 19: Fifth stage reactor dimensions, flow rate, and space velocities

Volume	0.760	m^3
Cross Sectional Area	0.232	m^2
Length	3.266	m
Diameter	0.544	m
v_0	104543	dm^3/s
Tau	0.007271	s
SV	137.537	s^{-1}

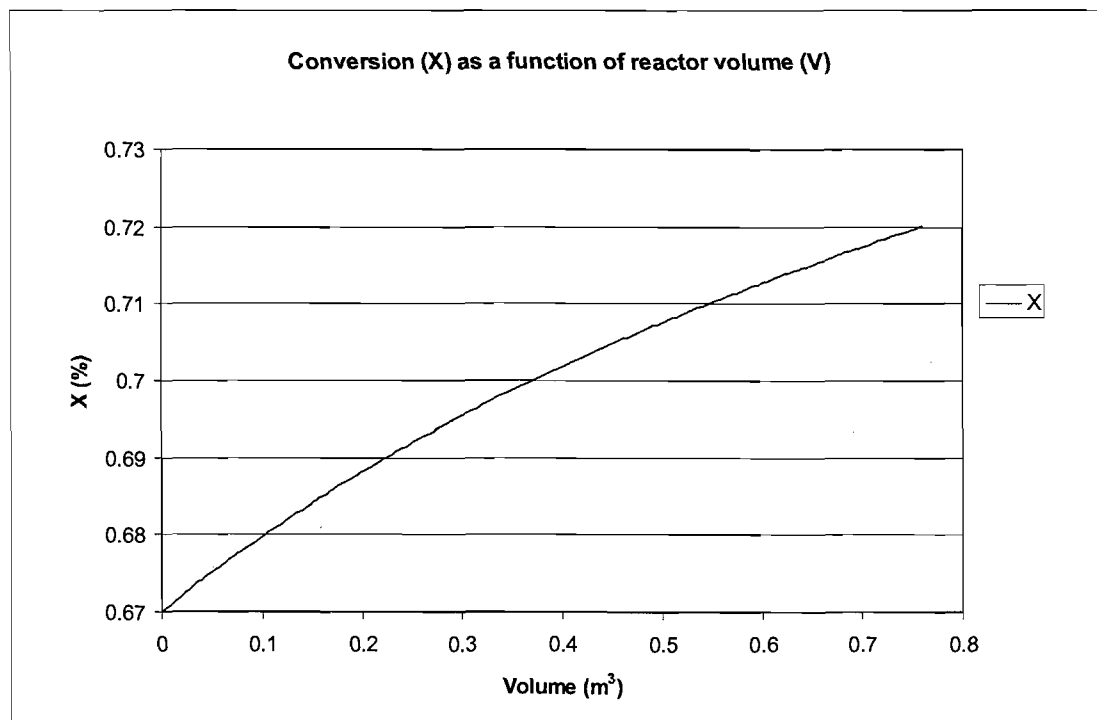


Figure 46: Conversion as a function of reactor volume of the fifth stage reactor

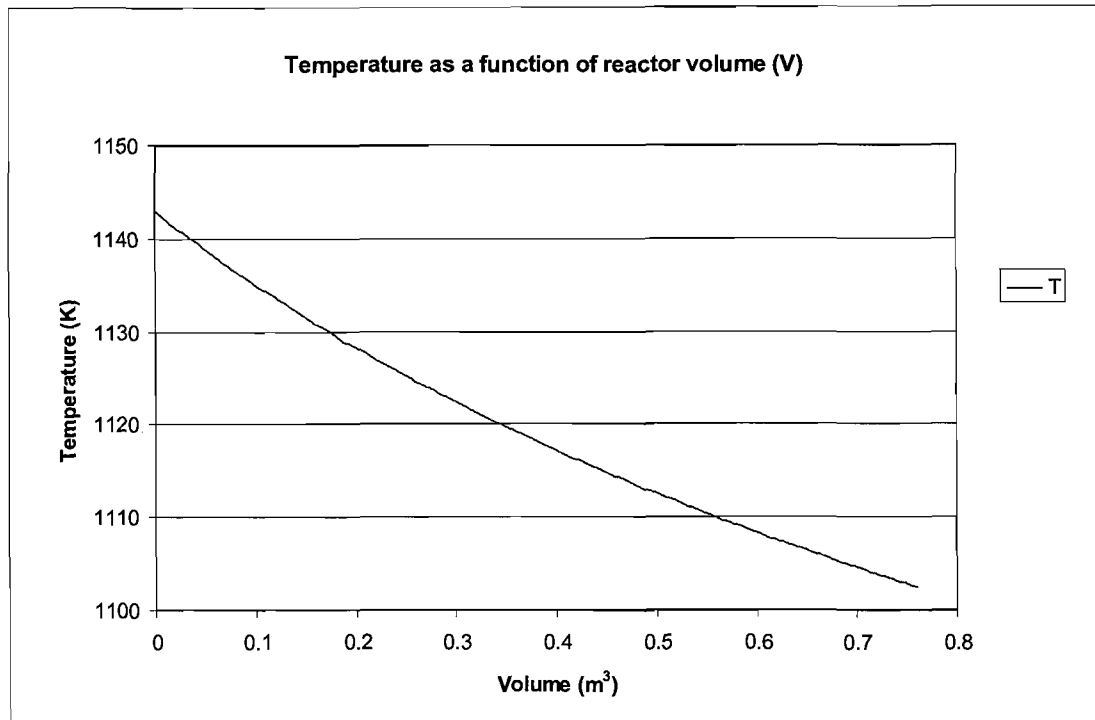


Figure 47: Temperature as a function of reactor volume for the fifth stage reactor

The temperature profile practically assumes a constant declining gradient with a total temperature drop of only 41 K in comparison with the 225 K temperature drop in the first reactor stage.

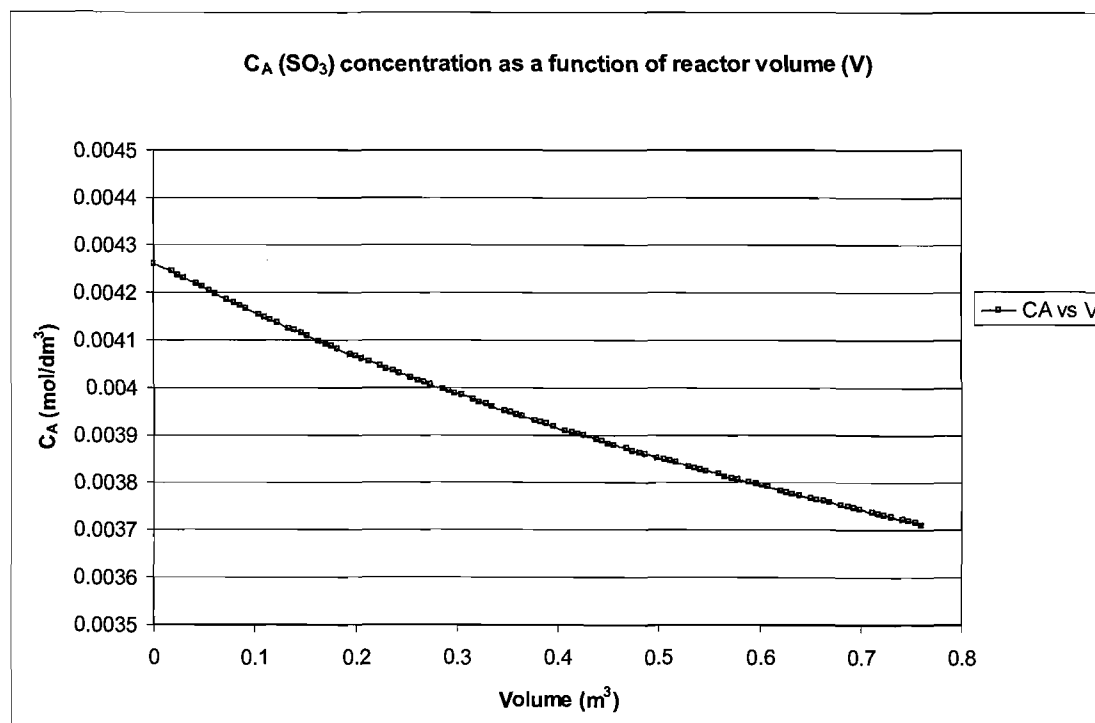


Figure 48: Concentration of SO_3 as a function of reactor volume for the fifth stage reactor

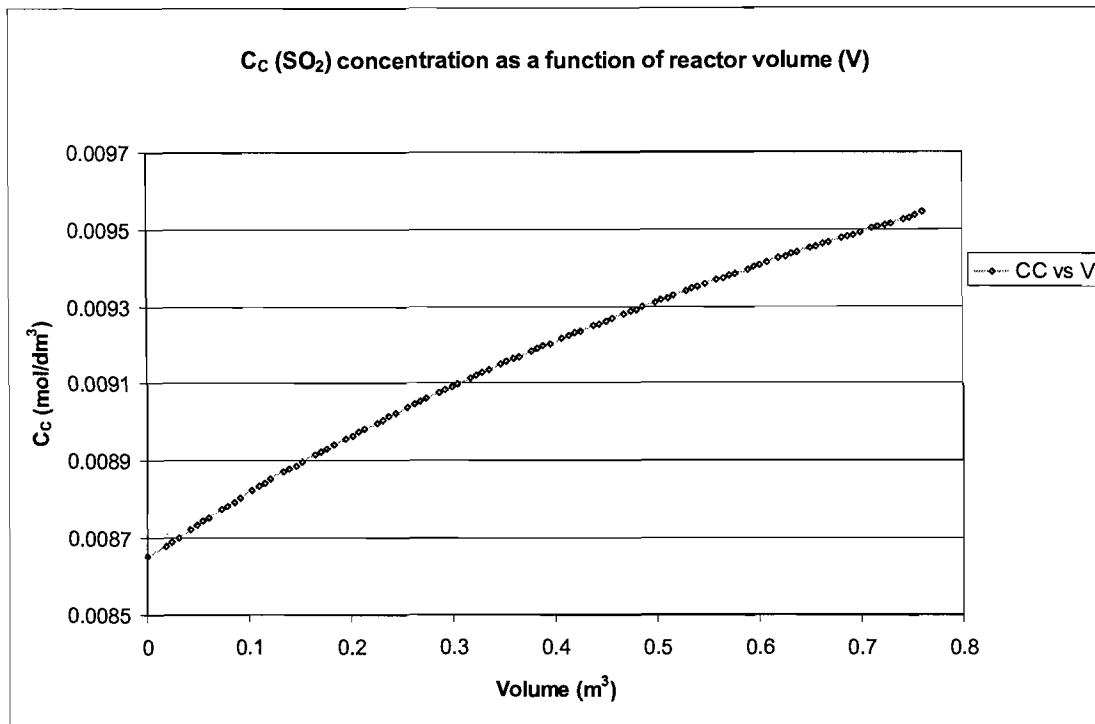


Figure 49: Concentration of SO_2 as a function of reactor volume for the fifth stage reactor

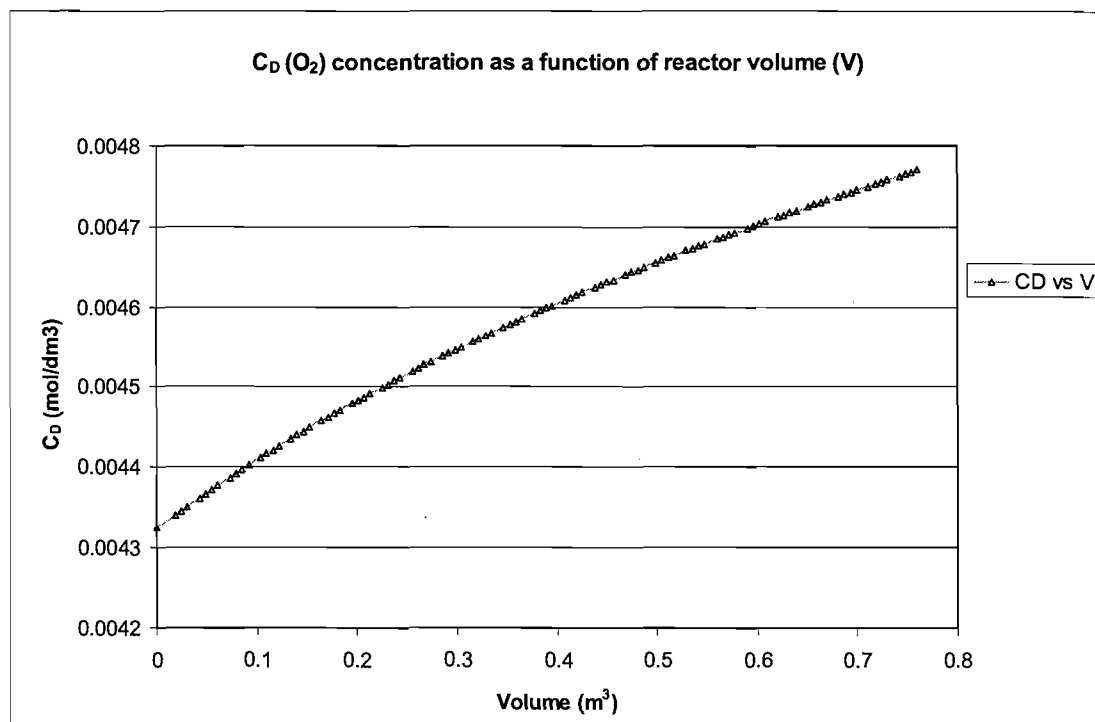


Figure 50: Concentration of O_2 as a function of reactor volume for the fifth stage reactor

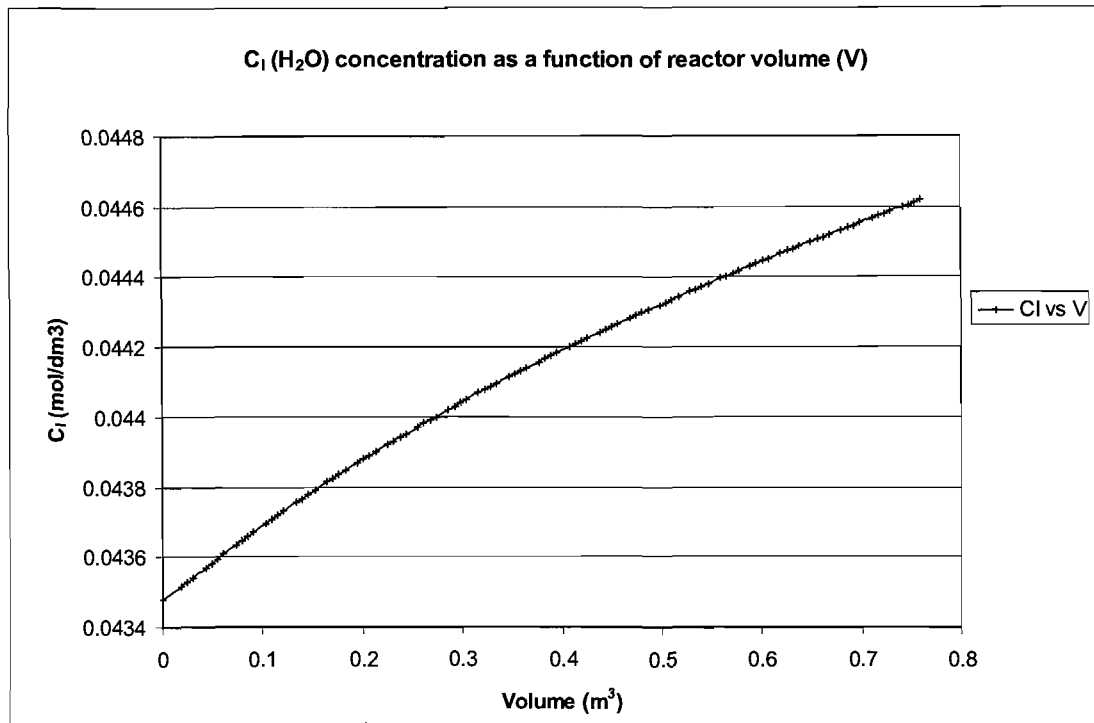


Figure 51: Concentration of H_2O as a function of reactor volume for the fifth stage reactor

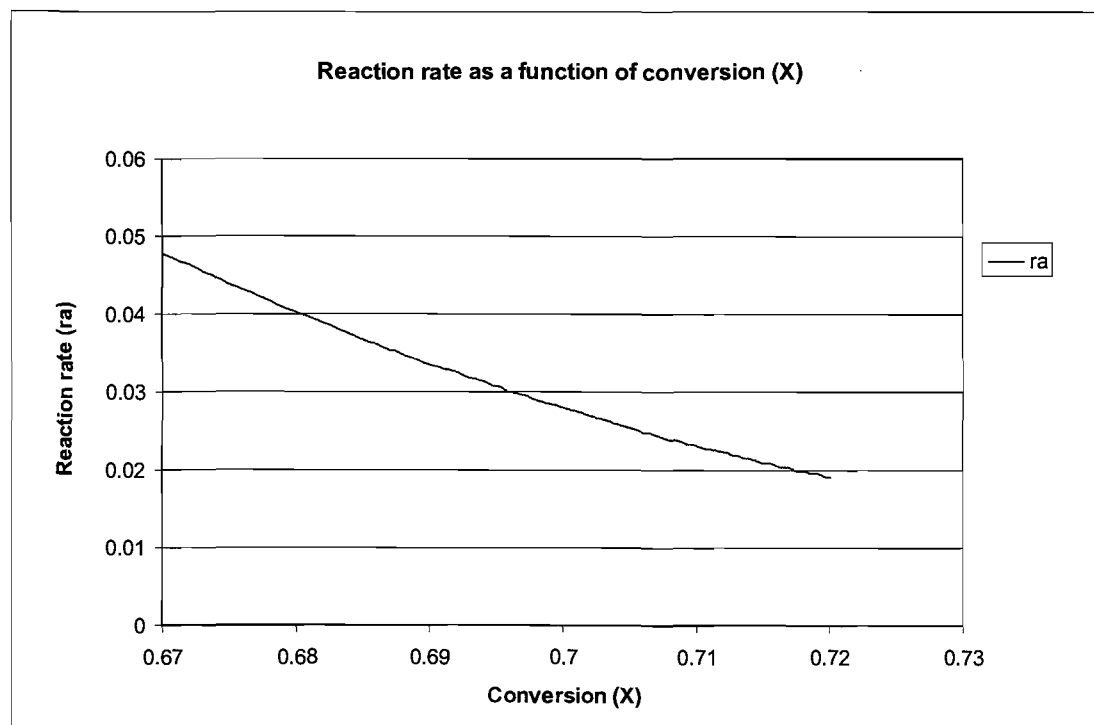


Figure 52: Reaction rate as a function of conversion for the fifth stage reactor

The reaction rate has decreased dramatically from the first reactor stage, and it is evident that the conversion achieved per m^3 of reactor volume is now almost constant. Although the reaction rate has decreased as expected, the actual drop in the reaction

rate is much less because of the higher average operating temperatures in the fifth stage of the reactor.

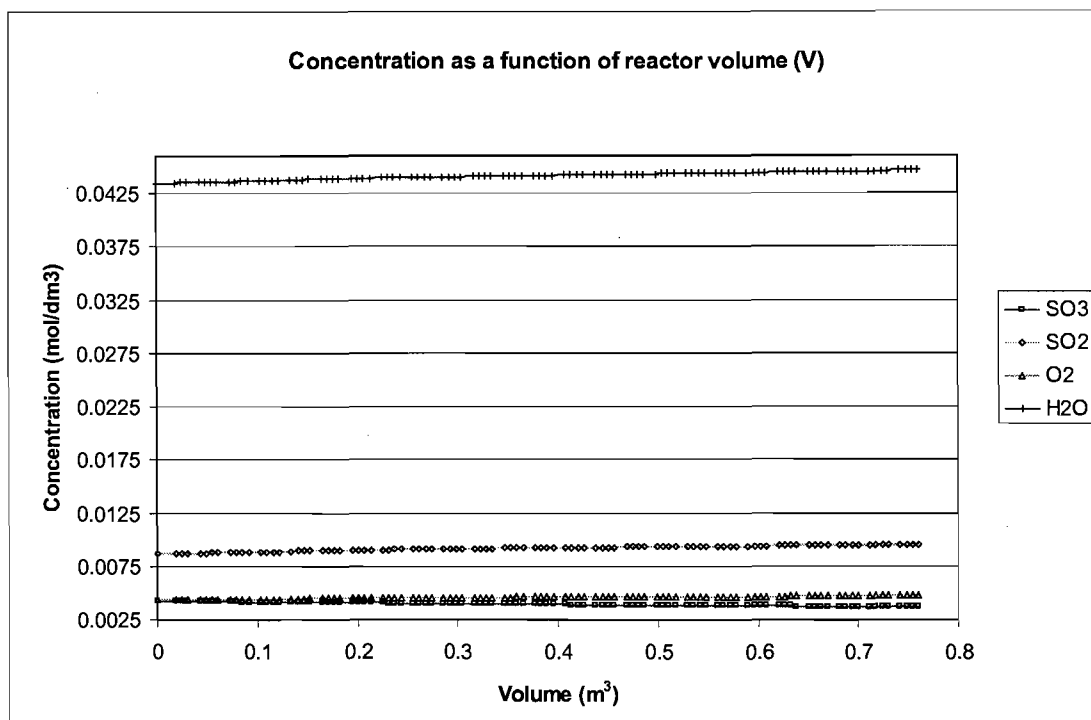


Figure 53: Concentration profile of all species as a function of reactor volume for the fifth stage reactor

5.3 Combined Reactor Stage Data Results

The design of the decomposition reactor focused primarily on the individual stages comprising the reactor. It is, however, important to remember that these stages still contribute to one reactor system and that the individual reactor stage data should still be viewed in light of this. All of the stage data and results are combined in this section, to provide a more general indication of the overall performance of the decomposition reactor system as a whole.

Table 20: Dimensions of multi-stage reactor at three-bar operating pressure

	Stage 1	Stage 2	Stage 3	Stage 4	Stage 5
Volume (m³)	69	12	3.66	1.52	0.76
Flowrate (dm³/s)	90220	96268	100267	102875	104543
SV (s⁻¹)	1.3	8.0	27.4	67.5	137.5

The reactor stage volumes required for reaction diminish from a volume of 69 m^3 for Stage 1 to a comparatively small volume of 0.76 m^3 for Stage 5. The total volume of the sulphur trioxide decomposition reactor amounts to 86.94 m^3 with a corresponding space-time of 0.948 seconds. The various reactor stage volumes, flow rates, and space velocities are shown in Table 20, while the combined illustrative conversion that is achieved down the length of the reactor is shown in Figure 54.

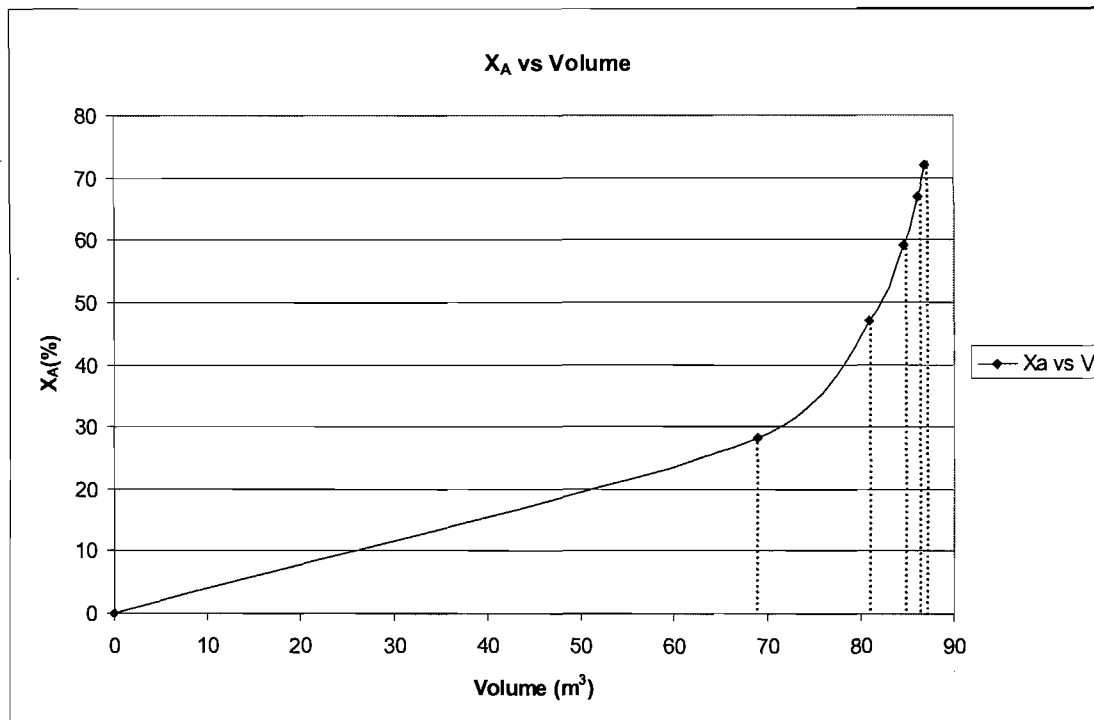


Figure 54: SO_3 conversion to SO_2 as a function of the total combined reactor system volume

The hourly space velocity of the multi-stage reactor system was calculated as 3797 h^{-1} which is within the range as recommended by Spewock et al. [22] and is explicated in Figure 5.

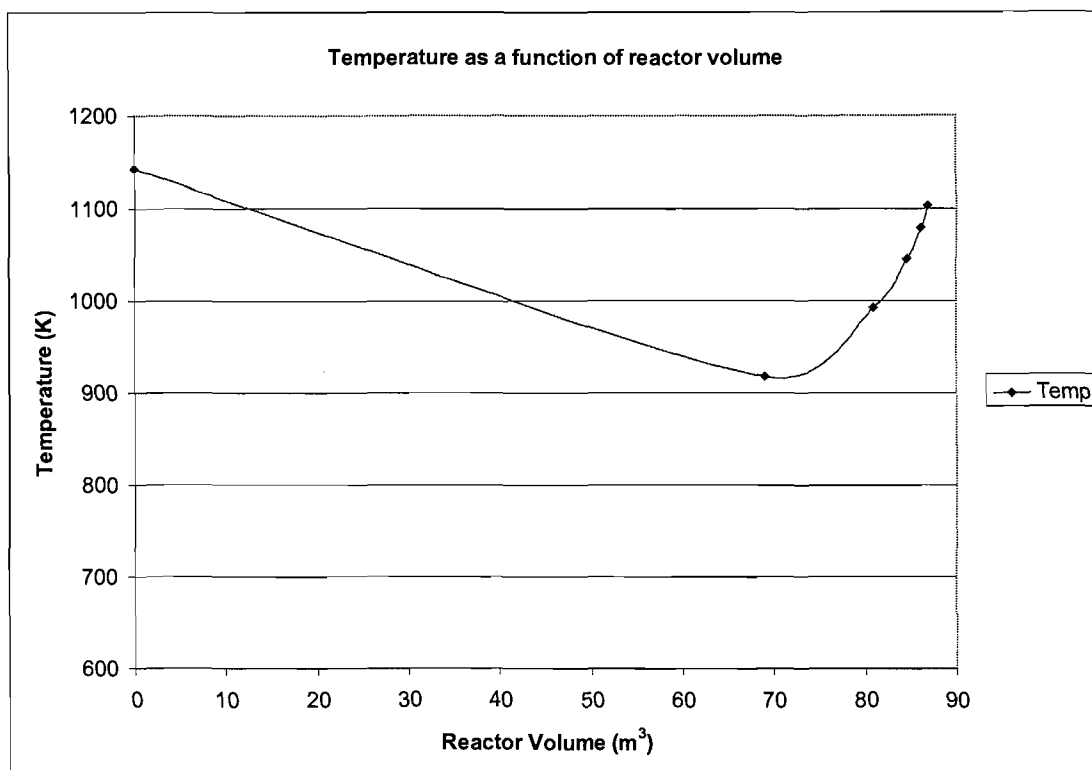


Figure 55: Temperature as a function of reactor volume

The strong endothermic nature of the SO_3 decomposition reaction is shown in Figure 55 as the temperature drops to a minimum along the length of the reactor. During the initial part of the reactor the reaction takes place very quickly (also evident in Figure 57) and in the process draws a lot of energy from the sensible heat of the helium gas supplied to the reaction mixture in the inter-stage heat exchanger. The consumption of reactants coupled with the reaction mixture temperature drop down the length of the reactor slows the reaction rate. Owing to the slower reaction rate, the inter-stage heat exchangers supply energy at a greater rate than the rate that the reaction draws energy from the helium gas supplied to it. This contributes to an increase in temperature again.

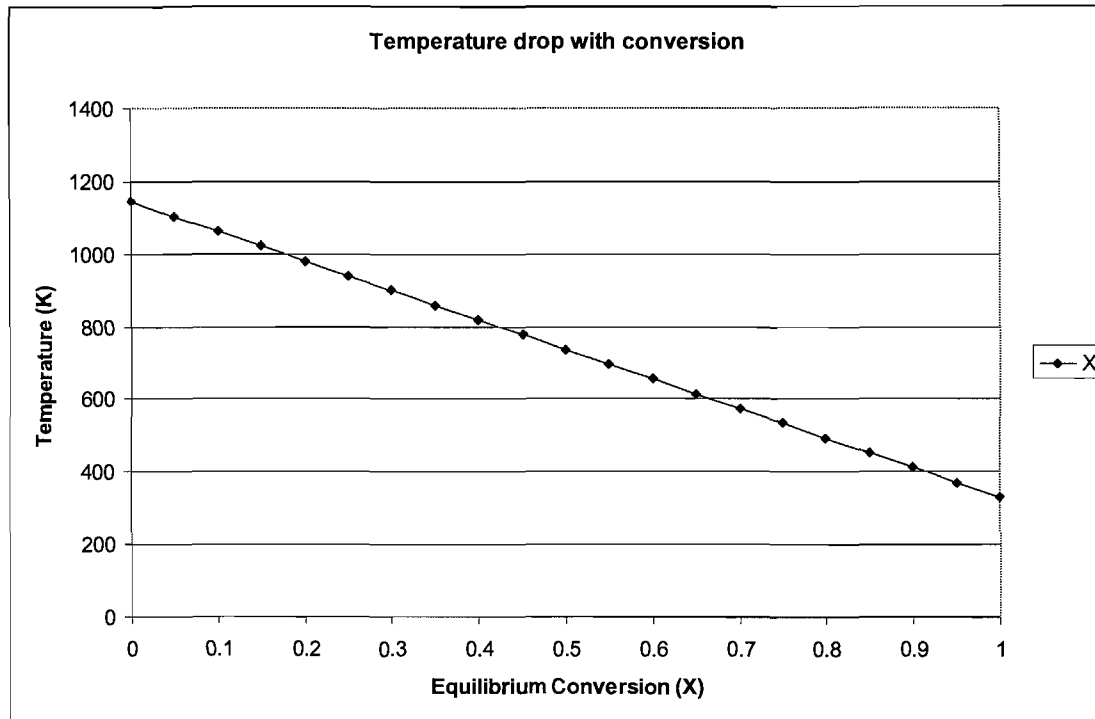


Figure 56: Temperature drop with conversion established from design equations

After performing an energy balance over the reactor system in Chapter 4 and solving the subsequent equations to establish conversion as a function of temperature the following equation was obtained:

$$X = \frac{(\sum \theta_i \cdot C_{p_i}) \cdot (T - T_0)}{-[\Delta H_{Rx}(T_R) + \Delta C_p(T - T_R)]} \quad (76)$$

Rearranging and substituting values provides:

$$T = T_0 - 812 \cdot X_A \quad (77)$$

Using this equation the temperature drop with conversion is presented in Figure 56 and the strong endothermic qualities of the reaction is once again highlighted indicating the extent of temperature drop for conversion achieved.

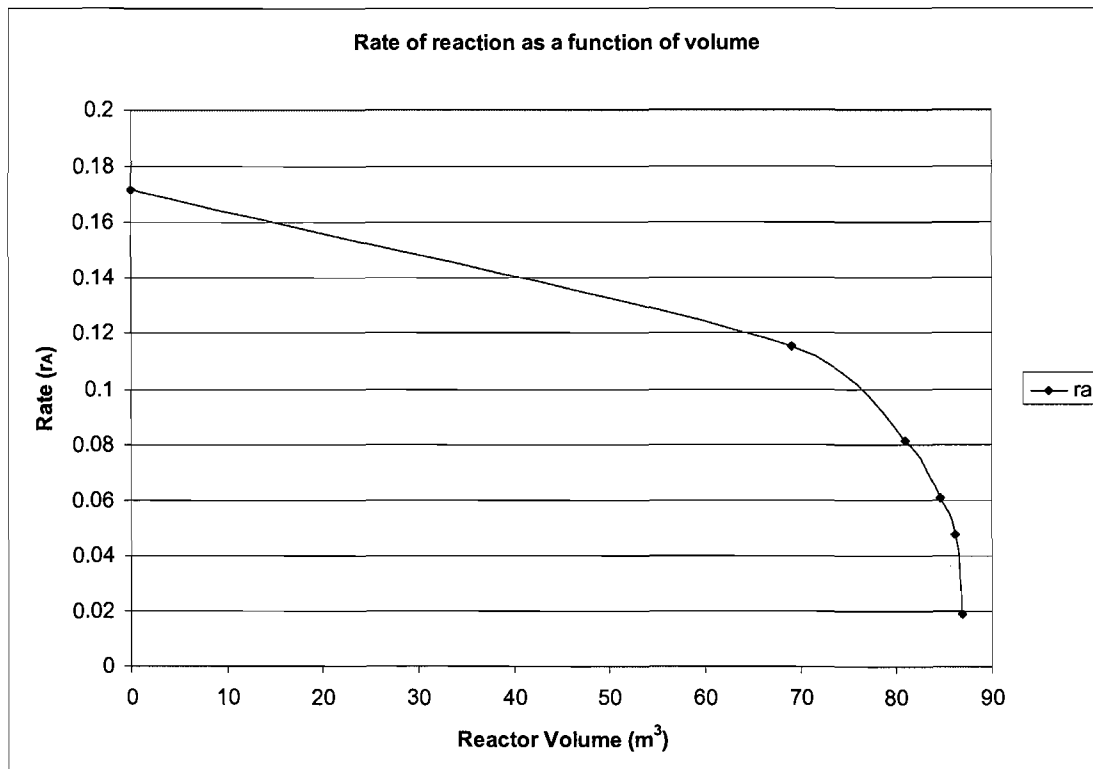


Figure 57: Rate of reaction as a function of reactor volume

The rate of the reaction can be seen to decrease down the length of the reactor, with the tempo of reduction in the rate increasing at a volume of approximately $70m^3$. The main reason for this drop in rate is because of the consumption of reactants in the front part of the reactor system, with a decreased amount of availability of reactants for conversion further down the reactor system. Although the overall reaction mixture temperature increases down the length of the reactor (Figure 55), the reaction rate steadily decreases, and this is an indication that the main driver for the reaction rate is the concentration of available reactants.

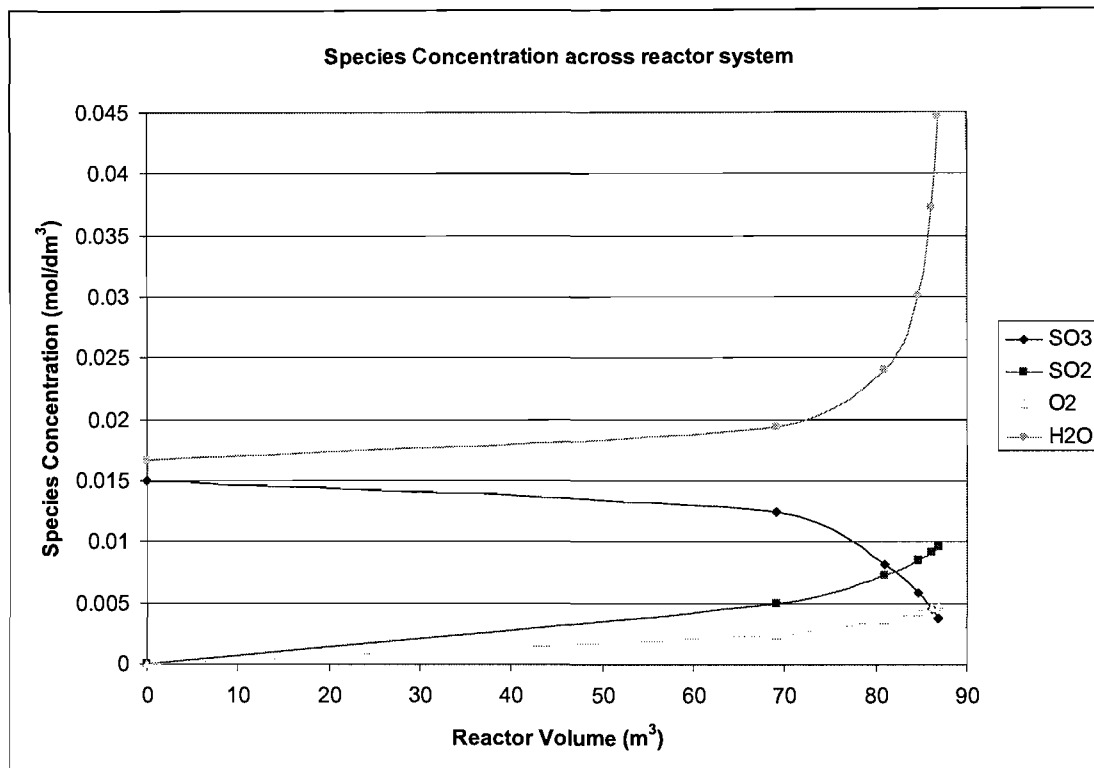


Figure 58: Species concentration as a function of reactor volume

The concentration profile of all the species down the length of the reactor system is shown in Figure 56. The sharp decrease in SO_3 concentration from 70 m^3 onwards is also an indicator of the reaction rate diminishing quite rapidly from that point onwards.

5.4 Process Unit Specification Data

The main process unit specification data is presented in tabulated format, with mass and energy balances performed over the H_2SO_4 decomposer both of the SO_3 pre-heaters as well as each reactor stage with its associated heat exchanger

5.4.1 H_2SO_4 Decomposer

Table 21: Mass and energy balance across the H_2SO_4 decomposition reactor

H_2SO_4 Decomposer					
H_2SO_4 side			Helium side		
In					
m_{in}	1500.00	mol/s	m	3223.27	mol/s
mass_{in}	135.00	kg/s	C_p	20.78	J/mol K
$m_{\text{H}_2\text{SO}_4}$	1350.00	mol/s	T_{in}	1046.00	K
$m_{\text{H}_2\text{SO}_4}$	0.90	mol	T_{out}	503.00	K
$C_{p_{\text{H}_2\text{SO}_4}}$	114.66	J/mol K	ΔT	543.00	K
$m_{\text{H}_2\text{O}}$	150.00	mol/s	Q	-36369865.16	Watt
$m_{\text{H}_2\text{O}}$	0.10	mol		-36.37	MWt
$C_{p_{\text{H}_2\text{O}}}$	36.16	J/mol K			
T_{in}	473.00	K	m	12.89	kg/s
Out					
m_{out}	2850.00	mol/s			
mass_{out}	135.00	kg/s			
m_{SO_3}	1350.00	mol/s			
m_{SO_3}	0.474	mol %			
m_{SO_3}	108.00	kg/s			
$m_{\text{H}_2\text{O}}$	1500.00	mol/s			
$m_{\text{H}_2\text{O}}$	0.526	mol %			
$m_{\text{H}_2\text{O}}$	27.00	kg/s			
T_{out}	700.00	K			
T_{cp}	0.59				
ΔT	-227.00	K			
Q	36369865.16	Watt			
Q	36.37	MWt (LH)			
Q	131679000.00	Watt			
Q	131.68	MWt (RH)			
Q_{TOT}	168.05	MWt			

5.4.2 SO₃ Pre-heatersTable 22: Mass and energy balance across the SO₃ Pre-Heater 1

SO ₃ Pre-heater 1					
Product stream side			Heater stream side		
In					
m _{in}	2850.00	mol/s	Conversion	0.72	x
mass _{in}	135.00	kg/s			
m _{SO3}	1350.00	mol/s	SO ₃	0.113	mol %
m _{SO3}	0.474	mol %	m	378.00	mol/s
Cp _{SO3}	74.38	J/mol K	m	30.24	kg/s
m _{H2O}	1500.00	mol/s	Cp	74.82	J/mol K
m _{H2O}	0.53	mol %			
Cp _{H2O}	39.83	J/mol K	SO ₂	0.291	mol %
T _{in}	700.00	K	m	972.00	mol/s
Out			m	62.21	kg/s
m _{out}	2850.00	mol/s	Cp	53.74	J/mol K
mass _{out}	135.00	kg/s			
m _{SO3}	1350.00	mol/s	H ₂ O	0.450	mol %
m _{SO3}	0.474	mol %	m	1500.00	mol/s
m _{SO3}	108.00	kg/s	m	27.00	kg/s
m _{H2O}	1500.00	mol/s	Cp	40.19	J/mol K
m _{H2O}	0.526	mol %			
m _{H2O}	27.00	kg/s	O ₂	0.146	mol %
T _{out}	1073.00	K	m	486.00	mol/s
T _{Cp}	0.89		m	15.55	kg/s
ΔT	-373.00	K	Cp	34.09	J/mol K
Q	59739433.58	Watt			
Q	59.74	MWt	m _{Tot}	3336.00	mol/s
			T _{in}	1105.00	K
			T _{avg}	915.00	K
			T _{Cp}	0.92	
			T _{out}	725.00	K
			ΔT	380.00	
			Q	59801288.82	Watt
				59.80	MWt
			m	135.00	kg/s

Table 23: Mass and energy balance across the SO₃ Pre-Heater 2

SO ₃ Pre-heater 2					
Product stream side			Helium side		
In					
m _{in}	2850.00	mol/s	m	8085.03	mol/s
mass _{in}	135.00	kg/s	Cp	20.78	J/mol K
m _{SO3}	1350.00	mol/s	T _{in}	1173.00	K
m _{SO3}	0.47	mol	T _{out}	1103.00	K
Cp _{SO3}	77.09	J/mol K	ΔT	70.00	K
m _{H2O}	1500.00	mol/s	Q	-11760491.00	Watt
m _{H2O}	0.53	mol		-11.76	MWt
Cp _{H2O}	42.62	J/mol K			
T _{in}	1073.00	K	m	32.34	kg/s
Out					
m _{out}	2850.00	mol/s			
mass _{out}	135.00	kg/s			
m _{SO3}	1350.00	mol/s			
m _{SO3}	0.474	mol %			
m _{SO3}	108.00	kg/s			
m _{H2O}	1500.00	mol/s			
m _{H2O}	0.526	mol %			
m _{H2O}	27.00	kg/s			
T _{out}	1143.00	K			
T _{Cp}	1.11				
ΔT	-70.00	K			
Q	11760491.01	Watt			
Q	11.76	MWt			

5.4.3 First Reactor Stage with Inter-stage Heating

Table 24: Mass and energy balance across Reactor 1 from Inter-Stage HX-1

Reactor 1		
Incoming Stream		
SO ₃	0.474	mol %
m	1350.00	mol/s
Cp	76.29	J/mol K
SO ₂	0.000	mol %
m	0.00	mol/s
Cp	54.70	J/mol K
H ₂ O	0.526	mol %
m	1500.00	mol/s
Cp	41.65	J/mol K
O ₂	0.000	mol %
m	0.00	mol/s
Cp	34.62	J/mol K
m _{Tot}	2850.00	mol/s
T _{in}	1143.00	K
Exiting Stream		
T _{avg}	1030.50	K
T _{Cp}	1.03	
T _{out}	918.00	K
ΔT	225.00	
Q	-37230803.67	Watt
	-37.23	MWt
m	135.00	kg/s

Table 25: Mass and energy balance across Inter-Stage HX-1 from Reactor 1

Heat Exchanger 1			
Product stream side			Helium side
Conversion	0.28	x	
SO ₃	0.318	mol %	
m	967.95	mol/s	
Cp	76.29	J/mol K	
SO ₂	0.126	mol %	
m	382.05	mol/s	
Cp	54.70	J/mol K	
H ₂ O	0.493	mol %	
m	1500.00	mol/s	
Cp	41.65	J/mol K	
O ₂	0.063	mol %	
m	191.03	mol/s	
Cp	34.62	J/mol K	
m _{Tot}	3041.03	mol/s	m 7884.25 mol/s
T _{in}	918.00	K	Cp 20.78 J/mol K
T _{avg}	1030.50	K	T _{in} 1173.00 K
T _{Cp}	1.03		T _{avg} 1060.50 K
T _{out}	1143.00	K	T _{Cp} 1.06
ΔT	-225.00		T _{out} 948.00 K
Q	36862795.11	Watt	ΔT 225.00 K
	36.86	MWt	Q -36862795.00 Watt
			-36.86 MWt
m	135.00	kg/s	m 31.54 kg/s

5.4.4 Second Reactor Stage with Inter-stage Heating

Table 26: Mass and energy balance across Reactor 2 from Inter-Stage HX-2

Reactor 2		
Incoming Stream		
SO ₃	0.318	mol %
m	967.95	mol/s
C _p	76.29	J/mol K
SO ₂	0.126	mol %
m	382.05	mol/s
C _p	54.70	J/mol K
H ₂ O	0.493	mol %
m	1500.00	mol/s
C _p	41.65	J/mol K
O ₂	0.063	mol %
m	191.03	mol/s
C _p	34.62	J/mol K
m _{Tot}	3041.03	mol/s
T _{in}	1143.00	K
Exiting Stream		
T _{avg}	1069.00	K
T _{Cp}	1.07	
T _{out}	995.00	K
ΔT	148.00	
Q	-24247527.45	Watt
	-24.25	MWt
m	135.00	kg/s

Table 27: Mass and energy balance across Inter-Stage HX-2 from Reactor 2

Heat Exchanger 2					
Product stream side			Helium side		
Conversion	0.47	x			
SO ₃	0.226	mol %			
m	715.50	mol/s			
Cp	76.70	J/mol K			
SO ₂	0.200	mol %			
m	634.50	mol/s			
Cp	54.97	J/mol K			
H ₂ O	0.474	mol %			
m	1500.00	mol/s			
Cp	42.13	J/mol K			
O ₂	0.100	mol %			
m	317.25	mol/s			
Cp	34.79	J/mol K			
m _{Tot}	3167.25	mol/s			
T _{in}	995.00	K			
T _{avg}	1069.00	K			
T _{Cp}	1.07				
T _{out}	1143.00	K			
ΔT	-148.00				
Q	24271687.80	Watt			
	24.27	MWt			
m	135.00	kg/s			

m	7892.10	mol/s
Cp	20.78	J/mol K
T _{in}	1173.00	K
T _{avg}	1099.00	K
T _{Cp}	1.10	
T _{out}	1025.00	K
ΔT	148.00	K
Q	-24271688.00	Watt
	-24.27	MWt
m	31.57	kg/s

5.4.5 Third Reactor Stage with Inter-stage Heating

Table 28: Mass and energy balance across Reactor 3 from Inter-Stage HX-3

Reactor 3		
Incoming Stream		
SO ₃	0.226	mol %
m	715.50	mol/s
Cp	76.70	J/mol K
SO ₂	0.200	mol %
m	634.50	mol/s
Cp	54.97	J/mol K
H ₂ O	0.474	mol %
m	1500.00	mol/s
Cp	42.13	J/mol K
O ₂	0.100	mol %
m	317.25	mol/s
Cp	34.79	J/mol K
m _{Tot}	3167.25	mol/s
T _{in}	1143.00	K
Exiting Stream		
T _{avg}	1094.00	K
T _{Cp}	1.09	
T _{out}	1045.00	K
ΔT	98.00	
Q	-16071793.27	Watt
	-16.07	MWt
m	135.00	kg/s

Table 29: Mass and energy balance across Inter-Stage HX-3 from Reactor 3

Heat Exchanger 3			
Product stream side			Helium side
Conversion	0.59	x	
SO ₃	0.169	mol %	
m	550.80	mol/s	
Cp	76.95	J/mol K	
SO ₂	0.246	mol %	
m	799.20	mol/s	
Cp	55.14	J/mol K	
H ₂ O	0.462	mol %	
m	1500.00	mol/s	
Cp	42.45	J/mol K	
O ₂	0.123	mol %	
m	399.60	mol/s	
Cp	34.89	J/mol K	
m _{Tot}	3249.60	mol/s	m 7895.46 mol/s
T _{in}	1045.00	K	Cp 20.78 J/mol K
T _{avg}	1094.00	K	T _{in} 1173.00 K
T _{Cp}	1.09		T _{avg} 1124.00 K
T _{out}	1143.00	K	T _{Cp} 1.12
ΔT	-98.00		T _{out} 1075.00 K
Q	16078634.87	Watt	ΔT 98.00 K
	16.08	MWt	Q -16078635.00 Watt
			-16.08 MWt
m	135.00	kg/s	m 31.58 kg/s

5.4.6 Fourth Reactor Stage with Inter-stage Heating

Table 30: Mass and energy balance across Reactor 4 from Inter-Stage HX-4

Reactor 4		
Incoming Stream		
SO ₃	0.17	mol %
m	550.80	mol/s
Cp	76.95	J/mol K
SO ₂	0.246	mol %
m	799.20	mol/s
Cp	55.14	J/mol K
H ₂ O	0.462	mol %
m	1500.00	mol/s
Cp	42.45	J/mol K
O ₂	0.123	mol %
m	399.60	mol/s
Cp	34.89	J/mol K
m _{Tot}	3249.60	mol/s
T _{in}	1143.00	K
Exiting Stream		
T _{avg}	1112.00	K
T _{Cp}	1.11	
T _{out}	1081.00	K
ΔT	62.00	
Q	-10172197.57	Watt
	-10.17	MWt
m	135.00	kg/s

Table 31: Mass and energy balance across Inter-Stage HX-4 from Reactor 4

Heat Exchanger 4			
Product stream side			Helium side
Conversion	0.67	x	
SO ₃	0.135	mol %	
m	445.50	mol/s	
Cp	77.13	J/mol K	
SO ₂	0.274	mol %	
m	904.50	mol/s	
Cp	55.25	J/mol K	
H ₂ O	0.454	mol %	
m	1500.00	mol/s	
Cp	42.67	J/mol K	
O ₂	0.137	mol %	
m	452.25	mol/s	
Cp	34.97	J/mol K	
m _{Tot}	3302.25	mol/s	m
T _{in}	1081.00	K	7900.04
T _{avg}	1112.00	K	mol/s
T _{Cp}	1.11		Cp
T _{out}	1143.00	K	20.78
ΔT	-62.00		J/mol K
Q	10178090.64	Watt	T _{in}
	10.18	MWt	1173.00
			K
			T _{avg}
m	135.00	kg/s	1142.00
			K
			T _{Cp}
			1.14
			T _{out}
			1111.00
			K
			ΔT
			62.00
			K
			Q
			-10178091.00
			Watt
			-10.18
			MWt
			m
			31.60
			kg/s

5.4.7 Fifth Reactor Stage

Table 32: Mass and energy balance across Reactor 5

Reactor 5		
Incoming Stream		
SO ₃	0.135	mol %
m	445.50	mol/s
Cp	77.13	J/mol K
SO ₂	0.274	mol %
m	904.50	mol/s
Cp	55.25	J/mol K
H ₂ O	0.454	mol %
m	1500.00	mol/s
Cp	42.67	J/mol K
O ₂	0.137	mol %
m	452.25	mol/s
Cp	34.97	J/mol K
m _{Tot}	3302.25	mol/s
T _{in}	1143.00	K
Exiting Stream		
T _{out}	1105.00	K
T _{avg}	1124.00	K
T _{Cp}	1.12	
ΔT	38.00	
Q	-6238184.59	Watt
	-6.24	MWt
m	135.00	kg/s

5.5 Sizing of Heat Exchanger

With the total volume of the adiabatic reactor system determined, the total heat exchanger volume of HX-1 was also determined as well as the total surface area of each heat exchanger. By investigating the difference in volume between the reactor system and the heat exchanger, the placement of the reactor in the tube side of the heat exchanger might be possible should the results indicate a substantially larger heat exchanger volume. The results are shown below:

Table 33: HX-1 Dimensions

Dimensions HX-1		
U	152	J/s·m ² ·K
Q	36862795	Watt
T _{h1}	949	K
T _{h2}	1173	K
T _{c1}	918	K
T _{c2}	1143	K
A	7952.135	m ²

Table 34: HX-2 Dimensions

Dimensions HX-2		
U	152	J/s·m ² ·K
Q	24271688	Watt
T _{h1}	1026	K
T _{h2}	1173	K
T _{c1}	995	K
T _{c2}	1143	K
A	5235.95	m ²

Table 35: HX-3 Dimensions

Dimensions HX-3		
U	152	J/s·m ² ·K
Q	16078635	Watt
T _{h1}	1076	K
T _{h2}	1173	K
T _{c1}	1045	K
T _{c2}	1143	K
A	3468.524	m ²

Table 36: HX-4 Dimensions

Dimensions HX-4		
U	152	J/s·m ² ·K
Q	10178091	Watt
T _{h1}	1112	K
T _{h2}	1173	K
T _{c1}	1081	K
T _{c2}	1143	K
A	2195.643	m ²

The total surface area of the heat exchanger system was determined to be 18852.24m². Large quantities of energy are required by the heat exchangers as a result of the strong endothermic decomposition reaction of SO₃ to SO₂ taking place. In order to quantify the volumetric size of the heat exchanger system in contrast to the reactor system, the volume of the multi-stage reactor was compared to that of HX-1. By making use of the results presented in Table 20 of section 5.3, the total reactor volume of the sulphur trioxide decomposition reactor amounts to 86.94 m³ with a corresponding space-time of 0.948 seconds. With this data the volume flow through the heat exchanger is determined to be 330 152 m³/h or 91.7m³/s. It is well documented from literature cited that acceptable gas velocities at atmospheric pressure should vary between 10 m/s to

30 m/s and for this reason the heat exchanger gas velocity should also be designed in such a way that it falls within this acceptable range. The number of pipes used in the tube section of the heat exchanger as well as the amount of tubes should also be chosen, keeping in mind that these choices will directly contribute to the heat transfer area of the heat exchanger and should amount to 7952 m². An industrial acceptable pipe ID size of 6 inches is selected and 200 pipes per HX. Dividing the volume flow of 91.7m³/s by the tube cross-sectional area of 0.0182m² multiplied with the 200 pipes provides the gas velocity of 25.19 m/s. This is within the acceptable gas velocity range. The heat transfer area can then be calculated by selecting a pipe length of 25m and using the formula:

$$A = N \cdot \Pi \cdot D \cdot L \quad (78)$$

Using the above dimensions a total heat transfer area of 2388m² is achieved, which is still less than the required 7952m². In order to achieve the required area, the HX can be connected in series to provide a sufficient area and connecting four of these heat exchangers in series, a total area of 9550m² is created. The associated volume of the HX can then be calculated with:

$$V = N \cdot \frac{\Pi}{4} \cdot D^2 \cdot L \quad (79)$$

A volume of 363m³ is produced with the dimensions described. With four heat exchangers connected in series the total area of 9550m² is more than required and can be reduced to give a clearer indication of the equivalent volume required by HX-1. This implies a heat exchanger volume equivalent to 83% (7952m²/9550m²) of the 363m³ volume will be needed by HX-1. The volume of HX-1 therefore amounts to 302m³ and on its own has a volume of nearly 3.5 times the total reactor volume (86.94 m³) The primary data concerning HX-1 is presented in Table 37.

Table 37: Process and dimensional data of HX-1

Volumetric Flowrate	91.71	m ³ /s
Gas Velocity	25.19	m/s
Inner Diameter	0.152	m
Number of tubes	200 x 4	-
Pipe Length	25 x 4	m
Volume	302	m ³

5.6 Production Rate of Products and Unreacted Reagents at Three-bar Operational Pressure

The maximum production of hydrogen and oxygen that could be obtained by a Hybrid Sulphur process at 3-bar operation making use of the reactor configuration as described is given in Table 38.

Table 38: Production rate of products and unreacted reagents at three-bar operational pressure

SO ₃ Production in kg/s	
378	mol/s
30.24	kg/s
SO ₂ Production in kg/s	
972	mol/s
62.208	kg/s
O ₂ Production in kg/s	
486	mol/s
15.552	kg/s
H ₂ O Production in kg/s	
1500	mol/s
27	kg/s
H ₂ Production in kg/s	
1.959	kg/s
169.3	TPD

The total amount of SO₂ produced in the multi-stage reactor system was 972 mol/s; therefore, the amount of H₂ produced will be 972 mol/s. With 1 mol of H₂ having a weight of 2.016g, the amount of H₂ produced was 1.96 kg/s or approximately 169.3 tonnes per day at a pressure of 3 bar and a temperature of 870°C.

5.7 Production Rate of Products and Unreacted Reagents at Ninety-bar Operational Pressure

The production of hydrogen and oxygen that can be obtained by a Hybrid Sulphur process at 90-bar operation, making use of the reactor configuration as described is given in Table 39.

Table 39: Production rate of products and unreacted reagents at ninety-bar operational pressure

SO ₃ Production in kg/s	
781.65	mol/s
62.53	kg/s
SO ₂ Production in kg/s	
568.35	mol/s
36.37	kg/s
O ₂ Production in kg/s	
284.18	mol/s
9.09	kg/s
H ₂ O Production in kg/s	
1500	mol/s
27	kg/s
H ₂ Production in kg/s	
1.15	kg/s
98.99	TPD

By operating the reactor at a pressure of 90 bar, the conversion of SO₃ is reduced. A total conversion of 42% was achieved over the multi-stage reactor system. In contrast with the production values achieved for the 3-bar operation scenario, only 568 mol/s of SO₂ was produced which amounts to 1.15 kg/s of H₂ production or approximately 98.99 tonnes per day, compared with almost 170 tonnes per day at the lower pressure. This lower output of H₂ is expected to have a significant effect on the process economics. The difference in production rates is, therefore, quite evident and supports the operation of the decomposition reactor at low-pressure operating conditions.

Chapter 6

Conclusion and Recommendations

CHAPTER 6 Conclusion and Recommendations

6.1 Summary

An overview of the world energy consumption was given in Chapter 1 with reference to the specific types of mainstream energy usage. This included the three main sources of energy: oil, coal, and gas. The negative impact these sources of energy have as well as the onset of several disadvantages in using them were discussed and acknowledged. It was highlighted that despite the negative impact of these fuels, there is a growing global demand for energy, and it was pointed out that this trend was not only limited to First World countries, but also extended to developing countries throughout the world. One of the solutions that was proposed to address the problem was the use of nuclear energy, in an effort to curb the large scale emissions of greenhouse gasses through coal-based electricity generation facilities. Hydrogen produced from nuclear energy was proposed as a viable and environmentally-attractive transportation fuel, in an effort to displace fossil fuels, which are firmly entrenched in the transportation sector. Techno-economic studies indicate that the decomposition reactor used in hydrogen production cycles has a significant influence on the efficiency of the system. The current field of interest is the investigation of the operation of the sulphuric acid decomposition reactor operating at pressure ranges between 8 and 9 MPa. The reduction of SO_3 to SO_2 is, however, favoured at low pressures, while maintaining high operating temperatures. It was therefore concluded that there is a need to investigate the possibility of operating at lower pressures in striving for higher process efficiencies.

The primary focus of Chapter 2 was to identify the most promising production cycles available for large-scale hydrogen production. The primary process means of commercial hydrogen production were identified and evaluated with a detailed account of the Hybrid Sulphur Cycle, selected as the most promising initiative. This was done in order to establish the optimum operating conditions, to enhance the overall system performance by means of the decomposition reactor.

As a first step in determining the possible success of an experimental investigation, a preliminary evaluation of the possible equilibrium conversions that can be attained for the specific reactions involved in the HYS process was undertaken. The effect of temperature and pressure on the equilibrium conversion of sulphur trioxide to sulphur dioxide was investigated and the favourable outcome of this analysis justified further investigation. This also provided a platform for measuring future improvements in the design process, by comparing the equilibrium conversions of the reactions achieved. The results and data generated in Chapter 3 were then used in Chapter 4 for expressing the rate of the reaction as a function of conversion, and subsequently solving the major design equations, to enable the sizing of the reactor system within the frame of the given design limits (3-bar operational pressure). The primary design equations addressed:

- reaction conversion as a function of the reactor volume;
- temperature profile across the reactor;
- rate equation for the decomposition reaction; and
- and establishing the concentration profiles of the species as a function of conversion along the reactor path.

The numerical solver Polymath was used to solve the equations in Chapter 5, and afforded greater insight into the effect of operating parameters, such as temperature and pressure, on the performance of the SO_3 decomposition reactor. In conjunction with this, the five major decomposition reactor stages, four intermediate heat exchangers, and the sulphuric acid decomposer were also designed by using the results obtained from Polymath.

6.2 Conclusion of the Research Project

It can be concluded from the literature review that energy is becoming an increasingly limited resource and that alternative sources of energy need to be investigated to address this demand, as well as lessen the environmental impact of fossil fuels. Nuclear-produced hydrogen could specifically serve as a viable alternative source of energy.

Techno-economic studies on the Hybrid Sulphur Cycle process showed that the performance of the decomposition reactor used in the cycle has a significant influence on the efficiency of the system. Therefore, this study was undertaken to develop a better understanding of the decomposition reactor and the reaction conditions that promote higher levels of conversion.

The objective of the research was to model the decomposition reactor as a multi-stage reactor system, operating under adiabatic process conditions. The results of the research indicate that operating at lower process pressures favourably enhances the overall conversion that can be achieved with the decomposition of SO_3 to SO_2 , and as a result, the overall production of H_2 .

By designing the reactor system separate from the heat exchanger system, the research showed that the volume ratio of the decomposition reactor to the heat exchanger is large to a point that the reactor can be built within the tube side of the heat exchanger. This could be a possible solution to lower the reactor costs and improve the overall economic viability.

The adiabatic operation of the multi-stage reactor system with inter-stage heating contributes to the simplicity of the reactor design. It is possible to determine the conversion, temperature, and concentration of the reacting species at any volume within the reactor. This system affords the researcher greater insight into the specific conditions that occur inside the reactor and a better understanding of the reaction mechanism.

One of the anticipated technical difficulties of the proposed concept design is the large pressure differential that will need to be addressed in the intermediate heat exchanger, to allow for the pressure drop of the hot helium gas exiting the PBMR from 90 bar to 3 bar. This problem could be partly overcome by first employing an initial set of high-pressure, multi-stage decomposition reactors with inter-stage heating, followed by a second phase of lower pressure operation. By doing this, the pressure differential can be used as an asset for attaining greater reaction conversions because of the reaction rate that is favoured by high pressures and conversion by low pressures.

It can be concluded that the SO_3 decomposition to SO_2 and O_2 is controlled to a much greater extent by heat transfer than by kinetics of the chemical reaction, as the total heat exchanger volume required is much larger than that required by the chemical reactor for achieving the necessary conversion.

6.3 Recommendations for Further Studies

The following recommendations are made with regard to a follow-up study:

- The decomposition reactor could consist of a two-reactor system, with the first reactor-system operating at high pressure (90 bar) followed by a second reactor-system operating at low pressure (3 bar). Most studies have however used an integral reactor – heat exchanger. An example of such an acid decomposer is the integral decomposer employed by the US Department of Energy at General Atomics which uses an all ceramic Bayonet configuration
- Heat could be added to the reactor vessel instead of adiabatic operation. Because the total heat exchanger volume required is much larger than that required by the chemical reactor for achieving the necessary conversion, sufficient residence time is available in the heat exchangers for conversion to take place. For this reason, the heat exchangers could possibly replace the reactors.
- Investigation into the availability of catalysts with sufficient activity to produce near-equilibrium conversions and the ability to maintain near-equilibrium conversions over extended periods could be furthered. An investigation into several metal oxide supported platinum catalysts were explored for the sulphuric acid decomposition reaction with regards to their activity and stability at Idaho National Laboratories to address the above mentioned issue [20].
- Due to the importance of cost implications and the influence it has on the selection of any process configuration or approach followed in the design, a cost analyses must be coupled to the design study to facilitate the selection of the most optimum process configuration. An economic analysis can be performed to investigate the cost implications of adiabatic reactor operation.

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Appendix A

Appendix A presents the thermodynamic values of SO_3 , SO_2 and O_2 at one-bar, three-bar, thirty-bar and ninety-bar operating pressure that was used for the calculation of equilibrium conversions in Chapter 3.

Table 40: Thermodynamic values of SO_3 at one-bar operating pressure

SO_3					
T (K)	T_r	P_r	B^0	B^1	Omega
300	0.611122	0.01218	-0.84491	-1.22179	0.973201
400	0.81483	0.01218	-0.50261	-0.26749	0.990834
500	1.018537	0.01218	-0.32678	-0.02023	0.995998
600	1.222245	0.01218	-0.2231	0.06496	0.998053
700	1.425952	0.01218	-0.15619	0.100249	0.999029
800	1.62966	0.01218	-0.11018	0.116883	0.999547
900	1.833367	0.01218	-0.077	0.125514	0.999842
1000	2.037075	0.01218	-0.05218	0.130336	1.000018
1100	2.240782	0.01218	-0.03306	0.133194	1.000127
1200	2.44449	0.01218	-0.01797	0.134972	1.000196
1300	2.648197	0.01218	-0.00584	0.136122	1.000239

Table 41: Thermodynamic values of SO_2 at one-bar operating pressure

SO_2					
T (K)	T_r	P_r	B^0	B^1	Omega
300	0.696379	0.012684	-0.66994	-0.64728	0.985023
400	0.928505	0.012684	-0.39218	-0.09587	0.994338
500	1.160631	0.012684	-0.24951	0.046995	0.997402
600	1.392758	0.012684	-0.16538	0.096219	0.998709
700	1.624884	0.012684	-0.11109	0.116609	0.999356
800	1.85701	0.012684	-0.07375	0.126221	0.999708
900	2.089136	0.012684	-0.04683	0.131208	0.999911
1000	2.321263	0.012684	-0.02669	0.133994	1.000034
1100	2.553389	0.012684	-0.01117	0.135645	1.00011
1200	2.785515	0.012684	0.001066	0.136672	1.000157
1300	3.017642	0.012684	0.010915	0.137337	1.000187

Table 42: Thermodynamic values of O₂ at one-bar operating pressure

O ₂					
T (K)	T _r	P _r	B ⁰	B ¹	Omega
300	1.940492	0.019829	-0.0631	0.128376	0.999384
400	2.587322	0.019829	-0.0092	0.135826	0.999952
500	3.234153	0.019829	0.01848	0.137757	1.000132
600	3.880983	0.019829	0.034805	0.138422	1.000193
700	4.527814	0.019829	0.045339	0.138697	1.000212
800	5.174644	0.019829	0.052584	0.138827	1.000213
900	5.821475	0.019829	0.057808	0.138895	1.000207
1000	6.468305	0.019829	0.061716	0.138932	1.000199
1100	7.115136	0.019829	0.064727	0.138955	1.000189
1200	7.761966	0.019829	0.067101	0.138969	1.000179
1300	8.408797	0.019829	0.069013	0.138978	1.00017

Table 43: Thermodynamic values of SO₃ at three-bar operating pressure

SO ₃					
T (K)	T _r	P _r	B ⁰	B ¹	Omega
300	0.611122	0.036541	-0.84491	-1.22179	0.921737
400	0.81483	0.036541	-0.50261	-0.26749	0.972753
500	1.018537	0.036541	-0.32678	-0.02023	0.988041
600	1.222245	0.036541	-0.2231	0.06496	0.994171
700	1.425952	0.036541	-0.15619	0.100249	0.997091
800	1.62966	0.036541	-0.11018	0.116883	0.998642
900	1.833367	0.036541	-0.077	0.125514	0.999526
1000	2.037075	0.036541	-0.05218	0.130336	1.000055
1100	2.240782	0.036541	-0.03306	0.133194	1.000382
1200	2.44449	0.036541	-0.01797	0.134972	1.000587
1300	2.648197	0.036541	-0.00584	0.136122	1.000716

Table 44: Thermodynamic values of SO₂ at three-bar operating pressure

SO ₂					
T (K)	T _r	P _r	B ⁰	B ¹	Omega
300	0.696379	0.038052	-0.66994	-0.64728	0.955737
400	0.928505	0.038052	-0.39218	-0.09587	0.983109
500	1.160631	0.038052	-0.24951	0.046995	0.992228
600	1.392758	0.038052	-0.16538	0.096219	0.996133
700	1.624884	0.038052	-0.11109	0.116609	0.998069
800	1.85701	0.038052	-0.07375	0.126221	0.999123
900	2.089136	0.038052	-0.04683	0.131208	0.999733
1000	2.321263	0.038052	-0.02669	0.133994	1.000101
1100	2.553389	0.038052	-0.01117	0.135645	1.000329
1200	2.785515	0.038052	0.001066	0.136672	1.000472
1300	3.017642	0.038052	0.010915	0.137337	1.000562

Table 45: Thermodynamic values of O₂ at three-bar operating pressure

O ₂					
T (K)	T _r	P _r	B ⁰	B ¹	Omega
300	1.940492	0.059488	-0.0631	0.128376	0.998154
400	2.587322	0.059488	-0.0092	0.135826	0.999857
500	3.234153	0.059488	0.01848	0.137757	1.000396
600	3.880983	0.059488	0.034805	0.138422	1.00058
700	4.527814	0.059488	0.045339	0.138697	1.000636
800	5.174644	0.059488	0.052584	0.138827	1.00064
900	5.821475	0.059488	0.057808	0.138895	1.000622
1000	6.468305	0.059488	0.061716	0.138932	1.000596
1100	7.115136	0.059488	0.064727	0.138955	1.000567
1200	7.761966	0.059488	0.067101	0.138969	1.000538
1300	8.408797	0.059488	0.069013	0.138978	1.00051

Table 46: Thermodynamic values of SO₃ at thirty-bar operating pressure

SO ₃					
T (K)	T _r	P _r	B ⁰	B ¹	Omega
300	0.611122	0.365408	-0.84491	-1.22179	0.442662
400	0.81483	0.365408	-0.50261	-0.26749	0.758621
500	1.018537	0.365408	-0.32678	-0.02023	0.886644
600	1.222245	0.365408	-0.2231	0.06496	0.943212
700	1.425952	0.365408	-0.15619	0.100249	0.971288
800	1.62966	0.365408	-0.11018	0.116883	0.9865
900	1.833367	0.365408	-0.077	0.125514	0.995272
1000	2.037075	0.365408	-0.05218	0.130336	1.000554
1100	2.240782	0.365408	-0.03306	0.133194	1.003826
1200	2.44449	0.365408	-0.01797	0.134972	1.005885
1300	2.648197	0.365408	-0.00584	0.136122	1.007184

Table 47: Thermodynamic values of SO₂ at thirty-bar operating pressure

SO ₂					
T (K)	T _r	P _r	B ⁰	B ¹	Omega
300	0.696379	0.380518	-0.66994	-0.64728	0.635894
400	0.928505	0.380518	-0.39218	-0.09587	0.843371
500	1.160631	0.380518	-0.24951	0.046995	0.924939
600	1.392758	0.380518	-0.16538	0.096219	0.961999
700	1.624884	0.380518	-0.11109	0.116609	0.980861
800	1.85701	0.380518	-0.07375	0.126221	0.991263
900	2.089136	0.380518	-0.04683	0.131208	0.99733
1000	2.321263	0.380518	-0.02669	0.133994	1.001007
1100	2.553389	0.380518	-0.01117	0.135645	1.003293
1200	2.785515	0.380518	0.001066	0.136672	1.004731
1300	3.017642	0.380518	0.010915	0.137337	1.005635

Table 48: Thermodynamic values of O₂ at thirty-bar operating pressure

O ₂					
T (K)	T _r	P _r	B ⁰	B ¹	Omega
300	1.940492	0.594884	-0.0631	0.128376	0.981691
400	2.587322	0.594884	-0.0092	0.135826	0.998572
500	3.234153	0.594884	0.01848	0.137757	1.003964
600	3.880983	0.594884	0.034805	0.138422	1.005819
700	4.527814	0.594884	0.045339	0.138697	1.006378
800	5.174644	0.594884	0.052584	0.138827	1.006417
900	5.821475	0.594884	0.057808	0.138895	1.006239
1000	6.468305	0.594884	0.061716	0.138932	1.005975
1100	7.115136	0.594884	0.064727	0.138955	1.005683
1200	7.761966	0.594884	0.067101	0.138969	1.005392
1300	8.408797	0.594884	0.069013	0.138978	1.005112

Table 49: Thermodynamic values of SO₃ at ninety-bar operating pressure

SO ₃					
T (K)	Tr	Pr	Bo	B1	Omega
300	0.611122	1.096224	-0.84491	-1.22179	0.08674
400	0.81483	1.096224	-0.50261	-0.26749	0.436591
500	1.018537	1.096224	-0.32678	-0.02023	0.697024
600	1.222245	1.096224	-0.2231	0.06496	0.839129
700	1.425952	1.096224	-0.15619	0.100249	0.916313
800	1.62966	1.096224	-0.11018	0.116883	0.960043
900	1.833367	1.096224	-0.077	0.125514	0.985882
1000	2.037075	1.096224	-0.05218	0.130336	1.001662
1100	2.240782	1.096224	-0.03306	0.133194	1.011522
1200	2.44449	1.096224	-0.01797	0.134972	1.017759
1300	2.648197	1.096224	-0.00584	0.136122	1.021708

Table 50: Thermodynamic values of SO₂ at ninety-bar operating pressure

SO ₂					
T (K)	Tr	Pr	Bo	B1	Omega
300	0.696379	1.141553	-0.66994	-0.64728	0.257131
400	0.928505	1.141553	-0.39218	-0.09587	0.599869
500	1.160631	1.141553	-0.24951	0.046995	0.791297
600	1.392758	1.141553	-0.16538	0.096219	0.890273
700	1.624884	1.141553	-0.11109	0.116609	0.943676
800	1.85701	1.141553	-0.07375	0.126221	0.974017
900	2.089136	1.141553	-0.04683	0.131208	0.99201
1000	2.321263	1.141553	-0.02669	0.133994	1.003025
1100	2.553389	1.141553	-0.01117	0.135645	1.009911
1200	2.785515	1.141553	0.001066	0.136672	1.01426
1300	3.017642	1.141553	0.010915	0.137337	1.017001

Table 51: Thermodynamic values of O₂ at ninety-bar operating pressure

O ₂					
T (K)	Tr	Pr	Bo	B1	Omega
300	1.940492	1.784652	-0.0631	0.128376	0.946072
400	2.587322	1.784652	-0.0092	0.135826	0.995721
500	3.234153	1.784652	0.01848	0.137757	1.011941
600	3.880983	1.784652	0.034805	0.138422	1.017557
700	4.527814	1.784652	0.045339	0.138697	1.019256
800	5.174644	1.784652	0.052584	0.138827	1.019374
900	5.821475	1.784652	0.057808	0.138895	1.018834
1000	6.468305	1.784652	0.061716	0.138932	1.018032
1100	7.115136	1.784652	0.064727	0.138955	1.017147
1200	7.761966	1.784652	0.067101	0.138969	1.016262
1300	8.408797	1.784652	0.069013	0.138978	1.015413

Appendix B

Appendix B presents the various reactor stage data as compiled from the numerical solver PolyMath for a reactor system operation at 3 bar.

Reactor Stage 1 Data

V	x	T	Ca	Cc	Cd	Ci	k1	Kc	rate	Fa	Fc	Fd	Fi
[m ³]	[-]	[K]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[s ⁻¹]	[-]	[mol/dm ³ ·s]	[mol/s]	[mol/s]	[mol/s]	[mol/s]
0.00	0.000	1143.00	0.014964	0	0	0.016605	11.471	0.2527	0.171645	1350.00	0.00	0.00	1500.00
1.43	0.086	1074.56	0.014288	0.001271	6.36E-04	0.017266	3.332	0.1354	0.047594	1239.71	110.29	55.15	1500.00
2.17	0.107	1058.54	0.014119	0.001601	8.00E-04	0.017444	2.399	0.1147	0.03386	1212.53	137.47	68.73	1500.00
3.21	0.127	1042.71	0.013948	0.001938	9.69E-04	0.017628	1.710	0.0967	0.023831	1185.34	164.66	82.33	1500.00
3.76	0.135	1036.11	0.013871	0.00209	0.001045	0.017713	1.465	0.0894	0.0203	1173.20	176.80	88.40	1500.00
4.31	0.142	1030.37	0.013805	0.002223	0.001112	0.017786	1.280	0.0836	0.017651	1162.75	187.25	93.62	1500.00
4.86	0.149	1025.31	0.013747	0.00234	0.00117	0.017852	1.136	0.0787	0.015594	1153.60	196.40	98.20	1500.00
5.97	0.159	1016.68	0.013648	0.002541	0.00127	0.017964	0.926	0.0709	0.01261	1138.14	211.86	105.93	1500.00
6.52	0.164	1012.94	0.013605	0.002627	0.001314	0.018013	0.847	0.0678	0.011496	1131.49	218.51	109.25	1500.00
7.07	0.168	1009.51	0.013566	0.002707	0.001354	0.018058	0.780	0.0651	0.010557	1125.41	224.59	112.29	1500.00
7.62	0.172	1006.34	0.01353	0.002781	0.001391	0.0181	0.723	0.0626	0.009754	1119.81	230.19	115.09	1500.00
8.73	0.180	1000.64	0.013465	0.002914	0.001457	0.018176	0.630	0.0584	0.008456	1109.79	240.21	120.10	1500.00
9.28	0.183	998.07	0.013435	0.002975	0.001487	0.01821	0.591	0.0566	0.007924	1105.27	244.73	122.36	1500.00
9.83	0.186	995.64	0.013408	0.003032	0.001516	0.018243	0.557	0.0549	0.007452	1101.03	248.97	124.48	1500.00
10.38	0.189	993.36	0.013382	0.003086	0.001543	0.018274	0.527	0.0534	0.007032	1097.04	252.96	126.48	1500.00
11.49	0.194	989.14	0.013334	0.003185	0.001593	0.018331	0.475	0.0507	0.006314	1089.68	260.32	130.16	1500.00
12.04	0.197	987.19	0.013311	0.003232	0.001616	0.018358	0.453	0.0495	0.006006	1086.29	263.71	131.86	1500.00
12.59	0.199	985.32	0.01329	0.003276	0.001638	0.018383	0.432	0.0483	0.005725	1083.05	266.95	133.48	1500.00
13.14	0.201	983.55	0.01327	0.003318	0.001659	0.018408	0.414	0.0473	0.005468	1079.96	270.04	135.02	1500.00
14.25	0.205	980.21	0.013232	0.003398	0.001699	0.018454	0.381	0.0453	0.005016	1074.18	275.82	137.91	1500.00

14.80	0.207	978.65	0.013214	0.003435	0.001718	0.018475	0.366	0.0444	0.004816	1071.47	278.53	139.27	1500.00
15.35	0.209	977.14	0.013197	0.003471	0.001736	0.018496	0.352	0.0436	0.00463	1068.86	281.14	140.57	1500.00
15.90	0.211	975.69	0.01318	0.003506	0.001753	0.018517	0.340	0.0428	0.004458	1066.35	283.65	141.82	1500.00
17.01	0.214	972.94	0.013149	0.003572	0.001786	0.018555	0.317	0.0413	0.004148	1061.61	288.39	144.20	1500.00
17.56	0.216	971.64	0.013134	0.003603	0.001802	0.018573	0.307	0.0406	0.004008	1059.36	290.64	145.32	1500.00
18.11	0.218	970.38	0.013119	0.003634	0.001817	0.018591	0.297	0.0400	0.003876	1057.18	292.82	146.41	1500.00
18.66	0.219	969.15	0.013105	0.003663	0.001832	0.018608	0.288	0.0394	0.003753	1055.08	294.92	147.46	1500.00
19.77	0.222	966.82	0.013079	0.00372	0.00186	0.018641	0.271	0.0382	0.003528	1051.06	298.94	149.47	1500.00
20.32	0.224	965.71	0.013066	0.003747	0.001874	0.018657	0.264	0.0376	0.003425	1049.14	300.86	150.43	1500.00
20.87	0.225	964.62	0.013054	0.003773	0.001887	0.018673	0.257	0.0371	0.003327	1047.28	302.72	151.36	1500.00
21.42	0.226	963.57	0.013042	0.003799	0.001899	0.018688	0.250	0.0366	0.003235	1045.47	304.53	152.27	1500.00
22.53	0.229	961.55	0.013018	0.003848	0.001924	0.018717	0.237	0.0357	0.003064	1041.99	308.01	154.00	1500.00
23.08	0.230	960.58	0.013007	0.003872	0.001936	0.018731	0.231	0.0352	0.002985	1040.32	309.68	154.84	1500.00
23.63	0.231	959.63	0.012996	0.003895	0.001948	0.018744	0.226	0.0348	0.00291	1038.69	311.31	155.65	1500.00
24.18	0.232	958.71	0.012986	0.003918	0.001959	0.018758	0.220	0.0344	0.002839	1037.11	312.89	156.45	1500.00
25.29	0.235	956.92	0.012965	0.003962	0.001981	0.018783	0.210	0.0336	0.002705	1034.05	315.95	157.98	1500.00
25.84	0.236	956.06	0.012955	0.003983	0.001991	0.018796	0.206	0.0332	0.002643	1032.57	317.43	158.71	1500.00
26.39	0.237	955.22	0.012946	0.004003	0.002002	0.018808	0.201	0.0328	0.002583	1031.13	318.87	159.43	1500.00
26.94	0.238	954.40	0.012936	0.004024	0.002012	0.01882	0.197	0.0325	0.002526	1029.72	320.28	160.14	1500.00
28.05	0.240	952.81	0.012918	0.004063	0.002031	0.018843	0.189	0.0318	0.002418	1026.99	323.01	161.50	1500.00
28.60	0.241	952.04	0.012909	0.004082	0.002041	0.018855	0.185	0.0315	0.002368	1025.67	324.33	162.16	1500.00
29.15	0.242	951.28	0.0129	0.004101	0.00205	0.018866	0.181	0.0312	0.002319	1024.38	325.62	162.81	1500.00
29.70	0.243	950.54	0.012892	0.004119	0.00206	0.018877	0.178	0.0309	0.002273	1023.11	326.89	163.44	1500.00
30.81	0.244	949.10	0.012875	0.004155	0.002077	0.018898	0.171	0.0303	0.002185	1020.65	329.35	164.67	1500.00
31.36	0.245	948.41	0.012867	0.004172	0.002086	0.018908	0.168	0.0300	0.002143	1019.46	330.54	165.27	1500.00
31.91	0.246	947.72	0.012859	0.004189	0.002095	0.018918	0.165	0.0297	0.002103	1018.28	331.72	165.86	1500.00
32.46	0.247	947.05	0.012851	0.004206	0.002103	0.018928	0.162	0.0295	0.002064	1017.13	332.87	166.43	1500.00
33.57	0.249	945.74	0.012836	0.004238	0.002119	0.018947	0.157	0.0289	0.001991	1014.90	335.10	167.55	1500.00
34.12	0.249	945.10	0.012829	0.004254	0.002127	0.018957	0.154	0.0287	0.001956	1013.81	336.19	168.10	1500.00
34.67	0.250	944.48	0.012821	0.00427	0.002135	0.018966	0.151	0.0285	0.001922	1012.74	337.26	168.63	1500.00
35.22	0.251	943.86	0.012814	0.004285	0.002143	0.018975	0.149	0.0282	0.00189	1011.68	338.32	169.16	1500.00

36.33	0.252	942.66	0.0128	0.004315	0.002158	0.018993	0.144	0.0278	0.001828	1009.63	340.37	170.18	1500.00
36.88	0.253	942.08	0.012794	0.00433	0.002165	0.019002	0.142	0.0276	0.001798	1008.63	341.37	170.68	1500.00
37.43	0.254	941.50	0.012787	0.004344	0.002172	0.019011	0.140	0.0273	0.001769	1007.65	342.35	171.18	1500.00
37.98	0.255	940.93	0.01278	0.004359	0.002179	0.019019	0.138	0.0271	0.001741	1006.68	343.32	171.66	1500.00
39.09	0.256	939.82	0.012767	0.004387	0.002193	0.019036	0.134	0.0267	0.001688	1004.79	345.21	172.61	1500.00
39.64	0.257	939.28	0.012761	0.0044	0.0022	0.019044	0.132	0.0265	0.001663	1003.86	346.14	173.07	1500.00
40.19	0.257	938.75	0.012755	0.004414	0.002207	0.019052	0.130	0.0263	0.001638	1002.95	347.05	173.52	1500.00
40.74	0.258	938.22	0.012749	0.004427	0.002213	0.01906	0.128	0.0262	0.001614	1002.05	347.95	173.97	1500.00
41.85	0.259	937.19	0.012737	0.004453	0.002226	0.019075	0.125	0.0258	0.001568	1000.30	349.70	174.85	1500.00
42.40	0.260	936.69	0.012731	0.004466	0.002233	0.019083	0.123	0.0256	0.001546	999.44	350.56	175.28	1500.00
42.95	0.261	936.19	0.012725	0.004478	0.002239	0.01909	0.121	0.0254	0.001524	998.59	351.41	175.70	1500.00
43.50	0.261	935.70	0.01272	0.004491	0.002245	0.019098	0.120	0.0253	0.001503	997.76	352.24	176.12	1500.00
44.61	0.262	934.74	0.012708	0.004515	0.002257	0.019112	0.117	0.0249	0.001463	996.12	353.88	176.94	1500.00
45.16	0.263	934.27	0.012703	0.004527	0.002263	0.01912	0.115	0.0248	0.001443	995.32	354.68	177.34	1500.00
45.71	0.264	933.81	0.012697	0.004539	0.002269	0.019127	0.114	0.0246	0.001424	994.52	355.48	177.74	1500.00
46.26	0.264	933.35	0.012692	0.00455	0.002275	0.019134	0.112	0.0245	0.001406	993.74	356.26	178.13	1500.00
47.37	0.265	932.45	0.012682	0.004573	0.002287	0.019147	0.110	0.0242	0.00137	992.21	357.79	178.89	1500.00
47.92	0.266	932.01	0.012676	0.004584	0.002292	0.019154	0.108	0.0240	0.001353	991.46	358.54	179.27	1500.00
48.47	0.266	931.58	0.012671	0.004595	0.002298	0.019161	0.107	0.0239	0.001337	990.72	359.28	179.64	1500.00
49.02	0.267	931.15	0.012666	0.004606	0.002303	0.019167	0.106	0.0237	0.00132	989.98	360.02	180.01	1500.00
50.13	0.268	930.30	0.012656	0.004628	0.002314	0.01918	0.103	0.0235	0.001289	988.54	361.46	180.73	1500.00
50.68	0.269	929.89	0.012652	0.004638	0.002319	0.019187	0.102	0.0233	0.001273	987.84	362.16	181.08	1500.00
51.23	0.269	929.48	0.012647	0.004649	0.002324	0.019193	0.101	0.0232	0.001258	987.14	362.86	181.43	1500.00
51.78	0.270	929.07	0.012642	0.004659	0.00233	0.019199	0.100	0.0231	0.001244	986.45	363.55	181.78	1500.00
52.89	0.271	928.27	0.012633	0.00468	0.00234	0.019211	0.098	0.0228	0.001216	985.09	364.91	182.45	1500.00
53.44	0.271	927.88	0.012628	0.00469	0.002345	0.019218	0.097	0.0227	0.001202	984.42	365.58	182.79	1500.00
53.99	0.272	927.50	0.012624	0.0047	0.00235	0.019223	0.096	0.0226	0.001189	983.76	366.24	183.12	1500.00
54.54	0.272	927.11	0.012619	0.004709	0.002355	0.019229	0.095	0.0224	0.001176	983.11	366.89	183.44	1500.00
55.65	0.273	926.36	0.01261	0.004729	0.002364	0.019241	0.093	0.0222	0.00115	981.83	368.17	184.09	1500.00
56.20	0.273	925.99	0.012606	0.004738	0.002369	0.019247	0.092	0.0221	0.001138	981.20	368.80	184.40	1500.00
56.75	0.274	925.62	0.012602	0.004748	0.002374	0.019252	0.091	0.0220	0.001126	980.57	369.43	184.71	1500.00

57.30	0.274	925.26	0.012597	0.004757	0.002379	0.019258	0.090	0.0219	0.001114	979.95	370.05	185.02	1500.00
58.41	0.275	924.54	0.012589	0.004775	0.002388	0.019269	0.088	0.0217	0.001091	978.73	371.27	185.63	1500.00
58.96	0.276	924.19	0.012585	0.004784	0.002392	0.019275	0.087	0.0215	0.00108	978.14	371.86	185.93	1500.00
59.51	0.276	923.84	0.012581	0.004793	0.002397	0.01928	0.086	0.0214	0.001069	977.54	372.46	186.23	1500.00
60.06	0.277	923.50	0.012577	0.004802	0.002401	0.019285	0.086	0.0213	0.001059	976.96	373.04	186.52	1500.00
61.17	0.277	922.82	0.012569	0.00482	0.00241	0.019296	0.084	0.0211	0.001038	975.80	374.20	187.10	1500.00
61.72	0.278	922.48	0.012565	0.004829	0.002414	0.019301	0.083	0.0210	0.001028	975.23	374.77	187.39	1500.00
62.27	0.278	922.15	0.012561	0.004837	0.002419	0.019307	0.082	0.0209	0.001018	974.66	375.34	187.67	1500.00
62.82	0.279	921.82	0.012557	0.004846	0.002423	0.019312	0.082	0.0208	0.001008	974.10	375.90	187.95	1500.00
63.93	0.279	921.17	0.012549	0.004862	0.002431	0.019322	0.080	0.0207	9.89E-04	973.00	377.00	188.50	1500.00
64.48	0.280	920.85	0.012546	0.004871	0.002435	0.019327	0.080	0.0206	9.80E-04	972.46	377.54	188.77	1500.00
65.03	0.280	920.54	0.012542	0.004879	0.002439	0.019332	0.079	0.0205	9.71E-04	971.92	378.08	189.04	1500.00
65.58	0.281	920.22	0.012538	0.004887	0.002444	0.019337	0.078	0.0204	9.62E-04	971.39	378.61	189.31	1500.00
66.69	0.281	919.60	0.012531	0.004903	0.002452	0.019346	0.077	0.0202	9.45E-04	970.33	379.67	189.83	1500.00
67.24	0.282	919.30	0.012527	0.004911	0.002456	0.019351	0.076	0.0201	9.36E-04	969.81	380.19	190.09	1500.00
67.79	0.282	919.00	0.012524	0.004919	0.002459	0.019356	0.076	0.0200	9.28E-04	969.30	380.70	190.35	1500.00
68.34	0.283	918.70	0.01252	0.004927	0.002463	0.019361	0.075	0.0199	9.20E-04	968.79	381.21	190.60	1500.00
69.00	0.283	918.34	0.012514	0.00494	0.00247	0.019369	0.074	0.0198	9.06E-04	967.94	382.06	191.03	1500.00

Reactor Stage 2 Data

V	x	T	Ca	Cc	Cd	Ci	k1	Kc	rate	Fa	Fc	Fd	Fi
[m ³]	[-]	[K]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[s ⁻¹]	[-]	[mol/dm ³ ·s]	[mol/s]	[mol/s]	[mol/s]	[mol/s]
0.00	0.283	1143.00	0.010055	0.003969	0.001984	0.021738	11.47	0.253	0.1152	967.95	382.05	191.03	1500.00
0.32	0.313	1118.88	0.009808	0.004397	0.002198	0.022019	7.77	0.208	0.0760	932.1259	417.8741	208.94	1500.00
0.42	0.320	1113.50	0.009741	0.004514	0.002257	0.022096	6.98	0.197	0.0678	922.5126	427.4874	213.74	1500.00
0.52	0.326	1108.65	0.00968	0.004619	0.00231	0.022166	6.34	0.187	0.0612	913.8905	436.1095	218.05	1500.00
0.61	0.332	1104.24	0.009625	0.004716	0.002358	0.022231	5.80	0.179	0.0556	906.0811	443.919	221.96	1500.00
0.80	0.341	1096.46	0.009529	0.004886	0.002443	0.022345	4.95	0.165	0.0470	892.3921	457.6079	228.80	1500.00
0.90	0.346	1093.00	0.009486	0.004962	0.002481	0.022396	4.62	0.160	0.0436	886.3263	463.6737	231.84	1500.00
1.00	0.350	1089.77	0.009446	0.005034	0.002517	0.022444	4.32	0.154	0.0407	880.6863	469.3137	234.66	1500.00
1.09	0.353	1086.75	0.009408	0.0051	0.00255	0.022489	4.06	0.150	0.0381	875.4185	474.5815	237.29	1500.00
1.28	0.360	1081.24	0.009339	0.005222	0.002611	0.022572	3.63	0.141	0.0337	865.8299	484.1701	242.09	1500.00
1.38	0.363	1078.71	0.009308	0.005279	0.002639	0.022611	3.44	0.138	0.0319	861.4411	488.5589	244.28	1500.00
1.48	0.366	1076.31	0.009278	0.005332	0.002666	0.022647	3.27	0.134	0.0302	857.2859	492.7141	246.36	1500.00
1.57	0.369	1074.03	0.009249	0.005383	0.002692	0.022682	3.12	0.131	0.0287	853.3416	496.6584	248.33	1500.00
1.76	0.375	1069.79	0.009196	0.005478	0.002739	0.022747	2.86	0.125	0.0261	846.0103	503.9897	251.99	1500.00
1.86	0.377	1067.80	0.009171	0.005523	0.002761	0.022778	2.74	0.123	0.0250	842.5914	507.4086	253.70	1500.00
1.96	0.379	1065.90	0.009147	0.005566	0.002783	0.022807	2.63	0.120	0.0239	839.3191	510.6809	255.34	1500.00
2.05	0.382	1064.08	0.009124	0.005607	0.002803	0.022835	2.53	0.118	0.0230	836.1817	513.8183	256.91	1500.00
2.24	0.386	1060.64	0.009081	0.005685	0.002842	0.022889	2.35	0.114	0.0212	830.272	519.728	259.86	1500.00
2.34	0.388	1059.02	0.009061	0.005722	0.002861	0.022914	2.27	0.112	0.0205	827.4824	522.5176	261.26	1500.00
2.44	0.390	1057.45	0.009041	0.005757	0.002879	0.022939	2.20	0.110	0.0197	824.7929	525.2071	262.60	1500.00
2.53	0.392	1055.94	0.009022	0.005792	0.002896	0.022963	2.13	0.108	0.0191	822.1967	527.8033	263.90	1500.00
2.72	0.395	1053.06	0.008986	0.005857	0.002929	0.023008	2.00	0.105	0.0178	817.2613	532.7387	266.37	1500.00
2.82	0.397	1051.69	0.008968	0.005889	0.002944	0.02303	1.94	0.103	0.0173	814.9115	535.0885	267.54	1500.00
2.92	0.399	1050.36	0.008951	0.005919	0.00296	0.023051	1.89	0.102	0.0167	812.6343	537.3658	268.68	1500.00
3.01	0.400	1049.06	0.008935	0.005949	0.002974	0.023072	1.83	0.100	0.0163	810.4253	539.5747	269.79	1500.00
3.20	0.404	1046.59	0.008904	0.006006	0.003003	0.023112	1.74	0.098	0.0153	806.1974	543.8026	271.90	1500.00

3.30	0.405	1045.41	0.008889	0.006033	0.003017	0.023131	1.69	0.096	0.0149	804.1717	545.8283	272.91	1500.00
3.40	0.406	1044.25	0.008874	0.00606	0.00303	0.023149	1.65	0.095	0.0145	802.2008	547.7992	273.90	1500.00
3.49	0.408	1043.13	0.00886	0.006086	0.003043	0.023167	1.61	0.094	0.0141	800.282	549.718	274.86	1500.00
3.68	0.411	1040.96	0.008832	0.006136	0.003068	0.023202	1.54	0.092	0.0134	796.5903	553.4097	276.70	1500.00
3.78	0.412	1039.92	0.008819	0.00616	0.00308	0.023219	1.50	0.091	0.0131	794.8129	555.1871	277.59	1500.00
3.88	0.413	1038.90	0.008806	0.006184	0.003092	0.023236	1.47	0.090	0.0128	793.0783	556.9217	278.46	1500.00
3.97	0.414	1037.91	0.008793	0.006207	0.003103	0.023252	1.44	0.089	0.0125	791.3846	558.6154	279.31	1500.00
4.16	0.417	1035.99	0.008769	0.006252	0.003126	0.023283	1.38	0.087	0.0119	788.1128	561.8872	280.94	1500.00
4.26	0.418	1035.06	0.008757	0.006273	0.003137	0.023299	1.35	0.086	0.0117	786.5314	563.4687	281.73	1500.00
4.36	0.419	1034.15	0.008745	0.006295	0.003147	0.023314	1.32	0.085	0.0114	784.9843	565.0157	282.51	1500.00
4.45	0.420	1033.26	0.008734	0.006315	0.003158	0.023328	1.30	0.084	0.0112	783.4701	566.5299	283.26	1500.00
4.64	0.422	1031.54	0.008712	0.006356	0.003178	0.023357	1.25	0.082	0.0107	780.5355	569.4645	284.73	1500.00
4.74	0.423	1030.70	0.008701	0.006376	0.003188	0.023371	1.22	0.082	0.0105	779.1126	570.8874	285.44	1500.00
4.84	0.424	1029.88	0.00869	0.006395	0.003197	0.023384	1.20	0.081	0.0103	777.7178	572.2822	286.14	1500.00
4.93	0.425	1029.08	0.00868	0.006414	0.003207	0.023397	1.18	0.080	0.0101	776.3501	573.6499	286.82	1500.00
5.12	0.427	1027.51	0.00866	0.006451	0.003225	0.023423	1.14	0.079	0.0097	773.692	576.308	288.15	1500.00
5.22	0.428	1026.75	0.00865	0.006469	0.003234	0.023436	1.12	0.078	0.0096	772.3998	577.6002	288.80	1500.00
5.32	0.429	1026.01	0.008641	0.006486	0.003243	0.023449	1.10	0.077	0.0094	771.1311	578.8689	289.43	1500.00
5.41	0.430	1025.27	0.008631	0.006504	0.003252	0.023461	1.08	0.077	0.0092	769.8849	580.1151	290.06	1500.00
5.60	0.432	1023.84	0.008613	0.006538	0.003269	0.023485	1.05	0.076	0.0089	767.4576	582.5424	291.27	1500.00
5.70	0.433	1023.15	0.008604	0.006554	0.003277	0.023496	1.03	0.075	0.0088	766.275	583.725	291.86	1500.00
5.80	0.434	1022.46	0.008595	0.00657	0.003285	0.023508	1.02	0.074	0.0086	765.1121	584.8879	292.44	1500.00
5.89	0.435	1021.79	0.008586	0.006586	0.003293	0.023519	1.00	0.074	0.0085	763.9685	586.0315	293.02	1500.00
6.08	0.436	1020.47	0.008569	0.006618	0.003309	0.023542	0.97	0.073	0.0082	761.7365	588.2635	294.13	1500.00
6.18	0.437	1019.83	0.008561	0.006633	0.003317	0.023552	0.96	0.072	0.0081	760.6469	589.3531	294.68	1500.00
6.28	0.438	1019.20	0.008553	0.006648	0.003324	0.023563	0.94	0.072	0.0079	759.5744	590.4256	295.21	1500.00
6.37	0.439	1018.58	0.008545	0.006663	0.003332	0.023574	0.93	0.071	0.0078	758.5183	591.4817	295.74	1500.00
6.56	0.440	1017.36	0.008529	0.006692	0.003346	0.023594	0.90	0.070	0.0076	756.4536	593.5464	296.77	1500.00
6.66	0.441	1016.76	0.008521	0.006706	0.003353	0.023604	0.89	0.070	0.0075	755.4441	594.5559	297.28	1500.00
6.76	0.442	1016.18	0.008513	0.00672	0.00336	0.023614	0.88	0.069	0.0074	754.4493	595.5507	297.78	1500.00
6.85	0.442	1015.60	0.008506	0.006734	0.003367	0.023624	0.87	0.069	0.0073	753.4688	596.5312	298.27	1500.00

7.04	0.444	1014.47	0.008491	0.006762	0.003381	0.023644	0.85	0.068	0.0071	751.549	598.451	299.23	1500.00
7.14	0.444	1013.91	0.008484	0.006775	0.003387	0.023653	0.84	0.067	0.0070	750.6091	599.3909	299.70	1500.00
7.24	0.445	1013.36	0.008477	0.006788	0.003394	0.023662	0.82	0.067	0.0069	749.6819	600.3181	300.16	1500.00
7.33	0.446	1012.82	0.00847	0.006801	0.003401	0.023672	0.81	0.067	0.0068	748.7673	601.2327	300.62	1500.00
7.52	0.447	1011.77	0.008456	0.006827	0.003413	0.02369	0.79	0.066	0.0066	746.9742	603.0258	301.51	1500.00
7.62	0.448	1011.25	0.008449	0.006839	0.00342	0.023699	0.79	0.065	0.0065	746.0952	603.9048	301.95	1500.00
7.72	0.448	1010.73	0.008443	0.006851	0.003426	0.023708	0.78	0.065	0.0064	745.2275	604.7725	302.39	1500.00
7.81	0.449	1010.23	0.008436	0.006864	0.003432	0.023716	0.77	0.065	0.0064	744.3707	605.6293	302.81	1500.00
8.00	0.450	1009.24	0.008423	0.006888	0.003444	0.023733	0.75	0.064	0.0062	742.6893	607.3107	303.66	1500.00
8.10	0.451	1008.75	0.008417	0.0069	0.00345	0.023742	0.74	0.063	0.0061	741.8641	608.1359	304.07	1500.00
8.20	0.451	1008.27	0.00841	0.006911	0.003456	0.02375	0.73	0.063	0.0061	741.0489	608.9511	304.48	1500.00
8.29	0.452	1007.79	0.008404	0.006923	0.003461	0.023759	0.72	0.063	0.0060	740.2435	609.7565	304.88	1500.00
8.48	0.453	1006.86	0.008392	0.006945	0.003473	0.023775	0.71	0.062	0.0058	738.6612	611.3388	305.67	1500.00
8.58	0.454	1006.40	0.008386	0.006957	0.003478	0.023783	0.70	0.062	0.0058	737.8838	612.1162	306.06	1500.00
8.68	0.454	1005.94	0.00838	0.006968	0.003484	0.023791	0.69	0.061	0.0057	737.1154	612.8846	306.44	1500.00
8.77	0.455	1005.49	0.008374	0.006979	0.003489	0.023798	0.69	0.061	0.0056	736.3557	613.6443	306.82	1500.00
8.96	0.456	1004.61	0.008362	0.007	0.0035	0.023814	0.67	0.060	0.0055	734.8619	615.1381	307.57	1500.00
9.06	0.456	1004.18	0.008357	0.007011	0.003505	0.023821	0.67	0.060	0.0055	734.1274	615.8726	307.94	1500.00
9.16	0.457	1003.75	0.008351	0.007021	0.003511	0.023829	0.66	0.060	0.0054	733.4009	616.5991	308.30	1500.00
9.25	0.458	1003.32	0.008346	0.007032	0.003516	0.023836	0.65	0.059	0.0053	732.6823	617.3177	308.66	1500.00
9.44	0.459	1002.49	0.008335	0.007052	0.003526	0.023851	0.64	0.059	0.0052	731.268	618.732	309.37	1500.00
9.54	0.459	1002.07	0.008329	0.007062	0.003531	0.023858	0.63	0.059	0.0052	730.572	619.428	309.71	1500.00
9.64	0.460	1001.67	0.008324	0.007072	0.003536	0.023865	0.63	0.058	0.0051	729.8833	620.1167	310.06	1500.00
9.73	0.460	1001.26	0.008318	0.007082	0.003541	0.023872	0.62	0.058	0.0051	729.2017	620.7983	310.40	1500.00
9.92	0.461	1000.47	0.008308	0.007101	0.003551	0.023886	0.61	0.057	0.0050	727.8592	622.1408	311.07	1500.00
10.02	0.462	1000.08	0.008303	0.007111	0.003555	0.023893	0.60	0.057	0.0049	727.1981	622.8019	311.40	1500.00
10.12	0.462	999.69	0.008298	0.00712	0.00356	0.0239	0.60	0.057	0.0049	726.5435	623.4565	311.73	1500.00
10.21	0.463	999.31	0.008293	0.00713	0.003565	0.023907	0.59	0.057	0.0048	725.8955	624.1046	312.05	1500.00
10.40	0.463	998.55	0.008283	0.007148	0.003574	0.02392	0.58	0.056	0.0047	724.6182	625.3818	312.69	1500.00
10.50	0.464	998.18	0.008278	0.007158	0.003579	0.023927	0.58	0.056	0.0047	723.9887	626.0113	313.01	1500.00
10.60	0.464	997.81	0.008273	0.007167	0.003583	0.023933	0.57	0.056	0.0046	723.3653	626.6347	313.32	1500.00

10.69	0.465	997.45	0.008268	0.007176	0.003588	0.02394	0.57	0.055	0.0046	722.7477	627.2523	313.63	1500.00
10.88	0.466	996.73	0.008259	0.007193	0.003597	0.023953	0.56	0.055	0.0045	721.5298	628.4702	314.24	1500.00
10.98	0.466	996.37	0.008254	0.007202	0.003601	0.023959	0.55	0.055	0.0045	720.9293	629.0707	314.54	1500.00
11.08	0.467	996.02	0.008249	0.007211	0.003605	0.023965	0.55	0.055	0.0044	720.3342	629.6658	314.83	1500.00
11.17	0.467	995.67	0.008245	0.00722	0.00361	0.023971	0.54	0.054	0.0044	719.7446	630.2554	315.13	1500.00
11.36	0.468	994.98	0.008236	0.007237	0.003618	0.023984	0.54	0.054	0.0043	718.581	631.419	315.71	1500.00
11.46	0.468	994.64	0.008231	0.007245	0.003623	0.02399	0.53	0.054	0.0043	718.007	631.993	316.00	1500.00
11.56	0.469	994.30	0.008227	0.007253	0.003627	0.023996	0.53	0.053	0.0042	717.4379	632.5621	316.28	1500.00
11.65	0.469	993.97	0.008222	0.007262	0.003631	0.024002	0.52	0.053	0.0042	716.8739	633.1262	316.56	1500.00
11.84	0.470	993.31	0.008213	0.007278	0.003639	0.024013	0.51	0.053	0.0041	715.7602	634.2398	317.12	1500.00
11.94	0.470	992.98	0.008209	0.007286	0.003643	0.024019	0.51	0.053	0.0041	715.2105	634.7895	317.39	1500.00
12.00	0.471	992.78	0.008204	0.007295	0.003648	0.024026	0.51	0.052	0.0040	714.5987	635.4013	317.70	1500.00

Reactor Stage 3 Data

V	x	T	Ca	Cc	Cd	Ci	k1	Kc	rate	Fa	Fc	Fd	Fi
[m ³]	[-]	[K]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[s ⁻¹]	[-]	[mol/dm ³ ·s]	[mol/s]	[mol/s]	[mol/s]	[mol/s]
0.00	0.470	1143.00	0.007136	0.006328	0.003164	0.028222	11.47	0.253	0.081398	715.50	634.50	317.25	1500.00
0.09	0.479	1135.54	0.007058	0.006458	0.003229	0.02833	10.23	0.239	0.071779	704.93	645.07	322.53	1500.00
0.12	0.482	1133.29	0.007029	0.006506	0.003253	0.028371	9.81	0.234	0.068518	701.06	648.94	324.47	1500.00
0.15	0.485	1131.13	0.007001	0.006552	0.003276	0.028409	9.42	0.229	0.065528	697.36	652.64	326.32	1500.00
0.21	0.490	1127.09	0.006949	0.006639	0.00332	0.028482	8.73	0.220	0.060238	690.42	659.58	329.79	1500.00
0.23	0.492	1125.18	0.006925	0.00668	0.00334	0.028517	8.42	0.216	0.057887	687.15	662.85	331.42	1500.00
0.26	0.494	1123.35	0.006901	0.006719	0.00336	0.02855	8.13	0.212	0.055705	684.02	665.98	332.99	1500.00
0.29	0.497	1121.58	0.006879	0.006758	0.003379	0.028582	7.86	0.209	0.053674	681.00	669.00	334.50	1500.00
0.35	0.501	1118.23	0.006836	0.00683	0.003415	0.028644	7.38	0.202	0.050008	675.27	674.73	337.36	1500.00
0.38	0.503	1116.64	0.006815	0.006864	0.003432	0.028673	7.16	0.199	0.048349	672.56	677.44	338.72	1500.00
0.41	0.505	1115.10	0.006795	0.006898	0.003449	0.028701	6.95	0.196	0.046791	669.93	680.07	340.04	1500.00
0.44	0.507	1113.61	0.006776	0.00693	0.003465	0.028729	6.75	0.193	0.045327	667.38	682.62	341.31	1500.00
0.50	0.510	1110.76	0.006739	0.006993	0.003496	0.028782	6.39	0.188	0.042644	662.53	687.47	343.74	1500.00
0.53	0.512	1109.40	0.006721	0.007022	0.003511	0.028807	6.22	0.186	0.041414	660.21	689.79	344.90	1500.00
0.56	0.513	1108.07	0.006704	0.007051	0.003526	0.028832	6.06	0.183	0.040249	657.95	692.05	346.02	1500.00
0.59	0.515	1106.78	0.006687	0.00708	0.00354	0.028856	5.91	0.181	0.039145	655.76	694.24	347.12	1500.00
0.64	0.518	1104.31	0.006655	0.007134	0.003567	0.028902	5.63	0.177	0.037102	651.55	698.45	349.23	1500.00
0.67	0.520	1103.12	0.006639	0.00716	0.00358	0.028925	5.50	0.174	0.036154	649.52	700.48	350.24	1500.00
0.70	0.521	1101.96	0.006624	0.007186	0.003593	0.028947	5.38	0.172	0.035252	647.55	702.45	351.22	1500.00
0.73	0.522	1100.82	0.00661	0.007211	0.003605	0.028968	5.26	0.171	0.034391	645.63	704.37	352.19	1500.00
0.79	0.525	1098.64	0.006581	0.007259	0.00363	0.02901	5.04	0.167	0.032785	641.92	708.08	354.04	1500.00
0.82	0.526	1097.58	0.006567	0.007283	0.003641	0.02903	4.94	0.165	0.032035	640.13	709.87	354.94	1500.00
0.85	0.528	1096.55	0.006554	0.007306	0.003653	0.029049	4.84	0.163	0.031316	638.38	711.62	355.81	1500.00
0.88	0.529	1095.54	0.00654	0.007328	0.003664	0.029069	4.74	0.162	0.030628	636.67	713.33	356.67	1500.00
0.94	0.531	1093.59	0.006515	0.007371	0.003686	0.029106	4.56	0.159	0.029334	633.36	716.64	358.32	1500.00
0.97	0.533	1092.64	0.006502	0.007393	0.003696	0.029124	4.48	0.157	0.028725	631.75	718.25	359.12	1500.00

1.00	0.534	1091.72	0.00649	0.007413	0.003707	0.029142	4.39	0.156	0.02814	630.18	719.82	359.91	1500.00
1.02	0.535	1090.81	0.006478	0.007434	0.003717	0.02916	4.31	0.154	0.027577	628.64	721.36	360.68	1500.00
1.08	0.537	1089.04	0.006455	0.007473	0.003737	0.029194	4.16	0.152	0.026513	625.65	724.35	362.17	1500.00
1.11	0.538	1088.19	0.006444	0.007492	0.003746	0.02921	4.09	0.150	0.02601	624.20	725.80	362.90	1500.00
1.14	0.539	1087.34	0.006432	0.007511	0.003756	0.029227	4.02	0.149	0.025525	622.78	727.22	363.61	1500.00
1.17	0.540	1086.52	0.006422	0.00753	0.003765	0.029243	3.96	0.148	0.025057	621.38	728.62	364.31	1500.00
1.23	0.542	1084.91	0.0064	0.007566	0.003783	0.029274	3.83	0.145	0.024168	618.66	731.34	365.67	1500.00
1.26	0.543	1084.13	0.00639	0.007584	0.003792	0.029289	3.77	0.144	0.023745	617.34	732.66	366.33	1500.00
1.29	0.544	1083.36	0.00638	0.007601	0.0038	0.029304	3.71	0.143	0.023337	616.04	733.96	366.98	1500.00
1.32	0.545	1082.60	0.00637	0.007618	0.003809	0.029319	3.66	0.142	0.022941	614.76	735.24	367.62	1500.00
1.38	0.547	1081.13	0.00635	0.007651	0.003826	0.029348	3.55	0.140	0.022187	612.27	737.73	368.87	1500.00
1.41	0.548	1080.41	0.006341	0.007668	0.003834	0.029362	3.50	0.139	0.021828	611.05	738.95	369.47	1500.00
1.43	0.549	1079.70	0.006331	0.007684	0.003842	0.029376	3.45	0.138	0.021479	609.86	740.14	370.07	1500.00
1.46	0.550	1079.01	0.006322	0.0077	0.00385	0.02939	3.40	0.137	0.021141	608.68	741.32	370.66	1500.00
1.52	0.551	1077.64	0.006304	0.007731	0.003865	0.029417	3.31	0.135	0.020494	606.38	743.62	371.81	1500.00
1.55	0.552	1076.98	0.006295	0.007746	0.003873	0.02943	3.26	0.134	0.020185	605.26	744.74	372.37	1500.00
1.58	0.553	1076.32	0.006286	0.007761	0.00388	0.029443	3.22	0.133	0.019884	604.15	745.85	372.92	1500.00
1.61	0.554	1075.68	0.006278	0.007775	0.003888	0.029456	3.18	0.132	0.019592	603.06	746.94	373.47	1500.00
1.67	0.555	1074.41	0.006261	0.007804	0.003902	0.029481	3.09	0.130	0.019031	600.93	749.07	374.54	1500.00
1.70	0.556	1073.80	0.006252	0.007818	0.003909	0.029493	3.06	0.130	0.018762	599.88	750.12	375.06	1500.00
1.73	0.557	1073.19	0.006244	0.007832	0.003916	0.029505	3.02	0.129	0.0185	598.85	751.15	375.57	1500.00
1.76	0.558	1072.58	0.006236	0.007846	0.003923	0.029517	2.98	0.128	0.018245	597.84	752.16	376.08	1500.00
1.82	0.559	1071.41	0.006221	0.007873	0.003937	0.029541	2.91	0.126	0.017755	595.85	754.15	377.08	1500.00
1.84	0.560	1070.83	0.006213	0.007886	0.003943	0.029552	2.87	0.126	0.017519	594.88	755.12	377.56	1500.00
1.87	0.560	1070.26	0.006205	0.007899	0.00395	0.029564	2.84	0.125	0.017289	593.91	756.09	378.04	1500.00
1.90	0.561	1069.70	0.006198	0.007912	0.003956	0.029575	2.81	0.124	0.017064	592.97	757.03	378.52	1500.00
1.96	0.562	1068.59	0.006183	0.007938	0.003969	0.029597	2.74	0.123	0.016632	591.10	758.90	379.45	1500.00
1.99	0.563	1068.05	0.006175	0.00795	0.003975	0.029608	2.71	0.122	0.016423	590.19	759.81	379.90	1500.00
2.02	0.564	1067.52	0.006168	0.007963	0.003981	0.029619	2.68	0.121	0.01622	589.29	760.71	380.36	1500.00
2.05	0.564	1066.99	0.006161	0.007975	0.003987	0.02963	2.65	0.121	0.016021	588.40	761.60	380.80	1500.00
2.11	0.566	1065.95	0.006147	0.007999	0.003999	0.029651	2.60	0.119	0.015637	586.65	763.35	381.68	1500.00

2.14	0.566	1065.44	0.00614	0.008011	0.004005	0.029661	2.57	0.119	0.015451	585.79	764.21	382.10	1500.00
2.17	0.567	1064.94	0.006134	0.008022	0.004011	0.029671	2.54	0.118	0.015269	584.94	765.06	382.53	1500.00
2.20	0.568	1064.44	0.006127	0.008034	0.004017	0.029681	2.52	0.118	0.015092	584.10	765.90	382.95	1500.00
2.25	0.569	1063.46	0.006114	0.008056	0.004028	0.029701	2.47	0.116	0.014749	582.46	767.54	383.77	1500.00
2.28	0.569	1062.98	0.006107	0.008068	0.004034	0.029711	2.44	0.116	0.014582	581.65	768.35	384.18	1500.00
2.31	0.570	1062.50	0.006101	0.008079	0.004039	0.029721	2.42	0.115	0.01442	580.84	769.16	384.58	1500.00
2.34	0.571	1062.03	0.006094	0.00809	0.004045	0.02973	2.39	0.115	0.014261	580.05	769.95	384.97	1500.00
2.40	0.572	1061.11	0.006082	0.008111	0.004056	0.029749	2.35	0.113	0.013952	578.49	771.51	385.75	1500.00
2.43	0.572	1060.65	0.006076	0.008122	0.004061	0.029759	2.32	0.113	0.013802	577.73	772.27	386.14	1500.00
2.46	0.573	1060.20	0.00607	0.008132	0.004066	0.029768	2.30	0.112	0.013656	576.97	773.03	386.52	1500.00
2.49	0.573	1059.76	0.006064	0.008143	0.004071	0.029777	2.28	0.112	0.013512	576.22	773.78	386.89	1500.00
2.55	0.575	1058.88	0.006052	0.008163	0.004082	0.029795	2.24	0.111	0.013233	574.74	775.26	387.63	1500.00
2.58	0.575	1058.45	0.006046	0.008173	0.004087	0.029804	2.22	0.110	0.013098	574.01	775.99	387.99	1500.00
2.61	0.576	1058.02	0.00604	0.008183	0.004092	0.029813	2.20	0.110	0.012965	573.29	776.71	388.35	1500.00
2.64	0.576	1057.60	0.006034	0.008193	0.004097	0.029821	2.18	0.109	0.012835	572.58	777.42	388.71	1500.00
2.69	0.577	1056.76	0.006023	0.008213	0.004106	0.029838	2.14	0.108	0.012582	571.18	778.82	389.41	1500.00
2.72	0.578	1056.35	0.006017	0.008222	0.004111	0.029847	2.12	0.108	0.012459	570.49	779.51	389.76	1500.00
2.75	0.578	1055.94	0.006012	0.008232	0.004116	0.029855	2.10	0.107	0.012338	569.80	780.20	390.10	1500.00
2.78	0.579	1055.54	0.006006	0.008241	0.004121	0.029864	2.09	0.107	0.012219	569.12	780.88	390.44	1500.00
2.84	0.580	1054.75	0.005996	0.00826	0.00413	0.02988	2.05	0.106	0.011988	567.78	782.22	391.11	1500.00
2.87	0.580	1054.35	0.00599	0.008269	0.004135	0.029888	2.03	0.106	0.011876	567.13	782.87	391.44	1500.00
2.90	0.581	1053.97	0.005985	0.008278	0.004139	0.029896	2.02	0.105	0.011766	566.47	783.53	391.76	1500.00
2.93	0.581	1053.58	0.00598	0.008287	0.004144	0.029904	2.00	0.105	0.011657	565.83	784.17	392.09	1500.00
2.99	0.582	1052.82	0.005969	0.008305	0.004153	0.02992	1.97	0.104	0.011446	564.55	785.45	392.73	1500.00
3.02	0.583	1052.45	0.005964	0.008314	0.004157	0.029928	1.95	0.103	0.011343	563.92	786.08	393.04	1500.00
3.05	0.583	1052.08	0.005959	0.008323	0.004161	0.029935	1.94	0.103	0.011242	563.30	786.70	393.35	1500.00
3.07	0.583	1051.71	0.005954	0.008331	0.004166	0.029943	1.92	0.103	0.011143	562.68	787.32	393.66	1500.00
3.13	0.584	1050.98	0.005944	0.008348	0.004174	0.029958	1.89	0.102	0.010949	561.46	788.54	394.27	1500.00
3.16	0.585	1050.63	0.005939	0.008357	0.004178	0.029966	1.88	0.101	0.010854	560.85	789.15	394.57	1500.00
3.19	0.585	1050.27	0.005935	0.008365	0.004183	0.029973	1.86	0.101	0.010761	560.26	789.74	394.87	1500.00
3.22	0.586	1049.92	0.00593	0.008374	0.004187	0.02998	1.85	0.101	0.010669	559.67	790.33	395.17	1500.00

3.28	0.587	1049.22	0.00592	0.00839	0.004195	0.029995	1.82	0.100	0.010491	558.50	791.50	395.75	1500.00
3.31	0.587	1048.88	0.005915	0.008398	0.004199	0.030002	1.81	0.099	0.010403	557.92	792.08	396.04	1500.00
3.34	0.587	1048.54	0.005911	0.008406	0.004203	0.030009	1.80	0.099	0.010318	557.35	792.65	396.33	1500.00
3.37	0.588	1048.20	0.005906	0.008414	0.004207	0.030016	1.78	0.099	0.010233	556.78	793.22	396.61	1500.00
3.43	0.589	1047.54	0.005897	0.00843	0.004215	0.03003	1.76	0.098	0.010068	555.66	794.34	397.17	1500.00
3.46	0.589	1047.21	0.005893	0.008438	0.004219	0.030037	1.74	0.098	0.009987	555.10	794.90	397.45	1500.00
3.48	0.589	1046.88	0.005888	0.008446	0.004223	0.030044	1.73	0.097	0.009908	554.55	795.45	397.72	1500.00
3.51	0.590	1046.56	0.005884	0.008453	0.004227	0.030051	1.72	0.097	0.009829	554.01	795.99	398.00	1500.00
3.57	0.591	1045.91	0.005875	0.008469	0.004234	0.030064	1.70	0.096	0.009676	552.93	797.07	398.53	1500.00
3.60	0.591	1045.60	0.00587	0.008476	0.004238	0.030071	1.69	0.096	0.009601	552.40	797.60	398.80	1500.00
3.63	0.591	1045.28	0.005866	0.008484	0.004242	0.030078	1.67	0.096	0.009527	551.87	798.13	399.06	1500.00
3.66	0.592	1044.97	0.00586	0.008495	0.004247	0.030088	1.66	0.095	0.009419	551.09	798.91	399.46	1500.00

Reactor Stage 4 Data

V	x	T	Ca	Cc	Cd	Ci	k1	Kc	rate	Fa	Fc	Fd	Fi
[m ³]	[-]	[K]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[s ⁻¹]	[-]	[mol/dm ³ ·s]	[mol/s]	[mol/s]	[mol/s]	[mol/s]
0.00	0.592	1143.00	0.005354	0.007769	0.003884	0.035758	11.47	0.253	0.060629	550.80	799.20	399.60	1500
0.04	0.596	1139.84	0.00532	0.007825	0.003912	0.035817	10.93	0.247	0.057392	546.37	803.63	401.81	1500
0.05	0.597	1138.84	0.005307	0.007846	0.003923	0.035839	10.74	0.244	0.056193	544.68	805.32	402.66	1500
0.06	0.598	1137.86	0.005294	0.007867	0.003934	0.035861	10.54	0.242	0.055039	543.01	806.99	403.49	1500
0.09	0.601	1135.95	0.005269	0.007908	0.003954	0.035904	10.18	0.238	0.052863	539.79	810.21	405.11	1500
0.10	0.602	1135.02	0.005256	0.007928	0.003964	0.035925	10.01	0.236	0.051835	538.22	811.78	405.89	1500
0.11	0.603	1134.11	0.005244	0.007947	0.003974	0.035946	9.84	0.234	0.050844	536.69	813.31	406.66	1500
0.12	0.604	1133.22	0.005233	0.007967	0.003983	0.035966	9.68	0.232	0.049888	535.18	814.82	407.41	1500
0.15	0.606	1131.48	0.00521	0.008004	0.004002	0.036006	9.37	0.228	0.048076	532.25	817.75	408.87	1500
0.16	0.607	1130.64	0.005198	0.008022	0.004011	0.036025	9.23	0.226	0.047216	530.83	819.17	409.59	1500
0.17	0.608	1129.81	0.005187	0.00804	0.00402	0.036044	9.08	0.225	0.046385	529.43	820.57	410.29	1500
0.18	0.609	1128.99	0.005177	0.008058	0.004029	0.036062	8.95	0.223	0.04558	528.05	821.95	410.97	1500
0.21	0.611	1127.41	0.005156	0.008092	0.004046	0.036099	8.69	0.220	0.044049	525.37	824.63	412.31	1500
0.22	0.612	1126.63	0.005145	0.008109	0.004055	0.036117	8.56	0.218	0.043319	524.07	825.93	412.97	1500
0.23	0.613	1125.87	0.005135	0.008126	0.004063	0.036134	8.44	0.216	0.042612	522.78	827.22	413.61	1500
0.24	0.614	1125.12	0.005125	0.008142	0.004071	0.036151	8.32	0.215	0.041927	521.52	828.48	414.24	1500
0.27	0.616	1123.65	0.005106	0.008174	0.004087	0.036185	8.10	0.212	0.040617	519.05	830.95	415.47	1500
0.28	0.617	1122.94	0.005096	0.008189	0.004095	0.036202	7.99	0.211	0.03999	517.85	832.15	416.08	1500
0.29	0.618	1122.23	0.005087	0.008205	0.004102	0.036218	7.88	0.209	0.039382	516.66	833.34	416.67	1500
0.31	0.619	1121.54	0.005078	0.00822	0.00411	0.036234	7.78	0.208	0.038791	515.49	834.51	417.25	1500
0.33	0.620	1120.18	0.005059	0.00825	0.004125	0.036266	7.58	0.205	0.037658	513.20	836.80	418.40	1500
0.34	0.621	1119.52	0.005051	0.008264	0.004132	0.036281	7.49	0.204	0.037115	512.09	837.91	418.96	1500
0.35	0.622	1118.87	0.005042	0.008278	0.004139	0.036296	7.40	0.203	0.036586	510.98	839.02	419.51	1500
0.37	0.623	1118.22	0.005033	0.008293	0.004146	0.036311	7.31	0.201	0.036072	509.90	840.10	420.05	1500
0.39	0.624	1116.96	0.005016	0.00832	0.00416	0.036341	7.13	0.199	0.035083	507.77	842.23	421.11	1500
0.40	0.625	1116.34	0.005008	0.008334	0.004167	0.036355	7.05	0.198	0.034608	506.73	843.27	421.64	1500

0.41	0.626	1115.73	0.005	0.008347	0.004174	0.03637	6.97	0.197	0.034144	505.70	844.30	422.15	1500
0.43	0.627	1115.12	0.004992	0.008361	0.00418	0.036384	6.89	0.195	0.033692	504.69	845.31	422.66	1500
0.45	0.628	1113.94	0.004976	0.008387	0.004193	0.036412	6.73	0.193	0.032822	502.70	847.30	423.65	1500
0.46	0.629	1113.36	0.004968	0.0084	0.0042	0.036425	6.66	0.192	0.032403	501.72	848.28	424.14	1500
0.48	0.629	1112.79	0.00496	0.008412	0.004206	0.036439	6.59	0.191	0.031993	500.76	849.24	424.62	1500
0.49	0.630	1112.22	0.004953	0.008425	0.004212	0.036452	6.52	0.190	0.031594	499.81	850.19	425.10	1500
0.51	0.631	1111.11	0.004938	0.008449	0.004225	0.036478	6.38	0.188	0.030822	497.94	852.06	426.03	1500
0.52	0.632	1110.57	0.00493	0.008461	0.004231	0.036491	6.31	0.187	0.030449	497.03	852.97	426.49	1500
0.54	0.633	1110.03	0.004923	0.008473	0.004237	0.036504	6.25	0.186	0.030085	496.12	853.88	426.94	1500
0.55	0.633	1109.50	0.004916	0.008485	0.004243	0.036517	6.18	0.185	0.029729	495.23	854.77	427.39	1500
0.57	0.635	1108.45	0.004902	0.008508	0.004254	0.036542	6.06	0.183	0.029041	493.47	856.53	428.26	1500
0.59	0.635	1107.94	0.004895	0.00852	0.00426	0.036554	6.00	0.182	0.028708	492.61	857.39	428.70	1500
0.60	0.636	1107.43	0.004888	0.008531	0.004266	0.036566	5.94	0.181	0.028382	491.75	858.25	429.12	1500
0.61	0.637	1106.93	0.004881	0.008542	0.004271	0.036578	5.89	0.180	0.028063	490.91	859.09	429.54	1500
0.63	0.638	1105.94	0.004868	0.008564	0.004282	0.036601	5.77	0.179	0.027445	489.25	860.75	430.37	1500
0.65	0.638	1105.45	0.004861	0.008575	0.004288	0.036613	5.72	0.178	0.027145	488.43	861.57	430.78	1500
0.66	0.639	1104.97	0.004855	0.008586	0.004293	0.036625	5.67	0.177	0.026852	487.63	862.37	431.19	1500
0.67	0.640	1104.50	0.004848	0.008596	0.004298	0.036636	5.61	0.176	0.026565	486.83	863.17	431.59	1500
0.70	0.641	1103.56	0.004836	0.008617	0.004309	0.036658	5.51	0.175	0.026007	485.26	864.74	432.37	1500
0.71	0.641	1103.10	0.004829	0.008628	0.004314	0.036669	5.46	0.174	0.025737	484.48	865.52	432.76	1500
0.72	0.642	1102.65	0.004823	0.008638	0.004319	0.03668	5.42	0.173	0.025471	483.72	866.28	433.14	1500
0.73	0.643	1102.19	0.004817	0.008648	0.004324	0.036691	5.37	0.172	0.025211	482.96	867.04	433.52	1500
0.76	0.644	1101.31	0.004805	0.008668	0.004334	0.036713	5.28	0.171	0.024706	481.47	868.53	434.27	1500
0.77	0.644	1100.87	0.004799	0.008678	0.004339	0.036723	5.23	0.170	0.02446	480.73	869.27	434.63	1500
0.78	0.645	1100.43	0.004793	0.008688	0.004344	0.036734	5.19	0.169	0.024219	480.00	870.00	435.00	1500
0.79	0.645	1100.00	0.004787	0.008697	0.004349	0.036744	5.14	0.169	0.023982	479.28	870.72	435.36	1500
0.82	0.646	1099.16	0.004776	0.008716	0.004358	0.036765	5.06	0.167	0.023522	477.86	872.14	436.07	1500
0.83	0.647	1098.74	0.00477	0.008726	0.004363	0.036775	5.02	0.167	0.023298	477.16	872.84	436.42	1500
0.84	0.647	1098.33	0.004765	0.008735	0.004367	0.036785	4.98	0.166	0.023078	476.47	873.53	436.76	1500
0.85	0.648	1097.92	0.004759	0.008744	0.004372	0.036795	4.94	0.165	0.022862	475.78	874.22	437.11	1500
0.88	0.649	1097.11	0.004748	0.008762	0.004381	0.036814	4.86	0.164	0.022441	474.43	875.57	437.79	1500

0.89	0.649	1096.71	0.004742	0.008771	0.004386	0.036824	4.82	0.163	0.022236	473.76	876.24	438.12	1500
0.90	0.650	1096.32	0.004737	0.00878	0.00439	0.036833	4.78	0.163	0.022035	473.10	876.90	438.45	1500
0.92	0.650	1095.93	0.004732	0.008789	0.004395	0.036843	4.75	0.162	0.021837	472.44	877.56	438.78	1500
0.94	0.651	1095.16	0.004721	0.008807	0.004403	0.036862	4.68	0.161	0.021451	471.15	878.85	439.43	1500
0.95	0.652	1094.78	0.004716	0.008815	0.004408	0.036871	4.64	0.160	0.021263	470.51	879.49	439.75	1500
0.96	0.652	1094.40	0.004711	0.008824	0.004412	0.03688	4.61	0.159	0.021077	469.88	880.12	440.06	1500
0.98	0.653	1094.02	0.004706	0.008832	0.004416	0.036889	4.57	0.159	0.020895	469.25	880.75	440.38	1500
1.00	0.654	1093.29	0.004696	0.008849	0.004425	0.036908	4.51	0.158	0.02054	468.01	881.99	440.99	1500
1.01	0.654	1092.92	0.004691	0.008857	0.004429	0.036916	4.47	0.157	0.020366	467.40	882.60	441.30	1500
1.02	0.654	1092.56	0.004686	0.008865	0.004433	0.036925	4.44	0.157	0.020196	466.79	883.21	441.60	1500
1.04	0.655	1092.20	0.004681	0.008874	0.004437	0.036934	4.41	0.156	0.020028	466.19	883.81	441.90	1500
1.06	0.656	1091.49	0.004671	0.00889	0.004445	0.036952	4.35	0.155	0.019699	465.00	885.00	442.50	1500
1.07	0.656	1091.14	0.004666	0.008898	0.004449	0.03696	4.32	0.154	0.019539	464.42	885.58	442.79	1500
1.09	0.657	1090.80	0.004661	0.008906	0.004453	0.036969	4.29	0.154	0.019381	463.83	886.17	443.08	1500
1.10	0.657	1090.45	0.004657	0.008913	0.004457	0.036977	4.26	0.153	0.019226	463.26	886.74	443.37	1500
1.12	0.658	1089.77	0.004647	0.008929	0.004465	0.036994	4.20	0.152	0.018921	462.12	887.88	443.94	1500
1.13	0.658	1089.43	0.004643	0.008937	0.004468	0.037002	4.17	0.152	0.018773	461.55	888.45	444.22	1500
1.15	0.659	1089.10	0.004638	0.008944	0.004472	0.03701	4.15	0.151	0.018626	460.99	889.01	444.50	1500
1.16	0.659	1088.77	0.004634	0.008952	0.004476	0.037019	4.12	0.151	0.018482	460.44	889.56	444.78	1500
1.18	0.660	1088.12	0.004624	0.008967	0.004483	0.037035	4.07	0.150	0.0182	459.34	890.66	445.33	1500
1.20	0.660	1087.79	0.00462	0.008974	0.004487	0.037043	4.04	0.149	0.018062	458.80	891.20	445.60	1500
1.21	0.661	1087.47	0.004616	0.008982	0.004491	0.037051	4.01	0.149	0.017925	458.26	891.74	445.87	1500
1.22	0.661	1087.15	0.004611	0.008989	0.004494	0.037059	3.99	0.148	0.017791	457.73	892.27	446.14	1500
1.24	0.662	1086.52	0.004603	0.009003	0.004502	0.037074	3.94	0.147	0.017528	456.67	893.33	446.66	1500
1.26	0.662	1086.21	0.004598	0.00901	0.004505	0.037082	3.91	0.147	0.0174	456.15	893.85	446.92	1500
1.27	0.663	1085.90	0.004594	0.009017	0.004509	0.03709	3.89	0.146	0.017273	455.63	894.37	447.18	1500
1.28	0.663	1085.59	0.00459	0.009025	0.004512	0.037097	3.87	0.146	0.017147	455.12	894.88	447.44	1500
1.31	0.664	1084.99	0.004581	0.009038	0.004519	0.037112	3.82	0.145	0.016902	454.10	895.90	447.95	1500
1.32	0.664	1084.69	0.004577	0.009045	0.004523	0.03712	3.80	0.145	0.016782	453.60	896.40	448.20	1500
1.33	0.665	1084.39	0.004573	0.009052	0.004526	0.037127	3.77	0.144	0.016663	453.10	896.90	448.45	1500
1.34	0.665	1084.09	0.004569	0.009059	0.00453	0.037135	3.75	0.144	0.016546	452.60	897.40	448.70	1500

1.37	0.666	1083.50	0.004561	0.009073	0.004536	0.037149	3.71	0.143	0.016317	451.62	898.38	449.19	1500
1.38	0.666	1083.21	0.004557	0.009079	0.00454	0.037157	3.69	0.142	0.016204	451.13	898.87	449.44	1500
1.39	0.666	1082.93	0.004553	0.009086	0.004543	0.037164	3.66	0.142	0.016093	450.65	899.35	449.68	1500
1.40	0.667	1082.64	0.004549	0.009092	0.004546	0.037171	3.64	0.142	0.015984	450.17	899.83	449.92	1500
1.43	0.667	1082.07	0.004541	0.009106	0.004553	0.037185	3.60	0.141	0.015769	449.22	900.78	450.39	1500
1.44	0.668	1081.79	0.004537	0.009112	0.004556	0.037192	3.58	0.140	0.015663	448.75	901.25	450.63	1500
1.45	0.668	1081.51	0.004533	0.009118	0.004559	0.037199	3.56	0.140	0.015559	448.28	901.72	450.86	1500
1.46	0.668	1081.24	0.004529	0.009125	0.004562	0.037206	3.54	0.140	0.015456	447.82	902.18	451.09	1500
1.49	0.669	1080.69	0.004522	0.009137	0.004569	0.03722	3.50	0.139	0.015254	446.90	903.10	451.55	1500
1.50	0.669	1080.42	0.004518	0.009144	0.004572	0.037227	3.48	0.138	0.015155	446.44	903.56	451.78	1500
1.51	0.670	1080.15	0.004514	0.00915	0.004575	0.037233	3.46	0.138	0.015057	445.99	904.01	452.00	1500
1.53	0.670	1079.88	0.004509	0.009159	0.00458	0.037244	3.44	0.138	0.014914	445.33	904.67	452.34	1500

Reactor Stage 5 Data

V	x	T	Ca	Cc	Cd	Ci	k1	Kc	rate	Fa	Fc	Fd	Fi
[m ³]	[-]	[K]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[s ⁻¹]	[-]	[mol/dm ³ ·s]	[mol/s]	[mol/s]	[mol/s]	[mol/s]
0.000	0.670	1143.00	0.004261	0.008652	0.004326	0.043478	11.47	0.2527	0.047758	445.50	904.50	452.25	1500.00
0.018	0.672	1141.43	0.004244	0.00868	0.00434	0.043514	11.20	0.2497	0.046426	443.31	906.69	453.34	1500.00
0.024	0.673	1140.93	0.004237	0.008691	0.004345	0.043528	11.10	0.2486	0.045917	442.46	907.54	453.77	1500.00
0.031	0.673	1140.43	0.00423	0.008702	0.004351	0.043541	11.00	0.2474	0.045418	441.62	908.38	454.19	1500.00
0.043	0.674	1139.44	0.004217	0.008723	0.004361	0.043568	10.80	0.2452	0.04445	439.97	910.03	455.02	1500.00
0.049	0.675	1138.95	0.004211	0.008733	0.004367	0.043582	10.71	0.2441	0.04398	439.15	910.85	455.42	1500.00
0.055	0.676	1138.47	0.004204	0.008744	0.004372	0.043595	10.61	0.2430	0.04352	438.35	911.65	455.83	1500.00
0.061	0.676	1138.00	0.004198	0.008754	0.004377	0.043608	10.52	0.2419	0.043069	437.55	912.45	456.23	1500.00
0.073	0.677	1137.06	0.004185	0.008774	0.004387	0.043634	10.34	0.2399	0.042192	435.98	914.02	457.01	1500.00
0.079	0.678	1136.60	0.004179	0.008784	0.004392	0.043646	10.26	0.2388	0.041767	435.20	914.80	457.40	1500.00
0.085	0.678	1136.14	0.004173	0.008794	0.004397	0.043659	10.17	0.2378	0.041349	434.44	915.56	457.78	1500.00
0.091	0.679	1135.69	0.004167	0.008804	0.004402	0.043671	10.09	0.2368	0.040939	433.68	916.32	458.16	1500.00
0.103	0.680	1134.80	0.004155	0.008823	0.004412	0.043696	9.92	0.2349	0.040142	432.19	917.81	458.91	1500.00
0.110	0.681	1134.36	0.004149	0.008833	0.004416	0.043708	9.84	0.2339	0.039754	431.45	918.55	459.27	1500.00
0.116	0.681	1133.92	0.004143	0.008842	0.004421	0.04372	9.76	0.2330	0.039373	430.72	919.28	459.64	1500.00
0.122	0.682	1133.49	0.004137	0.008852	0.004426	0.043732	9.69	0.2321	0.039	430.00	920.00	460.00	1500.00
0.134	0.683	1132.64	0.004126	0.00887	0.004435	0.043756	9.54	0.2302	0.038272	428.58	921.42	460.71	1500.00
0.140	0.683	1132.22	0.00412	0.008879	0.00444	0.043767	9.46	0.2293	0.037917	427.87	922.13	461.06	1500.00
0.146	0.684	1131.81	0.004114	0.008888	0.004444	0.043779	9.39	0.2284	0.037569	427.18	922.82	461.41	1500.00
0.152	0.684	1131.40	0.004109	0.008897	0.004449	0.04379	9.32	0.2276	0.037226	426.49	923.51	461.76	1500.00
0.164	0.685	1130.59	0.004098	0.008915	0.004457	0.043813	9.18	0.2258	0.036559	425.13	924.87	462.43	1500.00
0.170	0.686	1130.19	0.004092	0.008924	0.004462	0.043824	9.11	0.2250	0.036234	424.46	925.54	462.77	1500.00
0.176	0.686	1129.79	0.004087	0.008932	0.004466	0.043835	9.05	0.2242	0.035914	423.80	926.20	463.10	1500.00
0.183	0.687	1129.40	0.004082	0.008941	0.00447	0.043846	8.98	0.2233	0.035599	423.14	926.86	463.43	1500.00
0.195	0.688	1128.62	0.004071	0.008958	0.004479	0.043868	8.85	0.2217	0.034985	421.84	928.16	464.08	1500.00
0.201	0.688	1128.24	0.004066	0.008966	0.004483	0.043878	8.79	0.2209	0.034686	421.19	928.81	464.40	1500.00

0.207	0.689	1127.86	0.004061	0.008975	0.004487	0.043889	8.73	0.2201	0.034391	420.56	929.44	464.72	1500.00
0.213	0.689	1127.48	0.004056	0.008983	0.004491	0.0439	8.67	0.2194	0.034101	419.93	930.07	465.04	1500.00
0.225	0.690	1126.74	0.004046	0.008999	0.0045	0.04392	8.55	0.2178	0.033534	418.68	931.32	465.66	1500.00
0.231	0.691	1126.37	0.004041	0.009007	0.004504	0.043931	8.49	0.2171	0.033258	418.07	931.93	465.97	1500.00
0.237	0.691	1126.00	0.004036	0.009015	0.004508	0.043941	8.43	0.2163	0.032985	417.46	932.54	466.27	1500.00
0.243	0.691	1125.64	0.004031	0.009023	0.004512	0.043951	8.37	0.2156	0.032717	416.85	933.15	466.57	1500.00
0.255	0.692	1124.93	0.004021	0.009039	0.004519	0.043971	8.26	0.2142	0.032193	415.65	934.35	467.17	1500.00
0.262	0.693	1124.57	0.004016	0.009047	0.004523	0.043981	8.21	0.2134	0.031937	415.06	934.94	467.47	1500.00
0.268	0.693	1124.22	0.004011	0.009054	0.004527	0.043991	8.15	0.2127	0.031684	414.48	935.52	467.76	1500.00
0.274	0.694	1123.88	0.004007	0.009062	0.004531	0.044001	8.10	0.2120	0.031435	413.90	936.10	468.05	1500.00
0.286	0.694	1123.19	0.003997	0.009077	0.004539	0.04402	8.00	0.2107	0.030949	412.75	937.25	468.63	1500.00
0.292	0.695	1122.85	0.003993	0.009084	0.004542	0.04403	7.95	0.2100	0.030711	412.18	937.82	468.91	1500.00
0.298	0.695	1122.51	0.003988	0.009092	0.004546	0.044039	7.90	0.2093	0.030476	411.61	938.39	469.19	1500.00
0.304	0.696	1122.18	0.003984	0.009099	0.00455	0.044049	7.85	0.2087	0.030245	411.06	938.94	469.47	1500.00
0.316	0.697	1121.52	0.003975	0.009114	0.004557	0.044067	7.75	0.2074	0.029793	409.95	940.05	470.03	1500.00
0.322	0.697	1121.19	0.00397	0.009121	0.004561	0.044077	7.70	0.2067	0.029571	409.40	940.60	470.30	1500.00
0.328	0.697	1120.87	0.003966	0.009128	0.004564	0.044086	7.66	0.2061	0.029352	408.86	941.14	470.57	1500.00
0.335	0.698	1120.55	0.003961	0.009135	0.004568	0.044095	7.61	0.2055	0.029137	408.32	941.68	470.84	1500.00
0.347	0.699	1119.91	0.003952	0.009149	0.004575	0.044113	7.52	0.2042	0.028715	407.26	942.74	471.37	1500.00
0.353	0.699	1119.59	0.003948	0.009156	0.004578	0.044122	7.47	0.2036	0.028508	406.73	943.27	471.64	1500.00
0.359	0.699	1119.28	0.003944	0.009163	0.004582	0.044131	7.43	0.2030	0.028304	406.20	943.80	471.90	1500.00
0.365	0.700	1118.97	0.00394	0.00917	0.004585	0.04414	7.39	0.2024	0.028103	405.68	944.32	472.16	1500.00
0.377	0.700	1118.35	0.003931	0.009184	0.004592	0.044157	7.30	0.2012	0.027708	404.66	945.34	472.67	1500.00
0.383	0.701	1118.05	0.003927	0.009191	0.004595	0.044166	7.26	0.2006	0.027515	404.15	945.85	472.93	1500.00
0.389	0.701	1117.75	0.003923	0.009197	0.004599	0.044175	7.22	0.2000	0.027324	403.64	946.36	473.18	1500.00
0.395	0.702	1117.45	0.003919	0.009204	0.004602	0.044183	7.18	0.1995	0.027136	403.14	946.86	473.43	1500.00
0.407	0.702	1116.85	0.003911	0.009217	0.004609	0.0442	7.10	0.1983	0.026766	402.15	947.85	473.93	1500.00
0.414	0.703	1116.56	0.003907	0.009224	0.004612	0.044209	7.06	0.1978	0.026585	401.66	948.34	474.17	1500.00
0.420	0.703	1116.27	0.003903	0.00923	0.004615	0.044217	7.02	0.1972	0.026406	401.17	948.83	474.42	1500.00
0.426	0.703	1115.98	0.003899	0.009237	0.004618	0.044225	6.98	0.1967	0.026229	400.68	949.32	474.66	1500.00
0.438	0.704	1115.40	0.003891	0.009249	0.004625	0.044242	6.90	0.1956	0.025882	399.72	950.28	475.14	1500.00

0.444	0.704	1115.12	0.003887	0.009256	0.004628	0.04425	6.87	0.1951	0.025712	399.25	950.75	475.38	1500.00
0.450	0.705	1114.84	0.003883	0.009262	0.004631	0.044258	6.83	0.1945	0.025544	398.78	951.22	475.61	1500.00
0.456	0.705	1114.56	0.003879	0.009268	0.004634	0.044266	6.79	0.1940	0.025378	398.31	951.69	475.85	1500.00
0.468	0.706	1114.00	0.003871	0.009281	0.00464	0.044282	6.72	0.1930	0.025052	397.38	952.62	476.31	1500.00
0.474	0.706	1113.73	0.003868	0.009287	0.004643	0.04429	6.69	0.1925	0.024892	396.92	953.08	476.54	1500.00
0.480	0.706	1113.45	0.003864	0.009293	0.004646	0.044298	6.65	0.1920	0.024733	396.46	953.54	476.77	1500.00
0.487	0.707	1113.18	0.00386	0.009299	0.00465	0.044305	6.62	0.1915	0.024577	396.01	953.99	477.00	1500.00
0.499	0.707	1112.64	0.003853	0.009311	0.004656	0.044321	6.55	0.1905	0.02427	395.11	954.89	477.45	1500.00
0.505	0.708	1112.38	0.003849	0.009317	0.004659	0.044329	6.52	0.1900	0.024119	394.66	955.34	477.67	1500.00
0.511	0.708	1112.11	0.003845	0.009323	0.004661	0.044336	6.48	0.1895	0.02397	394.22	955.78	477.89	1500.00
0.517	0.708	1111.85	0.003842	0.009329	0.004664	0.044344	6.45	0.1890	0.023823	393.78	956.22	478.11	1500.00
0.529	0.709	1111.33	0.003834	0.00934	0.00467	0.044359	6.39	0.1881	0.023533	392.90	957.10	478.55	1500.00
0.535	0.709	1111.07	0.003831	0.009346	0.004673	0.044366	6.36	0.1876	0.023391	392.47	957.53	478.76	1500.00
0.541	0.710	1110.81	0.003827	0.009352	0.004676	0.044374	6.33	0.1871	0.02325	392.04	957.96	478.98	1500.00
0.547	0.710	1110.56	0.003824	0.009358	0.004679	0.044381	6.29	0.1867	0.023111	391.62	958.38	479.19	1500.00
0.559	0.711	1110.05	0.003817	0.009369	0.004685	0.044396	6.23	0.1858	0.022837	390.77	959.23	479.62	1500.00
0.566	0.711	1109.80	0.003813	0.009375	0.004687	0.044403	6.20	0.1853	0.022702	390.35	959.65	479.83	1500.00
0.572	0.711	1109.55	0.00381	0.00938	0.00469	0.04441	6.17	0.1849	0.022569	389.93	960.07	480.03	1500.00
0.578	0.712	1109.30	0.003806	0.009386	0.004693	0.044418	6.14	0.1844	0.022437	389.52	960.48	480.24	1500.00
0.590	0.712	1108.81	0.0038	0.009397	0.004699	0.044432	6.09	0.1835	0.022178	388.70	961.30	480.65	1500.00
0.596	0.713	1108.56	0.003796	0.009402	0.004701	0.044439	6.06	0.1831	0.022051	388.29	961.71	480.86	1500.00
0.602	0.713	1108.32	0.003793	0.009408	0.004704	0.044446	6.03	0.1827	0.021925	387.88	962.12	481.06	1500.00
0.608	0.713	1108.08	0.00379	0.009413	0.004707	0.044453	6.00	0.1823	0.0218	387.48	962.52	481.26	1500.00
0.620	0.714	1107.60	0.003783	0.009424	0.004712	0.044467	5.95	0.1814	0.021555	386.68	963.32	481.66	1500.00
0.626	0.714	1107.37	0.00378	0.009429	0.004715	0.044474	5.92	0.1810	0.021434	386.29	963.71	481.86	1500.00
0.632	0.714	1107.13	0.003776	0.009435	0.004717	0.044481	5.89	0.1806	0.021314	385.89	964.11	482.05	1500.00
0.639	0.715	1106.90	0.003773	0.00944	0.00472	0.044488	5.87	0.1802	0.021196	385.50	964.50	482.25	1500.00
0.651	0.715	1106.43	0.003767	0.009451	0.004725	0.044501	5.81	0.1794	0.020963	384.72	965.28	482.64	1500.00
0.657	0.715	1106.20	0.003763	0.009456	0.004728	0.044508	5.79	0.1790	0.020848	384.34	965.66	482.83	1500.00
0.663	0.716	1105.97	0.00376	0.009461	0.00473	0.044514	5.76	0.1786	0.020735	383.96	966.04	483.02	1500.00
0.669	0.716	1105.74	0.003757	0.009466	0.004733	0.044521	5.74	0.1782	0.020623	383.57	966.43	483.21	1500.00

0.681	0.717	1105.29	0.003751	0.009476	0.004738	0.044534	5.69	0.1774	0.020401	382.82	967.18	483.59	1500.00
0.687	0.717	1105.07	0.003748	0.009481	0.004741	0.044541	5.66	0.1770	0.020292	382.44	967.56	483.78	1500.00
0.693	0.717	1104.84	0.003745	0.009486	0.004743	0.044547	5.64	0.1766	0.020184	382.07	967.93	483.96	1500.00
0.699	0.717	1104.62	0.003741	0.009491	0.004746	0.044554	5.61	0.1762	0.020078	381.70	968.30	484.15	1500.00
0.711	0.718	1104.18	0.003735	0.009501	0.004751	0.044567	5.57	0.1755	0.019867	380.96	969.04	484.52	1500.00
0.718	0.718	1103.96	0.003732	0.009506	0.004753	0.044573	5.54	0.1751	0.019763	380.60	969.40	484.70	1500.00
0.724	0.718	1103.74	0.003729	0.009511	0.004756	0.04458	5.52	0.1747	0.019661	380.24	969.76	484.88	1500.00
0.730	0.719	1103.53	0.003726	0.009516	0.004758	0.044586	5.50	0.1743	0.019559	379.87	970.13	485.06	1500.00
0.742	0.719	1103.10	0.00372	0.009526	0.004763	0.044599	5.45	0.1736	0.019359	379.16	970.84	485.42	1500.00
0.748	0.720	1102.89	0.003717	0.009531	0.004765	0.044605	5.43	0.1732	0.01926	378.80	971.20	485.60	1500.00
0.754	0.720	1102.67	0.003714	0.009535	0.004768	0.044611	5.41	0.1729	0.019162	378.45	971.55	485.78	1500.00
0.760	0.720	1102.47	0.00371	0.009543	0.004771	0.04462	5.37	0.1724	0.019019	377.93	972.07	486.04	1500.00

Appendix C

Appendix C presents the various reactor stage data as compiled from the numerical solver PolyMath for a reactor system operation at 90 bar.

Reactor Stage 1 Data

V	x	T	Ca	Cc	Cd	Ci	k1	Kc	rate	Fa	Fc	Fd	Fi
[m ³]	[-]	[K]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[s ⁻¹]	[-]	[mol/dm ³ ·s]	[mol/s]	[mol/s]	[mol/s]	[mol/s]
0.00	0.000	1143.00	0.448916	0	0	0.498795	11.471	0.2527	5.149361	1350.00	0.00	0.00	1500.00
0.01	0.033	1116.66	0.441695	0.013356	0.006678	0.505612	7.482	0.2037	3.284375	1310.38	39.62	19.81	1500.00
0.02	0.050	1103.63	0.437592	0.021058	0.010529	0.509611	5.831	0.1796	2.515988	1288.02	61.98	30.99	1500.00
0.02	0.057	1098.05	0.435728	0.024585	0.012292	0.511459	5.199	0.1695	2.222549	1277.90	72.10	36.05	1500.00
0.03	0.063	1093.06	0.434068	0.02774	0.01387	0.513121	4.690	0.1609	1.986785	1268.91	81.09	40.55	1500.00
0.03	0.069	1088.56	0.432573	0.030593	0.015297	0.51463	4.271	0.1535	1.793427	1260.83	89.17	44.59	1500.00
0.04	0.079	1080.70	0.429974	0.035582	0.017791	0.517284	3.625	0.1413	1.49563	1246.82	103.18	51.59	1500.00
0.05	0.083	1077.23	0.42883	0.037787	0.018894	0.518464	3.370	0.1362	1.378704	1240.68	109.32	54.66	1500.00
0.05	0.087	1074.02	0.427772	0.039834	0.019917	0.519562	3.150	0.1316	1.277482	1235.00	115.00	57.50	1500.00
0.05	0.091	1071.03	0.426787	0.041744	0.020872	0.520589	2.957	0.1275	1.189047	1229.72	120.28	60.14	1500.00
0.06	0.098	1065.62	0.425005	0.045211	0.022606	0.522462	2.635	0.1203	1.042058	1220.20	129.80	64.90	1500.00
0.07	0.101	1063.16	0.424194	0.046795	0.023397	0.523321	2.500	0.1171	0.980368	1215.87	134.13	67.06	1500.00
0.07	0.104	1060.83	0.423429	0.048291	0.024146	0.524134	2.378	0.1142	0.924976	1211.80	138.20	69.10	1500.00
0.08	0.107	1058.63	0.422705	0.04971	0.024855	0.524906	2.268	0.1115	0.874978	1207.95	142.05	71.03	1500.00
0.08	0.112	1054.56	0.421367	0.05234	0.02617	0.526341	2.077	0.1067	0.788345	1200.84	149.16	74.58	1500.00
0.09	0.114	1052.67	0.420746	0.053563	0.026782	0.52701	1.993	0.1045	0.75059	1197.55	152.45	76.23	1500.00
0.09	0.116	1050.87	0.420154	0.054732	0.027366	0.527651	1.917	0.1024	0.715944	1194.41	155.59	77.80	1500.00
0.10	0.119	1049.15	0.419588	0.05585	0.027925	0.528265	1.846	0.1005	0.684046	1191.41	158.59	79.29	1500.00
0.11	0.123	1045.93	0.418527	0.057951	0.028976	0.529421	1.720	0.0970	0.627305	1185.81	164.19	82.10	1500.00
0.11	0.125	1044.41	0.418029	0.05894	0.02947	0.529966	1.664	0.0954	0.60197	1183.18	166.82	83.41	1500.00

0.11	0.126	1042.96	0.41755	0.059892	0.029946	0.530491	1.611	0.0938	0.578385	1180.65	169.35	84.67	1500.00
0.12	0.128	1041.56	0.41709	0.060808	0.030404	0.530997	1.562	0.0924	0.556378	1178.22	171.78	85.89	1500.00
0.13	0.131	1038.91	0.416218	0.062546	0.031273	0.531959	1.473	0.0897	0.516519	1173.64	176.36	88.18	1500.00
0.13	0.133	1037.66	0.415805	0.06337	0.031685	0.532416	1.433	0.0884	0.498418	1171.46	178.54	89.27	1500.00
0.14	0.135	1036.45	0.415406	0.064167	0.032084	0.532859	1.394	0.0872	0.481395	1169.37	180.63	90.32	1500.00
0.14	0.136	1035.27	0.41502	0.064939	0.03247	0.533288	1.359	0.0861	0.465357	1167.34	182.66	91.33	1500.00
0.15	0.139	1033.04	0.414285	0.066412	0.033206	0.534107	1.292	0.0840	0.435924	1163.49	186.51	93.26	1500.00
0.15	0.140	1031.98	0.413934	0.067115	0.033557	0.534499	1.262	0.0830	0.42239	1161.65	188.35	94.17	1500.00
0.16	0.141	1030.95	0.413594	0.067797	0.033899	0.534879	1.233	0.0820	0.409564	1159.87	190.13	95.06	1500.00
0.16	0.143	1029.95	0.413264	0.068461	0.03423	0.535249	1.206	0.0811	0.397394	1158.14	191.86	95.93	1500.00
0.17	0.145	1028.04	0.412632	0.069732	0.034866	0.53596	1.155	0.0793	0.374831	1154.84	195.16	97.58	1500.00
0.17	0.146	1027.12	0.412329	0.070342	0.035171	0.536301	1.131	0.0785	0.364357	1153.26	196.74	98.37	1500.00
0.18	0.147	1026.23	0.412035	0.070935	0.035468	0.536633	1.108	0.0777	0.354372	1151.72	198.28	99.14	1500.00
0.18	0.149	1025.36	0.411748	0.071514	0.035757	0.536957	1.087	0.0769	0.344843	1150.22	199.78	99.89	1500.00
0.19	0.151	1023.69	0.411197	0.072627	0.036314	0.537582	1.046	0.0755	0.327038	1147.35	202.65	101.32	1500.00
0.20	0.152	1022.89	0.410931	0.073163	0.036582	0.537883	1.027	0.0748	0.318709	1145.97	204.03	102.02	1500.00
0.20	0.153	1022.10	0.410673	0.073687	0.036843	0.538177	1.009	0.0741	0.310732	1144.62	205.38	102.69	1500.00
0.20	0.154	1021.34	0.41042	0.074197	0.037099	0.538464	0.992	0.0735	0.303085	1143.31	206.69	103.35	1500.00
0.21	0.155	1019.87	0.409933	0.075184	0.037592	0.539019	0.959	0.0722	0.288704	1140.78	209.22	104.61	1500.00
0.22	0.156	1019.16	0.409698	0.07566	0.03783	0.539287	0.943	0.0716	0.281936	1139.56	210.44	105.22	1500.00
0.22	0.157	1018.47	0.409469	0.076126	0.038063	0.53955	0.928	0.0711	0.275428	1138.36	211.64	105.82	1500.00
0.23	0.158	1017.79	0.409244	0.076582	0.038291	0.539807	0.914	0.0705	0.269166	1137.20	212.80	106.40	1500.00
0.23	0.160	1016.48	0.40881	0.077464	0.038732	0.540304	0.887	0.0694	0.257329	1134.94	215.06	107.53	1500.00
0.24	0.161	1015.84	0.4086	0.077891	0.038945	0.540546	0.874	0.0689	0.251729	1133.86	216.14	108.07	1500.00
0.24	0.161	1015.22	0.408395	0.078309	0.039155	0.540782	0.862	0.0684	0.246327	1132.79	217.21	108.61	1500.00
0.25	0.162	1014.62	0.408193	0.078719	0.039359	0.541013	0.849	0.0679	0.241114	1131.75	218.25	109.13	1500.00
0.26	0.164	1013.44	0.407803	0.079514	0.039757	0.541463	0.827	0.0670	0.231215	1129.73	220.27	110.14	1500.00
0.26	0.164	1012.87	0.407614	0.0799	0.03995	0.541682	0.816	0.0666	0.226512	1128.75	221.25	110.63	1500.00
0.26	0.165	1012.31	0.407428	0.080278	0.040139	0.541896	0.805	0.0661	0.221963	1127.79	222.21	111.11	1500.00
0.27	0.166	1011.76	0.407247	0.080649	0.040325	0.542106	0.795	0.0657	0.217561	1126.85	223.15	111.58	1500.00
0.28	0.167	1010.70	0.406893	0.08137	0.040685	0.542515	0.776	0.0649	0.209172	1125.02	224.98	112.49	1500.00

0.28	0.168	1010.18	0.406722	0.081721	0.04086	0.542714	0.766	0.0645	0.205171	1124.13	225.87	112.93	1500.00
0.28	0.168	1009.67	0.406553	0.082065	0.041033	0.542909	0.757	0.0641	0.201293	1123.26	226.74	113.37	1500.00
0.29	0.169	1009.18	0.406388	0.082403	0.041202	0.543101	0.749	0.0637	0.197532	1122.41	227.59	113.80	1500.00
0.30	0.170	1008.21	0.406066	0.083061	0.041531	0.543475	0.732	0.0630	0.19034	1120.75	229.25	114.63	1500.00
0.30	0.171	1007.74	0.40591	0.083382	0.041691	0.543657	0.724	0.0627	0.1869	1119.94	230.06	115.03	1500.00
0.31	0.171	1007.27	0.405756	0.083697	0.041848	0.543836	0.716	0.0623	0.183559	1119.15	230.85	115.43	1500.00
0.31	0.172	1006.82	0.405605	0.084006	0.042003	0.544012	0.708	0.0620	0.180311	1118.37	231.63	115.81	1500.00
0.32	0.173	1005.93	0.405311	0.084609	0.042305	0.544356	0.694	0.0613	0.174085	1116.85	233.15	116.57	1500.00
0.32	0.174	1005.50	0.405167	0.084904	0.042452	0.544523	0.687	0.0610	0.171098	1116.12	233.88	116.94	1500.00
0.33	0.174	1005.08	0.405026	0.085193	0.042596	0.544688	0.680	0.0607	0.168192	1115.39	234.61	117.31	1500.00
0.33	0.175	1004.66	0.404888	0.085478	0.042739	0.54485	0.673	0.0604	0.165363	1114.68	235.32	117.66	1500.00
0.34	0.176	1003.85	0.404617	0.086033	0.043017	0.545167	0.661	0.0598	0.159926	1113.28	236.72	118.36	1500.00
0.34	0.176	1003.45	0.404485	0.086304	0.043152	0.545322	0.655	0.0596	0.157311	1112.61	237.39	118.70	1500.00
0.35	0.177	1003.06	0.404355	0.086571	0.043286	0.545474	0.649	0.0593	0.154763	1111.94	238.06	119.03	1500.00
0.35	0.177	1002.68	0.404227	0.086834	0.043417	0.545624	0.643	0.0590	0.15228	1111.28	238.72	119.36	1500.00
0.36	0.178	1001.93	0.403978	0.087348	0.043674	0.545917	0.631	0.0585	0.147495	1110.00	240.00	120.00	1500.00
0.37	0.178	1001.57	0.403856	0.087599	0.043799	0.54606	0.626	0.0582	0.145189	1109.37	240.63	120.31	1500.00
0.37	0.179	1001.21	0.403736	0.087846	0.043923	0.546202	0.621	0.0580	0.142939	1108.75	241.25	120.62	1500.00
0.37	0.179	1000.85	0.403617	0.088089	0.044045	0.546341	0.615	0.0577	0.140743	1108.15	241.85	120.93	1500.00
0.38	0.180	1000.16	0.403386	0.088566	0.044283	0.546613	0.605	0.0573	0.136504	1106.96	243.04	121.52	1500.00
0.39	0.181	999.82	0.403273	0.088799	0.044399	0.546746	0.601	0.0570	0.134457	1106.38	243.62	121.81	1500.00
0.39	0.181	999.48	0.403162	0.089028	0.044514	0.546878	0.596	0.0568	0.132458	1105.81	244.19	122.10	1500.00
0.40	0.182	999.16	0.403052	0.089254	0.044627	0.547007	0.591	0.0566	0.130504	1105.25	244.75	122.38	1500.00
0.40	0.182	998.51	0.402837	0.089697	0.044849	0.547261	0.582	0.0561	0.126725	1104.15	245.85	122.93	1500.00
0.41	0.183	998.20	0.402732	0.089914	0.044957	0.547385	0.578	0.0559	0.124898	1103.61	246.39	123.20	1500.00
0.41	0.183	997.89	0.402629	0.090128	0.045064	0.547508	0.574	0.0557	0.123111	1103.08	246.92	123.46	1500.00
0.42	0.183	997.58	0.402527	0.090339	0.04517	0.547628	0.569	0.0555	0.121362	1102.55	247.45	123.72	1500.00
0.43	0.184	996.98	0.402327	0.090752	0.045376	0.547865	0.561	0.0551	0.117976	1101.53	248.47	124.24	1500.00
0.43	0.185	996.69	0.402229	0.090955	0.045477	0.547981	0.557	0.0549	0.116336	1101.03	248.97	124.49	1500.00
0.43	0.185	996.40	0.402132	0.091154	0.045577	0.548096	0.554	0.0547	0.114731	1100.53	249.47	124.73	1500.00
0.44	0.185	996.11	0.402037	0.091351	0.045676	0.548209	0.550	0.0545	0.113158	1100.05	249.95	124.98	1500.00

0.45	0.186	995.56	0.40185	0.091738	0.045869	0.548431	0.543	0.0542	0.110109	1099.09	250.91	125.45	1500.00
0.45	0.186	995.28	0.401758	0.091927	0.045963	0.548539	0.539	0.0540	0.10863	1098.62	251.38	125.69	1500.00
0.46	0.187	995.01	0.401668	0.092114	0.046057	0.548647	0.535	0.0538	0.107181	1098.16	251.84	125.92	1500.00
0.46	0.187	994.75	0.401579	0.092298	0.046149	0.548753	0.532	0.0537	0.10576	1097.71	252.29	126.15	1500.00
0.47	0.188	994.22	0.401404	0.09266	0.04633	0.54896	0.525	0.0533	0.103002	1096.81	253.19	126.59	1500.00
0.47	0.188	993.97	0.401319	0.092838	0.046419	0.549062	0.522	0.0531	0.101662	1096.37	253.63	126.81	1500.00
0.48	0.188	993.71	0.401234	0.093013	0.046507	0.549163	0.519	0.0530	0.100349	1095.94	254.06	127.03	1500.00
0.48	0.189	993.46	0.40115	0.093186	0.046593	0.549263	0.516	0.0528	0.09906	1095.51	254.49	127.24	1500.00
0.49	0.189	992.97	0.400986	0.093526	0.046763	0.549458	0.510	0.0525	0.096555	1094.68	255.32	127.66	1500.00
0.49	0.190	992.73	0.400906	0.093693	0.046846	0.549554	0.507	0.0524	0.095337	1094.27	255.73	127.87	1500.00
0.50	0.190	992.50	0.400827	0.093858	0.046929	0.549649	0.504	0.0522	0.094141	1093.86	256.14	128.07	1500.00
0.50	0.190	992.26	0.400748	0.09402	0.04701	0.549743	0.501	0.0521	0.092968	1093.46	256.54	128.27	1500.00
0.51	0.191	991.80	0.400594	0.09434	0.04717	0.549926	0.496	0.0518	0.090684	1092.68	257.32	128.66	1500.00
0.52	0.191	991.58	0.400518	0.094497	0.047248	0.550017	0.493	0.0516	0.089572	1092.29	257.71	128.86	1500.00
0.52	0.191	991.35	0.400444	0.094652	0.047326	0.550106	0.490	0.0515	0.088481	1091.91	258.09	129.05	1500.00
0.52	0.192	991.13	0.40037	0.094805	0.047403	0.550194	0.488	0.0513	0.087408	1091.53	258.47	129.23	1500.00
0.53	0.192	990.70	0.400225	0.095106	0.047553	0.550368	0.483	0.0511	0.085319	1090.79	259.21	129.60	1500.00
0.54	0.192	990.61	0.40016	0.095241	0.047621	0.550446	0.480	0.0510	0.08439	1090.46	259.54	129.77	1500.00

Reactor Stage 2 Data

V	x	T	Ca	Cc	Cd	Ci	k1	Kc	rate	Fa	Fc	Fd	Fi
[m ³]	[-]	[K]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[s ⁻¹]	[-]	[mol/dm ³ ·s]	[mol/s]	[mol/s]	[mol/s]	[mol/s]
0.000	0.192	1143.00	0.346937	0.08244	0.04122	0.590886	11.471	0.2527	3.530699	1090.80	259.20	129.60	1500.00
0.003	0.202	1135.33	0.344748	0.086292	0.043146	0.593174	10.191	0.2381	3.058108	1079.74	270.26	135.13	1500.00
0.004	0.204	1133.13	0.343986	0.087636	0.043818	0.593975	9.778	0.2331	2.906367	1075.90	274.10	137.05	1500.00
0.005	0.207	1131.03	0.34326	0.088919	0.044459	0.594741	9.398	0.2285	2.76757	1072.24	277.76	138.88	1500.00
0.007	0.212	1127.10	0.341905	0.091317	0.045659	0.596177	8.728	0.2202	2.522823	1065.44	284.56	142.28	1500.00
0.008	0.214	1125.27	0.34127	0.092442	0.046221	0.596852	8.429	0.2163	2.414429	1062.26	287.74	143.87	1500.00
0.009	0.216	1123.51	0.340662	0.093522	0.046761	0.597501	8.152	0.2127	2.314014	1059.21	290.79	145.39	1500.00
0.011	0.219	1121.83	0.340078	0.09456	0.04728	0.598126	7.894	0.2093	2.220748	1056.29	293.71	146.85	1500.00
0.013	0.223	1118.64	0.338977	0.096521	0.04826	0.599309	7.428	0.2030	2.052866	1050.80	299.20	149.60	1500.00
0.014	0.224	1117.14	0.338456	0.097449	0.048725	0.599869	7.217	0.2000	1.977074	1048.20	301.80	150.90	1500.00
0.015	0.226	1115.69	0.337954	0.098345	0.049173	0.600412	7.019	0.1972	1.906048	1045.70	304.30	152.15	1500.00
0.016	0.228	1114.30	0.337469	0.099211	0.049606	0.600936	6.832	0.1946	1.839361	1043.29	306.71	153.36	1500.00
0.018	0.231	1111.64	0.336547	0.10086	0.05043	0.601936	6.490	0.1896	1.717542	1038.71	311.29	155.65	1500.00
0.019	0.233	1110.38	0.336109	0.101645	0.050823	0.602414	6.333	0.1873	1.661776	1036.53	313.47	156.73	1500.00
0.020	0.235	1109.15	0.335684	0.102407	0.051204	0.602877	6.184	0.1850	1.609071	1034.43	315.57	157.79	1500.00
0.021	0.236	1107.97	0.335272	0.103146	0.051573	0.603327	6.043	0.1829	1.559189	1032.39	317.61	158.81	1500.00
0.023	0.239	1105.70	0.334484	0.104561	0.05228	0.604189	5.782	0.1789	1.467052	1028.49	321.51	160.75	1500.00
0.024	0.240	1104.62	0.334107	0.105238	0.052619	0.604603	5.661	0.1770	1.424426	1026.63	323.37	161.69	1500.00
0.025	0.242	1103.57	0.33374	0.105897	0.052949	0.605006	5.545	0.1751	1.383879	1024.82	325.18	162.59	1500.00
0.026	0.243	1102.55	0.333384	0.106538	0.053269	0.605398	5.435	0.1734	1.345265	1023.06	326.94	163.47	1500.00
0.028	0.245	1100.58	0.3327	0.107771	0.053886	0.606153	5.229	0.1700	1.273324	1019.69	330.31	165.15	1500.00
0.029	0.246	1099.64	0.332371	0.108364	0.054182	0.606516	5.133	0.1684	1.239766	1018.07	331.93	165.96	1500.00
0.030	0.248	1098.72	0.33205	0.108943	0.054471	0.606871	5.041	0.1669	1.207679	1016.50	333.50	166.75	1500.00
0.031	0.249	1097.83	0.331738	0.109507	0.054753	0.607217	4.952	0.1654	1.176973	1014.96	335.04	167.52	1500.00
0.033	0.251	1096.10	0.331136	0.110595	0.055297	0.607886	4.786	0.1626	1.119366	1012.00	338.00	169.00	1500.00
0.034	0.252	1095.27	0.330845	0.11112	0.05556	0.608209	4.708	0.1612	1.092316	1010.58	339.42	169.71	1500.00

0.035	0.253	1094.46	0.330562	0.111633	0.055816	0.608525	4.632	0.1599	1.066344	1009.19	340.81	170.40	1500.00
0.037	0.254	1093.67	0.330285	0.112134	0.056067	0.608833	4.560	0.1586	1.041389	1007.83	342.17	171.08	1500.00
0.039	0.256	1092.14	0.329749	0.113104	0.056552	0.609431	4.423	0.1562	0.994308	1005.21	344.79	172.39	1500.00
0.040	0.257	1091.40	0.32949	0.113574	0.056787	0.609721	4.358	0.1551	0.972079	1003.95	346.05	173.03	1500.00
0.041	0.258	1090.68	0.329237	0.114033	0.057017	0.610005	4.295	0.1539	0.950663	1002.71	347.29	173.65	1500.00
0.042	0.259	1089.97	0.328989	0.114483	0.057241	0.610282	4.235	0.1528	0.930017	1001.50	348.50	174.25	1500.00
0.044	0.260	1088.60	0.328509	0.115355	0.057677	0.610821	4.120	0.1507	0.890881	999.15	350.85	175.42	1500.00
0.045	0.261	1087.94	0.328276	0.115778	0.057889	0.611083	4.065	0.1497	0.872319	998.02	351.98	175.99	1500.00
0.046	0.262	1087.29	0.328048	0.116192	0.058096	0.611134	4.012	0.1487	0.854384	996.90	353.10	176.55	1500.00
0.047	0.263	1086.65	0.327824	0.116599	0.058299	0.611591	3.961	0.1478	0.837046	995.81	354.19	177.09	1500.00
0.049	0.264	1085.41	0.32739	0.117388	0.058694	0.612081	3.864	0.1459	0.804048	993.70	356.30	178.15	1500.00
0.050	0.265	1084.81	0.32718	0.117772	0.058886	0.612319	3.817	0.1450	0.788336	992.68	357.32	178.66	1500.00
0.051	0.266	1084.23	0.326973	0.118148	0.059074	0.612552	3.772	0.1442	0.773118	991.67	358.33	179.17	1500.00
0.052	0.267	1083.65	0.32677	0.118518	0.059259	0.612782	3.728	0.1433	0.758371	990.68	359.32	179.66	1500.00
0.054	0.268	1082.53	0.326375	0.119237	0.059619	0.613228	3.644	0.1417	0.730209	988.77	361.23	180.62	1500.00
0.055	0.269	1081.98	0.326183	0.119587	0.059794	0.613446	3.604	0.1409	0.716755	987.83	362.17	181.08	1500.00
0.056	0.269	1081.45	0.325995	0.119931	0.059966	0.61366	3.565	0.1401	0.703696	986.92	363.08	181.54	1500.00
0.057	0.270	1080.92	0.32581	0.120269	0.060134	0.61387	3.527	0.1394	0.691015	986.02	363.98	181.99	1500.00
0.059	0.271	1079.90	0.325449	0.120927	0.060464	0.61428	3.455	0.1379	0.666727	984.27	365.73	182.86	1500.00
0.060	0.272	1079.40	0.325274	0.121248	0.060624	0.614479	3.420	0.1372	0.65509	983.42	366.58	183.29	1500.00
0.061	0.272	1078.91	0.325101	0.121564	0.060782	0.614676	3.386	0.1365	0.643775	982.59	367.41	183.71	1500.00
0.063	0.273	1078.43	0.324931	0.121874	0.060937	0.614869	3.352	0.1358	0.632767	981.76	368.24	184.12	1500.00
0.065	0.274	1077.49	0.3246	0.12248	0.06124	0.615247	3.289	0.1345	0.611627	980.16	369.84	184.92	1500.00
0.066	0.275	1077.03	0.324438	0.122775	0.061388	0.615431	3.258	0.1339	0.601474	979.38	370.62	185.31	1500.00
0.067	0.275	1076.58	0.324279	0.123066	0.061533	0.615613	3.228	0.1333	0.591584	978.61	371.39	185.69	1500.00
0.068	0.276	1076.14	0.324123	0.123352	0.061676	0.615792	3.199	0.1327	0.581949	977.86	372.14	186.07	1500.00
0.070	0.277	1075.27	0.323818	0.123912	0.061956	0.616141	3.143	0.1315	0.563402	976.38	373.62	186.81	1500.00
0.071	0.278	1074.85	0.323669	0.124185	0.062092	0.616312	3.115	0.1309	0.554475	975.66	374.34	187.17	1500.00
0.072	0.278	1074.44	0.323522	0.124454	0.062227	0.61648	3.089	0.1303	0.545766	974.95	375.05	187.52	1500.00
0.073	0.279	1074.03	0.323377	0.124719	0.062359	0.616645	3.063	0.1298	0.537269	974.25	375.75	187.87	1500.00
0.075	0.280	1073.23	0.323095	0.125237	0.062618	0.61697	3.013	0.1287	0.520882	972.89	377.11	188.55	1500.00

0.076	0.280	1072.84	0.322956	0.12549	0.062745	0.617128	2.989	0.1282	0.512978	972.23	377.77	188.89	1500.00
0.077	0.281	1072.45	0.32282	0.12574	0.06287	0.617285	2.965	0.1277	0.505258	971.57	378.43	189.22	1500.00
0.078	0.281	1072.07	0.322686	0.125986	0.062993	0.617439	2.942	0.1272	0.497716	970.92	379.08	189.54	1500.00
0.080	0.282	1071.33	0.322424	0.126468	0.063234	0.61774	2.897	0.1262	0.483145	969.66	380.34	190.17	1500.00
0.081	0.282	1070.97	0.322296	0.126703	0.063352	0.617888	2.876	0.1257	0.476104	969.04	380.96	190.48	1500.00
0.082	0.283	1070.61	0.322169	0.126936	0.063468	0.618034	2.855	0.1253	0.469219	968.43	381.57	190.78	1500.00
0.083	0.283	1070.26	0.322044	0.127165	0.063582	0.618177	2.834	0.1248	0.462486	967.83	382.17	191.08	1500.00
0.085	0.284	1069.57	0.3218	0.127614	0.063807	0.618459	2.794	0.1239	0.449456	966.66	383.34	191.67	1500.00
0.086	0.285	1069.23	0.32168	0.127834	0.063917	0.618597	2.774	0.1235	0.443149	966.08	383.92	191.96	1500.00
0.087	0.285	1068.90	0.321562	0.128051	0.064025	0.618733	2.755	0.1230	0.436977	965.52	384.48	192.24	1500.00
0.089	0.285	1068.57	0.321446	0.128265	0.064132	0.618868	2.736	0.1226	0.430934	964.96	385.04	192.52	1500.00
0.091	0.286	1067.93	0.321218	0.128684	0.064342	0.619131	2.700	0.1218	0.419221	963.86	386.14	193.07	1500.00
0.092	0.287	1067.62	0.321106	0.12889	0.064445	0.61926	2.682	0.1214	0.413545	963.33	386.67	193.34	1500.00
0.093	0.287	1067.31	0.320996	0.129093	0.064546	0.619388	2.665	0.1210	0.407983	962.80	387.20	193.60	1500.00
0.094	0.287	1067.00	0.320887	0.129293	0.064647	0.619514	2.648	0.1206	0.402533	962.28	387.72	193.86	1500.00
0.096	0.288	1066.40	0.320674	0.129686	0.064843	0.619761	2.615	0.1198	0.391957	961.25	388.75	194.37	1500.00
0.097	0.289	1066.10	0.320569	0.129879	0.064939	0.619882	2.599	0.1195	0.386824	960.75	389.25	194.62	1500.00
0.098	0.289	1065.81	0.320466	0.130069	0.065034	0.620002	2.583	0.1191	0.381791	960.26	389.74	194.87	1500.00
0.099	0.289	1065.53	0.320364	0.130257	0.065128	0.62012	2.568	0.1187	0.376855	959.77	390.23	195.12	1500.00
0.101	0.290	1064.96	0.320164	0.130626	0.065313	0.620352	2.538	0.1180	0.367264	958.81	391.19	195.60	1500.00
0.102	0.290	1064.69	0.320066	0.130807	0.065403	0.620466	2.523	0.1177	0.362604	958.34	391.66	195.83	1500.00
0.103	0.291	1064.41	0.319969	0.130985	0.065493	0.620579	2.509	0.1174	0.358031	957.88	392.12	196.06	1500.00
0.104	0.291	1064.15	0.319873	0.131162	0.065581	0.62069	2.495	0.1170	0.353543	957.42	392.58	196.29	1500.00
0.106	0.292	1063.62	0.319685	0.131509	0.065754	0.620909	2.467	0.1164	0.344812	956.52	393.48	196.74	1500.00
0.107	0.292	1063.36	0.319593	0.131679	0.06584	0.621016	2.454	0.1160	0.340566	956.08	393.92	196.96	1500.00
0.108	0.292	1063.10	0.319502	0.131847	0.065924	0.621122	2.441	0.1157	0.336395	955.64	394.36	197.18	1500.00
0.109	0.293	1062.85	0.319411	0.132014	0.066007	0.621227	2.428	0.1154	0.332299	955.21	394.79	197.40	1500.00
0.111	0.293	1062.35	0.319234	0.13234	0.06617	0.621433	2.403	0.1148	0.324323	954.36	395.64	197.82	1500.00
0.112	0.294	1062.11	0.319148	0.132501	0.06625	0.621534	2.390	0.1145	0.32044	953.95	396.05	198.03	1500.00
0.113	0.294	1061.87	0.319062	0.132659	0.06633	0.621634	2.378	0.1142	0.316624	953.54	396.46	198.23	1500.00
0.115	0.294	1061.63	0.318977	0.132816	0.066408	0.621733	2.366	0.1139	0.312873	953.13	396.87	198.43	1500.00

0.117	0.295	1061.16	0.31881	0.133124	0.066562	0.621928	2.343	0.1134	0.305563	952.34	397.66	198.83	1500.00
0.118	0.295	1060.93	0.318728	0.133276	0.066638	0.622023	2.332	0.1131	0.302001	951.95	398.05	199.03	1500.00
0.119	0.295	1060.70	0.318647	0.133426	0.066713	0.622118	2.321	0.1128	0.298498	951.56	398.44	199.22	1500.00
0.120	0.296	1060.48	0.318567	0.133574	0.066787	0.622212	2.310	0.1126	0.295054	951.18	398.82	199.41	1500.00
0.122	0.296	1060.04	0.318409	0.133865	0.066932	0.622396	2.288	0.1120	0.288334	950.42	399.58	199.79	1500.00
0.123	0.296	1059.82	0.318332	0.134008	0.067004	0.622486	2.278	0.1118	0.285056	950.06	399.94	199.97	1500.00
0.124	0.297	1059.60	0.318255	0.13415	0.067075	0.622576	2.268	0.1115	0.281832	949.69	400.31	200.15	1500.00
0.125	0.297	1059.39	0.31818	0.13429	0.067145	0.622664	2.257	0.1113	0.278659	949.33	400.67	200.34	1500.00
0.127	0.297	1058.97	0.318031	0.134565	0.067283	0.622838	2.238	0.1108	0.272465	948.62	401.38	200.69	1500.00
0.128	0.298	1058.77	0.317957	0.134701	0.06735	0.622924	2.228	0.1105	0.269441	948.27	401.73	200.86	1500.00
0.129	0.298	1058.57	0.317885	0.134835	0.067418	0.623009	2.218	0.1103	0.266465	947.93	402.07	201.04	1500.00
0.130	0.298	1058.39	0.317786	0.135018	0.067509	0.623125	2.205	0.1100	0.26242	947.45	402.55	201.27	1500.00

Reactor Stage 3 Data

V	x	T	Ca	Cc	Cd	Ci	k1	Kc	rate	Fa	Fc	Fd	Fi
[m ³]	[-]	[K]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[s ⁻¹]	[-]	[mol/dm ³ ·s]	[mol/s]	[mol/s]	[mol/s]	[mol/s]
0.0000	0.298	1143.00	0.2943	0.1250	0.0625	0.6642	11.4707	0.2527	2.4349	947.70	402.30	201.15	1500.00
0.0016	0.302	1139.93	0.2934	0.1265	0.0633	0.6652	10.9402	0.2468	2.2717	943.27	406.73	203.36	1500.00
0.0020	0.3030	1139.03	0.2931	0.1271	0.0635	0.6656	10.7614	0.2447	2.2169	941.74	408.26	204.13	1500.00
0.0025	0.3041	1138.15	0.2928	0.1276	0.0638	0.6659	10.5894	0.2427	2.1642	940.24	409.76	204.88	1500.00
0.0030	0.3051	1137.30	0.2925	0.1281	0.0641	0.6663	10.4239	0.2408	2.1137	938.78	411.22	205.61	1500.00
0.0040	0.3072	1135.64	0.2919	0.1291	0.0646	0.6669	10.1108	0.2371	2.0183	935.95	414.05	207.03	1500.00
0.0044	0.3082	1134.84	0.2916	0.1296	0.0648	0.6673	9.9626	0.2354	1.9733	934.58	415.42	207.71	1500.00
0.0049	0.3092	1134.06	0.2914	0.1301	0.0651	0.6676	9.8195	0.2337	1.9300	933.25	416.75	208.38	1500.00
0.0054	0.3101	1133.30	0.2911	0.1306	0.0653	0.6679	9.6814	0.2320	1.8882	931.94	418.06	209.03	1500.00
0.0064	0.3120	1131.82	0.2906	0.1315	0.0657	0.6685	9.4189	0.2288	1.8089	929.41	420.59	210.29	1500.00
0.0068	0.3129	1131.10	0.2903	0.1319	0.0660	0.6688	9.2941	0.2273	1.7714	928.19	421.81	210.91	1500.00
0.0073	0.3138	1130.40	0.2901	0.1324	0.0662	0.6691	9.1734	0.2258	1.7351	926.99	423.01	211.51	1500.00
0.0078	0.3146	1129.71	0.2898	0.1328	0.0664	0.6694	9.0564	0.2243	1.7000	925.81	424.19	212.09	1500.00
0.0088	0.3163	1128.37	0.2893	0.1336	0.0668	0.6699	8.8333	0.2215	1.6332	923.53	426.47	213.23	1500.00
0.0092	0.3171	1127.73	0.2891	0.1340	0.0670	0.6702	8.7269	0.2201	1.6014	922.43	427.57	213.79	1500.00
0.0097	0.3179	1127.09	0.2889	0.1344	0.0672	0.6704	8.6236	0.2188	1.5706	921.34	428.66	214.33	1500.00
0.0102	0.3187	1126.47	0.2887	0.1348	0.0674	0.6707	8.5234	0.2175	1.5408	920.28	429.72	214.86	1500.00
0.0112	0.3202	1125.25	0.2882	0.1355	0.0678	0.6712	8.3315	0.2151	1.4838	918.21	431.79	215.90	1500.00
0.0116	0.3210	1124.66	0.2880	0.1359	0.0680	0.6714	8.2397	0.2139	1.4566	917.20	432.80	216.40	1500.00
0.0121	0.3217	1124.08	0.2878	0.1363	0.0681	0.6717	8.1504	0.2127	1.4302	916.21	433.79	216.89	1500.00
0.0126	0.3224	1123.51	0.2876	0.1366	0.0683	0.6719	8.0636	0.2115	1.4046	915.24	434.76	217.38	1500.00
0.0136	0.3238	1122.41	0.2872	0.1373	0.0687	0.6724	7.8969	0.2093	1.3554	913.36	436.64	218.32	1500.00
0.0140	0.3245	1121.87	0.2870	0.1376	0.0688	0.6726	7.8169	0.2082	1.3319	912.44	437.56	218.78	1500.00
0.0145	0.3251	1121.34	0.2868	0.1380	0.0690	0.6728	7.7390	0.2072	1.3090	911.53	438.47	219.23	1500.00
0.0150	0.3258	1120.81	0.2866	0.1383	0.0691	0.6731	7.6631	0.2062	1.2868	910.65	439.35	219.68	1500.00
0.0160	0.3270	1119.80	0.2863	0.1389	0.0695	0.6735	7.5170	0.2042	1.2440	908.91	441.09	220.54	1500.00

0.0164	0.3277	1119.30	0.2861	0.1392	0.0696	0.6737	7.4467	0.2032	1.2235	908.07	441.93	220.97	1500.00
0.0169	0.3283	1118.82	0.2859	0.1395	0.0698	0.6739	7.3781	0.2023	1.2035	907.24	442.76	221.38	1500.00
0.0174	0.3289	1118.34	0.2857	0.1398	0.0699	0.6741	7.3112	0.2013	1.1840	906.42	443.58	221.79	1500.00
0.0184	0.3300	1117.40	0.2854	0.1404	0.0702	0.6745	7.1822	0.1995	1.1466	904.83	445.17	222.59	1500.00
0.0188	0.3306	1116.94	0.2852	0.1407	0.0704	0.6747	7.1200	0.1987	1.1285	904.05	445.95	222.98	1500.00
0.0193	0.3312	1116.49	0.2851	0.1410	0.0705	0.6749	7.0592	0.1978	1.1109	903.28	446.72	223.36	1500.00
0.0198	0.3317	1116.05	0.2849	0.1413	0.0706	0.6751	6.9999	0.1970	1.0937	902.53	447.47	223.74	1500.00
0.0208	0.3328	1115.18	0.2846	0.1418	0.0709	0.6754	6.8852	0.1953	1.0606	901.05	448.95	224.47	1500.00
0.0212	0.3333	1114.76	0.2845	0.1421	0.0710	0.6756	6.8297	0.1945	1.0446	900.33	449.67	224.83	1500.00
0.0217	0.3339	1114.34	0.2843	0.1423	0.0712	0.6758	6.7755	0.1938	1.0290	899.63	450.37	225.19	1500.00
0.0222	0.3344	1113.93	0.2842	0.1426	0.0713	0.6760	6.7225	0.1930	1.0138	898.93	451.07	225.54	1500.00
0.0232	0.3354	1113.13	0.2839	0.1431	0.0715	0.6763	6.6198	0.1915	0.9843	897.56	452.44	226.22	1500.00
0.0236	0.3359	1112.73	0.2837	0.1433	0.0717	0.6765	6.5702	0.1908	0.9701	896.89	453.11	226.55	1500.00
0.0241	0.3364	1112.35	0.2836	0.1436	0.0718	0.6766	6.5215	0.1901	0.9562	896.23	453.77	226.88	1500.00
0.0246	0.3368	1111.97	0.2835	0.1438	0.0719	0.6768	6.4739	0.1893	0.9426	895.58	454.42	227.21	1500.00
0.0256	0.3378	1111.22	0.2832	0.1443	0.0721	0.6771	6.3816	0.1880	0.9163	894.31	455.69	227.84	1500.00
0.0260	0.3382	1110.85	0.2831	0.1445	0.0723	0.6773	6.3368	0.1873	0.9035	893.69	456.31	228.16	1500.00
0.0265	0.3387	1110.49	0.2829	0.1448	0.0724	0.6774	6.2929	0.1867	0.8910	893.07	456.93	228.46	1500.00
0.0270	0.3391	1110.13	0.2828	0.1450	0.0725	0.6776	6.2499	0.1860	0.8788	892.47	457.53	228.77	1500.00
0.0280	0.3400	1109.44	0.2825	0.1454	0.0727	0.6779	6.1665	0.1848	0.8552	891.28	458.72	229.36	1500.00
0.0284	0.3404	1109.09	0.2824	0.1456	0.0728	0.6780	6.1259	0.1841	0.8437	890.70	459.30	229.65	1500.00
0.0289	0.3409	1108.76	0.2823	0.1458	0.0729	0.6782	6.0862	0.1835	0.8324	890.13	459.87	229.94	1500.00
0.0294	0.3413	1108.42	0.2822	0.1461	0.0730	0.6783	6.0472	0.1829	0.8214	889.56	460.44	230.22	1500.00
0.0304	0.3421	1107.77	0.2819	0.1465	0.0732	0.6786	5.9714	0.1818	0.8001	888.45	461.55	230.77	1500.00
0.0308	0.3425	1107.45	0.2818	0.1467	0.0733	0.6787	5.9346	0.1812	0.7897	887.91	462.09	231.05	1500.00
0.0313	0.3429	1107.14	0.2817	0.1469	0.0734	0.6789	5.8984	0.1807	0.7795	887.37	462.63	231.31	1500.00
0.0318	0.3433	1106.82	0.2816	0.1471	0.0735	0.6790	5.8629	0.1801	0.7695	886.84	463.16	231.58	1500.00
0.0328	0.3440	1106.21	0.2814	0.1475	0.0737	0.6793	5.7938	0.1790	0.7502	885.80	464.20	232.10	1500.00
0.0332	0.3444	1105.91	0.2813	0.1476	0.0738	0.6794	5.7602	0.1785	0.7407	885.29	464.71	232.35	1500.00
0.0337	0.3448	1105.61	0.2812	0.1478	0.0739	0.6795	5.7272	0.1780	0.7315	884.79	465.21	232.61	1500.00
0.0342	0.3452	1105.32	0.2811	0.1480	0.0740	0.6796	5.6947	0.1775	0.7224	884.29	465.71	232.85	1500.00

0.0352	0.3459	1104.75	0.2808	0.1484	0.0742	0.6799	5.6315	0.1765	0.7048	883.31	466.69	233.34	1500.00
0.0356	0.3462	1104.46	0.2807	0.1486	0.0743	0.6800	5.6007	0.1760	0.6962	882.83	467.17	233.58	1500.00
0.0361	0.3466	1104.19	0.2806	0.1487	0.0744	0.6801	5.5704	0.1755	0.6878	882.36	467.64	233.82	1500.00
0.0366	0.3469	1103.91	0.2805	0.1489	0.0745	0.6802	5.5406	0.1750	0.6795	881.89	468.11	234.05	1500.00
0.0376	0.3476	1103.37	0.2804	0.1493	0.0746	0.6805	5.4826	0.1741	0.6634	880.97	469.03	234.51	1500.00
0.0380	0.3479	1103.10	0.2803	0.1494	0.0747	0.6806	5.4543	0.1737	0.6555	880.52	469.48	234.74	1500.00
0.0385	0.3483	1102.84	0.2802	0.1496	0.0748	0.6807	5.4264	0.1732	0.6478	880.08	469.92	234.96	1500.00
0.0390	0.3486	1102.58	0.2801	0.1498	0.0749	0.6808	5.3991	0.1728	0.6402	879.64	470.36	235.18	1500.00
0.0400	0.3492	1102.07	0.2799	0.1501	0.0750	0.6810	5.3456	0.1719	0.6254	878.77	471.23	235.61	1500.00
0.0404	0.3495	1101.82	0.2798	0.1502	0.0751	0.6812	5.3195	0.1715	0.6182	878.34	471.66	235.83	1500.00
0.0409	0.3498	1101.57	0.2797	0.1504	0.0752	0.6813	5.2938	0.1711	0.6112	877.92	472.08	236.04	1500.00
0.0414	0.3501	1101.33	0.2796	0.1506	0.0753	0.6814	5.2685	0.1706	0.6042	877.51	472.49	236.25	1500.00
0.0424	0.3507	1100.85	0.2794	0.1509	0.0754	0.6816	5.2192	0.1698	0.5906	876.69	473.31	236.65	1500.00
0.0428	0.3510	1100.61	0.2794	0.1510	0.0755	0.6817	5.1951	0.1694	0.5840	876.29	473.71	236.86	1500.00
0.0433	0.3513	1100.38	0.2793	0.1512	0.0756	0.6818	5.1713	0.1691	0.5775	875.89	474.11	237.05	1500.00
0.0438	0.3516	1100.14	0.2792	0.1513	0.0757	0.6819	5.1479	0.1687	0.5710	875.50	474.50	237.25	1500.00
0.0448	0.3522	1099.69	0.2790	0.1516	0.0758	0.6821	5.1022	0.1679	0.5585	874.73	475.27	237.64	1500.00
0.0452	0.3525	1099.47	0.2789	0.1517	0.0759	0.6822	5.0798	0.1675	0.5524	874.35	475.65	237.83	1500.00
0.0457	0.3528	1099.24	0.2789	0.1519	0.0759	0.6823	5.0578	0.1672	0.5464	873.97	476.03	238.02	1500.00
0.0462	0.3530	1099.02	0.2788	0.1520	0.0760	0.6824	5.0361	0.1668	0.5405	873.60	476.40	238.20	1500.00
0.0472	0.3536	1098.59	0.2786	0.1523	0.0762	0.6826	4.9937	0.1661	0.5289	872.87	477.13	238.57	1500.00
0.0476	0.3538	1098.38	0.2785	0.1524	0.0762	0.6826	4.9729	0.1657	0.5232	872.51	477.49	238.75	1500.00
0.0481	0.3541	1098.17	0.2785	0.1526	0.0763	0.6827	4.9525	0.1654	0.5177	872.15	477.85	238.92	1500.00
0.0486	0.3544	1097.96	0.2784	0.1527	0.0764	0.6828	4.9323	0.1651	0.5122	871.80	478.20	239.10	1500.00
0.0496	0.3549	1097.55	0.2782	0.1530	0.0765	0.6830	4.8928	0.1644	0.5014	871.10	478.90	239.45	1500.00
0.0500	0.3551	1097.35	0.2782	0.1531	0.0765	0.6831	4.8735	0.1641	0.4962	870.76	479.24	239.62	1500.00
0.0505	0.3554	1097.15	0.2781	0.1532	0.0766	0.6832	4.8544	0.1637	0.4910	870.43	479.57	239.79	1500.00
0.0510	0.3556	1096.96	0.2780	0.1533	0.0767	0.6833	4.8356	0.1634	0.4859	870.09	479.91	239.95	1500.00
0.0520	0.3561	1096.57	0.2779	0.1536	0.0768	0.6834	4.7988	0.1628	0.4760	869.43	480.57	240.28	1500.00
0.0524	0.3563	1096.38	0.2778	0.1537	0.0769	0.6835	4.7808	0.1625	0.4711	869.11	480.89	240.45	1500.00
0.0529	0.3566	1096.19	0.2777	0.1538	0.0769	0.6836	4.7630	0.1622	0.4663	868.79	481.21	240.61	1500.00

0.0534	0.3568	1096.00	0.2777	0.1540	0.0770	0.6837	4.7455	0.1619	0.4616	868.47	481.53	240.76	1500.00
0.0544	0.3573	1095.63	0.2775	0.1542	0.0771	0.6839	4.7111	0.1613	0.4523	867.85	482.15	241.08	1500.00
0.0548	0.3575	1095.45	0.2775	0.1543	0.0772	0.6839	4.6942	0.1610	0.4477	867.54	482.46	241.23	1500.00
0.0553	0.3577	1095.27	0.2774	0.1544	0.0772	0.6840	4.6776	0.1607	0.4433	867.23	482.77	241.38	1500.00
0.0558	0.3579	1095.09	0.2773	0.1545	0.0773	0.6841	4.6612	0.1604	0.4389	866.93	483.07	241.53	1500.00
0.0568	0.3584	1094.74	0.2772	0.1548	0.0774	0.6842	4.6290	0.1599	0.4302	866.34	483.66	241.83	1500.00
0.0572	0.3586	1094.57	0.2772	0.1549	0.0774	0.6843	4.6132	0.1596	0.4260	866.04	483.96	241.98	1500.00
0.0577	0.3588	1094.40	0.2771	0.1550	0.0775	0.6844	4.5976	0.1593	0.4218	865.75	484.25	242.12	1500.00
0.0582	0.3590	1094.23	0.2770	0.1551	0.0775	0.6845	4.5823	0.1590	0.4177	865.47	484.53	242.27	1500.00
0.0592	0.3594	1093.90	0.2769	0.1553	0.0777	0.6846	4.5521	0.1585	0.4096	864.90	485.10	242.55	1500.00
0.0596	0.3596	1093.73	0.2769	0.1554	0.0777	0.6847	4.5373	0.1583	0.4057	864.62	485.38	242.69	1500.00
0.0600	0.3598	1093.61	0.2768	0.1555	0.0778	0.6848	4.5191	0.1579	0.4008	864.28	485.72	242.86	1500.00

Reactor Stage 4 Data

V	x	T	Ca	Cc	Cd	Ci	k1	Kc	rate	Fa	Fc	Fd	Fi
[m ³]	[-]	[K]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[s ⁻¹]	[-]	[mol/dm ³ ·s]	[mol/s]	[mol/s]	[mol/s]	[mol/s]
0.0000	0.3590	1143.00	0.2652	0.1485	0.0743	0.7174	11.4707	0.2527	1.7240	865.35	484.65	242.33	1500.00
0.0012	0.3613	1141.18	0.2646	0.1495	0.0747	0.7181	11.1529	0.2492	1.6380	862.73	487.27	243.64	1500.00
0.0015	0.3619	1140.66	0.2644	0.1498	0.0749	0.7183	11.0466	0.2480	1.6094	861.83	488.17	244.08	1500.00
0.0019	0.3626	1140.14	0.2643	0.1501	0.0751	0.7186	10.9431	0.2468	1.5816	860.96	489.04	244.52	1500.00
0.0022	0.3632	1139.63	0.2641	0.1504	0.0752	0.7188	10.8422	0.2456	1.5545	860.10	489.90	244.95	1500.00
0.0029	0.3644	1138.65	0.2637	0.1510	0.0755	0.7192	10.6480	0.2434	1.5024	858.42	491.58	245.79	1500.00
0.0033	0.3650	1138.17	0.2635	0.1513	0.0757	0.7194	10.5545	0.2423	1.4774	857.60	492.40	246.20	1500.00
0.0036	0.3656	1137.69	0.2634	0.1516	0.0758	0.7196	10.4632	0.2413	1.4530	856.79	493.21	246.60	1500.00
0.0040	0.3662	1137.23	0.2632	0.1519	0.0759	0.7198	10.3742	0.2402	1.4293	856.00	494.00	247.00	1500.00
0.0047	0.3673	1136.32	0.2629	0.1525	0.0762	0.7202	10.2023	0.2382	1.3835	854.46	495.54	247.77	1500.00
0.0050	0.3679	1135.88	0.2627	0.1527	0.0764	0.7204	10.1194	0.2372	1.3615	853.70	496.30	248.15	1500.00
0.0054	0.3684	1135.44	0.2626	0.1530	0.0765	0.7206	10.0384	0.2363	1.3400	852.96	497.04	248.52	1500.00
0.0058	0.3690	1135.01	0.2624	0.1533	0.0766	0.7208	9.9592	0.2353	1.3191	852.23	497.77	248.88	1500.00
0.0065	0.3700	1134.17	0.2621	0.1538	0.0769	0.7212	9.8061	0.2335	1.2786	850.80	499.20	249.60	1500.00
0.0068	0.3705	1133.76	0.2620	0.1540	0.0770	0.7214	9.7321	0.2326	1.2591	850.11	499.89	249.95	1500.00
0.0072	0.3711	1133.36	0.2618	0.1543	0.0771	0.7215	9.6597	0.2317	1.2400	849.42	500.58	250.29	1500.00
0.0075	0.3715	1132.96	0.2617	0.1545	0.0773	0.7217	9.5889	0.2309	1.2214	848.74	501.26	250.63	1500.00
0.0082	0.3725	1132.18	0.2614	0.1550	0.0775	0.7221	9.4518	0.2292	1.1854	847.42	502.58	251.29	1500.00
0.0086	0.3730	1131.80	0.2612	0.1552	0.0776	0.7222	9.3854	0.2284	1.1680	846.78	503.22	251.61	1500.00
0.0089	0.3735	1131.42	0.2611	0.1555	0.0777	0.7224	9.3204	0.2276	1.1510	846.14	503.86	251.93	1500.00
0.0093	0.3739	1131.05	0.2610	0.1557	0.0779	0.7226	9.2567	0.2268	1.1344	845.51	504.49	252.24	1500.00
0.0100	0.3748	1130.33	0.2607	0.1562	0.0781	0.7229	9.1332	0.2253	1.1022	844.28	505.72	252.86	1500.00
0.0103	0.3753	1129.98	0.2606	0.1564	0.0782	0.7230	9.0733	0.2245	1.0866	843.68	506.32	253.16	1500.00
0.0107	0.3757	1129.63	0.2604	0.1566	0.0783	0.7232	9.0146	0.2238	1.0713	843.09	506.91	253.46	1500.00
0.0110	0.3761	1129.28	0.2603	0.1568	0.0784	0.7234	8.9571	0.2231	1.0564	842.50	507.50	253.75	1500.00
0.0117	0.3770	1128.61	0.2601	0.1572	0.0786	0.7237	8.8454	0.2217	1.0274	841.36	508.64	254.32	1500.00

0.0121	0.3774	1128.28	0.2600	0.1574	0.0787	0.7238	8.7911	0.2210	1.0134	840.80	509.20	254.60	1500.00
0.0124	0.3778	1127.95	0.2598	0.1576	0.0788	0.7240	8.7379	0.2203	0.9996	840.25	509.75	254.88	1500.00
0.0128	0.3782	1127.63	0.2597	0.1578	0.0789	0.7241	8.6857	0.2196	0.9861	839.70	510.30	255.15	1500.00
0.0135	0.3790	1127.00	0.2595	0.1582	0.0791	0.7244	8.5841	0.2183	0.9599	838.63	511.37	255.68	1500.00
0.0138	0.3794	1126.69	0.2594	0.1584	0.0792	0.7245	8.5348	0.2177	0.9472	838.11	511.89	255.95	1500.00
0.0142	0.3798	1126.39	0.2593	0.1586	0.0793	0.7247	8.4863	0.2171	0.9348	837.59	512.41	256.20	1500.00
0.0146	0.3801	1126.09	0.2592	0.1588	0.0794	0.7248	8.4387	0.2165	0.9226	837.08	512.92	256.46	1500.00
0.0153	0.3809	1125.50	0.2589	0.1592	0.0796	0.7251	8.3461	0.2152	0.8988	836.08	513.92	256.96	1500.00
0.0156	0.3812	1125.21	0.2588	0.1593	0.0797	0.7252	8.3010	0.2147	0.8873	835.59	514.41	257.21	1500.00
0.0160	0.3816	1124.92	0.2587	0.1595	0.0798	0.7253	8.2568	0.2141	0.8760	835.11	514.89	257.45	1500.00
0.0163	0.3819	1124.64	0.2586	0.1597	0.0799	0.7254	8.2132	0.2135	0.8649	834.63	515.37	257.69	1500.00
0.0170	0.3826	1124.09	0.2584	0.1600	0.0800	0.7257	8.1285	0.2124	0.8432	833.69	516.31	258.16	1500.00
0.0174	0.3830	1123.82	0.2583	0.1602	0.0801	0.7258	8.0872	0.2119	0.8327	833.23	516.77	258.39	1500.00
0.0177	0.3833	1123.55	0.2582	0.1604	0.0802	0.7259	8.0465	0.2113	0.8224	832.77	517.23	258.61	1500.00
0.0181	0.3836	1123.29	0.2581	0.1606	0.0803	0.7261	8.0066	0.2108	0.8123	832.33	517.67	258.84	1500.00
0.0188	0.3843	1122.77	0.2579	0.1609	0.0804	0.7263	7.9288	0.2097	0.7925	831.44	518.56	259.28	1500.00
0.0191	0.3846	1122.51	0.2579	0.1610	0.0805	0.7264	7.8908	0.2092	0.7829	831.01	518.99	259.49	1500.00
0.0195	0.3849	1122.26	0.2578	0.1612	0.0806	0.7265	7.8534	0.2087	0.7734	830.58	519.42	259.71	1500.00
0.0198	0.3852	1122.01	0.2577	0.1614	0.0807	0.7266	7.8167	0.2082	0.7642	830.16	519.84	259.92	1500.00
0.0205	0.3858	1121.52	0.2575	0.1617	0.0808	0.7269	7.7450	0.2073	0.7460	829.33	520.67	260.33	1500.00
0.0209	0.3861	1121.28	0.2574	0.1618	0.0809	0.7270	7.7100	0.2068	0.7372	828.92	521.08	260.54	1500.00
0.0212	0.3864	1121.04	0.2573	0.1620	0.0810	0.7271	7.6755	0.2063	0.7286	828.52	521.48	260.74	1500.00
0.0216	0.3867	1120.81	0.2572	0.1621	0.0811	0.7272	7.6416	0.2059	0.7200	828.12	521.88	260.94	1500.00
0.0223	0.3873	1120.35	0.2571	0.1624	0.0812	0.7274	7.5753	0.2050	0.7034	827.34	522.66	261.33	1500.00
0.0226	0.3876	1120.12	0.2570	0.1625	0.0813	0.7275	7.5430	0.2045	0.6953	826.96	523.04	261.52	1500.00
0.0230	0.3879	1119.90	0.2569	0.1627	0.0813	0.7276	7.5111	0.2041	0.6873	826.58	523.42	261.71	1500.00
0.0234	0.3881	1119.67	0.2568	0.1628	0.0814	0.7277	7.4797	0.2037	0.6794	826.20	523.80	261.90	1500.00
0.0241	0.3887	1119.24	0.2567	0.1631	0.0815	0.7279	7.4184	0.2028	0.6641	825.46	524.54	262.27	1500.00
0.0244	0.3889	1119.03	0.2566	0.1632	0.0816	0.7280	7.3884	0.2024	0.6566	825.10	524.90	262.45	1500.00
0.0248	0.3892	1118.81	0.2565	0.1634	0.0817	0.7281	7.3589	0.2020	0.6492	824.74	525.26	262.63	1500.00
0.0251	0.3895	1118.60	0.2564	0.1635	0.0817	0.7282	7.3298	0.2016	0.6420	824.39	525.61	262.81	1500.00

0.0258	0.3900	1118.19	0.2563	0.1638	0.0819	0.7284	7.2728	0.2008	0.6278	823.69	526.31	263.15	1500.00
0.0262	0.3902	1117.99	0.2562	0.1639	0.0819	0.7285	7.2450	0.2004	0.6208	823.35	526.65	263.33	1500.00
0.0265	0.3905	1117.79	0.2561	0.1640	0.0820	0.7285	7.2175	0.2000	0.6140	823.01	526.99	263.50	1500.00
0.0269	0.3907	1117.59	0.2561	0.1641	0.0821	0.7286	7.1905	0.1997	0.6073	822.67	527.33	263.66	1500.00
0.0276	0.3912	1117.20	0.2559	0.1644	0.0822	0.7288	7.1375	0.1989	0.5942	822.01	527.99	263.99	1500.00
0.0279	0.3915	1117.01	0.2558	0.1645	0.0822	0.7289	7.1116	0.1985	0.5878	821.69	528.31	264.16	1500.00
0.0283	0.3917	1116.82	0.2558	0.1646	0.0823	0.7290	7.0860	0.1982	0.5814	821.37	528.63	264.32	1500.00
0.0286	0.3919	1116.63	0.2557	0.1647	0.0824	0.7291	7.0608	0.1978	0.5752	821.05	528.95	264.48	1500.00
0.0293	0.3924	1116.27	0.2556	0.1650	0.0825	0.7292	7.0115	0.1971	0.5630	820.42	529.58	264.79	1500.00
0.0297	0.3926	1116.08	0.2555	0.1651	0.0825	0.7293	6.9873	0.1968	0.5570	820.12	529.88	264.94	1500.00
0.0300	0.3928	1115.90	0.2554	0.1652	0.0826	0.7294	6.9634	0.1964	0.5512	819.81	530.19	265.09	1500.00
0.0304	0.3931	1115.73	0.2554	0.1653	0.0827	0.7295	6.9399	0.1961	0.5454	819.51	530.49	265.24	1500.00
0.0311	0.3935	1115.38	0.2552	0.1655	0.0828	0.7297	6.8938	0.1955	0.5340	818.92	531.08	265.54	1500.00
0.0314	0.3937	1115.20	0.2552	0.1656	0.0828	0.7297	6.8712	0.1951	0.5285	818.63	531.37	265.69	1500.00
0.0318	0.3939	1115.03	0.2551	0.1657	0.0829	0.7298	6.8490	0.1948	0.5230	818.34	531.66	265.83	1500.00
0.0322	0.3941	1114.86	0.2551	0.1659	0.0829	0.7299	6.8270	0.1945	0.5176	818.05	531.95	265.97	1500.00
0.0329	0.3946	1114.53	0.2549	0.1661	0.0830	0.7300	6.7838	0.1939	0.5070	817.49	532.51	266.26	1500.00
0.0332	0.3948	1114.37	0.2549	0.1662	0.0831	0.7301	6.7627	0.1936	0.5019	817.21	532.79	266.39	1500.00
0.0336	0.3950	1114.21	0.2548	0.1663	0.0831	0.7302	6.7418	0.1933	0.4968	816.94	533.06	266.53	1500.00
0.0339	0.3952	1114.05	0.2548	0.1664	0.0832	0.7303	6.7212	0.1930	0.4917	816.67	533.33	266.67	1500.00
0.0346	0.3956	1113.73	0.2546	0.1666	0.0833	0.7304	6.6808	0.1924	0.4819	816.13	533.87	266.93	1500.00
0.0350	0.3958	1113.58	0.2546	0.1667	0.0833	0.7305	6.6610	0.1921	0.4770	815.87	534.13	267.07	1500.00
0.0353	0.3959	1113.42	0.2545	0.1668	0.0834	0.7306	6.6414	0.1918	0.4723	815.61	534.39	267.20	1500.00
0.0357	0.3961	1113.27	0.2545	0.1669	0.0834	0.7306	6.6221	0.1915	0.4676	815.35	534.65	267.33	1500.00
0.0364	0.3965	1112.97	0.2544	0.1671	0.0835	0.7308	6.5842	0.1910	0.4583	814.84	535.16	267.58	1500.00
0.0367	0.3967	1112.82	0.2543	0.1671	0.0836	0.7308	6.5656	0.1907	0.4538	814.59	535.41	267.71	1500.00
0.0371	0.3969	1112.67	0.2542	0.1672	0.0836	0.7309	6.5472	0.1904	0.4493	814.34	535.66	267.83	1500.00
0.0374	0.3971	1112.53	0.2542	0.1673	0.0837	0.7310	6.5291	0.1902	0.4449	814.10	535.90	267.95	1500.00
0.0381	0.3974	1112.24	0.2541	0.1675	0.0838	0.7311	6.4934	0.1896	0.4363	813.61	536.39	268.19	1500.00
0.0385	0.3976	1112.10	0.2540	0.1676	0.0838	0.7312	6.4760	0.1894	0.4321	813.37	536.63	268.31	1500.00
0.0388	0.3978	1111.96	0.2540	0.1677	0.0838	0.7312	6.4587	0.1891	0.4279	813.14	536.86	268.43	1500.00

0.0392	0.3979	1111.82	0.2539	0.1678	0.0839	0.7313	6.4416	0.1889	0.4237	812.90	537.10	268.55	1500.00
0.0399	0.3983	1111.55	0.2538	0.1680	0.0840	0.7314	6.4081	0.1884	0.4156	812.44	537.56	268.78	1500.00
0.0402	0.3984	1111.42	0.2538	0.1680	0.0840	0.7315	6.3916	0.1881	0.4117	812.21	537.79	268.89	1500.00
0.0406	0.3986	1111.29	0.2537	0.1681	0.0841	0.7315	6.3753	0.1879	0.4077	811.99	538.01	269.01	1500.00
0.0410	0.3988	1111.15	0.2537	0.1682	0.0841	0.7316	6.3592	0.1876	0.4038	811.77	538.23	269.12	1500.00
0.0417	0.3991	1110.89	0.2536	0.1684	0.0842	0.7317	6.3276	0.1872	0.3962	811.33	538.67	269.34	1500.00
0.0420	0.3993	1110.77	0.2535	0.1685	0.0842	0.7318	6.3121	0.1869	0.3925	811.11	538.89	269.44	1500.00
0.0424	0.3994	1110.64	0.2535	0.1685	0.0843	0.7318	6.2968	0.1867	0.3888	810.90	539.10	269.55	1500.00
0.0427	0.3996	1110.51	0.2535	0.1686	0.0843	0.7319	6.2816	0.1865	0.3852	810.68	539.32	269.66	1500.00
0.0434	0.3999	1110.27	0.2534	0.1688	0.0844	0.7320	6.2518	0.1860	0.3780	810.26	539.74	269.87	1500.00
0.0438	0.4000	1110.14	0.2533	0.1688	0.0844	0.7321	6.2372	0.1858	0.3745	810.06	539.94	269.97	1500.00
0.0440	0.4001	1110.06	0.2533	0.1689	0.0845	0.7321	6.2204	0.1856	0.3704	809.82	540.18	270.09	1500.00

Reactor Stage 5 Data

V	x	T	Ca	Cc	Cd	Ci	k1	Kc	rate	Fa	Fc	Fd	Fi
[m ³]	[-]	[K]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[mol/dm ³]	[s ⁻¹]	[-]	[mol/dm ³ ·s]	[mol/s]	[mol/s]	[mol/s]	[mol/s]
0.0000	0.4000	1143.00	0.2460	0.1640	0.0820	0.7593	11.47067	0.252721	1.203243	810.00	540.00	270.00	1500.00
0.0005	0.4007	1142.44	0.2459	0.1643	0.0821	0.7595	11.37722	0.251679	1.180397	809.24	540.76	270.38	1500.00
0.0008	0.4012	1142.04	0.2457	0.1645	0.0823	0.7597	11.29376	0.250746	1.16003	808.55	541.45	270.72	1500.00
0.0010	0.4014	1141.84	0.2456	0.1647	0.0823	0.7598	11.25278	0.250286	1.150038	808.21	541.79	270.89	1500.00
0.0012	0.4017	1141.64	0.2456	0.1648	0.0824	0.7599	11.21229	0.249831	1.140173	807.88	542.12	271.06	1500.00
0.0014	0.4019	1141.44	0.2455	0.1649	0.0825	0.7600	11.17226	0.249381	1.13043	807.54	542.46	271.23	1500.00
0.0017	0.4024	1141.05	0.2454	0.1651	0.0826	0.7602	11.09362	0.248493	1.111306	806.88	543.12	271.56	1500.00
0.0019	0.4027	1140.86	0.2453	0.1653	0.0826	0.7603	11.05498	0.248056	1.101921	806.56	543.44	271.72	1500.00
0.0021	0.4029	1140.67	0.2452	0.1654	0.0827	0.7604	11.01679	0.247623	1.09265	806.24	543.76	271.88	1500.00
0.0022	0.4031	1140.48	0.2451	0.1655	0.0827	0.7605	10.97903	0.247195	1.083493	805.92	544.08	272.04	1500.00
0.0026	0.4036	1140.11	0.2450	0.1657	0.0829	0.7606	10.90481	0.24635	1.065509	805.29	544.71	272.36	1500.00
0.0028	0.4038	1139.93	0.2449	0.1658	0.0829	0.7607	10.86832	0.245933	1.056678	804.98	545.02	272.51	1500.00
0.0029	0.4041	1139.74	0.2449	0.1660	0.0830	0.7608	10.83225	0.245521	1.047954	804.67	545.33	272.67	1500.00
0.0031	0.4043	1139.56	0.2448	0.1661	0.0830	0.7609	10.79658	0.245113	1.039333	804.36	545.64	272.82	1500.00
0.0035	0.4047	1139.21	0.2447	0.1663	0.0831	0.7610	10.72643	0.244308	1.022395	803.76	546.24	273.12	1500.00
0.0036	0.4050	1139.03	0.2446	0.1664	0.0832	0.7611	10.69193	0.243911	1.014075	803.46	546.54	273.27	1500.00
0.0038	0.4052	1138.85	0.2446	0.1665	0.0833	0.7612	10.65782	0.243518	1.005852	803.16	546.84	273.42	1500.00
0.0040	0.4054	1138.68	0.2445	0.1666	0.0833	0.7613	10.62408	0.243128	0.997724	802.87	547.13	273.57	1500.00
0.0043	0.4058	1138.34	0.2444	0.1668	0.0834	0.7615	10.55768	0.24236	0.981749	802.29	547.71	273.86	1500.00
0.0045	0.4060	1138.17	0.2443	0.1669	0.0835	0.7615	10.52503	0.241982	0.973899	802.00	548.00	274.00	1500.00
0.0047	0.4062	1138.00	0.2442	0.1670	0.0835	0.7616	10.49272	0.241606	0.966138	801.72	548.28	274.14	1500.00
0.0049	0.4064	1137.83	0.2442	0.1671	0.0836	0.7617	10.46076	0.241235	0.958465	801.43	548.57	274.28	1500.00
0.0052	0.4069	1137.50	0.2441	0.1673	0.0837	0.7618	10.39785	0.240501	0.943378	800.88	549.12	274.56	1500.00
0.0054	0.4071	1137.34	0.2440	0.1674	0.0837	0.7619	10.36689	0.24014	0.935961	800.60	549.40	274.70	1500.00
0.0056	0.4073	1137.18	0.2439	0.1675	0.0838	0.7620	10.33626	0.239781	0.928626	800.33	549.67	274.84	1500.00
0.0058	0.4075	1137.02	0.2439	0.1676	0.0838	0.7621	10.30595	0.239426	0.921373	800.06	549.94	274.97	1500.00

0.0061	0.4079	1136.70	0.2438	0.1678	0.0839	0.7622	10.24627	0.238726	0.907107	799.52	550.48	275.24	1500.00
0.0063	0.4081	1136.54	0.2437	0.1679	0.0840	0.7623	10.21689	0.23838	0.90009	799.26	550.74	275.37	1500.00
0.0065	0.4083	1136.39	0.2436	0.1680	0.0840	0.7624	10.18781	0.238037	0.89315	798.99	551.01	275.50	1500.00
0.0066	0.4084	1136.23	0.2436	0.1681	0.0841	0.7624	10.15903	0.237698	0.886286	798.73	551.27	275.63	1500.00
0.0070	0.4088	1135.93	0.2435	0.1683	0.0842	0.7626	10.10235	0.237027	0.872778	798.22	551.78	275.89	1500.00
0.0072	0.4090	1135.78	0.2434	0.1684	0.0842	0.7626	10.07444	0.236697	0.866133	797.96	552.04	276.02	1500.00
0.0073	0.4092	1135.63	0.2434	0.1685	0.0842	0.7627	10.04681	0.236369	0.859559	797.71	552.29	276.15	1500.00
0.0075	0.4094	1135.48	0.2433	0.1686	0.0843	0.7628	10.01945	0.236044	0.853054	797.46	552.54	276.27	1500.00
0.0079	0.4098	1135.18	0.2432	0.1688	0.0844	0.7629	9.965561	0.235402	0.840251	796.96	553.04	276.52	1500.00
0.0080	0.4099	1135.04	0.2432	0.1689	0.0844	0.7630	9.939015	0.235085	0.83395	796.71	553.29	276.64	1500.00
0.0082	0.4101	1134.90	0.2431	0.1690	0.0845	0.7631	9.912731	0.234771	0.827715	796.47	553.53	276.76	1500.00
0.0084	0.4103	1134.75	0.2430	0.1690	0.0845	0.7631	9.886705	0.23446	0.821545	796.23	553.77	276.89	1500.00
0.0087	0.4106	1134.47	0.2429	0.1692	0.0846	0.7633	9.835414	0.233845	0.809395	795.75	554.25	277.13	1500.00
0.0089	0.4108	1134.33	0.2429	0.1693	0.0847	0.7633	9.810141	0.233542	0.803415	795.51	554.49	277.24	1500.00
0.0091	0.4110	1134.19	0.2428	0.1694	0.0847	0.7634	9.785113	0.233241	0.797495	795.28	554.72	277.36	1500.00
0.0093	0.4112	1134.05	0.2428	0.1695	0.0847	0.7635	9.760326	0.232943	0.791636	795.05	554.95	277.48	1500.00
0.0096	0.4115	1133.78	0.2427	0.1696	0.0848	0.7636	9.711463	0.232353	0.780095	794.58	555.42	277.71	1500.00
0.0098	0.4117	1133.64	0.2426	0.1697	0.0849	0.7636	9.68738	0.232062	0.774412	794.36	555.64	277.82	1500.00
0.0100	0.4118	1133.51	0.2426	0.1698	0.0849	0.7637	9.663526	0.231774	0.768786	794.13	555.87	277.94	1500.00
0.0102	0.4120	1133.38	0.2425	0.1699	0.0849	0.7638	9.639897	0.231488	0.763217	793.91	556.09	278.05	1500.00
0.0105	0.4123	1133.12	0.2424	0.1701	0.0850	0.7639	9.593303	0.230922	0.752243	793.46	556.54	278.27	1500.00
0.0107	0.4125	1132.99	0.2424	0.1701	0.0851	0.7640	9.570333	0.230643	0.746838	793.24	556.76	278.38	1500.00
0.0109	0.4127	1132.86	0.2424	0.1702	0.0851	0.7640	9.547577	0.230366	0.741486	793.02	556.98	278.49	1500.00
0.0110	0.4128	1132.73	0.2423	0.1703	0.0851	0.7641	9.525032	0.230091	0.736187	792.81	557.19	278.60	1500.00
0.0114	0.4131	1132.47	0.2422	0.1705	0.0852	0.7642	9.480564	0.229549	0.725743	792.38	557.62	278.81	1500.00
0.0116	0.4133	1132.35	0.2422	0.1705	0.0853	0.7643	9.458636	0.229281	0.720597	792.16	557.84	278.92	1500.00
0.0117	0.4134	1132.22	0.2421	0.1706	0.0853	0.7643	9.436909	0.229015	0.715501	791.95	558.05	279.02	1500.00
0.0119	0.4136	1132.10	0.2421	0.1707	0.0853	0.7644	9.415379	0.228751	0.710455	791.75	558.25	279.13	1500.00
0.0123	0.4139	1131.86	0.2420	0.1708	0.0854	0.7645	9.372905	0.228229	0.700506	791.33	558.67	279.33	1500.00
0.0124	0.4141	1131.73	0.2419	0.1709	0.0855	0.7645	9.351955	0.227972	0.695602	791.13	558.87	279.44	1500.00
0.0126	0.4142	1131.61	0.2419	0.1710	0.0855	0.7646	9.331193	0.227716	0.690746	790.92	559.08	279.54	1500.00

0.0128	0.4144	1131.49	0.2419	0.1711	0.0855	0.7647	9.310617	0.227463	0.685935	790.72	559.28	279.64	1500.00
0.0131	0.4146	1131.26	0.2418	0.1712	0.0856	0.7648	9.270013	0.226961	0.676449	790.32	559.68	279.84	1500.00
0.0133	0.4148	1131.14	0.2417	0.1713	0.0856	0.7648	9.249981	0.226714	0.671773	790.12	559.88	279.94	1500.00
0.0135	0.4149	1131.02	0.2417	0.1714	0.0857	0.7649	9.230126	0.226468	0.667141	789.93	560.07	280.04	1500.00
0.0137	0.4151	1130.91	0.2416	0.1714	0.0857	0.7649	9.210446	0.226224	0.662551	789.73	560.27	280.13	1500.00
0.0140	0.4154	1130.68	0.2416	0.1716	0.0858	0.7650	9.171602	0.225742	0.6535	789.35	560.65	280.33	1500.00
0.0142	0.4155	1130.57	0.2415	0.1716	0.0858	0.7651	9.152434	0.225504	0.649037	789.16	560.84	280.42	1500.00
0.0144	0.4157	1130.46	0.2415	0.1717	0.0859	0.7651	9.133432	0.225268	0.644614	788.97	561.03	280.52	1500.00
0.0146	0.4158	1130.34	0.2414	0.1718	0.0859	0.7652	9.114595	0.225033	0.640233	788.78	561.22	280.61	1500.00
0.0149	0.4161	1130.12	0.2413	0.1719	0.0860	0.7653	9.077406	0.224569	0.631588	788.40	561.60	280.80	1500.00
0.0151	0.4162	1130.01	0.2413	0.1720	0.0860	0.7654	9.059051	0.22434	0.627325	788.22	561.78	280.89	1500.00
0.0153	0.4163	1129.90	0.2413	0.1721	0.0860	0.7654	9.040852	0.224112	0.6231	788.04	561.96	280.98	1500.00
0.0154	0.4165	1129.80	0.2412	0.1721	0.0861	0.7655	9.022809	0.223886	0.618913	787.85	562.15	281.07	1500.00
0.0158	0.4167	1129.58	0.2411	0.1723	0.0861	0.7656	8.987181	0.22344	0.610652	787.49	562.51	281.25	1500.00
0.0160	0.4169	1129.48	0.2411	0.1723	0.0862	0.7656	8.969592	0.223219	0.606577	787.31	562.69	281.34	1500.00
0.0161	0.4170	1129.37	0.2411	0.1724	0.0862	0.7657	8.952151	0.223	0.602537	787.14	562.86	281.43	1500.00
0.0163	0.4171	1129.27	0.2410	0.1724	0.0862	0.7657	8.934857	0.222782	0.598534	786.96	563.04	281.52	1500.00
0.0167	0.4174	1129.06	0.2410	0.1726	0.0863	0.7658	8.9007	0.222352	0.590633	786.61	563.39	281.69	1500.00
0.0168	0.4175	1128.96	0.2409	0.1726	0.0863	0.7659	8.883834	0.222139	0.586734	786.44	563.56	281.78	1500.00
0.0170	0.4176	1128.86	0.2409	0.1727	0.0864	0.7659	8.867109	0.221928	0.582869	786.27	563.73	281.87	1500.00
0.0172	0.4178	1128.76	0.2408	0.1728	0.0864	0.7660	8.850521	0.221719	0.579038	786.10	563.90	281.95	1500.00
0.0175	0.4180	1128.56	0.2408	0.1729	0.0864	0.7660	8.817754	0.221304	0.571476	785.76	564.24	282.12	1500.00
0.0177	0.4181	1128.46	0.2407	0.1730	0.0865	0.7661	8.801572	0.221099	0.567744	785.59	564.41	282.20	1500.00
0.0179	0.4183	1128.36	0.2407	0.1730	0.0865	0.7661	8.785522	0.220895	0.564044	785.43	564.57	282.29	1500.00
0.0181	0.4184	1128.26	0.2407	0.1731	0.0865	0.7662	8.769602	0.220693	0.560376	785.26	564.74	282.37	1500.00
0.0184	0.4186	1128.07	0.2406	0.1732	0.0866	0.7663	8.738149	0.220293	0.553133	784.94	565.06	282.53	1500.00
0.0186	0.4187	1127.97	0.2406	0.1733	0.0866	0.7663	8.722613	0.220096	0.549558	784.77	565.23	282.61	1500.00
0.0188	0.4189	1127.88	0.2405	0.1733	0.0867	0.7664	8.707202	0.219899	0.546013	784.61	565.39	282.69	1500.00
0.0190	0.4190	1127.78	0.2405	0.1734	0.0867	0.7664	8.691914	0.219704	0.542498	784.45	565.55	282.77	1500.00
0.0193	0.4192	1127.60	0.2404	0.1735	0.0867	0.7665	8.661705	0.219319	0.535557	784.14	565.86	282.93	1500.00
0.0195	0.4193	1127.50	0.2404	0.1736	0.0868	0.7665	8.64678	0.219128	0.53213	783.98	566.02	283.01	1500.00

0.0197	0.4194	1127.41	0.2403	0.1736	0.0868	0.7666	8.631974	0.218938	0.528732	783.83	566.17	283.09	1500.00
0.0198	0.4196	1127.32	0.2403	0.1737	0.0868	0.7666	8.617285	0.21875	0.525362	783.67	566.33	283.16	1500.00
0.0202	0.4198	1127.14	0.2402	0.1738	0.0869	0.7667	8.588253	0.218378	0.518706	783.36	566.64	283.32	1500.00
0.0204	0.4199	1127.05	0.2402	0.1738	0.0869	0.7668	8.573908	0.218194	0.515419	783.21	566.79	283.39	1500.00
0.0205	0.4200	1126.96	0.2402	0.1739	0.0869	0.7668	8.559675	0.218011	0.51216	783.06	566.94	283.47	1500.00
0.0207	0.4201	1126.87	0.2401	0.1739	0.0870	0.7668	8.545553	0.217829	0.508927	782.91	567.09	283.54	1500.00
0.0211	0.4203	1126.70	0.2401	0.1741	0.0870	0.7669	8.517638	0.21747	0.50254	782.62	567.38	283.69	1500.00
0.0212	0.4204	1126.61	0.2401	0.1741	0.0871	0.7670	8.503842	0.217292	0.499386	782.47	567.53	283.77	1500.00
0.0214	0.4206	1126.52	0.2400	0.1742	0.0871	0.7670	8.490153	0.217115	0.496257	782.32	567.68	283.84	1500.00
0.0216	0.4207	1126.44	0.2400	0.1742	0.0871	0.7671	8.476569	0.21694	0.493154	782.18	567.82	283.91	1500.00
0.0219	0.4209	1126.27	0.2399	0.1743	0.0872	0.7671	8.449713	0.216593	0.487022	781.89	568.11	284.05	1500.00
0.0220	0.4209	1126.24	0.2399	0.1744	0.0872	0.7672	8.438871	0.216453	0.484548	781.77	568.23	284.11	1500.00

Appendix D

Appendix D presents the PolyMath reactor stage data as well as the differential and explicit equations employed to solve the design equations used for a system operation at 3 bar.

Reactor Stage 1 Data

POLYMATH Results

No Title

11-21-2008, Rev5.1.232

Calculated values of the DEQ variables

<u>Variable</u>	<u>initial value</u>	<u>minimal value</u>	<u>maximal value</u>	<u>final value</u>
W	0	0	6.9E+04	6.9E+04
x	0	0	0.2830081	0.2830081
T	1143	918.3439	1143	918.3439
Fao	1350	1350	1350	1350
R	8.314	8.314	8.314	8.314
Po	300	300	300	300
To	1143	1143	1143	1143
Cto	0.0315693	0.0315693	0.0315693	0.0315693
theta_i	1.1097	1.1097	1.1097	1.1097
Epsilon	0.237	0.237	0.237	0.237
yao	0.474	0.474	0.474	0.474
Cao	0.0149638	0.0149638	0.0149638	0.0149638
Ca	0.0149638	0.0125142	0.0149638	0.0125142
Cc	0	0	0.0049396	0.0049396
Cd	0	0	0.0024698	0.0024698
Ci	0.0166054	0.0166054	0.0193685	0.0193685
Ea	1.96E+05	1.96E+05	1.96E+05	1.96E+05
A	1.04E+10	1.04E+10	1.04E+10	1.04E+10
Tin	1143	1143	1143	1143
kl	11.470668	0.0738436	11.470668	0.0738436

Tr	298	298	298	298
delta_A	12.23	12.23	12.23	12.23
delta_B	-42.04	-42.04	-42.04	-42.04
delta_C	36.04	36.04	36.04	36.04
delta_D	-10.55	-10.55	-10.55	-10.55
delta_E	0.0944	0.0944	0.0944	0.0944
Kc	0.2527205	0.0198024	0.2527205	0.0198024
Kc_onder	0.01458	0.0121932	0.01458	0.0121932
delta_Cp	-4.4190523	-4.4190523	-4.0415845	-4.0415845
delta_Hrx	9.892E+04	9.892E+04	9.892E+04	9.892E+04
Tgebruik	1.143	1.143	1.143	1.143
theta_i_C	125.20435	125.20435	125.20435	125.20435
Xeb	0	0	0.2843588	0.2843588
Fa	1350	967.9391	1350	967.9391
Fc	0	0	382.0609	382.0609
Fd	0	0	191.03045	191.03045
Fi	1500	1500	1500	1500
vo	9.022E+04	9.022E+04	9.022E+04	9.022E+04
F_SO2	0	0	24.451897	24.451897
Kc_bo1	0	0	0.0048129	0.0048129
Kc_bo2	0	0	0.0490554	0.0490554
Kc_var	0	0	0.0193629	0.0193629
ra	-0.1716454	-0.1716454	-9.064E-04	-9.064E-04
rate	0.1716454	9.064E-04	0.1716454	9.064E-04
Fao_op_mi	7865.054	7865.054	1.489E+06	1.489E+06
Ft	2850	2850	3041.0304	3041.0304

ODE Report (RK45)

Differential equations as entered by the user

- [1] $d(x)/d(W) = -ra/Fao$
- [2] $d(T)/d(W) = ((-ra)*(-1)*(delta_Hrx))/(Fao*((theta_i_Cp_i)+(x*delta_Cp)))$

Explicit equations as entered by the user

- [1] $Fao = 1350$
- [2] $R = 8.314$
- [3] $Po = 300$
- [4] $To = 1143$
- [5] $Cto = Po/(R*To)$

```

[6] theta_i = 1.1097
[7] Epsilon = 0.237
[8] yao = 0.474
[9] Cao = yao*Cto
[10] Ca = Cao*((1-x)/(1+(Epsilon*x)))*(To/T)
[11] Cc = (Cao*x)/(1+(Epsilon*x))*(To/T)
[12] Cd = (Cao*0.5*x)/(1+(Epsilon*x))*(To/T)
[13] Ci = (Cao*theta_i)/(1+(Epsilon*x))*(To/T)
[14] Ea = 1.96E+05
[15] A = 1.04E+10
[16] Tin = 1143
[17] k1 = A*exp(-Ea/(R*T))
[18] Tr = 298
[19] delta_A = 12.23
[20] delta_B = -42.04
[21] delta_C = 36.04
[22] delta_D = -10.55
[23] delta_E = 0.0944
[24] Kc = 0.041*exp((98920/R)*((1/973)-(1/T)))
[25] Kc_onder = 4.86e-5*Po*(((1-x)/(1+(0.237*x)))*Tin/T)
[26] delta_Cp = delta_A+(delta_B*(T/1000))+(delta_C*((T/1000)^2))+(delta_D*((T/1000)^3))+(delta_E*((T/1000)^4))
[27] delta_Hrx = (98920+(delta_A*(T-Tr)/1000))+((delta_B/2)*((T/1000)^2)-((Tr/1000)^2))+((delta_C/3)*((T/1000)^3)-((Tr/1000)^3))+((delta_D/4)*((T/1000)^4)-((Tr/1000)^4))-((delta_E*((T/1000)-(Tr/1000))))
[28] Tgebruik = Tin/1000
[29] theta_i_Cp_i = (24.02+(119.46*Tgebruik)-(94.38*Tgebruik^2)+(26.96*Tgebruik^3)-(0.117/(Tgebruik^2)))+((1.1097)*((30.09+(6.83*Tgebruik)+(6.79*Tgebruik^2)-(2.53*Tgebruik^3)+(0.0821/(Tgebruik^2))))))
[30] Xeb = ((theta_i_Cp_i*(T-Tin))/(-delta_Hrx))+0
[31] Fa = Fao*(1-x)
[32] Fc = Fao*x
[33] Fd = 0.5*Fao*x
[34] Fi = 1500
[35] vo = Fao/Cao
[36] F_SO2 = (Fc*64)/1000
[37] Kc_bo1 = ((4.86e-5)*Po*(x/(1+(0.237*x)))*Tin/T)
[38] Kc_bo2 = ((4.86e-5)*Po*((0.5*x)/(1+(0.237*x)))*(Tin/T))^0.5
[39] Kc_var = (Kc_bo1*Kc_bo2)/Kc_onder
[40] ra = -k1*((Ca)-((Ci*Cc*(Cd^0.5))/Kc))

```

```
[41] rate = -ra
[42] Fao_op_min_ra = Fao/rate
[43] Ft = Fa+Fc+Fd+Fi
```

Comments

```
[3] Fao =      1350
    mol/s
[18] Kc_var =    (Kc_bo1*Kc_bo2)/Kc_onder
    Korregeer Delta H
[19] Ea =      1.96E+05
    J/mol
[37] vo =      Fao/Cao
    dm3/s
[38] F_SO2 =    (Fc*64)/1000
    kg/s
```

Independent variable

variable name : W

initial value : 0

final value : 69000

Precision

Step size guess. h = 0.000001

Truncation error tolerance. eps = 0.000001

General

number of differential equations: 2

number of explicit equations: 43

Elapsed time: 1.1574 sec

Reactor Stage 2 Data

POLYMATH Results

No Title

11-21-2008, Rev5.1.232

Calculated values of the DEQ variables

<u>Variable</u>	<u>initial value</u>	<u>minimal value</u>	<u>maximal value</u>	<u>final value</u>
W	0	0	1.2E+04	1.2E+04
x	0.283	0.283	0.4706676	0.4706676
T	1143	992.78307	1143	992.78307
Fao	967.95	967.95	967.95	967.95
R	8.314	8.314	8.314	8.314
Po	300	300	300	300
To	1143	1143	1143	1143
Cto	0.0315693	0.0315693	0.0315693	0.0315693
theta_i	1.5501257	1.5501257	1.5501257	1.5501257
Epsilon	0.237	0.237	0.237	0.237
yao	0.474	0.474	0.474	0.474
Cao	0.0149638	0.0149638	0.0149638	0.0149638
Ca	0.0100547	0.0082042	0.0100547	0.0082042
Cc	0.0039686	0.0039686	0.0072949	0.0072949
Cd	0.0019843	0.0019843	0.0036475	0.0036475
Ci	0.0217379	0.0217379	0.0240256	0.0240256
Ea	1.96E+05	1.96E+05	1.96E+05	1.96E+05
A	1.04E+10	1.04E+10	1.04E+10	1.04E+10
Tin	1143	1143	1143	1143
k1	11.470668	0.5061129	11.470668	0.5061129
Tr	298	298	298	298
delta_A	12.23	12.23	12.23	12.23
delta_B	-42.04	-42.04	-42.04	-42.04
delta_C	36.04	36.04	36.04	36.04
delta_D	-10.55	-10.55	-10.55	-10.55
delta_E	0.0944	0.0944	0.0944	0.0944
Kc	0.2527205	0.0523128	0.2527205	0.0523128
Kc_onder	0.0097968	0.0079937	0.0097968	0.0079937

delta_Cp	-4.4190523	-4.4190523	-4.2123707	-4.2123707
delta_Hrx	9.892E+04	9.892E+04	9.892E+04	9.892E+04
Tgebruik	1.143	1.143	1.143	1.143
theta_i_C	125.20435	125.20435	125.20435	125.20435
Xeb	0	0	0.1901379	0.1901379
Fa	967.95	714.59869	967.95	714.59869
Fc	382.05	382.05	635.40131	635.40131
Fd	191.025	191.025	317.70066	317.70066
Fi	1500	1500	1500	1500
vo	6.469E+04	6.469E+04	6.469E+04	6.469E+04
F_SO2	24.4512	24.4512	40.665684	40.665684
Kc_bo1	0.0038668	0.0038668	0.0071078	0.0071078
Kc_bo2	0.0439704	0.0439704	0.0596146	0.0596146
Kc_var	0.0173551	0.0173551	0.0530077	0.0530077
ra	-0.1151597	-0.1151597	-0.0040498	-0.0040498
rate	0.1151597	0.0040498	0.1151597	0.0040498
Fao_op_mi	8405.2826	8405.2826	2.39E+05	2.39E+05
Ft	3041.025	3041.025	3167.7007	3167.7007

ODE Report (RK45)

Differential equations as entered by the user

- [1] $d(x)/d(W) = -ra/Fao$
- [2] $d(T)/d(W) = ((-ra)*(-1)*(delta_Hrx))/(Fao*((theta_i_Cp_i)+(x*delta_Cp)))$

Explicit equations as entered by the user

- [1] $Fao = 967.95$
- [2] $R = 8.314$
- [3] $Po = 300$
- [4] $To = 1143$
- [5] $Cto = Po/(R*To)$
- [6] $theta_i = 1.550125707$
- [7] $Epsilon = 0.237$
- [8] $yao = 0.474$
- [9] $Cao = yao*Cto$
- [10] $Ca = Cao*((1-x)/(1+(Epsilon*x)))*(To/T)$
- [11] $Cc = (Cao*x)/(1+(Epsilon*x))*(To/T)$
- [12] $Cd = (Cao*0.5*x)/(1+(Epsilon*x))*(To/T)$
- [13] $Ci = (Cao*theta_i)/(1+(Epsilon*x))*(To/T)$

```

[14] Ea = 1.96E+05
[15] A = 1.04E+10
[16] Tin = 1143
[17] k1 = A*exp(-Ea/(R*T))
[18] Tr = 298
[19] delta_A = 12.23
[20] delta_B = -42.04
[21] delta_C = 36.04
[22] delta_D = -10.55
[23] delta_E = 0.0944
[24] Kc = 0.041*exp((98920/R)*((1/973)-(1/T)))
[25] Kc_onder = 4.86e-5*Po*(((1-x)/(1+(0.237*x)))^Tin/T)
[26] delta_Cp = delta_A+(delta_B*(T/1000))+(delta_C*((T/1000)^2))+(delta_D*((T/1000)^3))+(delta_E*((T/1000)^4))
[27] delta_Hrx = (98920+(delta_A*(T-Tr/1000))+((delta_B/2)*((T/1000)^2)-(Tr/1000)^2))+((delta_C/3)*((T/1000)^3)-(Tr/1000)^3))+((delta_D/4)*((T/1000)^4)-(Tr/1000)^4))-((delta_E/((T/1000)-(Tr/1000))))
[28] Tgebruik = Tin/1000
[29] theta_i_Cp_i = (24.02+(119.46*Tgebruik)-(94.38*Tgebruik^2)+(26.96*Tgebruik^3)-(0.117/(Tgebruik^2)))+((1.1097)*((30.09+(6.83*Tgebruik)+(6.79*Tgebruik^2)-(2.53*Tgebruik^3)+(0.0821/(Tgebruik^2))))))
[30] Xeb = ((theta_i_Cp_i*(T-Tin))/(-delta_Hrx))+0
[31] Fa = 1350*(1-x)
[32] Fc = 1350*x
[33] Fd = 0.5*1350*x
[34] Fi = 1500
[35] vo = Fao/Cao
[36] F_SO2 = (Fc*64)/1000
[37] Kc_bo1 = ((4.86e-5)*Po*(x/(1+(0.237*x)))^Tin/T)
[38] Kc_bo2 = ((4.86e-5)*Po*((0.5*x)/(1+(0.237*x)))^Tin/T)^0.5
[39] Kc_var = (Kc_bo1*Kc_bo2)/Kc_onder
[40] ra = -k1*((Ca)-(Ci*Cc*(Cd^0.5))/Kc))
[41] rate = -ra
[42] Fao_op_min_ra = Fao/rate
[43] Ft = Fa+Fc+Fd+Fi

```

Comments

```

[3] Fao = 967.95
    mol/s
[18] Kc_var = (Kc_bo1*Kc_bo2)/Kc_onder

```


Korregeer Delta H
[19] Ea = 1.96E+05
J/mol
[37] vo = Fao/Cao
dm3/s
[38] F_SO2 = (Fc*64)/1000
kg/s

Independent variable

variable name : W

initial value : 0

final value : 12000

Precision

Step size guess. h = 0.000001

Truncation error tolerance. eps = 0.000001

General

number of differential equations: 2

number of explicit equations: 43

Reactor Stage 3 Data

POLYMATH Results

No Title

11-21-2008, Rev5.1.232

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
W	0	0	3660	3660
x	0.47	0.47	0.5917864	0.5917864
T	1143	1044.9721	1143	1044.9721
Fao	715.5	715.5	715.5	715.5
R	8.314	8.314	8.314	8.314
Po	300	300	300	300
To	1143	1143	1143	1143
Cto	0.0315693	0.0315693	0.0315693	0.0315693
theta_i	2.0960602	2.0960602	2.0960602	2.0960602
Epsilon	0.237	0.237	0.237	0.237
yao	0.474	0.474	0.474	0.474
Cao	0.0149638	0.0149638	0.0149638	0.0149638
Ca	0.007136	0.0058596	0.007136	0.0058596
Cc	0.0063281	0.0063281	0.0084947	0.0084947
Cd	0.0031641	0.0031641	0.0042474	0.0042474
Ci	0.0282215	0.0282215	0.0300876	0.0300876
Ea	1.96E+05	1.96E+05	1.96E+05	1.96E+05
A	1.04E+10	1.04E+10	1.04E+10	1.04E+10
Tin	1143	1143	1143	1143
k1	11.470668	1.6569084	11.470668	1.6569084
Tr	298	298	298	298
delta_A	12.23	12.23	12.23	12.23
delta_B	-42.04	-42.04	-42.04	-42.04
delta_C	36.04	36.04	36.04	36.04
delta_D	-10.55	-10.55	-10.55	-10.55
delta_E	0.0944	0.0944	0.0944	0.0944
Kc	0.2527205	0.0951812	0.2527205	0.0951812
Kc_onder	0.0069529	0.0057093	0.0069529	0.0057093
delta_Cp	-4.4190523	-4.4190523	-4.2980364	-4.2980364

delta_Hrx	9.892E+04	9.892E+04	9.892E+04	9.892E+04
Tgebruik	1.143	1.143	1.143	1.143
theta_i_C	125.20435	125.20435	125.20435	125.20435
Xeb	0	0	0.1240796	0.1240796
Fa	715.5	551.0883	715.5	551.0883
Fc	634.5	634.5	798.9117	798.9117
Fd	317.25	317.25	399.45585	399.45585
Fi	1500	1500	1500	1500
vo	4.782E+04	4.782E+04	4.782E+04	4.782E+04
F_SO2	40.608	40.608	51.130349	51.130349
Kc_bo1	0.0061658	0.0061658	0.0082768	0.0082768
Kc_bo2	0.0555238	0.0555238	0.0643304	0.0643304
Kc_var	0.0492381	0.0492381	0.0932597	0.0932597
ra	-0.0813983	-0.0813983	-0.0094189	-0.0094189
rate	0.0813983	0.0094189	0.0813983	0.0094189
Fao_op_mi	8790.1066	8790.1066	7.596E+04	7.596E+04
Ft	3167.25	3167.25	3249.4559	3249.4559

ODE Report (RK45)

Differential equations as entered by the user

- [1] $d(x)/d(W) = -ra/Fao$
- [2] $d(T)/d(W) = ((-ra)*(-1)*(delta_Hrx))/(Fao*((theta_i_Cp_i)+(x*delta_Cp)))$

Explicit equations as entered by the user

- [1] $Fao = 715.5$
- [2] $R = 8.314$
- [3] $Po = 300$
- [4] $To = 1143$
- [5] $Cto = Po/(R*To)$
- [6] $theta_i = 2.096060204$
- [7] $Epsilon = 0.237$
- [8] $yao = 0.474$
- [9] $Cao = yao*Cto$
- [10] $Ca = Cao*((1-x)/(1+(Epsilon*x)))*(To/T)$
- [11] $Cc = (Cao*x)/(1+(Epsilon*x))*(To/T)$
- [12] $Cd = (Cao*0.5*x)/(1+(Epsilon*x))*(To/T)$
- [13] $Ci = (Cao*theta_i)/(1+(Epsilon*x))*(To/T)$
- [14] $Ea = 1.96E+05$

```

[15] A = 1.04E+10
[16] Tin = 1143
[17] k1 = A*exp(-Ea/(R*T))
[18] Tr = 298
[19] delta_A = 12.23
[20] delta_B = -42.04
[21] delta_C = 36.04
[22] delta_D = -10.55
[23] delta_E = 0.0944
[24] Kc = 0.041*exp((98920/R)*((1/973)-(1/T)))
[25] Kc_onder = 4.86e-5*Po*(((1-x)/(1+(0.237*x)))^Tin/T)
[26] delta_Cp = delta_A+(delta_B*(T/1000))+(delta_C*((T/1000)^2))+(delta_D*((T/1000)^3))+(delta_E/((T/1000)^2))
[27] delta_Hrx = (98920+(delta_A*((T-Tr)/1000))+((delta_B/2)*((T/1000)^2)-((Tr/1000)^2))+((delta_C/3)*((T/1000)^3)-((Tr/1000)^3))+((delta_D/4)*((T/1000)^4)-((Tr/1000)^4))-((delta_E/((T/1000)-(Tr/1000))))
[28] Tgebruik = Tin/1000
[29] theta_i_Cp_i = (24.02+(119.46*Tgebruik)-(94.38*Tgebruik^2)+(26.96*Tgebruik^3)-(0.117/(Tgebruik^2)))+((1.1097)*((30.09+(6.83*Tgebruik)+(6.79*Tgebruik^2)-(2.53*Tgebruik^3)+(0.0821/(Tgebruik^2))))))
[30] Xeb = ((theta_i_Cp_i*(T-Tin))/(-delta_Hrx))+0
[31] Fa = 1350*(1-x)
[32] Fc = 1350*x
[33] Fd = 0.5*1350*x
[34] Fi = 1500
[35] vo = Fao/Cao
[36] F_SO2 = (Fc^64)/1000
[37] Kc_bo1 = ((4.86e-5)*Po*(x/(1+(0.237*x)))^Tin/T)
[38] Kc_bo2 = ((4.86e-5)*Po*((0.5*x)/(1+(0.237*x)))^Tin/T)^0.5
[39] Kc_var = (Kc_bo1*Kc_bo2)/Kc_onder
[40] ra = -k1*((Ca)-((Ci*Cc*(Cd^0.5))/Kc))
[41] rate = -ra
[42] Fao_op_min_ra = Fao/rate
[43] Ft = Fa+Fc+Fd+Fi

```

Comments

```

[3] Fao = 715.5
    mol/s
[18] Kc_var = (Kc_bo1*Kc_bo2)/Kc_onder
    Korregeer Delta H

```

[19] $E_a = 1.96E+05$
 J/mol
[37] $v_o = F_{ao}/C_{ao}$
 dm³/s
[38] $F_{SO_2} = (F_c \cdot 64)/1000$
 kg/s

Independent variable

variable name : W

initial value : 0

final value : 3660

Precision

Step size guess. h = 0.000001

Truncation error tolerance. eps = 0.000001

General

number of differential equations: 2

number of explicit equations: 43

Reactor Stage 4 Data

POLYMATH Results

No Title

11-21-2008, Rev5.1.232

Calculated values of the DEQ variables

<u>Variable</u>	<u>initial value</u>	<u>minimal value</u>	<u>maximal value</u>	<u>final value</u>
W	0	0	1525	1525
x	0.592	0.592	0.6701294	0.6701294
T	1143	1079.8807	1143	1079.8807
Fao	550.8	550.8	550.8	550.8
R	8.314	8.314	8.314	8.314
Po	300	300	300	300
To	1143	1143	1143	1143
Cto	0.0315693	0.0315693	0.0315693	0.0315693
theta_i	2.7249115	2.7249115	2.7249115	2.7249115
Epsilon	0.237	0.237	0.237	0.237
yao	0.474	0.474	0.474	0.474
Cao	0.0149638	0.0149638	0.0149638	0.0149638
Ca	0.0053541	0.0045086	0.0053541	0.0045086
Cc	0.0077686	0.0077686	0.0091592	0.0091592
Cd	0.0038843	0.0038843	0.0045796	0.0045796
Ci	0.0357582	0.0357582	0.0372435	0.0372435
Ea	1.96E+05	1.96E+05	1.96E+05	1.96E+05
A	1.04E+10	1.04E+10	1.04E+10	1.04E+10
Tin	1143	1143	1143	1143
k1	11.470668	3.4357653	11.470668	3.4357653
Tr	298	298	298	298
delta_A	12.23	12.23	12.23	12.23
delta_B	-42.04	-42.04	-42.04	-42.04
delta_C	36.04	36.04	36.04	36.04
delta_D	-10.55	-10.55	-10.55	-10.55
delta_E	0.0944	0.0944	0.0944	0.0944
Kc	0.2527205	0.1375309	0.2527205	0.1375309
Kc_onder	0.0052167	0.0043929	0.0052167	0.0043929
delta_Cp	-4.4190523	-4.4190523	-4.3450224	-4.3450224
delta_Hrx	9.892E+04	9.892E+04	9.892E+04	9.892E+04

Tgebruik	1.143	1.143	1.143	1.143
theta_i_C	125.20435	125.20435	125.20435	125.20435
Xeb	0	0	0.0798939	0.0798939
Fa	550.8	445.32528	550.8	445.32528
Fc	799.2	799.2	904.67472	904.67472
Fd	399.6	399.6	452.33736	452.33736
Fi	1500	1500	1500	1500
vo	3.681E+04	3.681E+04	3.681E+04	3.681E+04
F_SO2	51.1488	51.1488	57.899182	57.899182
Kc_bo1	0.0075693	0.0075693	0.0089242	0.0089242
Kc_bo2	0.0615197	0.0615197	0.066799	0.066799
Kc_var	0.0892639	0.0892639	0.1357017	0.1357017
ra	-0.0606288	-0.0606288	-0.0149138	-0.0149138
rate	0.0606288	0.0149138	0.0606288	0.0149138
Fao_op_mi	9084.796	9084.796	3.693E+04	3.693E+04
Ft	3249.6	3249.6	3302.3374	3302.3374
F_O2	12.7872	12.7872	14.474796	14.474796

ODE Report (RKF45)

Differential equations as entered by the user

- [1] $d(x)/d(W) = -ra/Fao$
- [2] $d(T)/d(W) = ((-ra)*(-1)*(delta_Hrx))/(Fao*((theta_i_Cp_i)+(x*delta_Cp)))$

Explicit equations as entered by the user

- [1] $Fao = 550.8$
- [2] $R = 8.314$
- [3] $Po = 300$
- [4] $To = 1143$
- [5] $Cto = Po/(R*To)$
- [6] $theta_i = 2.724911452$
- [7] $Epsilon = 0.237$
- [8] $yao = 0.474$
- [9] $Cao = yao*Cto$
- [10] $Ca = Cao*((1-x)/(1+(Epsilon*x)))*(To/T)$
- [11] $Cc = (Cao*x)/(1+(Epsilon*x))*(To/T)$
- [12] $Cd = (Cao*0.5*x)/(1+(Epsilon*x))*(To/T)$
- [13] $Ci = (Cao*theta_i)/(1+(Epsilon*x))*(To/T)$
- [14] $Ea = 1.96E+05$

```

[15] A = 1.04E+10
[16] Tin = 1143
[17] k1 = A*exp(-Ea/(R*T))
[18] Tr = 298
[19] delta_A = 12.23
[20] delta_B = -42.04
[21] delta_C = 36.04
[22] delta_D = -10.55
[23] delta_E = 0.0944
[24] Kc = 0.041*exp((98920/R)*((1/973)-(1/T)))
[25] Kc_onder = 4.86e-5*Po*(((1-x)/(1+(0.237*x)))^Tin/T)
[26] delta_Cp = delta_A+(delta_B*(T/1000))+(delta_C*((T/1000)^2))+(delta_D*((T/1000)^3))+(delta_E/((T/1000)^2))
[27] delta_Hrx = (98920+(delta_A*((T-Tr)/1000)))+(delta_B/2)*((T/1000)^2)-((Tr/1000)^2)+(delta_C/3)*((T/1000)^3)-((Tr/1000)^3)+(delta_D/4)*((T/1000)^4)-
((Tr/1000)^4)-(delta_E/((T/1000)-(Tr/1000))))
[28] Tgebruik = Tin/1000
[29] theta_i_Cp_i = (24.02+(119.46*Tgebruik)-(94.38*Tgebruik^2)+(26.96*Tgebruik^3)-(0.117/(Tgebruik^2)))+((1.1097)*((30.09+(6.83*Tgebruik)+(6.79*Tgebruik^2)-
(2.53*Tgebruik^3)+(0.0821/(Tgebruik^2))))))
[30] Xeb = ((theta_i_Cp_i*(T-Tin))/(-delta_Hrx))+0
[31] Fa = 1350*(1-x)
[32] Fc = 1350*x
[33] Fd = 0.5*1350*x
[34] Fi = 1500
[35] vo = Fao/Cao
[36] F_SO2 = (Fc*64)/1000
[37] Kc_bo1 = ((4.86e-5)*Po*(x/(1+(0.237*x)))^Tin/T)
[38] Kc_bo2 = ((4.86e-5)*Po*((0.5*x)/(1+(0.237*x)))^Tin/T)^0.5
[39] Kc_var = (Kc_bo1*Kc_bo2)/Kc_onder
[40] ra = -k1*((Ca)-((Ci*Cc*(Cd^0.5))/Kc))
[41] rate = -ra
[42] Fao_op_min_ra = Fao/rate
[43] Ft = Fa+Fc+Fd+Fi
[44] F_O2 = (Fd*32)/1000

```

Comments

```

[3] Fao = 550.8
    mol/s
[18] Kc_var = (Kc_bo1*Kc_bo2)/Kc_onder

```


Korregeer Delta H
[19] Ea = 1.96E+05
J/mol
[37] vo = Fao/Cao
dm3/s
[38] F_SO2 = (Fc*64)/1000
kg/s

Independent variable

variable name : W

initial value : 0

final value : 1525

Precision

Step size guess. h = 0.000001

Truncation error tolerance. eps = 0.000001

General

number of differential equations: 2

number of explicit equations: 44

Elapsed time: 1.1574 sec

Reactor Stage 5 Data

POLYMATH Results

No Title

11-21-2008, Rev5.1.232

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
W	0	0	760	760
x	0.67	0.67	0.7200537	0.7200537
T	1143	1102.4666	1143	1102.4666
Fao	445.5	445.5	445.5	445.5
R	8.314	8.314	8.314	8.314
Po	300	300	300	300
To	1143	1143	1143	1143
Cto	0.0315693	0.0315693	0.0315693	0.0315693
theta_i	3.3669385	3.3669385	3.3669385	3.3669385
Epsilon	0.237	0.237	0.237	0.237
yao	0.474	0.474	0.474	0.474
Cao	0.0149638	0.0149638	0.0149638	0.0149638
Ca	0.0042614	0.00371	0.0042614	0.00371
Cc	0.0086519	0.0086519	0.0095425	0.0095425
Cd	0.004326	0.004326	0.0047712	0.0047712
Ci	0.0434784	0.0434784	0.0446202	0.0446202
Ea	1.96E+05	1.96E+05	1.96E+05	1.96E+05
A	1.04E+10	1.04E+10	1.04E+10	1.04E+10
Tin	1143	1143	1143	1143
k1	11.470668	5.3735178	11.470668	5.3735178
Tr	298	298	298	298
delta_A	12.23	12.23	12.23	12.23
delta_B	-42.04	-42.04	-42.04	-42.04
delta_C	36.04	36.04	36.04	36.04
delta_D	-10.55	-10.55	-10.55	-10.55
delta_E	0.0944	0.0944	0.0944	0.0944
Kc	0.2527205	0.1723573	0.2527205	0.1723573
Kc_onder	0.0041521	0.0036148	0.0041521	0.0036148
delta_Cp	-4.4190523	-4.4190523	-4.3725612	-4.3725612

delta_Hrx	9.892E+04	9.892E+04	9.892E+04	9.892E+04
Tgebruik	1.143	1.143	1.143	1.143
theta_i_C	125.20435	125.20435	125.20435	125.20435
Xeb	0	0	0.0513056	0.0513056
Fa	445.5	377.92755	445.5	377.92755
Fc	904.5	904.5	972.07245	972.07245
Fd	452.25	452.25	486.03623	486.03623
Fi	1500	1500	1500	1500
vo	2.977E+04	2.977E+04	2.977E+04	2.977E+04
F_SO2	57.888	57.888	62.212637	62.212637
Kc_bo1	0.00843	0.00843	0.0092977	0.0092977
Kc_bo2	0.064923	0.064923	0.0681824	0.0681824
Kc_var	0.1318134	0.1318134	0.175373	0.175373
ra	-0.0477581	-0.0477581	-0.0190187	-0.0190187
rate	0.0477581	0.0190187	0.0477581	0.0190187
Fao_op_mi	9328.2529	9328.2529	2.342E+04	2.342E+04
Ft	3302.25	3302.25	3336.0362	3336.0362
F_O2	14.472	14.472	15.553159	15.553159

ODE Report (RK45)

Differential equations as entered by the user

- [1] $d(x)/d(W) = -ra/Fao$
- [2] $d(T)/d(W) = ((-ra)*(-1)*(delta_Hrx))/(Fao*((theta_i_Cp_i)+(x*delta_Cp)))$

Explicit equations as entered by the user

- [1] $Fao = 445.5$
- [2] $R = 8.314$
- [3] $Po = 300$
- [4] $To = 1143$
- [5] $Cto = Po/(R*To)$
- [6] $theta_j = 3.366938473$
- [7] $Epsilon = 0.237$
- [8] $yao = 0.474$
- [9] $Cao = yao*Cto$
- [10] $Ca = Cao*((1-x)/(1+(Epsilon*x)))*(To/T)$
- [11] $Cc = (Cao*x)/(1+(Epsilon*x))*(To/T)$
- [12] $Cd = (Cao*0.5*x)/(1+(Epsilon*x))*(To/T)$
- [13] $Ci = (Cao*theta_i)/(1+(Epsilon*x))*(To/T)$

```

[14] Ea = 1.96E+05
[15] A = 1.04E+10
[16] Tin = 1143
[17] k1 = A*exp(-Ea/(R*T))
[18] Tr = 298
[19] delta_A = 12.23
[20] delta_B = -42.04
[21] delta_C = 36.04
[22] delta_D = -10.55
[23] delta_E = 0.0944
[24] Kc = 0.041*exp((98920/R)*((1/973)-(1/T)))
[25] Kc_onder = 4.86e-5*Po*(((1-x)/(1+(0.237*x)))^Tin/T)
[26] delta_Cp = delta_A+(delta_B*(T/1000))+(delta_C*((T/1000)^2))+(delta_D*((T/1000)^3))+(delta_E*((T/1000)^4))
[27] delta_Hrx = (98920+(delta_A*(T-Tr)/1000))+((delta_B/2)*((T/1000)^2)-((Tr/1000)^2))+((delta_C/3)*((T/1000)^3)-((Tr/1000)^3))+((delta_D/4)*((T/1000)^4)-((Tr/1000)^4))-((delta_E/((T/1000)-(Tr/1000))))
[28] Tgebruik = Tin/1000
[29] theta_i_Cp_i = (24.02+(119.46*Tgebruik)-(94.38*Tgebruik^2)+(26.96*Tgebruik^3)-(0.117/(Tgebruik^2)))+((1.1097)*((30.09+(6.83*Tgebruik)+(6.79*Tgebruik^2)-(2.53*Tgebruik^3)+(0.0821/(Tgebruik^2))))))
[30] Xeb = ((theta_i_Cp_i*(T-Tin))/(-delta_Hrx))+0
[31] Fa = 1350*(1-x)
[32] Fc = 1350*x
[33] Fd = 0.5*1350*x
[34] Fi = 1500
[35] vo = Fao/Cao
[36] F_SO2 = (Fc*64)/1000
[37] Kc_bo1 = ((4.86e-5)*Po*(x/(1+(0.237*x)))^Tin/T)
[38] Kc_bo2 = ((4.86e-5)*Po*((0.5*x)/(1+(0.237*x)))^Tin/T)^0.5
[39] Kc_var = (Kc_bo1*Kc_bo2)/Kc_onder
[40] ra = -k1*((Ca)-((Ci*Cc*(Cd^0.5))/Kc))
[41] rate = -ra
[42] Fao_op_min_ra = Fao/rate
[43] Ft = Fa+Fc+Fd+Fi
[44] F_O2 = (Fd*32)/1000

```

Comments

```

[3] Fao = 445.5
    mol/s

```

```
[18] Kc_var =      (Kc_bo1*Kc_bo2)/Kc_onder  
      Korregeer Delta H  
[19] Ea =      1.96E+05  
      J/mol  
[37] vo =      Fao/Cao  
      dm3/s  
[38] F_SO2 =      (Fc*64)/1000  
      kg/s
```

Independent variable

variable name : W

initial value : 0

final value : 760

Precision

Step size guess. h = 0.000001

Truncation error tolerance. eps = 0.000001

General

number of differential equations: 2

number of explicit equations: 44

Appendix E

The heat capacity correlations of the reaction agents used in the study is presented in Table 52.

Table 52: Heat capacity correlations of reaction reagents

Variable Heat Capacity with Temperature - Correlation Constants											
H ₂ SO ₄		SO ₃		SO ₂		H ₂ O		O ₂		Helium	
A	47.28924	A	24.02503	A	21.43049	A	30.092	A	29.659	A	20.78603
B	190.3314	B	119.4607	B	74.35094	B	6.832514	B	6.137261	B	4.85E-10
C	-148.1299	C	-94.38686	C	-57.7522	C	6.793435	C	-1.18652	C	-1.6E-10
D	43.86631	D	26.96237	D	16.35534	D	-2.53448	D	0.09578	D	1.53E-11
E	-0.740016	E	-0.117517	E	0.086731	E	0.082139	E	-0.21966	E	3.2E-11
F	-758.9525	F	-407.8526	F	-305.769	F	-250.881	F	-9.86139		
G	301.2961	G	253.5186	G	254.8872	G	223.3967	G	237.948		
H	-735.1288	H	-395.7654	H	-296.842	H	-241.826	H	0		