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Modeling of Adiabatic Fixed Bed Reactor for Catalytic Oxidation of Sulphurdioxide to Sulphurtrioxide

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ABSTRACT

Models for predicting catalytic conversion of SO_2 to SO_3 were developed. The models were developed from the first principle using conservation of mass and energy respectively and the developed model is a set of ordinary differential equation that were solved using ODE 45 solver of MatLab and validated with literature data. The result yielded a minimum percentage absolute error (deviation) between predicted models and literature data of 4.20% and 5.00% for fractional conversion and temperature respectively. These shows that the model developed predicted the output of SO_2 catalytic conversion very closely. The developed models were used to study the effect of process parameters such as fractional conversion (concentration) and temperature (inlet and outlet) along the reactor length for adaiabatic fixed bed reactor at steady state.

KEYWORD: Adiabatic Fixed Bed. Steady State modeling, SO_2, SO_3, MatLab ODE45 Solver

I. INTRODUCTION

Sulphurdioxide (SO_2) is released into the atmosphere as a result of domestic and industrial activities by the oxidation of sulphur contained in fossil fuels and industrial processes that treat and produce sulphur containing compounds. The catalytic oxidation of sulphurdioxide appears in numerous industrial processes and has a significant environmental impact because of the associated sulphuroxide (SOx) emissions from processes such as burning molten waste elemental sulphur, high SO_2 strength metallurgical off-gases, decomposing spent sulphuric acid catalyst by smelting and roasting ores, crude oil refining. bleaching processes (foodstuffs, sugar, and textiles), papermaking and glass production, fumigation of vessels etc. This is of great concern as its accumulation with other harmful gases leads to greenhouse effect and ozone layer depletion, thus there is need for its reduction in the atmosphere[1] Sulphurdioxide is one of the most deadly gas in the universe and it is released into the atmosphere as a result of domestic and industrial activities. When SO_2 is released in the heart of densely populated areas, it does great damage to the respiratory organs of living entities and most importantly, it is one of the precursors of acid rain that damages buildings and also corrode other physical structures. Hence, there is need to minimize SO_2 release into the atmosphere. Thus, minimizing the release of SO_2 into the atmosphere, a model is developed in predicting its catalytic conversion in an adiabatic fixed bed reactor to produce SO_3, which is useful in producing some industrial chemicals[2]

One common configuration in the industrial practice of a catalytic process is the fixed bed reactor, which consists of stationary solid catalyst particles through which the reacting fluid flows at certain operating conditions. It is most widely used for gas phase reactions in large-scale production. Although the local flow characteristics in such a reactor are really complex, the macroscopic flow pattern can often be approached as plug flow. The analysis of these reactors spans from the micro scale, with the pellet and its pore structure where the phenomena of reaction and diffusion occur, to the macro scale, with the geometry and the characteristics of the reactor bed where the phenomena of heat and mass convection, dispersion, and transfer occur[3] Fixed bed reactor can be classified as adiabatic and non-adiabatic reactor. Adiabatic reactor and non-adiabatic reactor are thermodynamic terms that describe the energy exchange between the system and the surroundings. An adiabatic system exchanges work, but no heat transfer with its surrounding. Thus the wall of an adiabatic reactor are heat opaque; they are insulated: Also, system with no or poor insulation can be adiabatic if any change within them occurs more rapidly than does achieving a new energy equilibrium with their surroundings[4] Therefore, an adiabatic process is a thermodynamic process in which there is no heat transfer into or out of a system and is generally obtained by surrounding the entire system with a strongly insulating material or by carrying out the process so quickly that there is no time for a significant heat transfer to take place. Adiabatic process occurs within a system as a result of transfer of energy to or from the system in the form of work only, and is characterized by an increase in entropy or degree of disorderliness[5]

In addition, the importance of SO_3 gas to the chemical industry and the economy at large cannot be quantified, as it is used for the manufacturing of important products and chemicals such as fertilizers, paints, soaps, fibers, crude oil refining, paper production, sulphuric acid, linear Alkyl benzene-sulphonic acid etc. It is extremely hard to find any branch of the economy in which either SO_3 or products made from it are not used[6].

Also, several methods of removing sulphurdioxide from the atmosphere have been discussed by several authors, but this research study shall focus on SO_2 conversion to SO_3, which is a useful precursor in the production of sulfuric acid in the presence of Vanadium(V)oxide as a catalyst. Hence, the aim of this research study is to develop model equations for a steady state adiabatic fixed bed reactor for the oxidation of sulphurdioxide (SO_2) to sulphurtrioxide (SO_3) thereby reduce environmental pollution caused by the evolution of SO_2 that is detrimental to both living and non-living organism. Furthermore, the aim of this research study is achieved by determining the nature of the reaction, performing material and energy balance on the fixed bed reactor, thus analyzing the conversion at the exit temperature, solving the models with Matlab program to obtain conversion and exit temperature and analysis of the models' result.

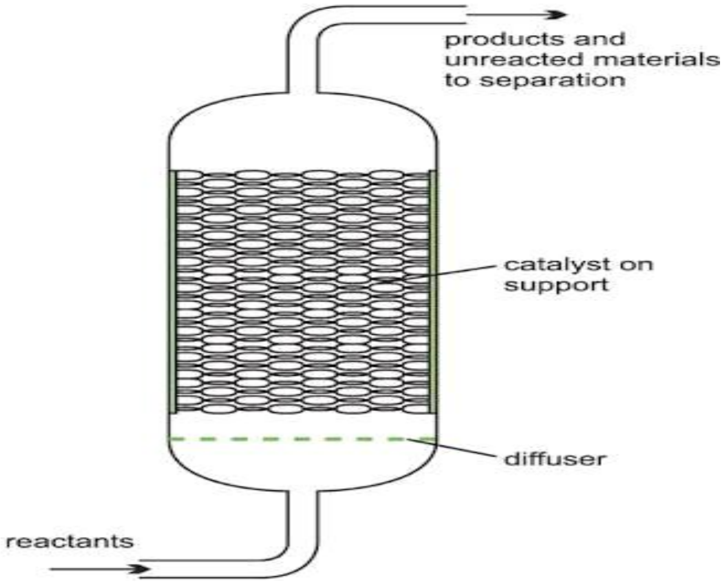

Figure 1: Catalytic Bed Reactor

II. MATERIAL AND METHOD

The materials applied in developing steady state model for adiabatic fixed bed reactor are SO_2, SO_3, MatLab, Runge-Kunta 4^{th} order etc.

Model Development

In describing the catalytic conversion of SO_2 to SO_3 in a fixed bed reactor over V_2O_5 catalyst, a mathematical analysis (model) of the fixed bed reactor is developed from the first principle with the application of the principles of conservation of mass and energy balances with these associated assumptions.

- The fixed bed reactor is a one-dimensional heterogeneous plug flow reactor with solid catalysts.
- Conversion reaction of SO_2 to SO_3 is exothermic as determined from its voidage value.
- Radial dispersion within the fixed bed reactor is negligible.
- The fixed bed reactor is adiabatic and steady state operational process is assumed in the reactor.
- Ideal gas behaviour was assumed at the operating conditions with the physical properties independent of temperature and pressure.

Nature of Reaction in Fixed Bed Reactor

The nature of the catalytic oxidation of SO_2 to SO_3 occurring in the fixed bed reactor is deduced from its voidage value as expressed thus[7]

$$\varepsilon = \frac{V_{XA=1} - V_{XA=0}}{V_{XA=0}} \quad (1)$$

The sum of the stoichiometric coefficients of the reactants and products are obtained from the balance catalytic oxidation reaction.

Kinetic Model

The reaction rate equation for the catalytic conversion of SO_2 to SO_3 over V_2O_5 catalyst as expressed thus[8]

$$r'_{SO_2} = K\sqrt{\frac{P_{SO\,2}}{P_{SO\,3}}}\left[P_{O_2} - \left(\frac{P_{SO\,3}}{K_p P_{SO\,2}}\right)^2\right] \tag{2}$$

This reaction rate equation can be written in terms of reacting concentration as

$$r'_{SO_2} = K\sqrt{\frac{C_{SO\,2}}{C_{SO\,3}}}\left[RTC_{O_2} - \left(\frac{C_{SO\,3}}{K_p C_{SO\,2}}\right)^2\right] \tag{3}$$

Reactor Model

Tubular reactor packed with a solid catalyst is widely applied as industrial reactor, which is called a fixed-bed reactor since the solid catalyst comprises a bed that is in a fixed position. The reaction takes place on the surface of the catalyst and the greater the catalyst mass, the higher the reactive surface area and the reaction is based on mass of solid catalyst other than that of the reactor volume. For heterogeneous reaction system, the rate of reaction of a particular specie is defined as moles of that specie reacting per time per mass of catalyst. Thus, the conversion or oxidation of SO_2 to SO_3 is an equilibrium reaction between SO_2 and oxygen in the presence of a solid catalyst usually vanadium pentaoxide (V_2O_5). The reaction equation is expressed as:

$$SO_2 + \frac{1}{2}O_2 \rightleftharpoons SO_3$$

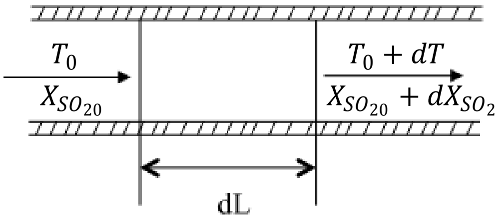

Figure 2: Tubular Fixed Bed Reactor

Mass transfer taking place in the fixed bed reactor was described by applying the principle of mass conservation on a differential element of the fixed bed reactor shown in Figure 2. Hence, this yields the model equation for predicting change in fractional conversion of SO_2 along the fixed bed reactor length as

$$C_{SO_{20}} U_0 \frac{dX_{SO\,2}}{dL} = K\rho_B\sqrt{\frac{C_{SO\,2}}{C_{SO\,3}}}\left[RTC_{O_2} - \left(\frac{C_{SO\,2}}{K_e C_{SO\,2}}\right)^2\right] \tag{4}$$

Similarly, temperature change along the fixed bed reactor length is evaluated by applying the principle of conservation of energy on the differential element of the reactor and temperature variation along the fixed bed reactor length is modeled as

$$\rho_{SO_2} U_0 C_{P_{SO\,2}} \frac{dT}{dL} = \left(-\Delta \mathrm{H}_{\mathrm{r}_{SO\,2}}\right) K\rho_B\sqrt{\frac{C_{SO\,2}}{C_{SO\,3}}}\left[RTC_{O_2} - \left(\frac{C_{SO\,2}}{K_e C_{SO\,2}}\right)^2\right] \tag{5}$$

III. METHOD

The developed model equations is a set of ordinary differential equations (ODE) which will be solved using the MatLab 7.5 ODE45 solver from Mathwork for non-stiff ordinary differential equations that uses the 4th order Runge-Kutta algorithm.

Determination of Model Parameters

Solving the developed model equations requires the evaluation of certain parameters and constants in the model. These parameters and constants were evaluated thus.

- Specific Heat Capacity

The specific heat capacity of SO_2 at any temperature was determined as stated thus[8]

$$C_{PSO_2} = 7.208 + 0.05633T + 0.000001343T^2 \qquad (6)$$

- Heat of Reaction

The heat of reaction for $S0_2$ conversion was evaluated at any temperature as described[8]

$$\Delta H_{R;SO_2}(T) = \Delta H_{R;SO_2}(T_R) + \Delta\gamma(T - T_R) + \frac{\Delta\beta}{2}(T^2 - T_R^2) + \frac{\Delta\alpha}{3}(T^3 - T_R^3) \qquad (7)$$

- Reaction Rate Constant

The reaction rate constant for the conversion of SO_2 is expressed as[8]

$$k = \exp\left[\frac{-176{,}000}{T} - (110.11 lnT) + 912.8\right] \qquad (8)$$

- Equilibrium Constant

The equilibrium constant is the ratio of the forward reaction rate constant to backward reaction rate constant. The equilibrium constant equation for catalytic oxidation of SO_2 to SO_3 at any temperature is evaluated thus[8]

$$K_e = \exp\left[\frac{42{,}311}{RT} - 11.24\right] \qquad (9)$$

Table 1: Operating and Thermodynamic Data[9]

Parameters	**Values**	**Unit**
C_{SO2}	3.236	mol/m^3
P_{SO2}	0.165	Pascal (Pa)
P_{SO3}	1	Pascal (Pa)
P_{O2}	0.755	Pascal (Pa)
ρ_{so2}	0.054	mol/m^3
ρ_B	33.8	mol/m^3
U_o	0.24	m/s
R	1.9861	Cal/mol.K
T	1260	Kelvin (K)

IV. RESULT AND DISCUSSION

The result obtained from the evaluation of the model equations for the fixed bed reactor are discuss thus.

Fractional Conversion Profile

The fractional conversion profile show a steady increase in SO_2 conversion up to 95% along the reactor length of 7ft as shown in Figure 3, after which there is sharp reduction in SO_2 conversion at reactor length above 7ft. This reduction in conversion rate may be as a result of catalyst deactivation due to particles or dirts on the catalyst surface as the conversion progresses along the reactor's length, thereby reducing catalyst's efficiency or effectiveness factor.

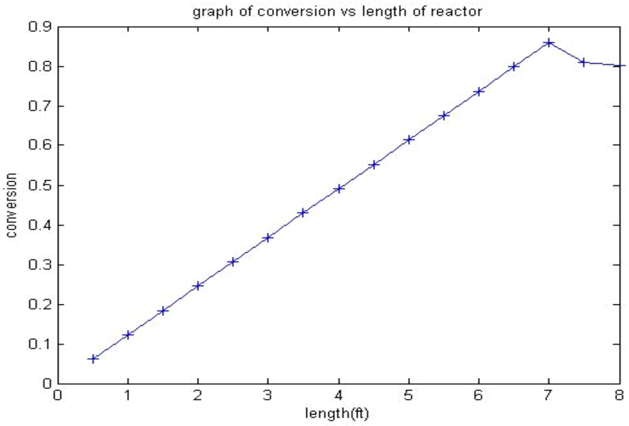

Figure 3: Plot of Fractional Conversion against Length

Temperature Profile

The predicted temperature profile along the fixed bed reactor length shows that SO_2 conversion to SO_3 is an exothermic reaction as heat is evolved along the reaction length path, thus, this deduction is in tandem with the voidage value evaluated from oxidation equilibrium equation.

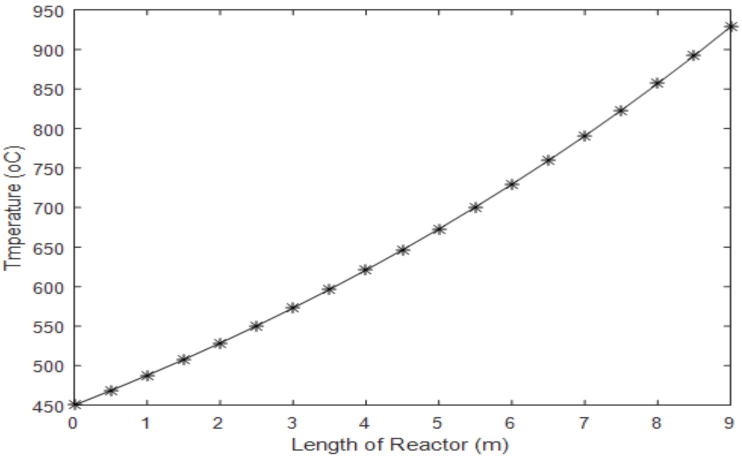

Figure 4: Plot of Temperature Variation along Reactor Length

Temperature and Conversion Profile

The temperature-conversion profile in Figure 5 shows an increase in SO_2 conversion as temperature progresses in the fixed bed reactor to a maximum temperature of 600^0C after which there is steady reduction in production of SO_3. Hence, the reaction temperature will be maintained at optimum of 600°C to optimize the production of SO_3 and since the process is exothermic, installation of cooling jacket to maintain the temperature at the desired level is required.

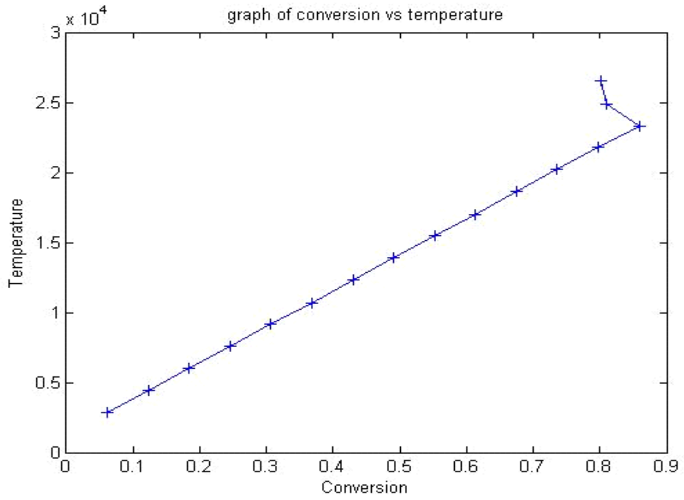

Figure 5: Plot of Temperature- Conversion Profile

Model Validation

The comparison of the model results with those obtained from previous work done (Literature data) are presented in Table 2

Table 2: Comparison of Model Result with Literature Data

Parameter	Literature Value	Model Prediction	Deviation (%)
Conversion	0.99	0.95	4.20
Temperature	1200	1260	5.00

As shown in Table 2, the maximum percentage absolute error (deviation) between the predicted models and literature data is 4.20% for fractional conversion and 5.00% for temperature effects on the fixed bed reactor. Hence, the developed model can be used to predict and simulate SO_2 catalytic conversion to SO_3.

Process Simulation.

The fixed bed reactor was simulated to evaluate the effect of temperature on fractional conversion of the feedstock as the reaction progresses with temperature. From the graph, increase in the inlet temperature increases the conversion to temperature of 1300K, after which there is drop in conversion. Thus, optimum conversion was obtained at 1300K. Above the optimum temperature, there is reduction in conversion by 0.14 due to probably catalyst deactivation resulting from deposition of particles on its surface thereby reducing its efficiency.

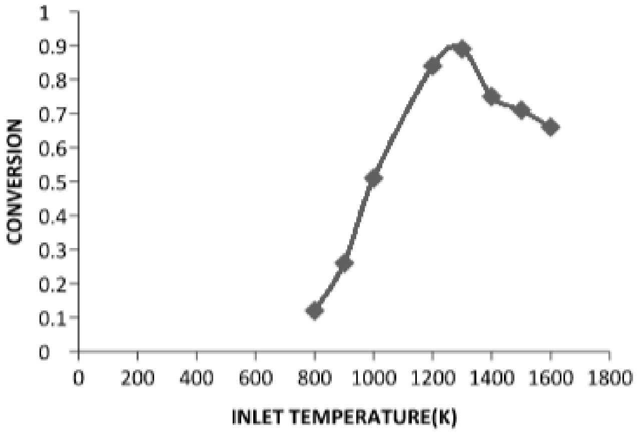

Figure 6: Plot of Conversion against Inlet Temperature

V. CONCLUSION

Models for the steady state adiabatic fixed bed reactor for catalytic oxidation or conversion of SO_2 to SO_3 were developed. The models predict fractional conversion and temperature progression along the length of adiabatic fixed bed reactor. The developed model was evaluated and compared with literature data and the percentage absolute error or deviation of 4.20% and 5.00% for fractional conversion and temperature respectively was deduced. This result yields a close mapping between model prediction and literature data, thus the developed model can be applied in simulating catalytic oxidation of SO_2 to SO_3 in an adiabatic fixed bed reactor at steady state.

REFERENCES

[1]. Kiss A. A., Bildea, C. S., &Grievink, J. (2010). Dynamic Modeling and Process Optimization of an Industrial Sulfuric Acid Plant. *Chemical Engineering Journal*, 158, 2, 241–249.

[2]. Gosiewski K., (2010). Dynamic Modelling of Industrial SO_2 Oxidation Reactors: Part 1 Model of Hot and Cold Start-ups of the Plant. *Chemical Engineering and Processing*, 32, 111–129.

[3]. Wu, H. S., Zhang, S. Z., & Li, C. Y. (1996). Study of Unsteady State Catalytic Oxidation of Sulfurdioxide by Periodic Flow Reversal. *Canadian Journal of Chemical Engineering*, 74, 5, 766–771,

[4]. Bailyn, M. (1994). A Survey of Thermodynamics. New-York: AIP Press. 21.

[5]. Mann R., Stavridis E., &Djamarani, K. (2009). Experimental Fixed-Bed Reactor Dynamics for SO_2 Oxidation. *Chemical Engineering Research and Design*, 64, 248–257

[6]. Sørensen, P. A., Møllerhøj, M., & Christensen, K. A. (2015). New Dynamic Models for Simulation of Industrial SO_2 Oxidation Reactors and Wet Gas Sulfuric Acid Plants. *Chemical Engineering Journal*, 278, 421–429.

[7]. Levenspiel O. (1999). Chemical Reaction Engineering. Singapore: John Wiley & Sons, 429 431

[8]. Donovan, J. R. &Salamone, J. M. (1984). In Kirk-Orhmer Encyclopedia of Chemical Technology. New-York: Wiley Publisher

[9]. Chase, M.W, (2011). Nist-JanafThemochemical Tables, *Journal of Physical and Chemical Reference Data, Monograph* 9, 1–1951,

VI. NOMENCLATURES

ε:: Voidage Value
$V_{XA=0}$: Sum of Reactant Stoichiometric Coefficients
$V_{XA=1}$: Sum of Product Stoichiometric Coefficients
P_{SO_2}, P_{O_2}, &P_{SO_3}: Partial Pressures of SO_2, O_2 and SO_3 respectively
C_{SO_2}, C_{O_2} *and* C_{SO_3}: Concentrations of SO_2, O_2 and SO_3 respectively.
R: Universal Gas Constant
T: Reaction Temperature
K: Reaction Rate Constant
K_e: Equilibrium constant.
$\left(-r'_{SO_2}\right)$: Heterogeneous Rate of Reaction expressed in unit mole per unit time per unit mass of catalyst
ρ_B: Bulk Density of Catalyst
A: Cross Sectional Area
U_0: Fluid Velocity
C_{PSO_2}: Specific Heat Capacity of $S0_2$

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