

Modelling of Semi Batch Reactor Adsorption Tower for Sulphur Trioxide Hydration using Vanadium Catalyst

Goodhead T.O and Abowei M.F.N

Abstract— A semi batch reactor for the production of sulphuric acid over a range of degree of conversion, $X_A = 0.95$ to 0.99 and reaction time $t = 30$ to 1800 sec have been designed. The reactor which operates at an optimum condition of 90°C and 1.5atm is capable of producing $10,000$ metric tons per year of sulphuric acid. This reactor is designed with hastelloy because it possesses an excellent corrosion and sulphuric acid resistance properties. The reactor performance equations are simulated with the aid of a Computer using MATLAB (R2007b). The results provided information for the functional parameters for the reactor which include; the reactor volume, reactor height, and rate of heat generation per unit volume of reactor. The results showed that the reactor volume which is dependent on the degree of conversion X_A would tend to infinity at 100% conversion. The relationship between the degree of conversion, reaction time and these functional parameters are presented graphically.

Index Terms— Sulphur, Vanadium, Modelling Semi-Batch Reactor.

1 INTRODUCTION

Sulphuric acid is a very important commodity chemical and indeed, a nation's sulphuric acid production is a good indicator of its industrial strength [1]. The search for the modification in sulphuric acid production is a global concern [2]. This is due to the importance attached to the use of the acid. Therefore, this work is focused on the development of reactor types at isothermal and non isothermal conditions. Reactor types addressed in this work at the above specified conditions include.

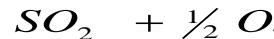
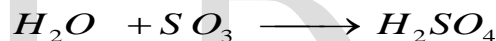
- Semi -batch reactor
- Continuous stirred tank reactors
- Plug flow reactors.

The design and operation of such equipment require rates of both physical and chemical process. The principles governing such physical process as energy transfer and mass transfer are often as important as those which govern chemical kinetics. This combination of physical and chemical operations is also a distinguishing feature of chemical engineering.

Industrial chemical reactors are used to carry out chemical reactions in commercial scale. Often times in reactor design we want to know the size, type of reactor and method of operation that are best for a given reaction.

Industrial scale production of sulphuric acid is dependent on the oxidation of sulphur dioxide to sulphur trioxide in fixed

bed thus as follows:



Through the years, several catalyst formulations have been employed, but one of the traditional catalytic agents has been Vanadium pent oxide (V_2O_5).

Its principal applications include; ore processing, fertilizer manufacturing, oil refining, waste water processing, chemical synthesis etc. [4]. The general schematic presentation for the production of sulphuric acid is given below.

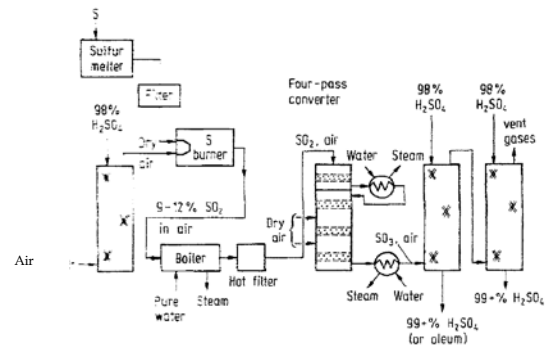


Figure 1.1: Contact process for making sulfuric acid and Oleum from sulfur.

It is worthwhile to continue to research on the best hypothetical reactor unit for the production of sulphuric acid. That actually formed the basis of this research. The task of this

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bed catalytic reactors [3].

The Chemistry for the production of sulphuric acid is present-

work is to design ideal fluid-fluid contactor units that would produce sulphuric acid in commercial quantity at the lowest possible cost from gaseous sulphur trioxide and water as absorbent. The production of the acid is considered on the three principal types of reactor – semi-batch reactor, continuous stirred tank reactor and plug flow absorption reactor in a view of selecting the best absorption reactor with the best operating condition that would give the minimum capital and operational cost to achieve maximum output.

In the industrial chemical process, heterogeneous fluid-fluid reactions are made to take place for one of three reasons. First, the product of reaction may be a desired material. Such reactions are numerous and can be found in practically all areas of the chemical industry where organic and inorganic syntheses are employed [5]. Fluid-fluid reactions may also be made to take place to facilitate the removal of an unwanted component from a fluid. Thus the absorption of a solute gas by water may be accelerated by adding a suitable material to the water which will react with the solute being absorbed. The third reason for using fluid-fluid systems is to obtain a vastly improved product distribution for homogeneous multiple reactions than is possible by using the single phase alone.

The area of interest in this study is of absorption with chemical reaction. Absorption is the process of removing one or more constituents of a gaseous mixture by treating it with a liquid. The necessary condition is the solubility of these constituents in the absorbing liquid. The soluble constituents of the gas mixture are called active components and the others, being practically insoluble, are called inert components [6], [7], [8]. The reverse process of removing a gas from a solution is called stripping or desorption. The direction of mass transfer depends on the way the liquid-gas composition deviates from the mutual equilibrium state. If the concentration of the active component in a gas is higher than its concentration when it is in equilibrium with the liquid, mass transfer occurs from the gas phase to the liquid phase. On the other hand, when its concentration in the gas is lower than that corresponding to its equilibrium with the liquid, mass transfer occurs from the liquid phase to the gas phase.

Absorption or stripping processes may be handled in two ways.

- a. **Statically:** This is done in order to know the equilibrium state between the phases and the deviation of the actual compositions of the two phases from the equilibrium state.
- b. **Kinetically:** This indicates the rate of the process under the given conditions or helps find conditions for running the process economically [7].

Gas absorption with reaction is usually carried out in columns. The process column requirement could be single unit, two units or multiple units, depending on choice and mixture composition. Absorption columns are vertical, cylindrical vessels containing devices that provide intimate contacting of the rising vapour (or gas) with the descending liquid. This contacting provides opportunity for the two streams to achieve some approach to thermodynamic equilibrium. Depending on the type of internal devices used, the contacting may occur in discrete steps called plates or trays, or in a continuous differ-

ential manner on the surface of a packing material [5]. The fundamental requirement of the column is to provide efficient and economic contacting at the required mass transfer rate. Individual column requirements vary from high vacuum to high pressure, from low to high liquid rates, from clean to dirty systems and so on. As a result a large variety of internal devices have been developed to fill these needs. [6].

For the case under investigation—gas absorption with chemical reaction, the following factors will determine the design method used.

- **The overall rate expression:** Since materials in the two separate phases must contact each other before reaction can occur, both the mass transfer and the chemical rates will enter the overall rate expression.
- **Equilibrium solubility:** The solubility of the reacting components will limit their movement from phase to phase. This factor will certainly influence the form of the rate equation since it will determine whether the reaction takes place in one or both phases.
- **The contacting scheme:** In gas-liquid systems semi-batch and counter current contacting schemes predominate. In liquid-liquid systems mixed flow and batch contacting are used in addition to counter and co current contacting. [5].

Many possible permutations of rate, equilibrium, and contacting pattern can be imagined; however, only some of these are important in the sense that they are widely used on the technical scale.

Sulphuric acid is an important commercial commodity. Related literatures have shown that its demand for consumption has exceeded its supply [9], [1]. The traditional methods of its production in pure form could not cope with the demand [10]. The lead chamber process and the contact process have been used to produce the acid in commercial quantity. The lead chamber process produces acid of very low grade, both in purity and concentration. However, the contact process produces acid of high concentration and purity but the process of its manufacture is very expensive. This process utilizes very expensive catalyst (Vanadium pent oxide). As a result the acid from this process is equally expensive.

Hence, to ensure availability and affordability of the product with acceptable quality, there is need to look for alternative methods of its production.

Substantial works had been done and documented on the kinetics of sulphuric acid production [2]. Literatures have shown that direct dissolution of sulphur trioxide in water to produce the acid is not done due to very high heat of reaction occasioned in the process. Instead sulphur trioxide is absorbed in concentrated sulphuric acid to form oleum, and subsequently diluted with water to form sulphuric acid of 98%-100% concentration.

Although the production of sulphuric acid is eminent and known globally, related literatures have shown that numerous treaties have been written and published on it [2]. The purpose of this research is to investigate into past works on the development of performance models for reactor types for the production of sulphuric acid, and to specifically identify and develop appropriate performance models for the areas that are

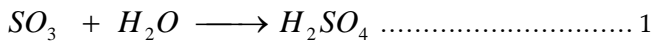
deficient in past work.

However, little or no known published work had been recorded for the development of performance models for the production of the acid using semi batch reactor, continuous stirred tank reactor, and plug flow reactor. This present work is aimed at addressing this seemingly neglected area.

2 KINETICS ANALYSIS

The reaction mechanism as presented in equation (1) showed chain reaction characteristics [11]. Gibney and ferracid reported on the photo-catalysed oxidation of SO₃²⁻ by (dimethyl-glyoximato) (SO₃)₂⁻ and its (Co(dimethyl-glyoximato) (SO₃)₂)²⁻[12].

The work showed that the reaction



is described as irreversible bimolecular chain reaction. Further research into the works of Erikson [13] and Huie, et al [15] established the reaction as second order reaction with rate constant K₂ = 0.3 mole/sec. Morokuma and Mugurama, performed abinitio calculation and determined the energetic barrier and established conclusively that the irreversible bi-molecular nature of the reaction have ΔH_r = -25kcal/mol at 250C [15].

Following the outcome of the work of Chenier as cited above, the rate expression for the formation and production of sulphuric acid is summarized as in equation (2) [1].

$$-R_A = K_2 [SO_3] [H_2O] \dots\dots\dots 2$$

Hence from equation (2.33) the amount of SO₃ and H₂O that have reacted at any time t can be presented as;

$$-R_A = K_2 [C_{A0} - C_{A0} X_A] [C_{B0} - C_{A0} X_A] \dots\dots\dots 3$$

Where

- CA₀ = Initial concentration of SO₃ (moles/Vol)
- CB₀ = Initial concentration of H₂O (moles/Vol)
- X_A = Fractional conversion of SO₃ (%)
- R_A = Rate of disappearance of SO₃ (mole/ Vol/t)

In this work, the rate expression (-R_A) as in equation (3) will be used to develop the hypothetical semi-batch reactor design equations with inculcation of the absorption coefficient factor as recommended in the works of Van-Krevelen and Hoftyger (1948) [17], [18] and [19]. This is achieved by modifying equation (3) as illustrated below. The hypothetical concentration profile of the absorption of sulphur trioxide by steam (H₂O) is represented in figure 2.

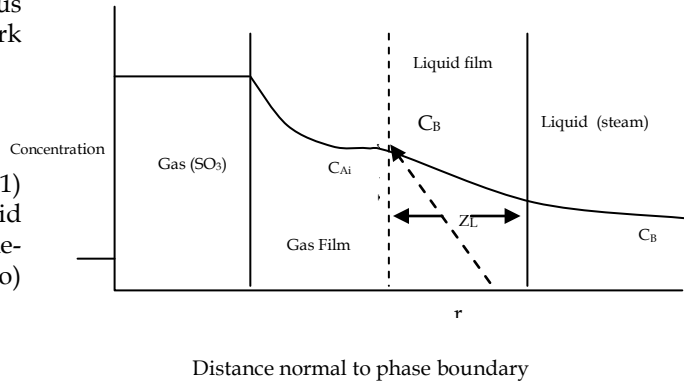


Figure 2: Absorption with chemical Reaction

Sulphur trioxide (A) is absorbed into the steam (B) by diffusion. Therefore the effective rate of reaction by absorption is defined by

$$-R_A = \frac{rD_L}{Z_L} (C_{Ai} - C_{AL}) = rK_L (C_{Ai} - C_{AL}) \dots\dots\dots 4$$

Invoking the works of Krevelen and Hoftyzer, the factor r is related to CA_i, D_L and K_L to the concentration of steam B in the bulk liquid C_{BL} and to the second order reaction rate constant K₂ for the absorption of SO₃ in steam solution. Thus

$$r = \frac{(K_2 D_L C_{BL})^{1/2}}{K_L} \dots\dots\dots 5$$

Substituting equation (5) into (4) results in

$$-R_A = (C_A) C_{BL}^{1/2} K_2^{1/2} D_L^{1/2} \dots\dots\dots 6$$

Previous reports Octave levenspiel [16] showed that the amount of SO₃ (C_A) and steam (C_{BL}) that have reacted in a bimolecular type reaction with conversion X_A is C_{A0} X_A. Hence equation (6) can be rewritten as

$$-R_A = K_2^{1/2} D_L^{1/2} (C_{B0} - C_{A0} X_A)^{1/2} (C_{A0} - C_{A0} X_A) = K_2^{1/2} D_L^{1/2} C_{A0}^{3/2} (m - X_A)^{1/2} (1 - X_A) \dots\dots\dots 7$$

Where

$$m = \frac{C_{B0}}{C_{A0}} \text{ - The initial molar ratio of reactants}$$

- R_A = Rate of disappearance of SO₃
- K₂ = Absorption reaction rate constant
- D_L = Liquid phase diffusivity of SO₃.
- K_L = Overall liquid phase mass transfer coefficient
- r = Ratio of effective film thickness for absorption with chemical reaction.

3. DEVELOPMENT OF PERFORMANCE MODEL

The fundamental design equations are algebraic descendants of the generalized material balance equation.

$$\left\{ \begin{matrix} \text{Rate of} \\ \text{Input} \end{matrix} \right\} = \left\{ \begin{matrix} \text{Rate of} \\ \text{Output} \end{matrix} \right\} + \left\{ \begin{matrix} \text{Rate of} \\ \text{Accumulation} \end{matrix} \right\} + \left\{ \begin{matrix} \text{Rate of disappearance} \\ \text{by reaction} \end{matrix} \right\} \dots (8)$$

For semi-flow reactors, rate of output = 0

If $F_{A0} = V_0 C_{A0}$ is the molar feed rate of SO_3 to the reactor, then considering the reactor as a whole we have.

Input of SO_3 , moles/time = $F_{A0} (1 - X_A) = F_{A0} \dots (9)$

Disappearance of SO_3 by reaction, moles/time = $(-R_A) V_R \dots (10)$

Rate of accumulation = $\frac{dN_A}{dt} \dots (11)$

Substituting equations (9), (10) and (11) in equation (8) gives

$$F_{A0} = \frac{dN_A}{dt} + (-R_A) V_R \dots (12)$$

But,

$$-R_A = K^{1/2} D^{1/2} C_{A0}^{3/2} (m - X_A)^{1/2} (1 - X_A) \dots (7)$$

Combining equations (12) and (7) and re-arranging we have

$$\frac{dN_A}{dt} = F_{A0} - V_R K^{1/2} D^{1/2} C_{A0}^{3/2} (m - X_A)^{1/2} (1 - X_A) \dots (13)$$

But,

$$N_A = N_{A0} (1 - X_A)$$

Differentiating we have

$$dN_A = -N_{A0} dX_A \dots (14)$$

Substituting equation (14) in equation (13)

$$\frac{dX_A}{dt} = K^{1/2} D^{1/2} C_{A0}^{3/2} (m - X_A)^{1/2} (1 - X_A) - \frac{F_{A0}}{N_{A0}} \dots (15)$$

But,

$$\frac{F_{A0}}{N_{A0}} = \frac{C_{A0} V_0}{C_{A0} V_R} = \frac{1}{t} \dots (16)$$

Where,

t is the residence time in seconds

$$\frac{dX_A}{dt} = K^{1/2} D^{1/2} C_{A0}^{3/2} (m - X_A)^{1/2} (1 - X_A) - \frac{1}{t} \dots (17)$$

Volume change of semi-Batch reactor with time

Recall that

$$V_R = V_0 (1 + \epsilon_A X_A) \dots (18)$$

Differentiating equation (18) with respect to time

$$dV_R = \epsilon_A V_0 dX_A \dots (19)$$

Substituting equation (17) in equation (19)

$$\frac{dV_R}{dt} = V_0 \epsilon_A \left[K^{1/2} D^{1/2} C_{A0}^{3/2} (m - X_A)^{1/2} (1 - X_A) - \frac{1}{t} \right] \dots (20)$$

Integrating equation (20) gives

$$V_R = V_0 \epsilon_A \left[K^{1/2} D^{1/2} C_{A0}^{3/2} (m - X_A)^{1/2} (1 - X_A) t - \ln t \right] \dots (21)$$

Reactor Height

Considering a reactor with cylindrical shape we have

$$V_R = \pi r^2 h_{sBr} \dots (22)$$

$$h_{sBr} = \frac{V_R}{\pi r^2} \dots (23)$$

Putting equation (21) into equation (23) results in

$$h_{sBr} = \frac{V_0 \epsilon_A \left[K^{1/2} D^{1/2} C_{A0}^{3/2} (m - X_A)^{1/2} (1 - X_A) t - \ln t \right]}{\pi r^2} \dots (24)$$

For $0.1m \leq r \leq 1.0m$

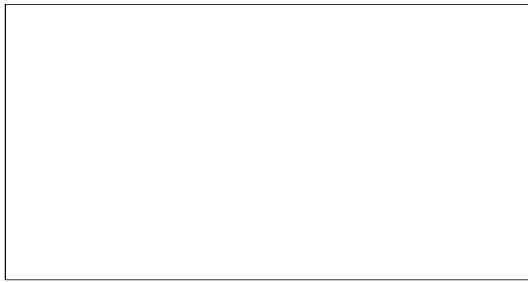


Fig. 3 Hypothetical model of Semi Batch Stirred Tank Reactor

3.3.3 Heat Generation Per Reactor Volume.

The rate of heat generation in a reactor is expressed as:

$$Q = (-\Delta H_R) F_{A0} X_A \dots\dots\dots(25)$$

Dividing both sides by the reactor volume, V_R

$$R_q = \frac{Q}{V_R} = \frac{(-\Delta H_R) F_{A0} X_A}{V_0 \epsilon_A \left[K^{1/2} D_L^{1/2} C_{A0}^{1/2} (m - X_A)^{1/2} (1 - X_A)t - \text{Int} \right]} \dots\dots\dots(26)$$

The computation of the functional parameters of the reactor as shown in figure 3 is implemented in MATLAB, and the computer flow chart describing the computation is illustrated in figure 4.

Algorithm Flow Chart for Semi-Batch Reactor

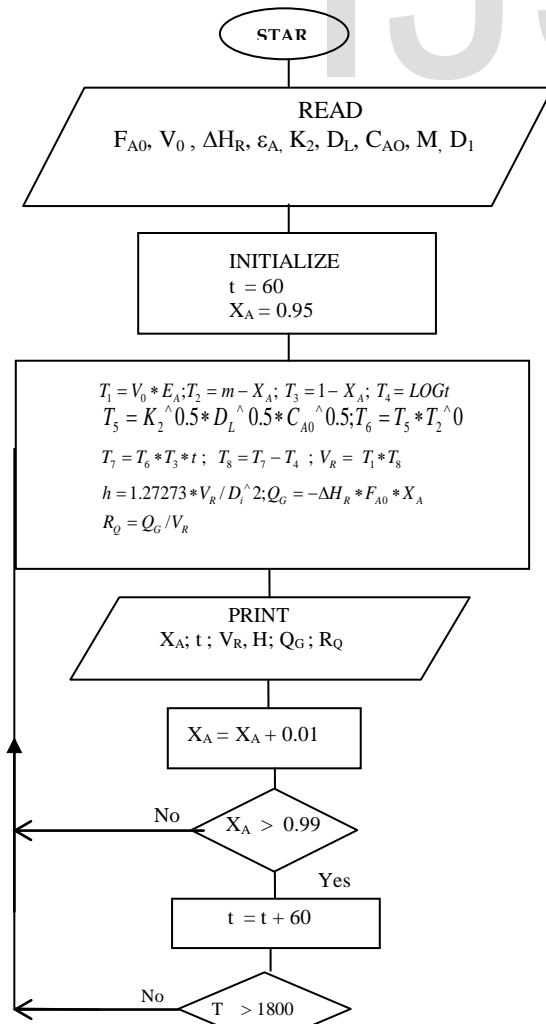


Figure 4: Flow chart describing the computation of semi-Batch Reactor functional parameters

THE REACTOR INPUT PARAMETERS

The reactor performance models developed in section 3 contain unknown parameters such as the molar flow rate, concentration etc. these parameters have to be determined before equation 21 – 26 can be evaluated.

Table 1: Design data sheet.

Quantity	Symbol	Value	Unit
Initial concentration of SO ₃	C _{A0}	16,759	mol/m ³
Fractional change in volume	ε _A	-0.5	
Heat of reaction	ΔH _R	-88	Kj/mol
Absorption reaction rate constant	K ₂	0.3	1/sec
Conversion degree	X _A	0.95 - 0.99	%
Reactant molar flow rate	F _{A0}	3.937	mol/sec
Molar ratio of reactants	m	1.0 to 1.5	
Radius of Semi batch reactor	r	0.1 to 1.0	m
Liquid phase diffusivity of SO ₃	D _L	17	m ² /Sec
Volumetric flow rate of reactants	V ₀	2.352 x10 ⁻⁴	m ³ /Sec
Residence time for semi-batch reactor	t	60 to 1800	Sec

DISCUSSION OF RESULTS

Industrial reactor for the production of sulphuric acid over a range of reaction time $t = 60$ to 1800 Sec, and degree of conversion $X_A = 0.95$ to 0.99 have been investigated and designed. This reactor has a capacity of 1.389×10^3 Kg/hr of sulphuric acid. The reactor was designed with hastelloy because it has excellent corrosion and sulphuric acid resistance properties.

The reactor performance models developed in section three were simulated with the aid of MATLAB R2007b. The results provided information for the functional reactor parameters viz: The reactor volume and the rate of heat generation per unit volume and the height of reactor. It is the purpose of this section to present and discuss the results of the reactor.

The functional parameters of the reactor are tabulated in appendices 1 and 2. The results showed that the reactor volume is dependent on the reaction time, t and degree of conversion X_A . The volume of the reactor would tend to infinity at 100% conversion. The variation of the reactor volume, reactor height and the rate of heat generation per reactor volume as a result of sulphur trioxide addition to water, with reaction time, and degree of conversion is illustrated in figures 5, 6, 7, and 8.

From the results it was observed that volume of the reactors increases with increasing reaction time and degree of conversion.

Figures 7 and 8 illustrated the variation of heat generation per unit volume of the reactors as a function of reaction time t , and degree of conversion within the limits t , and X_A as specified. A plot of heat generation RQ versus reaction time, t was observed to be curvilinear with negative gradient. The rate of heat generation per reactor volume RQ was found to be decreasing with increasing reaction time, t within the range of $X_A = 0.95$ to 0.99 . Similar plots were made RQ versus X_A within the range of $t = 60$ sec to 1800 sec. The graphs were also curvilinear with positive gradient. As reaction progresses, there was a sharp drop tending to the abscissa of the graph. At this stage the performance of the reactor approximate to the contact process of sulphuric acid production behavior. Finally the rate of heat generation per unit reactor volume decreases with increasing reaction time and degree of conversion.

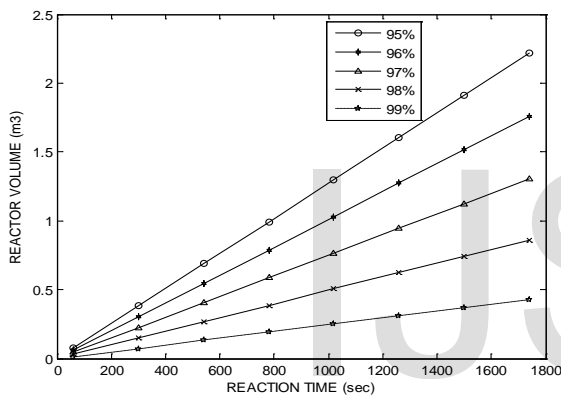


Figure 5: Plot of Reactor Volume against Reaction Time for Semi-Batch Reactor

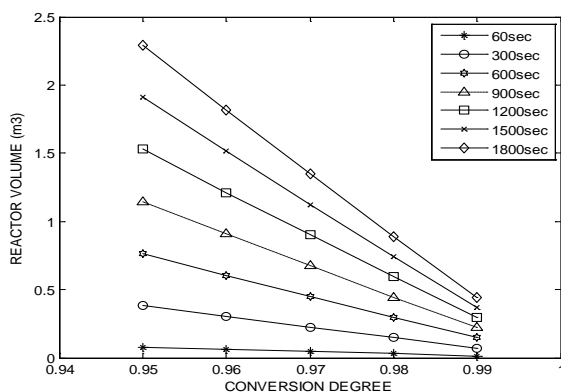


Figure 6: Plot of Reactor Volume against Conversion Degree for Semi-Batch Reactor

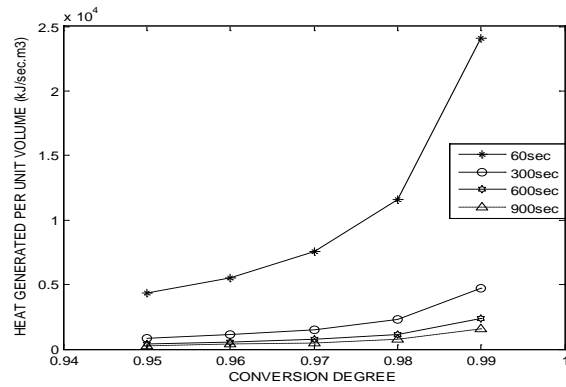


Figure 7: Plot of Heat Generated per unit Volume against Conversion Degree for Semi-Batch Reactor

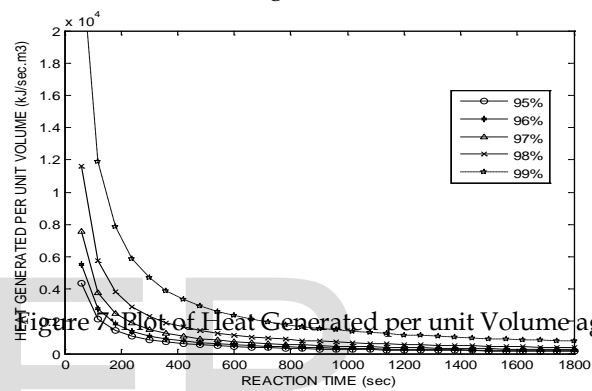


Figure 8: Plot of Heat Generated per unit Volume against Reaction Time for Semi-Batch Reactor

DISCUSSIONS

The consideration of non-isothermity of the reactors is a reasonable assumption as long as the operation of the reactors is within the sonic limit. An observation deduced from this work is that the operating temperature tends to influence the reactor performance. Generally the operation is favoured by low temperature. This confirms the reason why heat exchangers should be incorporated in the design. The consideration of the optimum limit of degree of conversion X_A from 0.95 to 0.99 is reasonable because at 100% conversion of sulphur trioxide, the functional parameters of the reactors will all tends to infinity. In this case the dimensions of the reactors have no limit.

Work free days of 65 is allowed to produce the specified quantity i.e. $1.389 \times 103\text{Kg/hr}$ of sulphuric acid. Sulphur trioxide, SO_3 can be produced by catalytic oxidation of sulphur dioxide using vanadium pentoxide as catalyst.

The semi-batch reactor results showed that, if the reaction time, t was 60 sec, and degree of conversion, X_A was 0.95 , the reactor volume, V_R were 0.0226m^3 and 0.0760m^3 when the reactant molar ratio, $m=1.0$ and 1.5 respectively but increase of t and X_A resulted in increase of the reactor volume up to 0.6910 to 0.0610 m^3 when $m=1.0$, $t=1800$ sec and $X_A=0.95$ to 0.99 and 2.2939 to 0.4411m^3 when $m=1.5$. At any given reaction time the semi-batch reactor volume decreases with in-

crease in degree of conversion. Similarly, at any given conversion degree the semi-batch reactor volume increases with increase in reaction time. This is due to its peculiar mode of operation. Such behaviour is expected of a semi-batch reactor since it holds a batch of one reactant while the second reactant is gradually introduced into the reactor during the processing period.

CONCLUSION

Reactors have been designed for the production of ten thousand metric tons per year of sulphuric acid. Computer programs were developed and utilized to simulate the reactors performance models over a temperature interval of T=313 to 363K, and conversion degree, XA=0.95 to 0.99. For the plug flow reactors and the semi-batch reactor, additional variable of reactor diameter of 0.02 to 0.1m and reaction time of 60 to 1800sec respectively were used.

From the results of computation, it is clearly established that:

For the semi-batch reactor

(a) When the degree of conversion, XA=0.95, reaction time, t=60sec, the reactor volume, VR are 2.26E-02m3 and 7.60E-02m2, the reactor height, h_{sbr} are 2.88E-02m and 9.68E-02m, and the rate of generation per reactor volume, RQ are 1.4593E04KJ/sec.m3 and 4.3353E03KJ/sec.m3 for the reactant molar ratio, m=1.0 and 15 respectively.

(b) When the degree of conversion, XA=0.99 for the same lower operating conditions as specified above, the reactor volume, VR are 1.5813E-03m3 and 1.425E-02m3, the reactor height, h_{sbr} are 2.0125E-03m and 1.8137E-02m, and the rate of heat generation per reactor volume, RQ are 2.1716E05KJ/sec.m3 and 2.4098E04KJ/sec.m3 for the reactant molar ratio, m=1.0 and 1.5 respectively.

(c) When the degree of conversion, XA=0.95, reaction time, t=1800sec, the reactor volume, VR are 0.6910m3 and 2.2939m3, the reactor height, h_{sbr} are 0.8798m and 2.9207m, and the rate of heat generation per reactor volume, RQ are 4.77E06KJ/sec.m3 and 1.437E04KJ/sec.m3 for the reactant molar ratio, m=1.0 and 1.5 respectively.

(d) When the degree of conversion, XA=0.99 for similar conditions as in (c) above, the reactor volume, VR are 6.10E-02m3 and 0.4411m3, the reactor height, h_{sbr} are 7.77E-02m and 0.5616m, and the rate of heat generation per reactor volume, RQ are 5.63E-07KJ/sec.m3 and 7.79E-06KJ/sec.m3 for the reactant molar ratio, m=1.0 and 1.5 respectively.

(e) From 3(a) - (d) above, the reactor volume and the reactor height were greater at the lower limits of conversion degree, and the rate of heat generation per reactor volume increases with conversion degree.

APPENDIX

APPENDIX 1a: SEMI-BATCH REACTOR

t (sec)	X _A	m	V _R (m ³)	h _{sbr} (m)	R _q (kJ/sec.m ³)*10 ⁴
60	.95	1	0.0226	0.0288	1.4593
120	.95	1	0.0456	0.0580	0.7232
180	.95	1	0.0686	0.0873	0.4805
240	.95	1	0.0916	0.1166	0.3597
300	.95	1	0.1146	0.1460	0.2874
360	.95	1	0.1377	0.1753	0.2393
420	.95	1	0.1607	0.2047	0.2050
480	.95	1	0.1838	0.2340	0.1793
540	.95	1	0.2068	0.2633	0.1593
600	.95	1	0.2299	0.2927	0.1433
660	.95	1	0.2529	0.3220	0.1303
720	.95	1	0.2760	0.3514	0.1194
780	.95	1	0.2990	0.3808	0.1102
840	.95	1	0.3221	0.4101	0.1023
900	.95	1	0.3452	0.4395	0.0955
960	.95	1	0.3682	0.4688	0.0895
1020	.95	1	0.3913	0.4982	0.0842
1080	.95	1	0.4143	0.5275	0.0795
1140	.95	1	0.4374	0.5569	0.0753
1200	.95	1	0.4604	0.5862	0.0716
1260	.95	1	0.4835	0.6156	0.0682
1320	.95	1	0.5065	0.6450	0.0651
1380	.95	1	0.5296	0.6743	0.0622
1440	.95	1	0.5527	0.7037	0.0596
1500	.95	1	0.5757	0.7330	0.0572
1560	.95	1	0.5988	0.7624	0.0550
1620	.95	1	0.6218	0.7918	0.0530
1680	.95	1	0.6449	0.8211	0.0511
1740	.95	1	0.6680	0.8505	0.0493
1800	.95	1	0.6910	0.8798	0.0477

APPENDIX 1b: SEMI-BATCH REACTOR

t (sec)	X _A	m	V _R (m ³)	h _{sbr} (m)	R _q (kJ/sec.m ³)*10 ⁴
60	.96	1	0.0160	0.0204	2.0785
120	.96	1	0.0324	0.0413	1.0264
180	.96	1	0.0489	0.0623	0.6810
240	.96	1	0.0654	0.0832	0.5094
300	.96	1	0.0818	0.1042	0.4069
360	.96	1	0.0983	0.1252	0.3387
420	.96	1	0.1148	0.1462	0.2900
480	.96	1	0.1313	0.1672	0.2536
540	.96	1	0.1478	0.1882	0.2253
600	.96	1	0.1643	0.2092	0.2027
660	.96	1	0.1808	0.2302	0.1842
720	.96	1	0.1973	0.2512	0.1688
780	.96	1	0.2138	0.2722	0.1558
840	.96	1	0.2302	0.2932	0.1446
900	.96	1	0.2467	0.3142	0.1350
960	.96	1	0.2632	0.3352	0.1265
1020	.96	1	0.2797	0.3562	0.1190
1080	.96	1	0.2962	0.3772	0.1124

1140	.96	1	0.3127	0.3982	0.1065
1200	.96	1	0.3292	0.4192	0.1011
1260	.96	1	0.3457	0.4402	0.0963
1320	.96	1	0.3622	0.4612	0.0919
1380	.96	1	0.3787	0.4822	0.0879
1440	.96	1	0.3952	0.5032	0.0843
1500	.96	1	0.4117	0.5242	0.0809
1560	.96	1	0.4282	0.5452	0.0778
1620	.96	1	0.4447	0.5662	0.0749
1680	.96	1	0.4612	0.5872	0.0722
1740	.96	1	0.4777	0.6082	0.0697
1800	.96	1	0.4942	0.6292	0.0674

360	.98	1	0.0343	0.0437	0.9906
420	.98	1	0.0401	0.0511	0.8470
480	.98	1	0.0460	0.0585	0.7398
540	.98	1	0.0518	0.0659	0.6566
600	.98	1	0.0576	0.0733	0.5902
660	.98	1	0.0634	0.0807	0.5360
720	.98	1	0.0692	0.0882	0.4909
780	.98	1	0.0751	0.0956	0.4528
840	.98	1	0.0809	0.1030	0.4202
900	.98	1	0.0867	0.1104	0.3920
960	.98	1	0.0925	0.1178	0.3673
1020	.98	1	0.0984	0.1253	0.3456
1080	.98	1	0.1042	0.1327	0.3262
1140	.98	1	0.1100	0.1401	0.3089
1200	.98	1	0.1159	0.1475	0.2934
1260	.98	1	0.1217	0.1549	0.2793
1320	.98	1	0.1275	0.1624	0.2666
1380	.98	1	0.1333	0.1698	0.2549
1440	.98	1	0.1392	0.1772	0.2442
1500	.98	1	0.1450	0.1846	0.2344
1560	.98	1	0.1508	0.1920	0.2254
1620	.98	1	0.1567	0.1995	0.2170
1680	.98	1	0.1625	0.2069	0.2092
1740	.98	1	0.1683	0.2143	0.2019
1800	.98	1	0.1742	0.2217	0.1952

APPENDIX 1c: SEMI-BATCH REACTOR

t (sec)	X _A	m	V _R (m ³)	h _{sbr} (m)	R _q (kJ/sec.m ³)* 10 ⁴
60	.97	1	0.0102	0.0130	3.2866
120	.97	1	0.0209	0.0266	1.6118
180	.97	1	0.0315	0.0402	1.0666
240	.97	1	0.0422	0.0538	0.7967
300	.97	1	0.0529	0.0674	0.6358
360	.97	1	0.0636	0.0810	0.5289
420	.97	1	0.0743	0.0946	0.4527
480	.97	1	0.0850	0.1083	0.3957
540	.97	1	0.0957	0.1219	0.3515
600	.97	1	0.1064	0.1355	0.3161
660	.97	1	0.1171	0.1492	0.2872
720	.97	1	0.1279	0.1628	0.2632
780	.97	1	0.1386	0.1764	0.2428
840	.97	1	0.1493	0.1901	0.2254
900	.97	1	0.1600	0.2037	0.2103
960	.97	1	0.1707	0.2173	0.1971
1020	.97	1	0.1814	0.2310	0.1855
1080	.97	1	0.1921	0.2446	0.1751
1140	.97	1	0.2028	0.2583	0.1659
1200	.97	1	0.2135	0.2719	0.1576
1260	.97	1	0.2243	0.2855	0.1500
1320	.97	1	0.2350	0.2992	0.1432
1380	.97	1	0.2457	0.3128	0.1370
1440	.97	1	0.2564	0.3265	0.1312
1500	.97	1	0.2671	0.3401	0.1260
1560	.97	1	0.2778	0.3537	0.1211
1620	.97	1	0.2885	0.3674	0.1166
1680	.97	1	0.2993	0.3810	0.1124
1740	.97	1	0.3100	0.3947	0.1085
1800	.97	1	0.3207	0.4083	0.1049

APPENDIX 1e: SEMI-BATCH REACTOR

t (sec)	X _A	m	V _R (m ³)	h _{sbr} (m)	R _q (kJ/sec.m ³)*10 ⁵
60	.99	1	0.0016	0.0020	2.1716
120	.99	1	0.0036	0.0045	0.9639
180	.99	1	0.0056	0.0071	0.6157
240	.99	1	0.0076	0.0097	0.4514
300	.99	1	0.0096	0.0123	0.3561
360	.99	1	0.0117	0.0149	0.2939
420	.99	1	0.0137	0.0175	0.2501
480	.99	1	0.0158	0.0201	0.2177
540	.99	1	0.0178	0.0227	0.1926
600	.99	1	0.0199	0.0253	0.1728
660	.99	1	0.0219	0.0279	0.1566
720	.99	1	0.0240	0.0305	0.1432
780	.99	1	0.0260	0.0331	0.1319
840	.99	1	0.0281	0.0358	0.1223
900	.99	1	0.0301	0.0384	0.1139
960	.99	1	0.0322	0.0410	0.1067
1020	.99	1	0.0343	0.0436	0.1003
1080	.99	1	0.0363	0.0462	0.0946
1140	.99	1	0.0384	0.0488	0.0895
1200	.99	1	0.0404	0.0515	0.0850
1260	.99	1	0.0425	0.0541	0.0808
1320	.99	1	0.0445	0.0567	0.0771
1380	.99	1	0.0466	0.0593	0.0737
1440	.99	1	0.0487	0.0619	0.0706
1500	.99	1	0.0507	0.0646	0.0677
1560	.99	1	0.0528	0.0672	0.0651
1620	.99	1	0.0548	0.0698	0.0626

APPENDIX 1d: SEMI-BATCH REACTOR

t (sec)	X _A	m	V _R (m ³)	h _{sbr} (m ³)	R _q (kJ/sec.m ³)*10 ⁴
60	.98	1	0.0054	0.0068	6.3502
120	.98	1	0.0111	0.0141	3.0607
180	.98	1	0.0169	0.0215	2.0123
240	.98	1	0.0227	0.0289	1.4979
300	.98	1	0.0285	0.0363	1.1927

1680	.99	1	0.0569	0.0724	0.0604
1740	.99	1	0.0589	0.0751	0.0583
1800	.99	1	0.0610	0.0777	0.0563

960	.96	1.5	0.9694	1.2342	0.3435
1020	.96	1.5	1.0300	1.3114	0.3233
1080	.96	1.5	1.0906	1.3886	0.3053
1140	.96	1.5	1.1512	1.4658	0.2892
1200	.96	1.5	1.2119	1.5430	0.2748
1260	.96	1.5	1.2725	1.6202	0.2617
1320	.96	1.5	1.3331	1.6974	0.2498
1380	.96	1.5	1.3938	1.7746	0.2389
1440	.96	1.5	1.4544	1.8518	0.2290
1500	.96	1.5	1.5150	1.9290	0.2198
1560	.96	1.5	1.5756	2.0062	0.2113
1620	.96	1.5	1.6363	2.0834	0.2035
1680	.96	1.5	1.6969	2.1606	0.1962
1740	.96	1.5	1.7575	2.2378	0.1895
1800	.96	1.5	1.8182	2.3150	0.1831

APPENDIX 2a: SEMI-BATCH REACTOR

t (sec)	X _A	m	V _R (m ³)	h _{sbr} (m)	R _q (kJ/sec.m ³)*10 ³
60	.95	1.5	0.0760	0.0968	4.3353
120	.95	1.5	0.1524	0.1941	2.1619
180	.95	1.5	0.2289	0.2914	1.4398
240	.95	1.5	0.3053	0.3888	1.0793
300	.95	1.5	0.3818	0.4861	0.8631
360	.95	1.5	0.4583	0.5835	0.7191
420	.95	1.5	0.5347	0.6808	0.6162
480	.95	1.5	0.6112	0.7782	0.5391
540	.95	1.5	0.6877	0.8756	0.4792
600	.95	1.5	0.7642	0.9730	0.4312
660	.95	1.5	0.8407	1.0704	0.3920
720	.95	1.5	0.9171	1.1677	0.3593
780	.95	1.5	0.9936	1.2651	0.3316
840	.95	1.5	1.0701	1.3625	0.3079
900	.95	1.5	1.1466	1.4599	0.2874
960	.95	1.5	1.2231	1.5573	0.2694
1020	.95	1.5	1.2996	1.6546	0.2536
1080	.95	1.5	1.3760	1.7520	0.2395
1140	.95	1.5	1.4525	1.8494	0.2269
1200	.95	1.5	1.5290	1.9468	0.2155
1260	.95	1.5	1.6055	2.0442	0.2052
1320	.95	1.5	1.6820	2.1416	0.1959
1380	.95	1.5	1.7585	2.2390	0.1874
1440	.95	1.5	1.8350	2.3364	0.1796
1500	.95	1.5	1.9115	2.4337	0.1724
1560	.95	1.5	1.9879	2.5311	0.1658
1620	.95	1.5	2.0644	2.6285	0.1596
1680	.95	1.5	2.1409	2.7259	0.1539
1740	.95	1.5	2.2174	2.8233	0.1486
1800	.95	1.5	2.2939	2.9207	0.1437

APPENDIX 2b: SEMI-BATCH REACTOR

t (sec)	X _A	m	V _R (m ³)	h _{sbr} (m)	R _q (kJ/sec.m ³)*10 ³
60	.97	1.5	0.0446	0.0568	7.5488
120	.97	1.5	0.0895	0.1140	3.7576
180	.97	1.5	0.1345	0.1713	2.5007
240	.97	1.5	0.1796	0.2286	1.8737
300	.97	1.5	0.2246	0.2860	1.4981
360	.97	1.5	0.2696	0.3433	1.2479
420	.97	1.5	0.3147	0.4006	1.0693
480	.97	1.5	0.3597	0.4580	0.9354
540	.97	1.5	0.4047	0.5153	0.8313
600	.97	1.5	0.4498	0.5727	0.7481
660	.97	1.5	0.4948	0.6300	0.6800
720	.97	1.5	0.5399	0.6874	0.6232
780	.97	1.5	0.5849	0.7447	0.5752
840	.97	1.5	0.6300	0.8021	0.5341
900	.97	1.5	0.6750	0.8594	0.4985
960	.97	1.5	0.7200	0.9168	0.4673
1020	.97	1.5	0.7651	0.9741	0.4398
1080	.97	1.5	0.8101	1.0315	0.4153
1140	.97	1.5	0.8552	1.0889	0.3934
1200	.97	1.5	0.9002	1.1462	0.3738
1260	.97	1.5	0.9453	1.2036	0.3559
1320	.97	1.5	0.9903	1.2609	0.3398
1380	.97	1.5	1.0354	1.3183	0.3250
1440	.97	1.5	1.0804	1.3756	0.3114
1500	.97	1.5	1.1255	1.4330	0.2990
1560	.97	1.5	1.1705	1.4904	0.2874
1620	.97	1.5	1.2156	1.5477	0.2768
1680	.97	1.5	1.2606	1.6051	0.2669
1740	.97	1.5	1.3057	1.6624	0.2577
1800	.97	1.5	1.3507	1.7198	0.2491

APPENDIX 2c: SEMI-BATCH REACTOR

t (sec)	X _A	m	V _R (m ³)	h _{sbr} (m)	R _q (kJ/sec.m ³)*10 ³
60	.96	1.5	0.0602	0.0766	5.5358
120	.96	1.5	0.1207	0.1537	2.7587
180	.96	1.5	0.1813	0.2308	1.8368
240	.96	1.5	0.2419	0.3080	1.3766
300	.96	1.5	0.3025	0.3852	1.1008
360	.96	1.5	0.3631	0.4623	0.9170
420	.96	1.5	0.4237	0.5395	0.7859
480	.96	1.5	0.4844	0.6167	0.6875
540	.96	1.5	0.5450	0.6939	0.6110
600	.96	1.5	0.6056	0.7711	0.5499
660	.96	1.5	0.6662	0.8483	0.4998
720	.96	1.5	0.7268	0.9255	0.4581
780	.96	1.5	0.7875	1.0026	0.4229
840	.96	1.5	0.8481	1.0798	0.3926
900	.96	1.5	0.9087	1.1570	0.3664

APPENDIX 2d: SEMI-BATCH REACTOR

t (sec)	X _A	m	V _R (m ³)	h _{sbr} (m)	R _q (kJ/sec.m ³)*10 ⁴
60	.98	1.5	0.0293	0.0373	1.1614
120	.98	1.5	0.0589	0.0750	0.5768

180	.98	1.5	0.0886	0.1129	0.3835
240	.98	1.5	0.1184	0.1507	0.2872
300	.98	1.5	0.1481	0.1885	0.2296
360	.98	1.5	0.1778	0.2264	0.1912
420	.98	1.5	0.2075	0.2643	0.1638
480	.98	1.5	0.2373	0.3021	0.1433
540	.98	1.5	0.2670	0.3400	0.1273
600	.98	1.5	0.2968	0.3778	0.1145
660	.98	1.5	0.3265	0.4157	0.1041
720	.98	1.5	0.3562	0.4536	0.0954
780	.98	1.5	0.3860	0.4914	0.0881
840	.98	1.5	0.4157	0.5293	0.0818
900	.98	1.5	0.4455	0.5672	0.0763
960	.98	1.5	0.4752	0.6051	0.0715
1020	.98	1.5	0.5049	0.6429	0.0673
1080	.98	1.5	0.5347	0.6808	0.0636
1140	.98	1.5	0.5644	0.7187	0.0602
1200	.98	1.5	0.5942	0.7565	0.0572
1260	.98	1.5	0.6239	0.7944	0.0545
1320	.98	1.5	0.6537	0.8323	0.0520
1380	.98	1.5	0.6834	0.8702	0.0497
1440	.98	1.5	0.7132	0.9080	0.0477
1500	.98	1.5	0.7429	0.9459	0.0458
1560	.98	1.5	0.7727	0.9838	0.0440
1620	.98	1.5	0.8024	1.0217	0.0424
1680	.98	1.5	0.8322	1.0595	0.0409
1740	.98	1.5	0.8619	1.0974	0.0394
1800	.98	1.5	0.8916	1.1353	0.0381

1560	.99	1.5	0.3822	0.4866	0.0899
1620	.99	1.5	0.3969	0.5053	0.0865
1680	.99	1.5	0.4116	0.5241	0.0834
1740	.99	1.5	0.4263	0.5428	0.0805
1800	.99	1.5	0.4411	0.5616	0.0779

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APPENDIX 2e: SEMI-BATCH REACTOR

t(sec)	X _A	m	V _R (m ³)	h _{sbr} (m)	R _q (kJ/sec.m ³)*10 ⁴
60	.99	1.5	0.0143	0.0181	2.4098
120	.99	1.5	0.0289	0.0368	1.1882
180	.99	1.5	0.0436	0.0555	0.7879
240	.99	1.5	0.0583	0.0742	0.5892
300	.99	1.5	0.0730	0.0929	0.4705
360	.99	1.5	0.0877	0.1117	0.3916
420	.99	1.5	0.1024	0.1304	0.3353
480	.99	1.5	0.1171	0.1491	0.2932
540	.99	1.5	0.1318	0.1679	0.2605
600	.99	1.5	0.1466	0.1866	0.2343
660	.99	1.5	0.1613	0.2054	0.2129
720	.99	1.5	0.1760	0.2241	0.1951
780	.99	1.5	0.1907	0.2428	0.1800
840	.99	1.5	0.2055	0.2616	
900	.99	1.5	0.2202	0.2803	0.1560
960	.99	1.5	0.2349	0.2991	0.1462
1020	.99	1.5	0.2496	0.3178	0.1376
1080	.99	1.5	0.2643	0.3366	0.1299
1140	.99	1.5	0.2791	0.3553	0.1231
1200	.99	1.5	0.2938	0.3741	0.1169
1260	.99	1.5	0.3085	0.3928	0.1113
1320	.99	1.5	0.3233	0.4116	0.1062
1380	.99	1.5	0.3380	0.4303	0.1016
1440	.99	1.5	0.3527	0.4491	0.0974
1500	.99	1.5	0.3674	0.4678	0.0935

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