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# MODELLING AND SIMULATION OF THE BATCH HYDROLYSIS OF ACETIC ANHYDRIDE TO PRODUCE ACETIC ACID

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**Abstract**

***The kinetic modelling of the batch synthesis of acetic acid from acetic anhydride was investigated. The kinetic data of the reaction was obtained by conducting the hydrolysis reaction in a batch reactor. A dynamic model was formulated for this process and simulation was carried out using gPROMS® an advanced process modelling and simulation software. The developed model was validated against experimental data by estimating the kinetic parameter (reaction rate constant $k=0.11302\ min^{-1}$) and comparing simulation results with experimental data. Results obtained show that the formulated model was able to predict the experimental data to a high level of confidence. The dynamic behaviour of the reaction process was assessed by simulating the validated model at the initial state to obtain time trajectories of all the variables of interest. The model developed in this work will provide insight as to how the process responds under dynamic conditions and its amenability to control.***

***Keywords:*** Acetic anhydride, acetic acid, reaction rate constant, kinetic modelling

## 1. Introduction

In trying to understand the dynamic behaviour of chemical processes involving reactions, it is important to have complete information on the kinetics of the process[1,2]. Understanding the kinetics of a reaction involves having a model of the reaction and the corresponding reaction parameters [3,4]. This is important because if the kinetics of a reaction is not fully understood, several problems may arise, such as ineffective reaction control, unsafe conditions and runaway reactions which can lead to equipment damage, explosion and the release of toxic substances into the environment [5]. For a majority of reactions, there is hardly any information regarding the kinetics, thermodynamics, and physical parameters that characterize such reactions which is rather inauspicious.

The hydrolysis of acetic anhydride to produce acetic acid is a fast exothermic reaction. This is an important reaction needed for the synthesis of an equally important chemical (acetic acid) hence the need for information about the progress of the reaction such as kinetic and thermodynamic parameters[6].

The kinetics of acetic anhydride hydrolysis to acetic acid has been studied with a number of techniques for measuring reaction rate reported in literature. Ampelli *et al,* [7] integrated an ultraviolet-visible (UV-Vis) spectrometer with an isoperibolic reaction calorimeter to study the kinetics of hydrolysis of acetic anhydride. An acid–base indicator was added to the reaction mixture and the change of its colour as the reaction progressed was followed by the UV-Vis spectrometer. Haji & Erkey, [8] developed a reaction set up that employed *in-situ* Fourier Transform Infrared Spectroscopy (FTIR) to monitor the kinetics of acetic anhydride hydrolysis to acetic acid. Kralj, [9] investigated the kinetics of acetic acid production from the hydrolysis of acetic anhydride. She estimated kinetic parameters such as reaction rate constant activation energy, and order of reaction by measuring the conductivity of a weak electrolyte (acetic acid). Hirota *et al,* [5] used calorimetric techniques to study the hydrolysis of acetic anhydride in an adiabatic reaction vessel by estimating kinetic and thermodynamic parameters such as reaction rate constant activation energy, and heat transfer coefficient.

In view of the foregoing, it can be seen that most of the techniques used for studying the kinetics of acetic anhydride hydrolysis reported in the literature involve the collection of experimental data from colorimetric, calorimetric, titration, conductivity and spectroscopy experiments and the data is subsequently subjected to differential or integral method of analysis to determine the kinetic parameters [10-14]. In spite of these experimental efforts aimed at determining the kinetics of the hydrolysis process, very little work has been done in modelling the process. Mathematical modelling of the hydrolysis process enables its representation in a mathematical sense. Dynamic simulation of the formulated model can be utilized in analyzing the behaviour of the process, provision of insights into the mechanisms that drive the process, understanding the response of the process to changes in operating conditions, design of controllers and design of entirely new processes thereby leading to vast improvements in process economics, design, operation and control [15, 16]. Model predictions make it possible to identify optimal design and operational parameters and this consequently leads to the maximisation of the system's performance [17].

The aim of this work is to estimate the kinetic parameters for the hydrolysis of acetic anhydride to acetic acid in an adiabatic batch reactor. A dynamic model of the process was developed and the kinetic parameters were estimated in the process of validating the model. The parameters were estimated using the parameter estimation tool of gPROMS®.

## 2. Materials and Methods

The equipment used for the experiments was a batch reactor integrated with a conductivity meter graduated in millisiemens. 500 $cm^3$ of distilled water was measured and poured into the reactor. Forty (40) $cm^3$ of acetic anhydride was then dispensed into the reactor using a syringe. The mains of the reactor were then connected and initial temperature and conductivity measurements were recorded. Sixteen (16) conductivity measurements were recorded at different times for 16 steps in the experiment.

## 3. Experimental Results

The conductivity measurements recorded were converted to concentration values by relating it to the conductivity of the solution as shown in Equation (1) (see Table 1).

$$\Lambda_m = \frac{\kappa}{c} \tag{1}$$

where $\Lambda_m$ is the molar conductivity of the solution. The molar concentration of the electrolyte $c$ is expressed in terms of the acid dissociation constant $K_a$ as follows [9]:

$$c = \frac{K_a(1-\alpha)}{\alpha^2} \tag{2}$$

The fraction of ion present in the solution $\alpha$ is given as [9]:

$$\alpha = \frac{1}{\left(1+\frac{\kappa}{K_a\Lambda_m^o}\right)} \tag{3}$$

where $\Lambda_m^o$ is the molar conductivity at infinite dilution. The values $\Lambda_m^o$ and $K_a$ are reasonably constant at the initial temperature of the reaction. They are respectively 39.1 $Sm^2 mol^{-1}$ and $1.8\times10^{-5}$ [18].

*Table 1: Experimental data for acetic anhydride hydrolysis*

| t (min) | κ (mS/cm) | c (mol/dm³) | $C_{AA(reacted)}$ (mol/dm³) | $C_{AA(unreacted)}$ (mol/dm³) | $C_{A(produced)}$ (mol/dm³) | $X_{AA}$ |
|---|---|---|---|---|---|---|
| Time | Conductivity | Ion conc. | Reacted Acetic Anhydride | Unreacted Acetic Anhydride | Produced Acetic Acid | Conversion of Acetic Anhydride |
| 0 | 0.000 | 0.00 | 0.00 | 0.41 | 0.00 | 0.00 |
| 1 | 0.432 | 0.07 | 0.04 | 0.37 | 0.08 | 0.09 |
| 3 | 0.692 | 0.18 | 0.09 | 0.32 | 0.18 | 0.22 |
| 4 | 0.874 | 0.28 | 0.14 | 0.26 | 0.28 | 0.35 |
| 6 | 1.051 | 0.42 | 0.21 | 0.20 | 0.42 | 0.51 |
| 8 | 1.163 | 0.51 | 0.26 | 0.15 | 0.52 | 0.63 |
| 10 | 1.244 | 0.58 | 0.29 | 0.12 | 0.58 | 0.72 |
| 13 | 1.323 | 0.66 | 0.33 | 0.10 | 0.66 | 0.81 |
| 15 | 1.354 | 0.69 | 0.35 | 0.10 | 0.70 | 0.85 |
| 16 | 1.370 | 0.71 | 0.36 | 0.10 | 0.70 | 0.87 |
| 18 | 1.391 | 0.73 | 0.36 | 0.04 | 0.72 | 0.89 |
| 20 | 1.406 | 0.75 | 0.37 | 0.03 | 0.74 | 0.91 |
| 23 | 1.420 | 0.76 | 0.38 | 0.03 | 0.76 | 0.93 |
| 25 | 1.427 | 0.77 | 0.38 | 0.02 | 0.76 | 0.94 |
| 29 | 1.435 | 0.78 | 0.39 | 0.02 | 0.78 | 0.95 |
| 31 | 1.438 | 0.78 | 0.39 | 0.02 | 0.78 | 0.96 |
| 35 | 1.442 | 0.78 | 0.39 | 0.02 | 0.78 | 0.96 |

## 4. Model Development

The liquid phase hydrolysis reaction of acetic anhydride to produce acetic acid was carried out in a constant volume adiabatic batch reactor whose schematic is shown in Figure 1. The reaction is exothermic and proceeds according to the following stoichiometry:

$$\left(CH_3CO\right)_2 + H_2O \longrightarrow 2CH_3COOH + Heat \qquad (4)$$

In formulating the model, the following assumptions were made:

- The volume of the reactor is fixed
- No nuclear reaction occurs; hence rate of material generation is zero.
- The content of the reactor is perfectly mixed (lumped system).

The implication of the last assumption is that all intensive properties of the stream leaving the reactor system are identical to those inside the system [19].

The reactor model was obtained from material and energy conservation laws applied to the reactor. The general form of the conservation law for mass is written as (5) below. Equation (5) is applied to all the components within the reactor to obtain (6) also given below.

### *4.1 Material balance:*

The equations describing the material balance of acetic anhydride and acetic acid in the reactor are given as:

$$\frac{dC_{AA}}{dt} = -r_{AA} \qquad (7)$$

$$\frac{dC_{AC}}{dt} = 2r_{AA} \qquad (8)$$

Fractional conversion of acetic anhydride to acetic acid is given as:

$$X_{AA} = \frac{C_{AA}^{O} - C_{AA}}{C_{AA}^{O}} \qquad (9)$$

The rate of the hydrolysis reaction is described by the following equation:

$$r_{AA} = kC_{AA} \qquad (10)$$

### *4.2 Energy balance:*

The equation describing the energy balance of the reactor obtained from applying the law of conservation of energy to the reactor is given as:

$$\left[\sum M_i C_{pi}\right]\frac{dT}{dt} = r_{AA}(-\Delta H_r)V \qquad (11)$$

Equation (11) can be expanded to obtain:

$$\left[M_{AA}C_{pAA} + M_{AC}C_{pAC} + M_W C_{pW}\right]\frac{dT}{dt} = r_{AA}(-\Delta H_r)V \qquad (12)$$

*$M_i$* and *$C_{pi}$* are the moles and molar specific heat capacities of the chemical species in the reactor. *$\Delta H_r$ (J/mol)* is the heat of reaction.

The reactor model is described by the system of equations (7) to (12) which is a set of non-linear differential and algebraic equations (DAEs) and describes the dynamic behaviour of the concentration of all chemical species present in the batch reactor and the temperature profile of the reactor content.

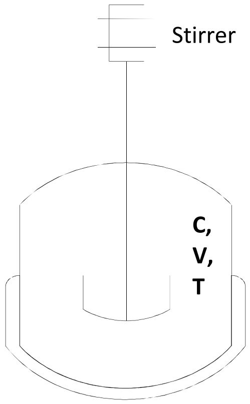

*Figure 1: Schematic of adiabatic batch reactor with variables*

### *4.3 Degree of freedom analysis*

The degree of freedom analysis is used to determine the completeness of a model. The number of degrees of freedom gives an indication of the extra variables or equations that must be specified in order to have a complete model. In common chemical engineering terminology, the degree of freedom is defined in (13) below [20,21]

For the process under consideration, we have the following:

Number of Model Variables : 15

Number of Model Independent Equations: 5

From equation (13), the number of degrees of freedom is given as: DOF= (15) - (5) = 10

Since the number of degrees of freedom is 10, it means we are at liberty to specify 10 variables.

$$\begin{pmatrix}\text{Rate of accumulation}\\ \text{of component i within}\\ \text{the reactor}\end{pmatrix} = \begin{pmatrix}\text{Rate of flow of}\\ \text{component i into}\\ \text{the reactor}\end{pmatrix} - \begin{pmatrix}\text{Rate of flow of}\\ \text{component i out of}\\ \text{the reactor}\end{pmatrix} + \begin{pmatrix}\text{Rate of generation}\\ \text{of component i within}\\ \text{the reactor}\end{pmatrix} \qquad (5)$$

$$\begin{pmatrix}\text{Rate of accumulation}\\ \text{of component i within}\\ \text{the reactor}\end{pmatrix} = \begin{pmatrix}\text{Rate of generation}\\ \text{of component i within}\\ \text{the reactor}\end{pmatrix} \qquad (6)$$

## 5. Model Validation and Estimation of Kinetic Parameters

Parameter estimation has to do with the validation of a model against the results of an experiment. This is done by estimating some of the model parameters which are not known to a high level of accuracy. An experimental validation of the formulated reactor model was carried out by estimating the reaction rate constant *k*. The reactor model was simulated and the result of the simulation was compared with experimental results to determine validity.The numerical solver used for the parameter estimation exercise is 'MAXLKHD' which is based on a sequential quadratic programming code. The parameter estimation was based on the maximum likelihood formulation, which attempts to determine values for the uncertain physical and variance model parameters that maximize the probability that the model will predict the measurement values obtained from the experiments.

Table 3 shows the estimated parameter *k*, optimal estimated value, confidence intervals, 95% t-value and standard deviation. The t-value shows the percentage accuracy of the estimated parameter *k* with respect to the 95% confidence interval. The 95% confidence interval shows that an estimated parameter will have a 95% probability of being within the stated interval. The small magnitude of the confidence intervals and the standard deviation indicates that the estimated parameter is accurate to a high level of confidence.

The weighted residual and $\chi^2$-value are statistical tools used to test how well a model fits experimental data. A good fit results if the weighted residual is less than the $\chi^2$-value. As shown in Table 3, the $\chi^2$-value was 44.9805 while the weighted residual was 28.9080. Since the weighted residual is less than the $\chi^2$-value, then it can be inferred that the model results show a good fit and proper correlation with the experimental results.

Table 4 shows the value of reaction rate constant *k* estimated as well as values of *k* reported in literature. Comparing the value of *k* obtained in this work with those reported in literature, it can be observed that they are very similar. Therefore it is logical to infer that the method of estimation adopted was effective. Figures 2 and 3 respectively show the overlay plots of acetic anhydride and acetic acid concentrations. These plots display a comparison between the experimental results and the model predicted results in terms of trend and correlation. Figure 2 shows the variation of acetic anhydride concentration with time for both experimental and model results. It is evident from the plot that the model was able to replicate the experimental concentration of acetic anhydride in the reactor to a high level of confidence.

This is an indication that the model exhibits a good fit with the experimental data as seen in the excellent correlation between the experimental and model predicted results. In spite of the difference in trend showed in Figure 3 compared with Figure 2, similar correlation was however observed i.e. the model was also able to replicate the experimental concentration of acetic acid produced in the reactor to a high level of confidence.

$$\begin{pmatrix}\text{Number of Degrees}\\ \text{of freedom}\end{pmatrix} = \begin{pmatrix}\text{Number of Model Variables}\\ \text{excluding inputs}\end{pmatrix} - \begin{pmatrix}\text{Number of Model}\\ \text{Independent Equation}\end{pmatrix} \quad (13)$$

*Table 2: Summary of model equations, variables and corresponding assumptions*

| Equations | Number of Equations | New Variables | Number of New Variables | Assumptions |
|---|---|---|---|---|
| $\frac{dC_{AA}}{dt} = -r_{AA}$ | 1 | $C_{AA}, r_{AA}$ | 2 | Perfect mixing of the material content |
| $\frac{dC_{AC}}{dt} = 2r_{AA}$ | 1 | $C_{AC}$ | 1 | Perfect mixing of the material content |
| $r_{AA} = kC_{AA}$ | 1 | $k$ | 1 | N/A |
| $X_{AA} = \frac{C_{AA}^{O} - C_{AA}}{C_{AA}^{O}}$ | 1 | $X_{AA}$, $C_{AA}{}^{O}$ | 2 | N/A |
| $\left[\sum M_i C_{pi}\right]\frac{dT}{dt} = r_{AA}(-\Delta H_r)V$ | 1 | $M_i, C_{pi},$<br>$\Delta H$, $V$, $T$ | 9 | Adiabatic operation |
| Total | 5 | | 15 | |

## 6. Model Implementation and Simulation Results

In order to investigate the dynamic behaviour of the batch hydrolysis of acetic anhydride, the formulated reactor model was implemented in gPROMS®. The data utilized for the simulation of the model is presented in Table 5.

*Table 3: Statistical information for parameter estimation*

| Parameter | Optimal Estimate | Confidence Intervals | | | 95% t-value | Standard Deviation |
|---|---|---|---|---|---|---|
| | | 90% | 95% | 99% | | |
| *k* | 0.11302 | 0.0064 | 0.0077 | 0.0104 | 14.61 | 0.0038 |
| Weighted residual | | $\chi^2$-value | Comment | | | |
| 28.9080 | | 44.9850 | Weighted residual less than $\chi^2$-value imply | | | |

*Table 4: Comparison of estimated value of k with values reported in literature*

| Value of rate constant *k* (min$^{-1}$) | Reference |
|---|---|
| 0.11302 | This work |
| 0.11354 | Kralj, [9] |
| 0.11015 | Haji and Erkey,[8] |
| 0.10824 | Shatynski and Hanesian,[22] |
| 0.13522 | Lavertu et al, [23] |

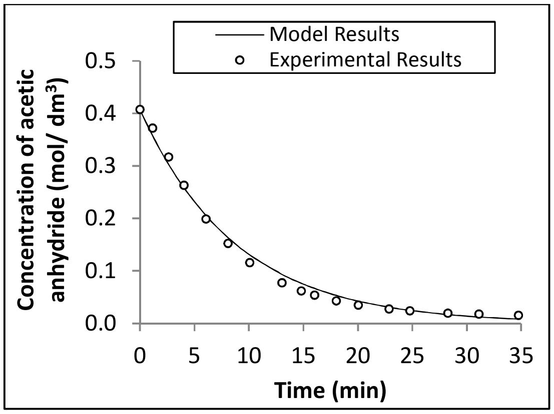

*Figure 2: Comparison between model and experimental results for acetic anhydride*

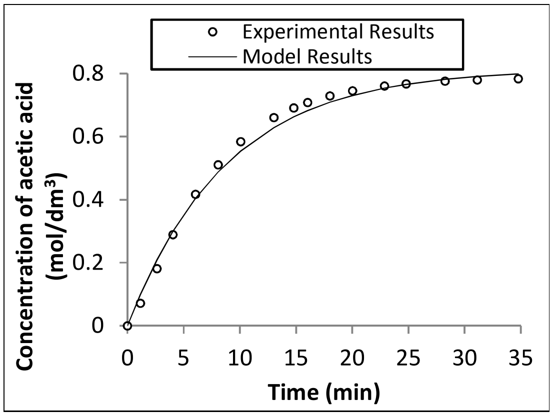

*Figure 3: Comparison between model and experimental results for acetic acid*

*Table 5: Data for the dynamic simulation of the CSTR reactor* [18]

| Parameter | Value |
|---|---|
| $C_{pAA}$ | 1870 J/kg |
| $C_{pAC}$ | 2043 J/kg |
| $C_{pW}$ | 4184 J/kg |
| $M_{AA}$ | 0.04324kg |
| $M_{AC}$ | 0.001kg |
| $M_W$ | 1kg |
| $\Delta H_r$ | 56000 J/mol |
| $C_{AA}^0$ | 0.41 mol/dm$^3$ |
| V | 1040 cm$^3$ |
| Initial conditions | |
| $C_{AA}$ | 0.41 mol/dm$^3$ |
| $C_{AC}$ | 0 mol/dm$^3$ |
| Temperature | 23°C |

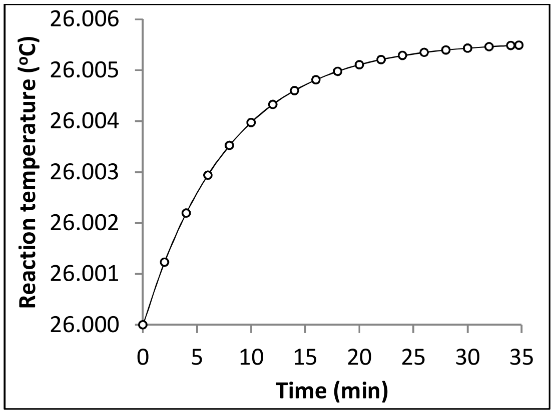

*Figure 4: Time trajectory of reaction temperature*

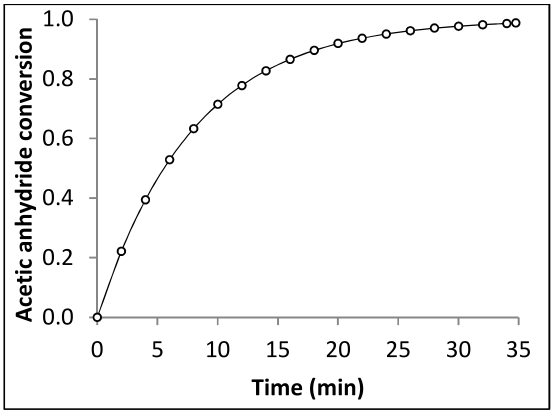

*Figure 5: Time trajectory of acetic anhydride conversion*

The time trajectory of acetic anhydride concentration as predicted by the reactor model is shown in Figure 2. It can be observed that there was a rapid and progressive decrease in the concentration of acetic anhydride as the reaction progressed. The trend observed indicates that the acetic anhydride initially charged to the reactor is consumed as a result of the stoichiometric formation of acetic acid.

The variation of the concentration of acetic acid produced during the reaction as predicted by the reactor model is also presented in Figure 3. The trend observed indicates a rapid and progressive increase in the concentration of acetic acid for the first 15 minutes of the reaction. This increase corresponds to an equally rapid decrease in the concentration of acetic anhydride for the first 15 minutes of the reaction as shown in Figure 2 suggesting that most of the acetic anhydride was converted to acetic acid.

Figure 4 shows the change in the reaction temperature as a function of time. From the plot, it can be observed that though there is an increase in temperature since the reaction is exothermic, however the change was not very significant.

Figure 5 shows the trend in the conversion of acetic anhydride to acetic acid with respect to time. It can be observed that there was a rapid and progressive increase in the conversion of acetic anhydride for the first 15 minutes of the reaction similar to the trend observed in Figure 3. This indicates that the acetic anhydride was being consumed stoichiometrically to produce acetic acid.

## 7. Conclusions

Kinetic modelling is gaining interest in different fields of research due to its wide range of application. The following conclusions can be drawn from this study.

- The use of modelling tools to describe the trends in the hydrolysis of acetic anhydride to produce acetic acid has been demonstrated.
- The hydrolysis of acetic anhydride to produce acetic acid in a batch reactor was accurately represented by a dynamic reaction model
- Kinetic parameters can be estimated accurately using experimentally validated models.
- The reaction model upon validation was able to replicate the results of the experiment to a high level of confidence as seen in the excellent correlation between model and experimental results.
- As part of model validation, the reaction rate constant was estimated to be 0.11302 $\text{min}^{-1}$. This value was within the range of values reported in literature

## Nomenclature

| | |
|---|---|
| $c$ | Concentration of ions in solution (mol/ $\text{dm}^3$) |
| $C_{AA}$ | Concentration of acetic anhydride (mol/ $\text{dm}^3$) |
| $C_{AC}$ | Concentration of acetic anhydride (mol/ $\text{dm}^3$) |
| $C_{PAA}$, $C_{PAC}$, $C_{PW}$ | Specific heat capacities of acetic anhydride, acetic acid and water respectively (kJ/kg) |
| $M_{AA}$, $M_{AC}$, $M_W$ | Mass of acetic anhydride, acetic acid and water respectively (kg) |
| $X_{AA}$ | Conversion of acetic anhydride to acetic acid |
| $r_{AA}$ | Rate of reaction (mol/ $\text{dm}^3$.min) |
| $T$ | Reaction temperature (°C) |
| $V$ | Reactor volume ($\text{cm}^3$) |
| $k$ | Reaction rate constant ($\text{min}^{-1}$) |
| $Ka$ | Acid dissociation constant |

| | |
|---|---|
| $\alpha$ | Fraction of ions present in solution |
| $\Lambda_m$ | Molar conductivity (Sm$^2$ mol$^{-1}$) |
| $\Lambda_m^o$ | Molar conductivity at infinite dilution (Sm$^2$ mol$^{-1}$) |
| $\kappa$ | Conductivity (mS/cm$^{-1}$) |
| $\Delta H_r$ | Heat of reaction (J/mol) |

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