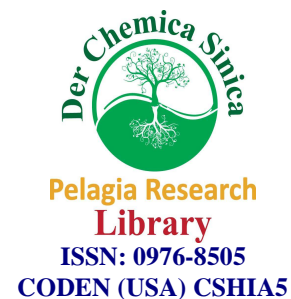




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Flow parameters (heat generated/pressure drop) in the simulated model design of isothermal plug-flow reactor for acid hydrolysis of cellulose

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ABSTRACT

An isothermal plug flow reactor model was developed to study the behaviour of acid hydrolysis of Cellulosic substrates. The Kinetic parameters in a model which gives the glucose formation from purified cellulose (Solka-flock), were obtained over the following range of independent variables temperature, 4833% sulfuric acid concentration 0.0102M, fractional conversion (XA) form 0.10 to 0.91. It was also determined that the volume of reactor (VR) length of reactor (LR) and internal diameter (Di) etc. directly increased with fractional conversion (XA) with values as 1.87, 11.4, 0.45 respectively. A computer programme using C-machine Language was used to simulate the models. The production of glucose in this work tells us that, the continuous acid hydrolysis of cellulose from cellulose may be a process of commercial interest and may alleviate our environmental problems.

Keywords: Cellulose, Hydrolysis, Plug-flow reactor

INTRODUCTION

Cellulose constitutes approximately a fluid of all vegetable matter and thus it exists in far greater quantity than any other polysaccharide. It is also produced by some macro organisms, in a few cases reaching amounts of 20 – 30% cellulose for chemical modification particularly for derivation, is often obtained from cotton linters by boiling with 1% sodium hydroxide solution [1].

Recent studies have shown that researchers in this field have successfully converted many cellulosic materials. Such as saw dust, solid animal wastes, crop residue etc [1,2,4,6] to more valuable products such as fermentable sugars.

Ethanol which can be produced from cellulose is used as an automobile combustible and its production by fermentation of glucose is a promising alternative. In spite of relatively low current petroleum prices, interest given to ethanol derived combustibles persist [9], mainly due to the attention paid to environmental causes.

Acid hydrolysis of cellulose from past researchers work were not without limitation/deficiencies. The apparatus set up for cellulose acid hydrolysis by Grethlein and Thompson (1978) has a diameter of the carvary tubing in the heat exchanger which fixes the maximum particles diameter to 0.35mm (42 meshes) in the slurry.

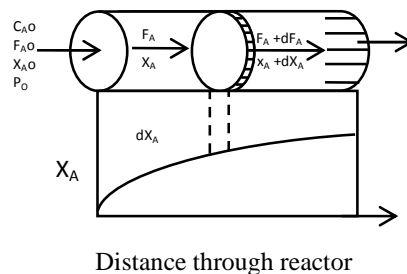
Commercial derivative of cellulose are ethers that among other properties, provide water solubility and esters which in high degree of substitution, provide organic solubility needed for spinning cellulose into fibres or molding it into shaped object.

Cellulose acetate is the principal commercial ester. Reaction is usually conducted in a mixture of acetic anhydride, acetic acid and sulfuric acid as the catalyst to produce a degree of substitution of about 2.4, resulting in a product soluble in acetone. This has application as a quick – drying adhesive, for film formation or for use in cigarette filters.

In this study, a novel method of evaluating the reactor flow parameters (heat generated/pressure drops) in the simulated model design of isothermal slug – flow reactor for acid hydrolysis of cellulose is introduced. This method is simple and straight forward and can be applied to any acid hydrolysis of cellulose with any level of crystallinity.

MATERIALS AND METHODS

The reactor volume VR used in this work is otherwise known as slug – flow or steady state flow reactor as shown in figure 1.



In slug – flow reactor, the composition of the fluid varies from point to point along a flow path. Consequently the material balance for a reaction component must be made different. To obtain a simulation model for reactor flow parameters, space time (S_{TP}), space velocity (S_{VP}), rate of heat generated (Q1), Rate of heat generated per volume (Q2) and pressure drop along reactor tube (ΔP) must be calculated.

Space Time (S_{TP})

This is the time required to process one reactor volume of feed at a specified condition (I), given the volumetric flow rate of reactant as V_o, the space time become

$$S_{TP} = V_R/V_O \tag{1}$$

$$\text{but } V_R = \frac{F_{A0}}{V_O(K_1C_{A0} - K_2C_{A0})} \ln (1 - X_{AF})^{-1} \tag{2}$$

Substituting (2) into (1) and simplifying; results into:

$$S_{TP} = \frac{F_{A0}}{V_O \left(\frac{K_1C_{A0}(1-X_A)}{1 + 3X_A} - K_2K_1C_{A0} \left(\frac{e^{-K_1 t}}{K_2-K_1} + \frac{e^{-K_2 t}}{K_1-K_2} \right) \right)} \ln (1 - X_{AF})^{-1} \tag{3}$$

Space Velocity (S_{VP})

Space velocity is the inverse of space time which is the flow velocity required to processes a unit reactor volume

$$SVP = \frac{V_O}{V_R} = S_{TP}^{-1} \tag{4}$$

Hence substituting (4) into (3) yields:

$$S_{VP} = \frac{F_{AO}}{V_O \left(\frac{K_1 C_{AO}(1-X_A)}{1+3X_A} - K_2 K_1 C_{AO} \left(\frac{e^{-K_1 t}}{K_2-K_1} + \frac{e^{-K_2 t}}{K_1-K_2} \right) \right)} \ln(1 - X_{AF}) \quad (5)$$

Rates of Heat Generated (Q1)

In any chemical process, material balances are accompanied by energy balance. Changes in heat content are determined by taking energy balances over an elemental volume due for steady state flow reactor as

$$\text{Sensible heat Inflow to reactor volume} = \left\{ \begin{array}{l} \text{Sensible heat} \\ \text{Outflow from} \\ \text{reactor volume} \end{array} \right\} + \left\{ \begin{array}{l} \text{Heat generated} \\ \text{in reactor volume} \end{array} \right\} + \left\{ \begin{array}{l} \text{Heat accumulating} \\ \text{in the reactor} \\ \text{volume} \end{array} \right\}$$

Since the process under consideration is isothermal, the heat terms cancel out leaving the equation as

$$\left\{ \begin{array}{l} \text{heat accumulation} \\ \text{in reactor volume} \end{array} \right\} = \left\{ \begin{array}{l} \text{Heat generated} \\ \text{in the reactor volume} \end{array} \right\} \quad (6)$$

$$dQ_1 = (\Delta H_R) F_{AO} dX_A \quad (7)$$

Integrating equation (7) over the entire reactor volume

$$Q_1 = (\Delta H_R) F_{AO} dX_{AF} \quad (8)$$

Rate of heat generated per unit volume (Q2)

This is calculated as follows

$$Q_2 = \frac{Q_1}{V_R} \quad (9)$$

$$\text{But } V_R = \frac{F_{AO}}{\frac{K_1 C_{AO}(1-X_A)}{1+3X_A} - K_2 K_1 C_{AO} \left(\frac{e^{-K_1 t}}{K_2-K_1} + \frac{e^{-K_2 t}}{K_1-K_2} \right)} \ln \frac{1}{(1 - X_{AF})} \quad (10)$$

Substituting equation (8) and (10) into (9) result in the heat generation per unit volume equation. Thus

$$Q_2 = \frac{(\Delta H_R) F_{AO} X_{AF} K_1 C_{AO} - k_2 C_{AO} \ln(1 - X_{AF})}{F_{AO}} \quad (11)$$

$$Q_2 = \Delta H_R k_1 C_A - k_2 C_A X_{AF} \ln(1 - X_{AF}) \quad (12)$$

Pressure drop along reactor (ΔP)

The heat of reaction (ΔH_R) is computed from the work of James and Kastner (1972). Pressure drop is one of the functional parameters in reactor design. It's important is based on the stability of the system. The flow rigime analysis of the system is very important, knowing that pressure analysis gives impulse function (force x Time) of the system which is mathematically defined as F.T.

In the design of steady state reactor, pressure drop computation must be made to enable the engineer to control the system in question. Pressure drop (also called frictional head loss) is mathematically defined as

$$DP = \frac{FLP_m U^2}{2Di} \tag{13}$$

Where

- F = frictional factor, U = mean velocity
- m = Density of reaction mixture, D = Diameter of the tube
- L = Length of the reactor

Using the Fanning or Dacey equation for pressure drop in circular pipe under isothermal flow (3), ΔP is

$$DP = \frac{32FLR_p V_o^2}{\bar{\lambda}^2 g C D i^5} \tag{14}$$

For a two phase pressure drop due to friction, estimation can be done using the Lockhart and Martinelli Correlation. (25)

$$\left(\frac{D_P}{D_L} \right)_{TP} = Y_L \left(\frac{D_P}{D_L} \right)_L \tag{15}$$

$$X = \left(\frac{(D_P/D_L)_L}{(D_P/D_L)_6} \right) \tag{16}$$

$X \gg 1$, as the gas liquid phase is considered in the kinetic evaluation. Two phase pressure drop in the system thus become

$$Y_6 = Y_L \tag{17}$$

F in equation (14) is a function of the flow regime given by the Reynolds number Re [4] as

$$F = 0.184 Re^{-0.2} \tag{18}$$

So replacing F in equation (14) and applying necessary conversion factors for dimensional consistency yields.

$$DP_A = \frac{2.78 \times 10^{-3} Re^{-0.2} L_R P_A V_o^2}{\bar{\lambda}^2 g C D i^5} \tag{19}$$

$$\text{but } Re = \frac{P_A V_A D i}{\mu A} \tag{20}$$

while the mean linear velocity V_A is given by

$$V_A = \frac{\text{Volumetric Flow rate}}{\text{Cross sectional area of the tube}}$$

$$V_A = \frac{4V}{\bar{\lambda}^2 D i^2} \tag{21}$$

RESULTS AND DISCUSSION

The simulated model equation obtained were used to produce 300, 000m³ per year capacity of glucose and the result obtained for reactor flow parameter/ heat generated is shown in Table 1 while the pressure drops is presented in Table 2.

Table 1: Reactor Flow Parameters/ Heat Generated

XA	St	Sv	Q1	Q2
0.1000	70.4511	0.00141942	0.0013962	0.0001886
0.2000	149.2087	0.0067020	0.0027924	0.0007990
0.3000	238.4968	0.0041929	0.0041886	0.0019156
0.4000	341.5722	0.0029276	0.0055848	0.0036580
0.5000	463.4847	0.0021576	0.0069810	0.0062045
0.6000	612.6934	0.0016321	0.0083772	0.0098422
0.7000	805.0569	0.0012421	0.0097734	0.0150877
0.8000	1076.1780	0.0009292	0.0125658	0.0230501
0.9000	1539.6627	0.0006495	0.0125658	0.0370995
0.9100	1610.1138	0.0006211	0.0127054	0.0392281

Table 2: Reactor Flow Parameter/ Pressure Drop

Xa	Va	Re	Delta Pa
0.1000	0.2320	10757.2502	0.00000064255
0.2000	0.1407	8378.6572	0.00000052612
0.3000	0.1030	7167.1457	0.00000046432
0.4000	0.0811	6359.1374	0.00000042195
0.5000	0.0662	5744.5780	0.00000038900
0.6000	0.0549	5234.7497	0.00000036113
0.7000	0.0458	4779.7772	0.00000033579
0.8000	0.0378	4339.4080	0.00000031080
0.9000	0.0297	3851.5468	0.00000028252
0.9100	0.0289	3794.5883	0.00000027917

The space time which by definition is the time taken for the reactor volume feed to be completely processed, grew exponentially with length. Anyway, this is not unexpected, since even the volume of the reactor has similar profile with length.

Space velocity was shown to be reciprocal of space time. The profile with a positive exponential growth (exponential decay) reassures our confidence in this work.

This result obtained is consistent with previous works on design of P F R's[5,7,10] which indicates a negligence effect of pressure drop in the reactor. Pressure drop is expected since an increase in conversion definitely leads to an increase in volume of the reactor which correspondingly increases the reactor length and consequently reduces the pressure drop. Mathematically stated as:

$$XA \propto VRLR / \Delta P$$

$$XA = K VRLR / \Delta P$$

$$\text{and } K = XA \Delta P / VRLR$$

Where K= proportionality constant.

CONCLUSION

The study reveals that the pressure drop which is an undesirable property is negligibly small as can be seen from the results. The plug flow reactor can therefore be used to obtain the kinetics of acid hydrolysis for any cellulose biomass environmentally, high temperature, short reaction time and varying acid concentrations/rate constants non-isothermally.

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