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Heat exchange dimensions of simulated model of isothermal plug-flow reactor in acid hydrolysed 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) from 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

Biotechnology of cellulose and hemicellulose began in early 1980's, first in animal feed followed by food applications [1,2,3]. Since last two decades, the use of cellulases, hemicellulases and pectinase has increased considerably, especially in textile, food, brewery and wine as well as in pulp and paper industries [4,5,6,7].

Hydrolysis of cellulose in the production of bioethanol, a clean and renewable energy source which can be produced through fermentation and acid hydrolysis from renewable biomass has drawn much attention from government and researchers [8]. Based on specific lignocellulosic structure, the common bioethanol process employs three steps including substrate pre- treatment [9] hydrolysis and sugar fermentation.

Over the years, the future need to replace petroleum has simulated interest in the conversion of cellulose to a liquid fuel and chemical feed stocks [8]. Moreover, the possibility for converting cellulose from sources such as municipal refuse, agricultural waste, and wood waste may be a way of turning a waste disposal problem into a resource opportunity.

Acid hydrolysis of cellulose followed by fermentation of the sugars to ethanol is one method for accomplishing this conversion. In the past, numerous attempts at hydrolysing cellulose with low concentrations of sulphuric acid have been tried commercially. For example, Saeman's work in the 1940's led to the Madison process – a semi – batch process for wood hydrolysis [9] using transient batch experiments, demonstrated that the kinetics model developed by Saeman could also be used for paper.

As a result, flow sheets for a new large scale continuous process have been prepared [9] using a plug flow reactor and the kinetic data on paper hydrolysis. In this type of process analysis made some reasonable but untested assumptions to evaluate the economic subsential of the acid hydrolysis.

In order to obtain reliable kinetic information in the economic region of the design space of temperature, acid concentration, and slurry concentration, a laboratory scale continuous plug – flow reactor was developed for acid hydrolysis [5]. Although the work was not without limitation, yet a reasonable yield of glucose ranging from 50 to 55% was repeatedly realized with 1% acid and temperature range of 235 – 240°C while residence time was 0.22 minutes.

This study was aimed at introducing the best condition for simulation model of heat exchange dimension in isothermal plug – flow reactor of acid hydrolysis of cellulose. This is geared towards models functionality check as per the results obtained in correlation to the work of Grethlein and Thompson (1978).

Design

Usually the material balance equation governs the basis for the development of model equation for reaction functional parameter system. Engineering design is the foundation of modern technological equipment development and uses either physical or mathematical model as its references.

For this reactor, the conservation principle of material, for species in a volume element can be expresses as:

$$\begin{aligned} \text{Rate of species} \\ \text{Input to volume} \\ \text{element} \end{aligned} = \left\{ \begin{array}{l} \text{Rate of species} \\ \text{output of volume} \\ \text{element} \end{array} \right\} + \left\{ \begin{array}{l} \text{Rate of disappearance} \\ \text{of species within volume} \\ \text{element} \end{array} \right\} \\ \left\{ \begin{array}{l} \text{Rate of accumulation of} \\ \text{Species within volume element} \end{array} \right\} \quad \text{————— (1)}$$

And the conservation of energy principle can be expressed as:

$$\begin{aligned} \text{Energy in stream} \\ \text{entering volume} \\ \text{element} \end{aligned} = \left\{ \begin{array}{l} \text{Energy streams} \\ \text{leaving volume} \\ \text{element} \end{array} \right\} + \left\{ \begin{array}{l} \text{Energy Transferred} \\ \text{from Surrounding} \\ \text{to volume element} \end{array} \right\} \\ \left\{ \begin{array}{l} \text{Accumulation of the Energy} \\ \text{Within volume element} \end{array} \right\} \quad \text{————— (2)}$$

Models for the different reactor types are directly derivation of equation (1) and (2). Using the rate equation from the work of Grethlein and Thompson given in equation (3), model equation for the design of PF reactor for the production of glucose and its simulated heat generated is achieved.

$$r_{C_6H_{10}O_5} = \frac{K_1 C_{AO}(1-X_A)}{1 + 3X_A - K_2 K_1 C_{AO}} \left[\frac{e^{-K_1} +}{K_1 - K_2} + \frac{e^{-K_2} +}{K_1 - K_2} \right] \quad \text{———— (3)}$$

where $C_{AO} = C_{OC_6H_{10}O_6}$: $X_A = X_{C_6H_{10}O_5}$

Model for Design of Heat Exchanger (Cooling Jacket)

Heat exchanger unit is designed to control the heat generation per unit volume of the reactor. Hence heat exchange dimension is also a function of the kinetic of the rate of reaction. The fundamental modelling formular for heat exchanger unit is given in equation (4).

$$Q_1 = M_w C P_w (T_{wO} - T_{wI}) \quad \text{———— (4)}$$

M_w = Mass flow rate of cooling fluid

CP_w = specific heat capacity of cooling fluid

T_{wO} = outlet temperature of cooling fluid

T_{wI} = inlet temperature of cooling fluid

The mass flow rate per unit volume of cooling fluid (water) is:

$$M_w = V_R \frac{Q_1}{CP_w (T_{wO} - T_{wI})} \quad (5)$$

And the volumetric flow rate of the cooling water (V_{ow}) is

$$V_{ow} = \frac{M_w}{P_w} \quad (6)$$

Cross Sectional Area of Cooling Jacket (AC)

The cross sectional areas of the shell cooling

$$\text{jacket AC is Area} = \text{width, height (all internal)} \quad (7)$$

So, for a cooling jacket of

$$\text{cross sectional area AC} = \quad (8)$$

Area of flow of cooling water (AF)

The area of flow of cooling water is

$$A_f = AC - \frac{DO^2}{4} \lambda \quad (9)$$

For cross section of a jacket

$$D_o = D_i + 2R \quad (10)$$

Substitute equation (8) and (10) into (9)

$$AF = 3.2(D_i + 2x)^2 \quad (11)$$

Hydraulic mean diameter (D_m)

This is given by

$$D_m = \frac{4 \times \text{free area of flow}}{\text{wetted perimeter}} \quad (12)$$

$$D_m = \frac{[4 \times 3.2(D_i + 2x)^2]}{[(2H_j + W_j) + D_o] \lambda} \quad (13)$$

By relevant substitution, equation (13) becomes

$$D_m = 0.51(D_i + 2x) \quad (14)$$

Required Heat transfer area (A_R)

The heat load Q_1 can be expressed as

$$Q_1 = H.A_R.T_m \quad (15)$$

Therefore the required heat transfer area, A_R becomes

$$A_R = \frac{Q_1}{H.T_m} \quad (16)$$

Where H = overall heat transfer coefficient

T_m = log mean temperature difference

Total Surface Area of Jacket (AS)

$$AS = 2(W_j H_j - D_o^2/4)\bar{\Delta} + 2H_j L_j + 2W_j L_j \quad (17)$$

Therefore

$$AS = 2[H_j W_j + H_j L_j + W_j L_j - D_o^2/4] \bar{\Delta} \quad (18)$$

RESULTS AND DISCUSSION

The result of heat exchange dimension of the simulated model obtained in this work is presented in Table 1 which shows area of flow of cooling water (A_F), Hydraulic mean diameter (D_m), Required heat transfer area (A_R) and total surface area of jacket (A_S).

Table 1: Heat Exchange Dimension

X_a	D_m	A_f	A_s	A_r
0.1000	0.0874	0.0940	42.3187	0.2773279
0.2000	0.1108	0.1510	42.2907	0.5546558
0.3000	0.1287	0.2037	42.2649	0.8319837
0.4000	0.1444	0.2564	42.2390	1.1093116
0.5000	0.1593	0.3121	42.2116	1.3866396
0.6000	0.1743	0.3737	42.1814	1.6639675
0.7000	0.1904	.4459	42.1459	1.9412954
0.8000	0.2092	0.5383	42.1005	2.2186233
0.9000	0.2350	0.6796	42.0311	2.4959512
0.9100	0.2385	0.6997	42.0213	2.5236840

The heat generated over the entire reactor volume is directly proportional to fractional conversion (X_a). It is not unexpected since the reaction with H_2SO_4 and Cellulose is an exothermic reaction; Hence, as the reaction goes to completion, more heat is given out. Our results are in consonant with past work [5,9] and have similar trends, therefore it is evident that the required heat transfer area has a more direct dependence on conversion than any other measure of area in this work.

CONCLUSION

The study so far carried out reveals that the plug flow reactor can be used to obtain the Kinetics of acid hydrolysis for any cellulose biomass environmentally, at high temperature, short reaction time and varying acid concentrations.

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