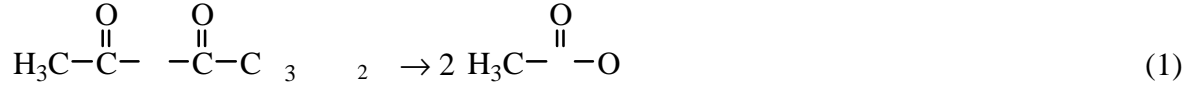


Abbreviated Theory for a Transient CSTR

Acetic anhydride is converted to acetic acid by reaction with water as given in equation (1).



in equation (2). AAn is not ionic and so it does not appreciably affect the electrical conductivity of a solution containing it. On the other hand, AAc is ionic, and so as its concentration changes,

of the electrical conductivity of the solution leaving the reactor can be used to find the concentration of AAc in that solution (using a pre-measured calibration curve).

there is only a single reaction taking place in the system. Therefore, if the instantaneous flow rate at which any one of the species exits the reactor is measured, the stoichiometry of the reaction

done using a mole table like the one given in Table 1 where \mathbf{x} is the extent of reaction.

Table 1. A mole table for acetic anhydride hydrolysis.

Species	Inlet Flow Rate	Outlet Flow Rate
AAn	\dot{n}_{AAn}^0	$\dot{n}_{AAn}^0 - \mathbf{x}$
H ₂ O	$\dot{n}_{H_2O}^0$	$\dot{n}_{H_2O}^0 - \mathbf{x}$
AAc	\dot{n}_{AAc}^0	$\dot{n}_{AAc}^0 + 2\mathbf{x}$
Total	\dot{n}_{Total}^0	\dot{n}_{Total}^0

A mole balance on the CSTR can be written for any species, denoted by i , as in equation (3). In equation (3) the first term is the molar rate of input of i and the second term is the net rate of generation of i . These terms are set equal to the molar rate of output of i (third term) and its

rate of accumulation (fourth term). Note that in the absence of chemical reaction the second term is zero, and alternatively, at steady state the fourth term is zero.

$$\dot{n}_i^0 + V_{fluid} \mathbf{n}_i r = \dot{n}_i + \frac{d}{dt} \left(\frac{\dot{n}_i V_{fluid}}{V} \right) \quad (3)$$

In your project the literature and other company reports suggest that the rate expression is given by equation (4). The hypothesis that you are testing is that when H₂O is present in excess, its concentration will be essentially constant. Under such circumstances the rate coefficient and the (constant) H₂O concentration can be combined into a pseudo first order rate coefficient, k , as in equation (5).

$$r = k' [AAn] [H_2O] \quad (4)$$

$$r = k [AAn] \quad (5)$$

Note also that the concentration is related to the flow rates according to equation (6).

$$[i] = \frac{\dot{n}_i}{V} \quad (6)$$

The rate coefficient in an equation like equation (4) or equation (5) is normally expected to depend upon temperature as given by the Arrhenius expression, equation (7).

$$k = A e^{-E/RT} \quad (7)$$

To analyze the data for any one isothermal run, the rate expression can be substituted into the mole balance. The relationship between molar flow rate and concentration, along with the mole table, can be used to rewrite the resulting equation so that the only dependent variable is the outlet molar flow rate of one of the species. At this point the differential equation can be integrated to give an algebraic equation. The algebraic equation can then be fit to the experimental data to obtain a value for the rate coefficient, k . A statistical analysis can be used to assess the quality of the resulting fit. Data for other temperatures can be similarly analyzed, leading to a set of rate coefficients and their corresponding temperatures. The values of the Arrhenius parameters, A and E , can then be found from these data by plotting the logarithm of k

versus the inverse of T . It can be seen from equation (7) that this plot should be a straight line, the slope and intercept of which can be used to find the desired parameters.

Nomenclature

A , pre-exponential factor

E , activation energy

k' , true second order rate coefficient

k , apparent first order rate coefficient

\dot{n}_i^0 , total molar inlet flow rate of i

\dot{n}_i , total molar outlet flow rate of i

r , rate of reaction per unit volume

R , ideal gas constant

T , absolute temperature

V_{fluid} , total volume of fluid within the reactor

V , total outlet volumetric flow rate

$[i]$, molar concentration of i

x , extent of reaction

n_i , stoichiometric coefficient of i (positive for products and negative for reactants)