APPENDIX A

Estimation of Concentrations of Vari

The term $k_{L,iC4}$ a_v in the equation A.3 is the mass transfer term. This constant term was assumed to be a constant value, $2000s^{-1}$.

The concentration of isobutane in the hydrocarbon phase is calculated from reactant feed flow rate. The concentration of isobutane in hydrocarbon phase is equal to the molar flow rate of isobutane divided by the volumetric flow rate of hydrocarbon.

The rate of isobutane consumption is calculated from component mass balance in the reactor. This rate value is equal to the rate of consumption of isobutane divided by volume of acid in the reactor

The volume of acid in the reactor can be determined by the definition of olefin space velocity. Olefin space velocity is defined as the volume of olefin charged per hour divided by the volume of acid in reactor.

Olefin Concentration in Acid Phase

Since olefins are well solvated by acid phase, their concentrations in the acid phase would be proportional to their concentra

The olefin concentration in feed can be determined from a mass balance equation, similar to that used for isobutane. At steady state, the rate of formation of paraffin (i) in the acid phase must equal to the rate of its mass transfer out of the acid phase.

$$k \quad a \; C \qquad C \qquad r \quad Ha \qquad (A.7)$$

to be 2000 s^{-1}

The consumption of iso-butylene is:

$$iC_4 \ X \quad iC_4 \quad iC_8 \ X \tag{A.15}$$

But the only reaction involved for the iso-octane carbonium ion is:

-

, so

equation A.14 can be arranged to:

From equations A.14 and A.18, the simplest functional form to determine the concentration of iso-butylene is a proportion. So the form to be used for the concentration

Where Y is the m

Concentrations of the other olefinic intermediates may be derived in a similar way.

2. Iso-pentylene concentration in the acid phase

and

$$iC_{10}\ X \qquad iC_5 \qquad iC_5\ X \tag{A.21}$$

Thus, the concentration of iso-pentylene is a function of the concentrations of isodecane carbonium ion and iso-heptylene.

The consumption of iso-pentylenes is given by:

$$[iC_5\ ]_a \quad f([iC_7\ ]_a \quad [iC_{10}X\ \ ]_a) \tag{A.22}$$

$$iC_5 \quad HX \quad iC_5\ X \tag{A.23}$$

$$iC_4 \quad iC_5\ X \qquad iC_5 \quad iC_4\ X$$

$$iC_5 \quad iC_4\ X \qquad iC_9\ X \tag{A.24}$$

$$iC_4 \quad iC_9\ X \qquad iC_9 \quad iC_4\ X$$

and

Thus, the concentration of iso-pentylene is a function of isopentane and isononane:

$$[iC_5\ ]_a \quad f([iC_5]_a \quad [iC_9]_a) \tag{A.25}$$

So, the equation for calculating the iso-pentylene is:

$$[iC_5\ ]_a \quad (Y_{iC5} \quad Y_{iC9})([iC_7\ ]_a \quad [iC_{10}\ \ X\ \ ]_a) \tag{A.26}$$

3. Iso-heptylene concentration in the acid phase

The reaction forming iso-heptylene is:

$$iC_7\ X \qquad iC_7 \quad HX \tag{A.27}$$

4. Iso-butylene concentration in the acid phase

$$iC_4 \quad X \qquad iC_4 \qquad HX \qquad \text{(A.33)}$$

The reaction forming iso-butylene is:

The consumption of iso-butylene is:

$$iC_4 \quad X \qquad iC_4 \qquad iC_8 \quad X$$

Thus, the equation used to calculate the concentration of iso-butylene is:

The reaction

and

So, the equation for calculating the iso-pentylene concentration is:

5 a $iC5$ $iC9$ 8 a 11 a

6. Iso-octylene concentration in the acid phase

The reaction forming iso-octylene is:

he other reac

he con

In pentyl

ion in acid phase

he consumption

hus, the concentration of iso-butylene can be calculated as:

Thus, the concentration of iso-he

By following the above procedure, concentrations of all the species in the acid phase were obtained. Substituting these concentrations into the rate equations in Tables 2.1, and 2.2, reaction rates were determined.

Estimation of Concentrations of the contactor components

The concentrations of the contactor components in the acid phase are calculated using the equations in Table 2.2 given the following concentrations

Acid Concentration:

$$C_{C623}^{HX} \quad \frac{{}_{AC09}x_{AC09}^{11}}{MW^{11}}$$

Isobutane Concentration:

$$C_{C623}^{3} \quad \frac{{}_{AC09}x_{AC09}^{3}}{MW^{3}}$$

Butene Concentration:

$$C_{C623}^{2} \quad \frac{{}_{AC09}x_{AC09}^{2}}{MW^{2}}$$