V. CONCLUSIONS

A. Review of Tanks-in-Series Model: Assumptions & Conclusions

Below is a review of the major assumptions used in the tanks-in-series analysis. For the gas phase tracer analysis:

1. The model uses a series of equal volume CSTR's with no backmixing for the slurry region. For the freeboard section of the reactor, the plug flow reactor model was assumed for the rest of the analysis.

2. For a system approaching a single CSTR, up to a 10% error in the normalization factor could occur if the tail of radiation on the detector curves is cut off at an inappropriate point.

3. No micromixing effects were assumed.

4. The analysis used only the inlet, slurry level and outlet radiation detectors.

5. A uniform velocity profile was assumed at the slurry level.

6. The solubility of the argon in the liquid was neglected in the analysis.

For the slurry phase mixing:

1. The inlet pulse was assumed to be a Gaussian impulse.

2. The tanks-in-series model with backmixing was used with no outlet stream.

3. The Mn_2O_3 particles were assumed to closely follow that of the catalyst particles in the liquid.

4. The backmixing flowrate in the liquid was set equal to the forward flow rate.

The first analysis was the first step in modeling the LPMEOH three phase slurry system. The major conclusions of the tanks-in-series model are:

1. For the liquid mixing analysis, a 3-cell model was best fitted to the data. The model predicts equilibrium values in 60 seconds and, although the data shows the bulk of the liquid is well mixed by then, the data shows a slower approach to equilibrium than that predicted by the model.

2. For the gas phase, the mixing could be characterized as a series of CSTR's in the slurry region with the freeboard section of the reactor modeled as a plug flow reactor. The model showed

two important trends: as the superficial gas velocity increased, the number of CSTR's increased (approaching a plug flow reactor) and as the L/D decreased, the number of CSTR's decreased (approaching a single well mixed tank).

B. Review of the Axial Dispersion Model: Assumptions & Conclusions

In the axial dispersion analysis, mixing in the slurry is characterized separately from the gas phase. For the slurry phase tracer analysis, the following assumptions and results are applicable:

1. The Mn_2O_3 particles were assumed to closely follow that of the catalyst particles in the liquid.

2. An axial dispersion model was used to visually fit the concentration model with the curves for the two slurry tracer injections. This produced a value for $\mathscr{D}_L$ of 3.7 ± 0.2 ft^2/sec at the superficial inlet gas velocity of 0.5 ft^2/sec. A dependency of $\mathscr{D}_L$ on U_G to the power of 1/3 was recommended such that:

$$\mathscr{D}_L = 0.667\ (g\ D^4 U_G)^{1/3}$$

To analyze the gas phase tracer data, the following assumptions were made and the results included:

1. An axial dispersion model was used which accounted for phase transfer between the liquid and gas. The gas dispersion coefficient was calculated by simultaneously fitting the effective dispersion coefficient and the effective velocity.

2. Correlations available in the literature do not match the tracer data. In addition, the literature correlations vary widely among themselves. Based on literature correlation groupings, the gas tracer data were fit to the following relationship for $\mathscr{D}_G$:

$$\mathscr{D}_G = 4.42\ D^{1.5}\ U_G^{1.8}$$

3. The gas dispersion coefficient may be translated to the number of CSTR's by a relationship reported in Levenspiel:

$$n^{-1} = 2\ Pe^{-1} - 2\ Pe^{-2}\ (1-\exp(-Pe))$$

The number of CSTR's based on the gas dispersion shows no trend with changing superficial velocity due to scatter in the data. However, using the effective dispersion coefficient (equation 21) and an effective Peclet number, an effective number of CSTRs was calculated which shows the same dependency as the tanks-in-series model; i.e. as the gas velocity increases, the number of CSTR's increase.

C. Recommendations

Figures IV.C.3-2 and IV.C.3-3 show the comparison of the two models in predicting the effective number of CSTR's versus the outlet gas velocity for the LaPorte data. Although the tanks-in-series model offers a simpler approach to analyzing the mixing characteristics, it has a few shortcomings. Only the liquid level and outlet detectors were used to analyze the residence time distribution (RTD) of the gas tracer. The applicability of the plug flow assumption to the zone between the slurry level and the outlet detectors is suspect since the gas must bypass a demister at the top of the reactor. Therefore, more credence is placed on the slurry level detectors. A model that utilizes only 4 slurry detectors out of 20 imposes a significant limitation on the analysis. Although the tanks-in-series analysis was used on the gas phase and a 3-cell mixing model was applied to the liquid phase, there is no direct relationship between the two models. In addition, the tanks-in-series model offers no reliable means for scaleup of the reactor. Its primary purpose is to allow the user to characterize the mixing in the present, studied system.

The dispersion model separates the mixing of the gas and liquid phases into two scaleable relationships and offers a means to combine the mixing of the two phases into an effective mixing parameter, also scaleable. Although it is phenomonological, like the tanks-in-series model, the dispersion model simplifies the characteristics of mixing and makes use of the bulk of the detector data from all heights along the reactor. The dispersion model also accounts for phase transfer between the gas and liquid, an important factor for the argon/LPMEOH reactor study as seen in the Henry's Law constant analysis. For these reasons, the dispersion model is the recommended method for characterizing the LPMEOH system.

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Nomenclature

Area	=	area under the response curve
Baseline	=	baseline of the response curve
$\bar{C}_A$	=	outlet reactor concentration of species A
C	=	concentration
C_A	=	concentration of species A
C_{AN}	=	concentration of species A in last tank
C_{An}	=	concentration of species A in nth tank
d	=	particle diameter
D	=	Column diameter
E(t)	=	exit age distribution
F	=	fraction of a tank
g	=	gravitational acceleration 32 ft/sec^2
H	=	Henry's Law constant
$K_l a$	=	Mass transfer coefficient
L	=	slurry height
N	=	number of CSTR's
$norm_i$	=	value of data point after normalization
Pe	=	Peclet number defined as ($uL/\mathcal{D}$)
Q	=	reactor volumetric flow rate
r_A	=	reaction rate
Re_p	=	particle Reynolds number (Equation 1)
t	=	the residence time of each tank in the tanks-in-series model with uniform tanks
$\bar{t}$	=	total reactor residence time
t_i	=	residence time of each tank in the liquid mixing model with non-uniform tanks

Nomenclature

t_n	=	residence time of n^{th} tank
t_o	=	time of injection
U_G	=	superficial gas velocity based on outlet gas composition and reactor temperature and pressure
V, V_n	=	reactor volume, volume of n^{th} cell
ΔT	=	time interval between data points
X_i	=	value of data point before normalization
z	=	height along the reactor
α	=	as defined in Equation 27
β	=	ratio of mixing time of liquid to response time of solid particle in Equation 2
$\mathcal{D}$	=	dispersion coefficient
ε	=	holdup (gas, liquid or solid in the slurry)
∂	=	partial derivative
ρ	=	density
υ	=	kinematic viscosity ($\frac{\mu}{\rho}$)

Subscripts

EFF	=	effective
G	=	gas
L	=	liquid
p	=	particle
s	=	solid