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**LIQUID PHASE METHANOL LAPORTE PROCESS DEVELOPMENT UNIT:
MODIFICATION, OPERATION, AND SUPPORT STUDIES**

Topical Report Revision #1

Task 2.3: Tracer Studies in the LaPorte LPMEOH PDU

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U.S. Department of Energy
Pittsburgh Energy Technology Center
Pittsburgh, Pennsylvania**

**By
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Allentown, Pennsylvania**

and

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ABSTRACT

A gas phase and a slurry phase radioactive tracer study was performed on the 12 ton/day Liquid Phase Methanol (LPMEOH) Process Development Unit (PDU) in LaPorte, Texas. To study the gas phase mixing characteristics, a radioactive argon tracer was injected into the feed gas and a residence time distribution was generated by measuring the response at the reactor outlet. Radioactive manganese oxide powder was independently injected into the reactor to measure the slurry phase mixing characteristics.

A tanks-in-series model and an axial dispersion model were applied to the data to characterize the mixing in the reactor. From the axial dispersion model, a translation to the number of CSTR's (continuous stirred tank reactors) was made for comparison purposes with the first analysis. Dispersion correlations currently available in the literature were also compared.

The tanks-in-series analysis is a simpler model whose results are easily interpreted. However, it does have a few drawbacks; among them, the lack of a reliable method for scaleup of a reactor and no direct correlation between mixing in the slurry and gas phases.

The dispersion model allows the mixing in the gas and slurry phases to be characterized separately while including the effects of phase transfer. This analysis offers a means for combining the gas and slurry phase dispersion models into an effective dispersion coefficient, which, in turn, can be related to an equivalent number of tanks-in-series. The dispersion methods reported are recommended for scaleup of a reactor system.

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I. INTRODUCTION

A gas phase and a slurry phase radioactive tracer study were performed on the Liquid Phase Methanol (LPMEOH*) Process Development Unit (PDU) in LaPorte, Texas. The LPMEOH reactor is operated as a three phase slurry bubble column with an internal diameter of 22.5 inches and an L/D (Length over Diameter) of approximately 10. The slurry phase is operated batch and contains an inert hydrocarbon oil and a powdered methanol catalyst. Synthesis gas is bubbled through the slurry via a gas sparger. A freeboard section is present above the slurry to allow for oil disengagement. To study the gas phase mixing characteristics, a radioactive argon tracer was injected into the feed gas and a residence time distribution was generated by measuring the response at the reactor outlet. Radioactive manganese oxide powder was independently injected into the reactor to measure the slurry phase mixing characteristics.

Two separate analyses were done on the data. The first employed a tanks-in-series model and the second an axial dispersion model. From the axial dispersion model, a translation to the number of CSTR's was made for comparison purposes with the first analysis. Correlations currently available in the literature are also compared. However, since most of the literature correlations are based on air-water bubble columns, these data and analyses provide an interesting comparison.

This report summarizes the experimental testing methods used, the two models studied and those available in the literature. A recommended procedure is offered for calculating the number of CSTR's from a dispersion model which is applicable for reactor scaleup.

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II. DESCRIPTION OF EXPERIMENT

A. Gas Tracer

Mixing studies were performed on the LPMEOH reactor located in LaPorte, Texas. The reactor is a stainless steel column with an internal diameter of 22.5 inches and a possible liquid height of 25 feet. The slurry phase is stationary and contains an inert hydrocarbon oil and a powdered methanol synthesis catalyst. Synthesis gas is bubbled through the slurry via a gas sparger. Oil becomes disengaged from the gas in a space above the liquid and the gas exits from the reactor through the top of the column. A detailed description of the LPMEOH PDU has been presented in several previous DOE program reports [23,24] and will not be repeated here.

The gas phase residence time distribution was measured by ICI TracerCo of Houston, Texas. For each experimental condition, the gas holdup, liquid level, temperature, pressure and gas flow rate were measured prior to injection of the radioactive tracer. Argon (Ar-41) was irradiated at Texas A&M University and transported to LaPorte on the day of the test. Radioactive Ar-41 (chosen for its half-life of 1.8 hours) was transferred to a gas sampling bomb which was connected to the gas feed line through a sampling valve near the reactor bottom. At the start of the experiment, the contents of the bomb were injected into the gas feed line using a purge of high pressure nitrogen. The radioactive gas was vented to the atmosphere in accordance with Texas state law.

Twenty detectors were located around the reactor to measure the response for 10 minutes after the injection. The most important detectors were on the inlet, outlet and directly above the slurry level. This allowed measurement of the residence time distribution (RTD) for the entire reactor and also the RTD of the gas in the slurry portion of the reactor. Mixing of the gas in the liquid portion of the reactor is of most interest because that is where the catalyst is located and the reaction occurs. The response was recorded digitally at a rate of 4000 points per 10 minute period per detector. At least three injections were made at each condition to check consistency of results. After the injections were made for a given condition, the gas holdup, liquid level, temperature, pressure and gas flow rate were measured.

Over a two day period, six conditions were studied for the gas tracer as shown by the first six entries of Table II.A-1. Three gas velocities were studied at full slurry height and three gas velocities were studied at half slurry height. This information was used to determine mixing effects as a function of L/D and of gas velocity.

Table II.A-1

Nominal Conditions for Tracer Studies

<u>Tracer</u>	<u>Case</u>	<u>Inlet Gas Velocity (ft/sec)</u>	<u>L/D</u>
Ar-41	1	.25	10
Ar-41	2	.5	10
Ar-41	3	.6	10
Ar-41	4	.5	6.5
Ar-41	5	.25	6.5
Ar-41	6	.18	6.5
Mn ₂ O ₃	7	.5	11

T = 250°C

P = 750 psig

B. Liquid Tracer

The slurry mixing test was also performed by ICI TracerCo. Manganese oxide (Alpha Chemicals, Mn₂O₃, 98% pure, -325 mesh) was supplied to Texas A&M for irradiation. Mn₂O₃ was selected as the tracer since it would not interfere with the methanol reaction. A particle size less than 44 microns was chosen to match the size of the catalyst particles. The degree to which suspended particles follow turbulent liquid mixing in a bubble column is discussed in a recent paper by Matsumoto et al.[9] on the basis of mixing length theory. For the present case, the particle Reynolds number for a 44 micron particle, based on the fluctuation velocity, is about 6. This number is defined by

$$Re_p = \frac{d_p (gDe_g)^{1/2}}{v_L \sqrt{2}} \quad (1)$$

(written here for the case of zero bulk liquid velocity). The ratio of the mixing time associated with a turbulent fluid eddy to the response time of a suspended particle is characterized by the group β defined below. A large value of β would indicate that the response time of the particle is small compared with the mixing time of the fluid.

$$\beta = \frac{\phi L P_L}{(1 - \epsilon_g) v_L \rho_p Re_p^2} \quad (2)$$

β_L is the liquid dispersion coefficient based on total volume. For our case, β is about 400 for a 44 micron particle, and it is even larger for smaller particles. In this range, it is clear that the particle closely follows the fluid.

A pretest was performed by Texas A&M to verify the half-life of 2.5 hours. Unlike the gas tracer, the solid powder would remain in the reactor, so a short half-life was important. Since the tracer remained in the reactor, only one injection per day was permitted by Texas state law.

Approximately 0.1 gm of radioactive Mn_2O_3 was loaded into a gas sample bomb and mixed with reactor oil. The gas bomb was connected to a 2" reactor inlet pipe at the bottom of the reactor. Although DME Solid Tracer Studies done in the past have injected the powder at the top of the reactor, the current reactor configuration would not allow this. For future tracer study tests, modifications to the reactor will be considered which would allow this method of testing. Experimental conditions were measured before and after the injections as was done in the gas tracer tests. The conditions for the liquid tracer test are listed in Table II.A-1. At the start of the experiment, the contents of the bomb were injected into the reactor using a purge of high pressure nitrogen. Twenty detectors were located around the reactor to measure the response for 10 minutes after the injection.

C. Run Summary

The cases in Table II.A-1 were performed during February and March of 1989. On February 24, 1989 cases 1, 2, and 3 were conducted at full slurry level. To maintain a constant concentration of solids, the slurry level had to be varied slightly with gas flow rate. Three injections were made for each case. Due to equipment problems during case 3, four injections were made. On February 28, 1989, cases 4, 5, and 6 were conducted at the lower slurry level. The liquid tracer, Case 7, was performed on March 30, 1989. Detectors 3, 5, 6, 7, 8, 9, 13, and 16 malfunctioned and the injection was repeated by blowing in the remaining Mn_2O_3 that lay in the injection line. The second injection did not contain enough radioactivity to provide a strong signal for the detectors. However, enough detectors had worked during the first injection to provide data at each reactor level. Additional Mn_2O_3 injections were not possible on March 30 due to a state-imposed limit on radiation dosage. Actual conditions for all these cases are listed in Table II.C-1 and the position of the detectors for each case is reported in Appendix A.

D. Data Reduction

The data analyzed in this report consisted of 4000 points per detector taken over a ten minute time span for each injection. During each injection, there were 20 detectors mounted on the reactor at various elevations. Each point represents the relative amount of radioactive material that was present at that position in the reactor at that instant in time.

The original data were received in the form of 21 sets of numerical strings roughly 1.4 megabytes in length. Each continuous numerical string represented a single injection and consisted of 4000 points from each of the 20 detectors. This initial data set was reduced to a set of 20 files per injection with 4000 points per file.

Figure II.D-1 shows a detector file plotted on a real time scale. Notice that the radiation increases at long times. At the LaPorte PDU, a portion of the gas product is recycled and mixed with fresh syngas feed. The "tail" seen in the detector data is due to radiation returning in the recycle; it was omitted in the data analysis. Many of the response curves reached a baseline that was less than 10% of the maximum value before the recycle radiation was detected. Depending on the type of curve, omitting the tail could introduce a 10% error in the normalization factor if the mixing is characterized by a single CSTR, or as low as a 3% error if the mixing is plug flow. The plots of all the data resulted in a thick curve that was very difficult to integrate and fit to a model because of the "noise" and the number of data points involved.

Therefore, a method was required to normalize, and if possible, smooth each response curve. The three different types of curves that were analyzed were the impulse spike, the gas phase detector response curves, and the liquid phase detector response curves.

The first five minutes of data from the impulse spike was integrated using the trapezoidal rule and the baseline (background) radiation determined. The baseline radiation was subtracted from the data points and the data were normalized by dividing the value by the peak area.

The noise in the gas phase response curves was eliminated by using the Fourier transform. The Fourier transform converts the data from the time domain to the frequency domain. With the data in the frequency domain, the high frequency points (noise) were omitted and the inverse Fourier transform was performed. The resulting smooth curve overlays the original curve and has a low degree of noise (Figure II.D-2). With the data in this form, it was possible to subtract the baseline radiation from the data. The data were integrated using the trapezoidal rule and normalized using the following equation:

$$\text{norm}_i = (X_i - \text{Baseline}) / (\text{Area} - \text{Baseline} * \text{No. data points})$$

where norm_i is the normalized data, X_i is the transformed data, "Area" is the integrated area under the transformed curve and "Baseline" is the baseline radiation.

Similar techniques were used to reduce and normalize the liquid tracer data. However, since the tracer powder remained in the reactor, the radiation counts leveled out, not at zero as in the gas phase tests, but at a value which represents a well-mixed system. Therefore, the response curve was not normalized by the integrated area, but rather by the value termed well-mixed so that the curves leveled out at a value of 1.0.

Table II.C-1
Actual Conditions for Tracer Studies

Case	Injection Number	Slurry Level (tape)* at Injection	Gas Flow scfh	Inlet Superficial Gas Velocity ft/s	Ave. Temp F	Ave. Press psig	Fraction Gas Holdup	Catalyst Inventory Kg	wt % Cat (oxide)
1	1	185	73040	.25	482	753	.286	362	36.3
	2	185							
	3	184							
2	4	206	146640	.50	483	753	.363	362	37.
	5	205							
	6	205							
3	7	210	175940	.60	484	753	.378	362	36.4
	8	207							
	9	207							
4	10	205							
	b1	135	145210	.50	481	753	.353	256	37.2
	b2	135							
5	b3	134							
	b4	117	72640	.25	482	753	.273	256	37.5
	b5	115							
6	b6	115							
	b7	108	54370	.18	482	753	.227	256	37.5
	b8	108							
7	b9	108							
	L1	216	146600	.50	482	753	.439	301	34.2
	L2	218							

* The zero of the tape measure is 32" above the bottom of the reactor.

Figure II.D.1 LAPORTE LPMEOH TRACER STUDY
TYPICAL RADIATION COUNTS vs TIME FOR REACTOR OUTLET

FIGURE II.D.2 : LAPORTE LPMEOH TRACER STUDY
NORM. RADIATION COUNTS vs TIME AT REACTOR OUTLET

III. TANKS-IN-SERIES ANALYSIS

The initial analysis of the experimental data, by J. H. Frey and G. N. Brown, used a tanks-in-series model [1]. This section summarizes the theory and results of that analysis.

A. Background

1. Mixing in Continuous Systems (Gas Phase Mixing)

Macromixing is a term used to describe the distribution of residence times of fluid elements through a reactor. The degree of macromixing is quantified by the residence time distribution (RTD) or exit age distribution $E(t)$ defined so that the fraction of fluid in the exit stream with age less than t_1 is

$$\int_0^{t_1} E(t) dt \quad (3)$$

The mean residence time is given by

$$\bar{\tau} = \int_0^{\infty} t E(t) dt \quad (4)$$

$$= V/Q \quad (5)$$

The exit age distribution is obtained experimentally by injecting a pulse of tracer and measuring the response at the reactor outlet.

$$E(t) = \frac{C(t)}{\int_0^{\infty} C(t) dt} \quad (6)$$

where $C(t)$ is the concentration at the reactor outlet. $E(t)$ is simply the normalized reactor outlet concentration.

The use of classical residence time distribution theory for predicting reaction conversion in reactors is valid for linear reaction systems, such as first order reactions. The conversion of a first order reaction depends only on the time allowed for reaction. In this case, two extremes of macromixing can occur. One extreme of macromixing is represented by the CSTR, which has an exponential distribution of residence times. The other extreme of macromixing is represented by the plug flow reactor (PFR). In a PFR, since every element travels through the reactor with exactly the same residence time, $E(t)$ would be a spike if a perfect impulse were injected.

Residence time distribution theory can be used with non-linear reaction systems if a premixed feed stream is available. However, macromixing characterization is not sufficient to determine reaction conversion in the non-linear reaction case. Micromixing, defined as the mixing of molecules of one age with molecules of another age, is also important for non-linear reaction kinetics. For a PFR, molecules of different ages cannot mix, so micromixing effects cannot occur. For a CSTR, Nauman and Buffman [18] state that micromixing can affect the conversion of a second order reaction by only 7%. For the LPMEOH PDU, micromixing effects were neglected and the characterization of macromixing in terms of the PFR and CSTR extremes was studied.

Once the macromixing information is experimentally obtained, the age distribution function can be used to predict reactor performance in two ways. The first way is to calculate the outlet concentration ($\bar{C}_A$) based on

$$\bar{C}_A = \int_0^{\infty} C_A(t) E(t) dt \quad (7)$$

$$\text{where } \frac{dC_A}{dt} = r_A$$

$$\text{with } C_A|_{t=0} = \text{feed concentration}$$

($C_A(t)$ is the concentration of A in a batch reactor.)

The alternative method is to fit the measured $E(t)$ function to a tanks-in-series model. The number of tanks and the tank residence times are used as adjustable parameters in fitting the model to the data. If the reactor behaves as a CSTR, then the model will predict one tank. If the reactor behaves as a PFR, then there will be an infinite number of tanks-in-series. The tanks-in-series model can be used to predict reactor performance by these equations.

$$\frac{dC_{An}}{dt} = \frac{C_{A(n-1)} - C_{An}}{\tau_n} - r_a \quad n = 1, \dots, N \quad (8)$$

$$\text{with } \tau_n = V_n/Q \quad (9)$$

$$\text{and } \bar{C}_A = C_{AN}$$

The number of tanks (N) and the tank residence time is evaluated by fitting the normalized data (E_N) from an impulse/response experiment to the following equations.

$$\frac{dE_1}{dt} = \frac{E_0 - E_1}{tF} \quad (10)$$

$$\frac{dE_n}{dt} = \frac{E_{(n-1)} - E_n}{\tau} \quad n = 2, \dots, N \quad (11)$$

where F = fraction of a tank
 E_0 = a Gaussian impulse

$$E_0 = \exp \left[-\frac{1}{2} \frac{(t - \bar{t})^2}{\sigma^2 (2\pi)^{1/2}} \right] \quad (12)$$

The adjustable parameters (τ , number of tanks) are adjusted by a Newton-Raphson algorithm or a two variable search algorithm until the error between the response data and E_N is a minimum.

2. Mixing in Batch Systems (Slurry Mixing)

Since the slurry phase does not leave or enter the reactor, a residence time distribution analysis is not possible. A numerical solution to a cell model with a Gaussian impulse was chosen as the mixing model to provide an analysis of the slurry consistent with the gas phase analysis. The cell model chosen for the liquid phase is similar to the gas phase model except backmixing occurs from the upper cells to lower cells and there is no outlet stream. The equations are:

$$\frac{dC_1}{dt} = \frac{C_0 + C_2 - C_1}{\tau_1} \quad (13)$$

$$\frac{dC_i}{dt} = \frac{C_{i-1} - 2C_i + C_{i+1}}{\tau_i} \quad i = 2, \dots, N-1 \quad (14)$$

$$\frac{dC_N}{dt} = \frac{C_{N-1} - C_N}{\tau_N} \quad (15)$$

(Where C_0 is given by equation 12)

The adjustable parameters in this model are N and $t_1, 2, \dots, t_N$ and are determined using a Newton-Raphson algorithm.

3. Literature Background

An excellent review of mixing in gas-liquid reactors is provided by Shah, et al. [20]. In this review, methods for measuring residence time distributions, mixing models, data analysis, and various mixing studies are discussed. It is apparent from this review that much of the mixing work has been done with air-water systems, small columns, or low gas velocities.

Mixing references citing large scale, multiphase reactors at high temperature and pressure include articles by Nalitham and Davies [17], Tarmy, et al [21], and Field and Davidson [2]; however, the highest superficial gas velocities reported were 0.05, 0.22, and 0.18 ft/s, respectively. A mixing study on the liquid phase methanol reactor provides needed mixing data for large scale, multiphase reactors operating at high temperature, high pressure and high gas velocity with organic liquids and gases.

B. Results of Numerical Analysis

1. Gas Mixing Numerical Analysis

The most suitable place to measure the residence time distribution (RTD) is at the reactor outlet where there exists a uniform velocity profile [22]. In the LPMEOH reactor, however, gas mixing information obtained at the reactor outlet includes the mixing behavior of the gas in the slurry section and also the mixing behavior of the gas in the freeboard section. Mixing of the gas in the slurry section is of primary importance for predicting reactor behavior. To satisfy the condition of a uniform velocity profile at the measurement location and to satisfy the requirement of obtaining an RTD for the slurry section, the numerical analysis assumes the freeboard is a plug flow reactor (PFR). The response from the outlet detector is shifted in time by a time equivalent to the height of the freeboard divided by the gas velocity. The resulting RTD should be the RTD of the gas in the slurry region if the freeboard is a PFR.

The normalized data were fit to a two dimensional model. As discussed by Shah, et al. [20], evaluation of mixing parameters from the variance of an RTD curve can be inaccurate when there is uncertainty in the tail of the response curve. To minimize this error, mixing parameters were evaluated by comparing the numerical solution of a tanks-in-series model to the actual data. In this way, each point carries an equal weight in the optimization routine. For the gas phase data, the model (equation 10, 11) was a series of CSTRs of equal volume with no backmixing between CSTRs. The number of CSTRs in series and the individual residence time of each CSTR were the two parameters that were adjusted to minimize the difference between the experimental curve and the calculated curve.

The inlet impulse was defined by a time lag, a spike width, and equation 12. A lag-time parameter was used in the model fitting algorithm to account for the time which elapsed between time zero and the actual injection time. These parameters were determined for each injection by direct examination of the normalized impulse spike data. The spike lag time was determined by the following:

$$\text{Spike lag} = (\text{spike peak point} \# - 1) * \Delta T \text{ (sec)}$$

The spike width was determined by:

$$\text{Sigma} = \frac{(\text{Back Edge Point \#} - \text{Leading Edge Point \#}) * \Delta T (\text{sec})}{2}$$

For the analysis of the slurry level detectors, an additional time lag was included that represented the time the gas took to travel from the liquid level to the detectors above liquid level. This was done to account for the detectors not being precisely at the liquid level. In these cases, the additional time lag was estimated assuming the gas behaved like a PFR in the reactor freeboard. An example of a typical model fit from this analysis is shown in Figure III.B.1-1. For the gas phase, the analysis of the detectors directly above liquid level and the reactor outlet were of most interest and the model fits were determined using each response.

The results for the number of CSTRs in series for the gas in the slurry region are reported in Table III.B.1-1. Note that based on the outlet detectors, the number of CSTRs in the slurry increases with an increase in gas velocity and the number of CSTRs in the slurry decreases with a decrease in L/D.

The detectors directly above the slurry level were also used to analyze the gas mixing in the slurry section. The number of tanks-in-series as a function of gas velocity calculated from the slurry level detectors for cases 1-6 are illustrated in Figure III.B.1-2 and listed in Table III.B.1-1. The calculated model parameters (N, τ) are listed in Appendix C for each liquid level detector and each case. As gas velocity and L/D increases, the slurry region behaves more like a PFR. This trend agrees with that predicted by the outlet detectors. Note that in all cases except for the high velocity case, the number of CSTRs calculated from the outlet detector is slightly less than the number calculated from the liquid level detector, indicating that some degree of mixing is occurring in the gas space. Although some mixing is present, a majority of the cases show agreement in the number of CSTRs calculated from the two different detectors. Therefore, the assumption of plug flow in the gas space does not have a large impact on the number of CSTRs calculated.

Figure III.B.1-3 shows the number of CSTRs per L/D as a function of gas velocity calculated from the slurry level detectors. The two curves of Figure III.B.1-2 do not collapse perfectly into one curve when divided by L/D because there appears to be a stronger dependence on gas velocity at the lower L/D than at the higher L/D. The curve of Figure III.B.1-3 could be used for calculating reactor performance within the bounds of the outlet gas velocities ($.17 < V < .5$ ft/s) and L/Ds ($6.7 < L/D < 10.2$) studied.

FIGURE III.B.1-1: LAPORTE LPMEOH TRACER STUDY
TYPICAL CURVE FIT TO EXPERIMENTAL DATA

LEGEND

● EXPERIMENTAL DATA

— CURVE FIT DATA

FIGURE III.B.1-2 **LaPorte LPMEOH Tracer Study**
CSTRs in Series vs Superficial Gas Velocity

FIGURE III.B.1-3 LaPorte LPMEOH Tracer Study
CSTRs in Series per L/D vs Superficial Gas Velocity

LEGEND

○ AVG L/D=10.2A

□ AVG L/D=6.7A

By assuming that the freeboard may be modeled as plug flow, the response of the detectors from above the liquid level may be used without interference from tracer that has backmixed from the upper gas space. If the assumption is correct, the response from the reactor outlet should be identical to the response from the liquid level but shifted by a time representing the time to travel between detectors. If the assumption is incorrect, mixing will occur in the upper gas space and the outlet detector response will be much broader than the liquid level detector's response.

Figure III.B.1-4 illustrates that at high gas velocities and L/D, the assumption is good since the outlet detector response is only slightly broader than the liquid level response. At the lower gas velocities and especially when there is a small L/D (large freeboard), the outlet detector response appears to be much broader than the liquid level response and the freeboard plug flow assumption may be in jeopardy. (See Figure III.B.1-5.)

The total residence time for the slurry section using the two detectors described above was calculated by multiplying the individual tank residence time by the number of tanks. The values of the total residence time are listed in Table III.B.1-1. The total residence time from the outlet detector should be identical to the residence time from the slurry level detector since the outlet response was already shifted in time by the freeboard residence time. In all cases, the residence times calculated from the outlet detector are larger than the times calculated from the slurry level detector. At least three effects could be responsible for this:

- 1) The radioactive argon is not passing through in plug flow in the freeboard, but rather some is remaining for longer times and contributing to a higher residence time for the outlet detector. The total residence time is probably quite sensitive to a small amount of tailing because the product $tE(t)$ will contribute significantly to the integral $\tau = \int_0^{\infty} tE(t)dt$ at large times.
- 2) Shielding and the width of the reactor may cause the liquid level detector to miss the low levels of radiation that pass through in the tail, while the outlet detector may detect this tail.
- 3) As discussed by Levenspiel and Turner [22], a nonuniform velocity profile at the slurry level may contribute to a different residence time than observed where a uniform velocity profile exists.

The plug flow assumption in the freeboard is a good assumption to use as a first approximation. For the slurry residence time, the results that obey the assumption very well are the results at

Table III.B.1-1

Gas Mixing Behavior of the Slurry Volume
Based on Two Different Responses

<u>Case</u>	<u>Gas Velocity</u> <u>ft/s</u>	<u>Based on</u> <u>Slurry Level Detector</u>		<u>Based on</u> <u>Outlet Detector</u>	
		<u>Number</u> <u>of CSTRs</u>	<u>Total</u> <u>Residence</u> <u>Time (sec)</u> <u>for slurry</u> <u>section</u>	<u>Number</u> <u>of CSTRs</u>	<u>Total</u> <u>Residence</u> <u>Time (sec)</u> <u>for slurry</u> <u>section*</u>
1	.25	2.8 ± .4	48 ± 3.	2.2 ± .1	64.6 ± .8
2	.5	3.6 ± .5	25 ± 1.	3.3 ± .2	31.4 ± .8
3	.6	4.1 ± .9	22 ± 2.	4.2 ± .1	26.8 ± .6
4	.5	2.8 ± .3	18 ± 1.	2.2 ± .1	27.6 ± .7
5	.25	1.6 ± .5	40 ± 9	1.01 ± .01	71.1 ± .8
6	.18	1.2 ± .1	61 ± 11	1.02 ± .01	108 ± 3

* times have been reduced to account for gas volume above slurry

Table III.B.1-2

Theoretical Residence Time (V/Q)

<u>Case</u>	<u>Gas Velocity</u> <u>ft/s</u>	<u>L/D**</u>	<u>V/Q (sec)</u> <u>Using Gas</u> <u>Volume in Slurry</u> <u>Section</u>	<u>V/Q (sec)</u> <u>Using Total Gas</u> <u>and Slurry Volume</u> <u>in Slurry Section</u>
1	.25	9.6	20.6	72.1
2	.5	10.5	14.2	39.2
3	.6	10.6	12.4	32.9
4	.5	7.4	9.9	27.9
5	.25	6.5	13.5	49.3
6	.18	6.2	14.4	63.4

**total L/D of reactor = 13.3

FIGURE III.B.1-4: LAPORTE LPMEOH GAS PHASE TRACER STUDY
EXTENT OF MIXING IN REACTOR FREEBOARD

FIGURE III.B.1-5 : LAPORTE LPMEOH TRACER STUDY
 LIQUID LEVEL DETECTOR RESPONSE and REACTOR OUTLET RESPONSE
 $L/D = 10.2$; GAS VELOCITY = 0.25 FT/S

inlet gas velocities greater than or equal to 0.5 ft/s at the high L/D. The residence times for the low velocity cases at the low L/D with the plug flow assumption are in poor agreement for the two different detectors.

A theoretical residence time (V/Q) was calculated and compared to the residence time calculated in the curve fitting. Unfortunately, the volume (V) that the tracer gas "sees" is not well defined for the liquid phase methanol reactor. The theoretical residence times based on the gas holdup volume in the slurry and based on the total reactor volume in the slurry section are listed in Table III.B.1-2. In all cases the theoretical residence times calculated using these two volumes shown in Table III.B.1-2 provides bounds to the curve fit residence time from the liquid level detector shown in Table III.B.1-1. This indicates that argon gas (like CO and H₂) is soluble in the slurry and that the volume the argon "sees" is between the gas holdup volume and the total slurry volume. The Air Products' thermodynamic data base (Peng-Robinson equation of state) predicts that gases such as Ar, CO, and H₂ are 10-20 mol% soluble in the oil at the operating conditions.

2. Liquid Mixing Numerical Analysis

A 3-cell model (equations 12 - 14) was compared to the liquid mixing data at elevations of 44, 86, and 230 inches. The reverse flow rate was set to be equal to the forward flow rate. The analysis for the liquid tracer concentrated on finding mixing time constants for each mixing cell. The experimental data at all elevations are shown in Figure III.B.2-1. A Gaussian curve centered at 11.4 seconds, with a width defined by sigma of 5.9 seconds, was used to simulate the non-ideal impulse spike. The result of the model fit to the data is shown in Figure III.B.2-2 with cell time constants of 7.4, 20.6, and 13.4 seconds. The 3-cell model qualitatively accounts for the observed behavior. However, the model curves do not reproduce the mixing behavior precisely. The model reaches an equilibrium, concentration at 60 seconds, but the observed behavior shows a slow approach to the equilibrium value. Nevertheless, a majority of the Mn₂O₃ is well mixed within 60 seconds. However, since it appears that a significant amount of the gas is dissolved in the liquid, some of the effects of liquid mixing are accounted for in the gas residence time distribution.

FIGURE III.B.2-1 LAPORTE LPMEOH LIQUID TRACER STUDY REACTOR LIQUID MIXING

NOTE: HEIGHTS SHOWN ABOVE ARE FROM INJECTION POINT.

FIGURE III.B.2-2 LAPORTE LPMEOH LIQUID TRACER STUDY
REACTOR LIQUID MIXING MODEL

IV. AXIAL DISPERSION MODEL

A. Introduction

The analysis which begins below is a follow-up report to the tanks-in-series analysis. R. E. Larson examined the same tracer data in terms of an axial dispersion model [15]. Although the tanks-in-series analysis was useful, a dispersion model offers the additional benefit of scaleability. The principal results of this study are the values of the axial dispersion coefficient in both the liquid and gas phases. The effects of phase transfer are taken into account in the measurement of gas phase dispersion, and a measure of the Henry's law constant for argon in the slurry is given. An effective dispersion coefficient is calculated from the liquid and gas coefficients and translated to the number of effective CSTR's in series. This analysis and data provides a method to determine the degree of dispersion in the LPMEOH reactor for use in scale-up.

B. Background: Axial Dispersion Model

The mixing characteristics of the LaPorte slurry bubble column reactor are not expected to be simple. The reactor is currently operated batch-wise with respect to the slurry, neglecting a small loss of mineral oil overhead and consequent retrieval and makeup (about 0.226 gal/min, or 2×10^{-4} ft/sec superficial velocity). Gas enters the reactor through a sparger at the bottom of the reactor. At some height above the sparger, a bubble size and radial distribution of gas may be achieved which are not greatly influenced by the sparger.

In the upper section of the column, a flow pattern which is driven by the buoyancy of the gas phase is probably established. The largest scale of this flow, often referred to as gulf streaming, has been observed in bubble columns to consist of a number of circulation cells limited in size by the radius of the column [8].

Despite the complexities of the actual mixing process, the full simplicity of the dispersion model is retained and the mixing of the liquid phase is described in terms of uniform dispersion along the entire slurry height. The mixing of the gas phase is also described as uniform dispersion superimposed upon plug flow. This simplicity makes scale-up of the model possible. Like the tanks-in-series model, the dispersion model is phenomenological. It is very useful as a description of the mixing, adequate for reactor design, but it is not a faithful representation of the complexities of the actual flow.

One advantage of the dispersion model over the tanks-in-series model is that detector responses at several axial positions along the reactor can be matched for each injection. Tracer signals were, in fact, measured at several heights along the reactor vessel as a basis for measuring both liquid and gas phase mixing. The tanks-in-series model utilized only the data from the inlet, outlet and slurry level detectors.

Radioactive argon, which was used as the gas phase tracer, dissolves significantly into the liquid. Phase transfer must therefore be accounted for in an attempt to characterize the gas phase mixing from argon tracer data. The inherent gas phase dispersion coefficient can be estimated, however, from the overall effective dispersion of argon by making use of the independently measured liquid phase dispersion coefficient.

1. Axial Dispersion Liquid Mixing Model

For the liquid slurry, considered a batch system, the concentration of tracer at any axial position is modeled by

$$\mathcal{D}_L \frac{\partial^2 C}{\partial z^2} = \frac{\partial C}{\partial t}, \quad t > t_0, \quad 0 \leq z \leq L \quad (16)$$

where $C(z,t)$ is the radially averaged concentration of tracer at axial position z , time t . The axial dispersion coefficient, $\mathcal{D}_L$, has units of diffusivity, length²/time.

The initial condition for a pulse injection is $C(z,t_0) = \delta(z)$, and the boundary conditions for $t > t_0$ are $\partial C / \partial z = 0$ at $z = 0$ and $z = L$. $\delta(z)$ is the Dirac delta function centered on $z = 0$. The solution is:

$$\frac{C}{C_0} = 1 + \sum_{n=1}^{\infty} 2 \cos \left(\frac{n\pi z}{L} \right) \exp \left[- \frac{n^2 \pi^2 \mathcal{D}_L (t-t_0)}{L^2} \right] \quad (17)$$

C_0 is the final concentration of tracer, uniform throughout the column. (See Appendix D for the derivation.) The normalized response curves from the radiation detectors are equated to C/C_0 , a good assumption under sufficient radial mixing.

The injection pulse was also measured with a detector mounted on the injection line as close to the reactor vessel as possible. The finite width and shape of this pulse are taken into account by summing the ideal response over a series of impulse functions of appropriate weight.

A computer program was written which carries out the model calculations for a given injection pulse and dispersion coefficient. A visual fit of the two injections is sufficient to

find the best possible fit of the data. A least squares fit of the dispersion coefficient would be appropriate if more data were available or more accuracy possible. However, with 8 of the detectors failing on the first injection and the second injection being, in reality, the injection of the residual powder from the first attempt which remained in the inlet line, the accuracy of the detector data would not merit these numerical fits.

2. Axial Dispersion Gas Phase Mixing Model

The model equation for dispersion under plug flow, applied to the gas phase, is

$$D_G \frac{\partial^2 C_G}{\partial z^2} - \frac{U_G}{\epsilon_G} \frac{\partial C_G}{\partial z} + K_L a (H C_L - C_G) = \frac{\partial C_G}{\partial t} \quad (18)$$

U_G is the superficial gas velocity and ϵ_G is the gas phase volume fraction. An interphase transfer term is included: $(K_L a)$ is the mass transfer coefficient and H is the Henry's Law coefficient. Dispersion in the gas phase is coupled with dispersion in the liquid by the following:

$$D_L \frac{\partial^2 C_L}{\partial z^2} - \frac{\epsilon_G}{\epsilon_L} K_L a (H C_L - C_G) = \frac{\partial C_L}{\partial t} \quad (19)$$

Phase transfer does not affect the superficial concentration $\epsilon_G C_G + \epsilon_L C_L$, so multiplying (18) by ϵ_G and (19) by ϵ_L and adding eliminates the term. Assuming mass transfer resistance is small, $C_G = H C_L$ at every point. This simplifies to (See Appendix E):

$$D_{EFF} \frac{\partial^2 C_G}{\partial z^2} - U_{EFF} \frac{\partial C_G}{\partial z} = \frac{\partial C_G}{\partial t} \quad (20)$$

where

$$D_{EFF} = \frac{D_G + \frac{\epsilon_L}{H \epsilon_G} D_L}{1 + \frac{\epsilon_L}{H \epsilon_G}} \quad (21)$$

and

$$U_{EFF} = \frac{U_G}{\epsilon_G + \frac{\epsilon_L}{H}} \quad (22)$$

Equation (20) is simply the plug flow dispersion equation. Here ϵ_L is the overall volume fraction of liquid in the dispersion, equal to $[(1-\epsilon_G)(1-\epsilon_{SL})]$ where ϵ_{SL} is the fractional volume of solids in the slurry. The first term, $(1-\epsilon_G)$ represents the fraction of the slurry volume divided by the total volume and the second term, $(1-\epsilon_{SL})$, is the volume fraction of liquid in the slurry.

The solution of (3), due to Brenner [4,6], is (See Appendix F)

$$C = \bar{C} \sum_{n=1}^{\infty} f_n \exp(-A_n(t-t_0)) D_{EFF}/L^2 \quad (23)$$

$$f_n = \frac{8 \alpha_n}{4 (\alpha_n^2 + Pe) + Pe^2} \left(\alpha_n \cos \frac{\alpha_n Z}{L} + \frac{Pe}{2} \sin \frac{\alpha_n Z}{L} \right) \exp \left(\frac{Pe Z}{2L} \right) \quad (24)$$

$$A_n = \alpha_n^2 + \frac{Pe^2}{4} \quad (25)$$

$$Pe = \frac{U_{EFF} L}{D_{EFF}} \quad (26)$$

where α_n are the positive roots, taken in order, of

$$\frac{\alpha_n}{2} \tan \left(\frac{\alpha_n}{2} \right) - \frac{Pe}{4} = 0 \quad (27)$$

and

$$\frac{\alpha_n}{2} \cot \left(\frac{\alpha_n}{2} \right) + \frac{Pe}{4} = 0 \quad (28)$$

respectively.

This solution is for a pulse input at time t_0 , and $z = 0$. The boundaries are closed: the boundary conditions are $C_G U_{EFF} = D_{EFF} \partial C / \partial z$ at $z = 0$ and $\partial C / \partial z = 0$ at $z = L$. The latter boundary condition is an approximation which ensures that the solute concentration does not pass through a minimum or a maximum while in the slurry.

The normalization factor $\bar{C}$ is the integral of concentration at a fixed height with respect to dimensionless time:

$$\bar{C} = \frac{U_{EFF}}{L} \int_{t_0}^{\infty} C(L,t) dt \quad (29)$$

Where t_0 is the time of injection

The model requires that two adjustable parameters, D_{EFF} and U_{EFF} , be simultaneously fit to the actual response curves.

Consistent with the tanks-in-series analysis, the freeboard region of the reactor is treated as a plug flow reactor. Model response curves for those detectors above the slurry height, i.e., $z > L$, are taken as equivalent to that at $z = L$ shifted in time by $t_{LAG} = (z-L)/U_G$. A very small time shift is included for the time it takes the tracer to pass from the injection detector to the sparger.

As with the liquid tracer, the injection pulse was monitored with a detector mounted on the injection line. The finite time span of injection is again taken into account by summing the ideal pulse response over a series of impulse functions of appropriate weight.

A computer program was developed which carries out the simultaneous fit of dispersion coefficient and bulk velocity. The sum of the squares of residuals between the model and an actual detector response curve are calculated as a function of dispersion coefficient and bulk holdup time.

Several of the detectors appear to have been faulty or to simply not fit the model very well. As a basis for disregarding certain detectors, it is assumed that only fits for which the sum of squares is within a certain tolerance represent a valid fit.

Note that by rearranging equation 22, the Henry's Law coefficient for argon may be calculated from the tracer data by the effective velocity, along with the measurements of gas holdup:

$$H = \frac{\epsilon_L U_{EFF}}{U_G - \epsilon_G U_{EFF}} \quad (30)$$

H varies between zero and infinity as U_{EFF} varies between zero and U_G/ϵ_G .

C. Axial Dispersion Model Fit

1. Liquid Phase Measurements

Dispersion coefficients were fit first to the liquid tracer data. These data were taken at the conditions listed in Table IV.C.1-1

as case 7. Response curves were first smoothed by Laplace transform filtering [1], then added together at a given height. Figures IV.C.1-1, IV.C.1-2, IV.C.1-3, and IV.C.1-4 show the response curves out to 120 seconds. Five positions are given: $z = 44, 86, 140, 188,$ and 230 inches above the reactor bottom. Note that, except for the detector at 44 inches, the fit is reasonably good and seems to fall between the two values of dispersion coefficient plotted, $\mathcal{D}_L = L^2 0.008 \text{ sec}^{-1}$ and $\mathcal{D}_L = L^2 0.009 \text{ sec}^{-1}$, or $\mathcal{D}_L = 3.7 \pm 0.2 \text{ ft}^2/\text{sec}$. This fit is best for the uppermost detectors.

Several correlations exist in the literature for liquid dispersion coefficients measured primarily in bubble columns. The three-phase slurry bubble column is an extension of the two-phase column discussed in the literature, particularly in the limit of very small solid particle sizes. However, most of the data reported in the literature is for small diameter reactor systems operating at superficial gas velocities below those of the LaPorte reactor.

Akita [7] measured dispersion in 3.0, 6.0, and 11.9 inch diameter bubble columns of air in various liquids and presented a correlation for the experimental data:

$$\frac{\mathcal{D}_L}{DU_G} = \frac{(Dg)^{1/2}}{U_G} \left[0.06 + 0.55 \left(\frac{U_G}{(Dg)^{1/2}} \right)^{0.7} \right] \quad (31)$$

Baird and Rice [3,12] showed the following correlation by dimensional analysis:

$$\frac{\mathcal{D}_L}{DU_G} = K \left[\frac{(Dg)^{1/2}}{U_G} \right]^{2/3} \quad (32)$$

and set $K = 0.35$ according to a fit of literature data. The tabulated data included bubble columns as large as 17.3 inches in diameter operated at superficial gas velocities as high as .67 ft/sec.

The two correlations above both predict $\mathcal{D}_L$ near $2.0 \text{ ft}^2/\text{sec}$, 45% low relative to the measurement for case 7. The scatter in the data to which the correlations are fit is about 50%, and it is interesting that both correlations also underpredict the dispersion for the larger columns tabulated by Baird and Rice.

TABLE IV.C.1-1
REACTOR CONDITIONS FOR EACH INJECTION

Injection #	Inlet Superficial Gas Velocity ft/sec	Outlet Superficial Gas Velocity ft/sec	Slurry Level [*] ft	Gas Holdup	Catalyst Inventory (Oxide) kg	Solids Holdup Overall (Reduced Catalyst)	Solids Holdup in Slurry
Case 1	1	0.25	.209	18.08	0.286	362	0.036
	2			18.08	0.286	362	0.036
	3			18.00	0.286	362	0.036
Case 2	4	0.50	.415	19.83	0.363	362	0.033
	5			19.75	0.363	362	0.033
	6			19.75	0.363	362	0.033
Case 3	7	0.60	.504	20.16	0.378	362	0.032
	8			19.91	0.378	362	0.032
	9			19.91	0.378	362	0.032
	10			19.75	0.378	362	0.033
Case 4	1B	0.50	.435	13.91	0.353	256	0.033
	2B			13.91	0.353	256	0.033
	3B			13.83	0.353	256	0.033
Case 5	4B	0.25	.224	12.41	0.273	256	0.037
	5B			12.25	0.273	256	0.037
	6B			12.25	0.273	256	0.037
Case 6	7B	0.19	.171	11.66	0.227	256	0.039
	8B			11.66	0.227	256	0.039
	9B			11.66	0.227	256	0.039
Case 7	1L	0.50	.415	20.67	0.439	301	0.026
	2L			20.75	0.439	301	0.026

Reactor Temperature: 482° ±5°F
Reactor Pressure: 753 psig

* relative to reactor bottom

FIGURE IV.C.1-1

Signal - First Pulse

FIGURE IV.C.1-2

Signal - First Pulse

FIGURE IV.C.1-3

Signal - Second Pulse

FIGURE IV.C.1-4

Signal - Second Pulse

Matsumoto et al. [9,10] derived a mechanistic equation for $\mathcal{D}_L$ based on mixing length theory. This equation, in the limit of zero bulk liquid velocity, is

$$\mathcal{D}_L = K (gD^3 \epsilon_G)^{1/2} \quad (33)$$

$K = 0.3$ is given, again fit to two-phase bubble column data. For the diameter of the LaPorte column and a gas holdup value as measured for case 7, this correlation gives a value of 2.89 ft²/sec, 38% low relative to the measurement.

The first two correlations, (31) and (32), are in close agreement in the neighborhood of our test conditions and suggest an extrapolation of the dispersion coefficient proportional to $D^{4/3} U_G^{1/3}$. The third correlation, (33), suggests an extrapolation of $\epsilon_G^{1/2} D^{3/2}$ which is not a simple function of superficial gas velocity since the gas holdup, ϵ_G , is also a function of slurry properties. Since the data from LaPorte did not test a wide range of gas holdups, a correlation of the form suggested by Baird and Rice (equation 32) is recommended.

2. Gas Phase Measurements

The quantity of data available from gas tracer measurements made a more rigorous fit of the data possible. The dispersion coefficients and slurry holdup times for each detector are given in **Appendix G**. The norm of residuals may vary between 0 (a perfect fit) and 1. Certain fits must be rejected so that a dispersion coefficient is chosen based only on those response curves that fit the model quite well. As indicated in the last column of **Appendix F**, any detector for which the norm of residuals is greater than 0.09 is rejected. The remaining fits are averaged and tabulated in **Table IV.C.2-1**.

Figure IV.C.2-1 is a plot of the averaged dispersion coefficient for each injection. $\mathcal{D}_{EFF}$ varies between about 1.5 ft²/sec and 3 ft²/sec, increasing with increasing superficial gas velocity. The value of $\mathcal{D}_L$, for dispersion due to liquid mixing alone, measured for case 7 is also shown in **Figure IV.C.2-1**. From this point, an extrapolation was made according to the dependence suggested by Baird and Rice, i.e., $\mathcal{D}_L$ proportional to $U_G^{1/3}$. This approximation of the liquid dispersion as a function of superficial gas velocity is shown as a dashed line. The plot shows that the mixing due to the liquid phase is more intense than that measured by the gas tracer.

TABLE IV.C.2-1
Averaged Results for Effective Dispersion

	Injection	D/(L*L) Average (1/sec)	M.R.T. Average (sec)	D/(L*L) Std Dev (1/sec)	M.R.T. Std Dev (sec)	Number of Detectors Used
Case 1	1	0.00646	47.8	0.00102	7.5	11
	2	0.00621	44.7	0.00109	9.0	10
	3	0.00590	41.7	0.00057	5.8	4
Case 2	4	0.00733	25.3	0.00124	3.4	9
	5	0.00813	25.4	0.00154	3.7	9
	6	—	—	—	—	0
Case 3	7	0.00863	22.3	0.00150	2.7	6
	8	0.00846	22.3	0.00201	2.9	6
	9	0.00812	21.1	0.00133	1.4	6
	10	0.00809	21.6	0.00162	1.1	3
Case 4	1b	0.01337	16.5	0.00161	1.9	6
	2b	0.01412	17.2	0.00053	1.3	4
	3b	0.01464	16.3	0.00277	1.5	7
Case 5	4b	0.00954	23.7	0.00131	2.6	4
	5b	0.01186	23.3	0.00110	1.9	4
	6b	0.01095	23.5	0.00177	2.9	2
Case 6	7b	0.01150	38.0	0.00224	16.5	5
	8b	0.01307	35.2	0.00522	11.1	5
	9b	0.01001	30.2	0.00125	3.8	4

FIGURE IV.C.2-1
Effective Dispersion vs Outlet Superficial Gas Velocity

We calculate the gas dispersion coefficient, $\mathcal{D}_G$, using the definition of $\mathcal{D}_{EFF}$:

$$\mathcal{D}_G = \mathcal{D}_{EFF} (1 + \eta) - \mathcal{D}_L, \quad \eta = \frac{U_G - \epsilon_G \mathcal{D}_{EFF}}{\epsilon_G U_{EFF}} \quad (34)$$

Values of $\mathcal{D}_G$ are plotted in Figure IV.C.2-2 for the individual injections as a function of superficial gas velocity. One injection gives a slightly negative dispersion coefficient, an anomaly due to the combination of experimental error and uncertainty in the prediction of the liquid phase dispersion. On average, $\mathcal{D}_G$ roughly follows a $U_G^{3/2}$ curve, and varies between zero and 3.5 ft²/sec.

There are few correlations in the literature for dispersion coefficients in the gas phase. For a recent review of the available correlations, see Fan [11] p.270. These correlations are made largely from air-water data, and they predict gas phase mixing far greater than that measured in our system. As an example, Field and Davidson [2] give

$$\mathcal{D}_G = 1.82 D^{1.33} \left(\frac{U_G}{\epsilon_G} \right)^{3.56} \quad (35)$$

(D - units of feet)
(U_G - units of feet/second)

For our system, at $U_G = 0.5$ ft/sec and $\epsilon_G = 0.363$ (case 2), this predicts a $\mathcal{D}_G = 12.33$ ft²/sec. Towell and Ackerman [12] give

$$\mathcal{D}_G = 6.0 D^2 U_G \quad (36)$$

(D - units of feet)
(U_G - units of feet/second)

For our system, at case 2 conditions, $\mathcal{D}_G = 9.64$ ft²/sec.

After examining the available gas dispersion correlations, the LPMEOH data were fit to different variable groupings. The best fit resulted in a correlation of the following form (average error of 21.4% for cases 1 through 5):

$$\mathcal{D}_G = 4.64 D^{1.5} U_G^{1.8} \quad (37)$$

The data did not exhibit a strong dependency on gas holdup, so the data were fit only to outlet gas velocity. The various column diameter dependencies reported in the literature range from 1.3 to 2.0, with several authors using 1.5. Since our data were from one column, the column diameter dependency is arbitrary.

As previously noted, the Henry's Law coefficient may be inferred from the bulk velocity in the slurry. Figure IV.C.2-3 is a plot of the Henry's Law coefficient for each injection versus the slurry height for that injection. Each cluster of points corresponds to

FIGURE IV.C.2-2

Gas Dispersion vs Outlet Superficial Velocity

Curve Fit $D_g = a \cdot (U_g)^{0.75}$: All Cases

Figure: IV.C.2-3
Apparent Henry's Law Coefficient

one injection of case 1 through 6 as labeled. The value of the experimental coefficient H varies between 2 and 4.5 with the bulk of the data predicting values between 3.2 and 4.0. The Peng-Robinson equation of state places the value for Argon at 5.4. This thermodynamic model has previously shown good reliability. The increasing scatter at low slurry levels (cases 4, 5, and 6) suggest that the bottom 10 feet of the reactor behave differently than the rest of the column. The lower measured values of H may imply that more argon is dissolving into the slurry than expected. Adsorption onto the catalyst might account for the enhanced phase transfer, though the effect has not been quantified.

3. Equivalent CSTR Models

The gas phase mixing was described earlier using the series-of-CSTR's model. The translation of a plug flow dispersion model to a series of CSTR's is given by Levenspiel [13] as

$$n^{-1} = 2 Pe^{-1} - 2 Pe^{-2} (1 - \exp(-Pe)) \quad (38)$$

where the Peclet number is defined as $(U_G L)/(e_G D_G)$. Figure IV.C.3-1 is a plot of the number of tanks per unit length for gas phase mixing versus superficial gas velocity. The number of tanks, n , is calculated from the dispersion coefficients reported above for the gas phase. The more reliable measurements, based on the scatter of data, are those of cases 1, 2 and 3, the high slurry level runs.

The number of tanks varies between about 0.20 per foot and 0.35 per foot for cases 1, 2, 3 and 4. There is considerable scatter for the other 2 cases. While the tanks-in-series analysis done previously showed an increasing number of CSTR's with increasing gas velocity, this translation of gas dispersion to number of tanks shows no strong trend. The scatter in the data is too strong to suggest any effect of gas velocity.

To relate the number of tanks to the liquid dispersion coefficient, the relationship between the backflow cells model and the dispersion model must be utilized [14]. A comparison with the finite difference form of the dispersion equation suggests that, for uniform backflow cells, the axial dispersion coefficient is given by the equation

$$D_L = (f_i L^2)/(n V_{TOTAL}) = f_i L_i^2/V_i \quad (39)$$

where V_i is the single cell volume, f_i is the flow rate between cells, and L_i is the axial length of a cell. The number of identical cells into which a given system is divided may be increased arbitrarily keeping the ratio f_i/n constant. The ability to break the column into zones of different mixing intensity without introducing great complexity is an advantage of

FIGURE IV.C.3-1 Number of CSTRs per Length
Based on Gas Dispersion vs Outlet Gas Velocity

LEGEND

○ $L/D = 10$

■ $L/D = 6$

the backflow cell model. The measured value of the liquid dispersion coefficient, $\mathcal{D}_L = 3.7 \text{ ft}^2/\text{sec}$ for case 7, translates to $V_1/f_1 = 13 \text{ sec}$ for a three cell model. The average holdup time of the three cells in the model reported earlier was 13.8 sec, which is in good agreement. The backflow model could be used to iterate on the number of mixing cells given the dispersion characteristics of the liquid.

The number of CSTR's was next calculated from the effective dispersion coefficients used to determine $\mathcal{D}_G$. The statistical fit of $\mathcal{D}_{EFF}$ from all the detectors for each injection was used to calculate the effective Peclet number (based on U_{EFF} and $\mathcal{D}_{EFF}$) and the number of effective CSTR's. The calculated number of CSTRs are compared in Table IV.C.3-1 and illustrated in Figures IV.C.3-2 and IV.C.3-3. By using $\mathcal{D}_{EFF}$ to calculate the number of CSTR's, the trends predicted by the tanks-in-series model were duplicated. That is, as superficial gas velocity increases, the number of CSTR's increases.

4. Scaleup Using the Axial Dispersion Model

The axial dispersion coefficients in both gas and liquid phases have been measured for the LaPorte methanol synthesis reactor, a slurry bubble column, and correlations were selected for scaleup.

The slurried catalyst solids and the solid tracer powder closely follow the liquid. Therefore, dispersion of the solids need not be considered separately. The liquid dispersion coefficient was determined to be $3.7 \pm 0.2 \text{ ft}^2/\text{sec}$ for a superficial gas velocity of 0.5 ft/sec, the single run condition studied. For scale-up, equation (32) is recommended with $K = 0.667$ to fit the measured value. In this way, the liquid dispersion coefficient is

$$\mathcal{D}_L = 0.667 (g D^4 U_G)^{1/3} \quad (40)$$

In the absence of a generally agreed upon or reliable correlation for gas dispersion in the literature, the LPMEOH data were fit to a dependency on outlet superficial gas velocity. The following correlation is recommended as the best available to characterize the dispersion of the gas phase in the LPMEOH slurry. The dependency on column diameter was chosen from literature recommendations, since the data analyzed was for one column diameter.

$$\mathcal{D}_G = 4.42 D^{1.5} U_G^{1.8} \quad (41)$$

These correlations were tested for scaleup to a commercial scale reactor. Conditions for a typical commercial application are shown in Table IV.C.4-1 [16]. The reactor feed gas conditions are based on a 1000 psig Texaco gasifier firing Illinois No. 6 coal and are

taken from an EPRI sponsored report (No. AP2212). The dispersion coefficients for the gas and liquid phase were calculated using the previously recommended correlations (equations 40 & 41). From these values, an effective dispersion coefficient, as defined in equation 21, was estimated. This was translated to an effective number of tanks-in-series, using the Levenspiel relationship (equation 38). See Appendix H for the detailed calculations.

For the liquid phase D_L was estimated at 56.16 ft²/sec and for the gas phase, D_G was calculated to be 106.52 ft²/sec. The effective dispersion coefficient for the commercial scale reactor was 96.35 ft²/sec and this translates to 1.22 CSTRs.

FIGURE IV.C.3-2

Number of CSTRs vs Outlet Superficial Velocity Dispersion vs Tanks in Series Model: $L/D = 9.5 - 10.8$

FIGURE IV.C.3-3

Number of CSTRs vs Outlet Superficial Velocity
Dispersion vs Tanks in Series Model: $L/D = 6.18 - 7.56$

TABLE IV.C.3-1

COMPARISON OF THE NUMBER OF CSTR'S
CALCULATED FROM AN "EFFECTIVE" DISPERSION
COEFFICIENT WITH THE TANKS-IN-SERIES MODEL

Case No.	Inlet Gas Superficial Velocity ft/sec	Outlet Gas Superficial Velocity ft/sec	L/D	Axial Dispersion Model Ncstr	Tanks in Series Model Ncstr
6	0.19	0.171	6.22	1.99 ± 0.34	1.20 ± 0.1
1	0.25	0.209	9.64	2.43 ± 0.26	2.80 ± 0.4
5	0.25	0.224	6.53	2.65 ± 0.19	1.60 ± 0.5
2	0.50	0.415	10.53	3.18 ± 0.14	3.60 ± 0.5
4	0.50	0.435	7.42	2.79 ± 0.10	2.80 ± 0.3
3	0.60	0.504	10.62	3.35 ± 0.17	4.10 ± 0.9

TABLE IV.C.4-1
COMMERCIAL OPERATING AND PERFORMANCE PREDICTION

	Commercial Application
Reactor Feed Gas Conditions	
Flowrate, MSCFH	9024
Composition, mol%	
Hydrogen	36.6
Carbon Monoxide	53.5
Carbon Dioxide	8.8
Methane	0.1
Methanol	--
Nitrogen/Inerts	1.0
Reactor Design Conditions	
Temperature, °F	482
Pressure, psia	895
Internal Diameter, ft	12.8
Liquid Height, ft	42.8
L/D Ratio, ft/ft	3.4
Liquid Volume, cubic ft	5500
Gas Velocity, ft/sec	0.7
Space Velocity, SI/hr kg	8000
Slurry Catalyst Conc., wt%	35
Reactor Performance	
Production Rate, TPD	560
Catalyst Productivity, gmol/hr kg	23.0
Conversion, %	
BTU (LHV)	17.1
Feed Gas Flow (SCFH)	12.9
Carbon Monoxide	11.9
Hydrogen	35.3

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 $\mathcal{D}_L$ of 3.7 ± 0.2 ft^2/sec at the superficial inlet gas velocity of 0.5 ft^2/sec . A dependency of $\mathcal{D}_L$ on U_G to the power of $1/3$ was recommended such that:

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

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 $\mathcal{D}_G$:

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

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 phenomenological, 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_1a	=	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/D)
Q	=	reactor volumetric flow rate
r_A	=	reaction rate
Rep	=	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_0	=	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
D	=	dispersion coefficient
ϵ	=	holdup (gas, liquid or solid in the slurry)
∂	=	partial derivative
ρ	=	density
ν	=	kinematic viscosity ($\frac{\mu}{\rho}$)

Subscripts

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

Appendices

APPENDIX A: Diagrams of Reactor with Detector Locations for Each Injection

LPMEOH REACTOR AT LAPORTE PDU

Argon Tracer Study

Case 1

LPMEOH REACTOR AT LAPORTE PDU

Argon Tracer Study

Cases 2 & 3

LPMEOH REACTOR AT LAPORTE PDU

Argon Tracer Study

Case 4

LPMEOH REACTOR AT LAPORTE PDU

Argon Tracer Study

Case 5

LPMEOH REACTOR AT LAPORTE PDU

Argon Tracer Study

Case 6

LPMEOH REACTOR AT LAPORTE PDU

Mn203 Tracer Study

Case 7

APPENDIX B: Summary of Log Sheets

Summary of Tracer Study Data
 ess 2/13/90

Tracer Case Injection Date Time	1 Begin 24-Feb-89 15:43	End 17:18	2 Begin 24-Feb-89 18:00	End 20:02	3 Begin 24-Feb-89 22:14	End 25-Feb-89 0:37	4 Begin 28-Feb-89 15:05	End 17:24
Temperature oF	481.7	482.9	482.7	482.9	482.7	484	481.8	480.5
Pressure psig	752.5	753.1	753.1	753.1	752.5	752.5	751.9	753.1
Slurry Height in	192	181.5	206	204	211	203.5	138	132
Wt % catalyst		36.254	37.006	36.138		37.36		37.206
Catalyst Loading kg		361.9	361.9	355.1		361.9		255.9
%		28.58	36.33	35.58		37.84		35.3
Gas Holdup SCFH	71567.73	74514.71	145879.7	147398.1	176400.5	175472.7	145594.4	144826.5
FT-187 Reactor flow ft/sec	0.245	0.255	0.500	0.505	0.605	0.602	0.499	0.495
Inlet Sup Velocity ft/sec	0.205	0.214	0.414	0.419	0.508	0.506	0.434	0.430
Outlet Sup Velocity								
Outlet GC analysis -1								
H2	101.049	99.965	99.629	99.684	100.309	99.789	99.619	99.379
N2	21.982	21.980	24.027	26.736	26.467	27.512	27.623	28.524
CH4	0.611	0.622	0.556	0.718	0.685	0.669	0.478	0.462
CO	0.265	0.210	0.137	0.236	0.334	0.303	0.218	0.181
CO2	55.410	53.632	53.617	51.545	53.168	51.437	52.170	51.968
H2O	13.570	13.744	13.482	13.161	13.282	12.962	13.079	12.606
MeOH	0.013	0.000	0.015	0.045	0.003	0.026	0.012	0.015
DME	9.197	8.777	7.745	7.243	6.370	6.880	6.039	5.623
ETOH	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Outlet GC analysis -2		mole %									
H2	100.151	99.626	99.626	100.025	99.595	99.805	99.643	99.472			
N2	21.802	22.028	22.028	26.350	27.064	26.956	28.736	28.334			
CH4	0.604	0.612	0.612	0.675	0.695	0.672	0.457	0.463			
CO	0.237	0.192	0.192	0.206	0.324	0.294	0.194	0.166			
CO2	54.773	53.280	53.280	52.194	52.014	52.151	51.855	51.743			
H2O	13.781	14.514	14.514	13.250	13.130	12.983	12.399	12.756			
MeOH	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000			
DME	8.954	9.000	9.000	7.350	6.368	6.749	6.002	6.010			
EtOH	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000			
	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000			
Average GC analysis		(Norm.)									
H2	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000			
N2	21.761	22.049	23.114	26.582	26.780	27.289	28.284	28.593			
CH4	0.604	0.618	0.586	0.698	0.690	0.672	0.469	0.465			
CO	0.249	0.201	0.190	0.221	0.329	0.299	0.207	0.175			
CO2	54.763	53.565	53.648	51.945	52.615	51.899	52.205	52.155			
H2O	13.595	14.659	14.050	13.225	13.212	12.999	12.786	12.754			
MeOH	0.006	0.000	0.008	0.023	0.001	0.013	0.006	0.008			
DME	9.021	8.907	8.404	7.307	6.372	6.828	6.043	5.850			
EtOH	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000			
	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000			
Average Outlet GC		(Norm.)									
H2	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000			
N2	21.905	21.905	23.114	24.848	26.780	27.035	28.439	28.439			
CH4	0.611	0.611	0.586	0.642	0.690	0.681	0.467	0.467			
CO	0.225	0.225	0.190	0.206	0.329	0.314	0.191	0.191			
CO2	54.164	54.164	53.648	52.797	52.615	52.257	52.180	52.180			
H2O	14.127	14.127	13.638	13.638	13.212	13.106	12.770	12.770			
MeOH	0.003	0.003	0.015	0.015	0.001	0.007	0.007	0.007			
DME	8.964	8.964	7.855	7.855	6.368	6.600	5.946	5.946			
EtOH	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000			
	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000			

Avg Feed GC	(Norm.)				
H2	100.000	100.000	100.000	100.000	100.000
N2	33.822	35.001	35.423	35.815	35.815
CH4	0.502	0.562	0.607	0.408	0.408
CO	0.191	0.181	0.271	0.179	0.179
CO2	53.554	52.199	51.905	51.691	51.691
H2O	11.683	11.857	11.580	11.716	11.716
MeOH	0.000	0.000	0.000	0.000	0.000
DME	0.249	0.201	0.214	0.191	0.191
EtOH	0.000	0.000	0.000	0.000	0.000
density corr. outlet/inlet	1.196	1.206	1.191	1.150	1.150

Summary of Tracer Study Data
 ess 2/13/90

Tracer Case Injection Date Time	5 Begin 28-Feb-89 18:05	End 19:53	6 Begin 28-Feb-89 20:32	End 22:12	7 Begin 30-Mar-89 14:55	End 19:10
Temperature oF	482.7	481.2	481.5	482.1	483	482.1
Pressure psig	753.1	752.5	752.5	752.5	752.5	752.5
Slurry Height in	118.5	114	109.5	107	211	219
wt % catalyst		37.506		37.468		35
kg catalyst		255.9		255.9		301.4
Catalyst Loading %		27.3		22.67		43.9
Gas Holdup %						
FT-187 Reactor flow SCFH	73388.6	71884.84	54640.67	54101.82	148702.4	148180.1
Inlet Sup Velocity ft/sec	0.251	0.246	0.187	0.185	0.510	0.508
Outlet Sup Velocity ft/sec	0.225	0.221	0.168	0.167	0.430	0.428
Outlet GC analysis -1 mole %						
H2	99.399	99.463	99.372	99.536	99.944	99.060
N2	28.900	25.340	25.244	23.120	23.876	23.078
CH4	0.470	0.481	0.472	0.490	0.869	1.018
CO	0.181	0.188	0.185	0.208	0.386	0.364
CO2	51.311	51.565	51.610	51.296	50.428	50.607
H2O	12.777	14.009	14.071	16.230	15.249	14.857
MeOH	0.010	0.009	0.011	0.013	0.019	0.007
DME	5.750	7.871	7.779	8.179	9.111	9.129
ETOH	0.000	0.000	0.000	0.000	0.006	0.000
	0.000	0.000	0.000	0.000	0.000	0.000

Feed GC analysis -1	mole %	100.019	100.060	100.060	100.060	100.238	100.082	99.169
H2		36.629	35.415	35.415	35.415	33.904	35.595	34.740
N2		0.394	0.391	0.391	0.391	0.394	0.688	0.853
CH4		0.166	0.170	0.170	0.170	0.182	0.324	0.308
CO		51.070	51.649	51.649	51.649	51.342	50.255	50.402
CO2		11.495	12.203	12.203	12.203	14.187	12.833	12.482
H2O		0.000	0.000	0.000	0.000	0.000	0.000	0.000
MeOH		0.265	0.232	0.232	0.232	0.229	0.387	0.384
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000
EtOH		0.000	0.000	0.000	0.000	0.000	0.000	0.000

Feed GC analysis -2	mole %	99.990	100.055	99.991	99.536	99.946	98.688
H2		35.858	35.230	35.056	33.338	35.320	34.416
N2		0.432	0.424	0.414	0.425	0.737	0.812
CH4		0.154	0.146	0.149	0.173	0.324	0.295
CO		51.577	51.741	51.783	51.114	50.420	50.492
CO2		11.794	12.362	12.462	14.353	12.882	12.429
H2O		0.000	0.000	0.000	0.000	0.000	0.000
MeOH		0.175	0.152	0.127	0.133	0.263	0.244
DME		0.000	0.000	0.000	0.000	0.000	0.000
EtOH		0.000	0.000	0.000	0.000	0.000	0.000

Avg Feed GC analysis (Norm.)	100.000	36.242	0.413	0.160	51.321	11.644	0.000	0.220	0.000	0.000
H2										
N2										
CH4										
CO										
CO2										
H2O										
MeOH										
DME										
EtOH										

Avg Feed GC	(Norm.)		
H2	100.000	100.000	100.000
N2	35.772	34.442	35.202
CH4	0.410	0.406	0.777
CO	0.159	0.169	0.314
CO2	51.493	51.495	50.662
H2O	11.960	13.308	12.723
MeOH	0.000	0.000	0.000
DME	0.206	0.180	0.321
ETOH	0.000	0.000	0.000
density corr. outlet/inlet	0.000	1.111	1.185

APPENDIX C: Tanks-in-Series Model Calculations

APPENDIX C

Model Parameters Based on Slurry Level Detectors

LIN VEL AVG L/D CSTRS IN RES TIME TOT RES TM CSTR/L/D
(FT/S) SERIES (S) (S)

0.25	9.66	2.40	20.21	48.51	0.25 CSTR AVG
0.25	9.66	2.40	20.77	49.85	0.25 2.77
0.25	9.66	2.40	20.27	48.65	0.25 0.37
0.25	9.63	3.10	14.41	44.67	0.32 CSTR/L/D AVG
0.25	9.63	3.20	13.99	44.78	0.33 0.29
0.25	9.63	3.20	14.10	45.12	0.33 0.04
0.25	9.60	3.10	14.53	45.04	0.32 RES TIM AVG
0.25	9.60	2.40	20.49	49.18	0.25 17.41
0.25	9.60	2.40	20.07	48.17	0.25 2.97
0.25	9.60	3.10	15.24	47.24	0.32 TOT RES TIM AVG
					47.12
					1.92

0.50	10.56	3.40	7.07	24.02	0.32 CSTR AVG
0.50	10.56	3.30	7.74	25.54	0.31 3.59
0.50	10.56	3.30	7.65	25.25	0.31 0.38
0.50	10.56	3.40	7.31	24.84	0.32 CSTR/L/D AVG
0.50	10.53	4.10	6.24	25.56	0.39 0.34
0.50	10.53	4.20	6.54	27.46	0.40 0.04
0.50	10.53	4.20	6.38	26.78	0.40 RES TIM AVG
0.50	10.53	4.10	6.29	25.78	0.39 7.18
0.50	10.52	3.40	7.36	25.02	0.32 0.59
0.50	10.52	3.50	7.35	25.74	0.33 TOT RES TIM AVG
0.50	10.52	3.20	8.03	25.70	0.30 25.52
0.50	10.52	3.20	7.72	24.71	0.30 0.84
0.50	10.52	3.33	7.62	25.29	0.32

0.60	10.75	3.22	7.36	23.70	0.30 CSTR AVG
0.60	10.75	3.28	7.35	24.12	0.31 4.09
0.60	10.75	3.35	7.72	25.87	0.31 0.73
0.60	10.61	3.63	5.66	20.83	0.35 CSTR/L/D AVG
0.60	10.61	3.53	6.02	21.25	0.33 0.39
0.60	10.61	3.49	6.05	21.11	0.33 0.07
0.60	10.61	3.54	5.99	21.20	0.33 RES TIM AVG
0.60	10.60	4.44	4.62	20.52	0.42 5.61
0.60	10.60	4.23	5.06	21.39	0.40 1.14
0.60	10.60	4.60	4.36	20.06	0.43 TOT RES TIM AVG
0.60	10.60	4.22	5.08	21.42	0.40 22.23
0.60	10.52	5.40	4.27	23.06	0.51 1.62
0.60	10.52	5.15	4.61	23.73	0.49
0.60	10.52	5.16	4.46	22.99	0.49

0.50	7.43	3.20	5.39	17.25	0.43 CSTR AVG
0.50	7.43	2.40	7.96	19.10	0.32 2.89
0.50	7.43	2.50	7.29	18.23	0.34 0.56
0.50	7.43	2.70	6.50	17.55	0.36 CSTR/L/D AVG
0.50	7.40	4.40	4.11	18.35	0.59 0.39
0.50	7.40	3.10	5.92	18.35	0.42 0.08
0.50	7.40	3.10	5.67	17.58	0.42 RES TIM AVG
0.50	7.40	3.20	5.10	16.32	0.43 6.45
0.50	7.39	2.90	5.70	16.53	0.39 1.33
0.50	7.39	2.30	8.76	20.15	0.31 TOT RES TIM AVG
0.50	7.39	2.30	8.21	18.88	0.31 17.97

0.50	7.39	2.60	6.69	17.40	0.35	1.05
0.25	6.62	1.40	24.42	34.19	0.21	CETR AVG
0.25	6.62	1.25	32.89	41.11	0.19	1.59
0.25	6.62	1.20	39.70	47.64	0.18	0.45
0.25	6.62	1.30	30.01	39.01	0.20	CETR/L/D AVG
0.25	6.64	1.30	30.18	39.24	0.20	0.24
0.25	6.64	1.20	40.41	48.49	0.18	0.07
0.25	6.64	1.20	43.32	51.99	0.19	FEE TIM AVG
0.25	6.64	1.30	33.03	42.93	0.20	27.29
0.25	6.62	2.30	12.04	27.69	0.35	10.99
0.25	6.62	2.20	13.91	30.59	0.34	TOT RES TIM AVG
0.25	6.62	2.20	13.57	29.86	0.34	38.62
0.25	6.62	2.20	13.96	30.71	0.34	7.78
0.19	6.24	1.20	48.79	58.55	0.19	CETR AVG
0.19	6.24	1.10	66.26	72.88	0.19	1.23
0.19	6.24	1.10	74.27	81.63	0.18	0.10
0.19	6.24	1.20	58.22	69.97	0.19	CETR/L/D AVG
0.19	6.23	1.30	36.94	40.41	0.24	0.20
0.19	6.23	1.30	36.02	46.82	0.21	0.02
0.19	6.23	1.20	44.99	53.93	0.19	FEE TIM AVG
0.19	6.23	1.30	45.25	58.82	0.21	50.50
0.19	6.22	1.20	47.16	56.59	0.19	12.07
0.19	6.22	1.20	50.37	60.45	0.19	TOT RES TIM AVG
0.19	6.22	1.20	56.69	68.03	0.19	61.21
0.19	6.22	1.30	51.10	66.44	0.21	10.92

APPENDIX D: Axial Dispersion: Equation (16) Derivation

APPENDIX D

Solution of equation (16):

$$\partial_L \frac{\partial^2 C}{\partial z^2} = \frac{\partial C}{\partial t} \quad t > t_0 \quad 0 \leq z \leq L \quad (1)$$

Rewrite as:

$$C_t - \partial_L C_{zz} = 0 \quad (2)$$

$$C(z, t) = f(z) \quad (3)$$

$$C_z(0, t) = 0 \quad (4)$$

$$C_z(L, t) = 0 \quad (5)$$

Use the method of separation of variables:

$$C = Z(z) T(t) \quad (6)$$

$$C_z = Z'(z) T(t) \quad (7)$$

$$C_{zz} = Z''(z) T(t) \quad (8)$$

$$C_t = Z(z) T'(t) \quad (9)$$

Substitute (6) through (9) into (2):

$$Z(z) T'(t) - \partial_L Z''(z) T(t) = 0 \quad (10)$$

Divide by equation (6) to get:

$$\frac{T'(t)}{T(t)} - \partial_L \frac{Z''(z)}{Z(z)} = 0 \quad (11)$$

$$\frac{T'(t)}{T(t)} = \lambda \quad \frac{Z''(z)}{Z(z)} = -\frac{\lambda}{\partial_L} \quad (12)$$

$$T'(t) - \lambda T(t) = 0 \quad Z''(z) - \frac{\lambda}{\partial_L} Z(z) = 0 \quad (13, 14)$$

Solve for T(t):

$$T(t) = \exp(\lambda t) \quad (15)$$

$$T'(t) = \lambda \exp(\lambda t) \quad (16)$$

$$\frac{T'(t)}{T(t)} = \lambda \quad (17)$$

Solve for Z(z):

$$Z(z) = +\cos \sqrt{-\frac{\lambda}{\partial_L}} z \quad Z(z) = -\cos \sqrt{-\frac{\lambda}{\partial_L}} z \quad (18, 19)$$

$$Z'(z) = -\sqrt{-\frac{\lambda}{D_L}} \sin \sqrt{-\frac{\lambda}{D_L}} z \quad Z'(z) = \sqrt{-\frac{\lambda}{D_L}} \sin \sqrt{-\frac{\lambda}{D_L}} z \quad (20,21)$$

$$Z''(z) = \frac{\lambda}{D_L} \cos \sqrt{-\frac{\lambda}{D_L}} z \quad Z''(z) = -\frac{\lambda}{D_L} \cos \sqrt{-\frac{\lambda}{D_L}} z \quad (22,23)$$

$$\frac{Z''(z)}{Z(z)} = -\frac{\lambda}{D_L} \quad \text{for both solutions} \quad (24)$$

Apply boundary conditions:

$$C = Z(z) T(t) \quad (25)$$

$$C = \pm \cos \sqrt{-\frac{\lambda}{D_L}} z \exp(\lambda t) \quad (26)$$

$$C_z = Z'(z) T(t) \quad (27)$$

$$C_z = -\sqrt{-\frac{\lambda}{D_L}} \sin \sqrt{-\frac{\lambda}{D_L}} z \exp(\lambda t) \quad (28)$$

$$C_z(0,t) = -\sqrt{-\frac{\lambda}{D_L}} \sin 0 \exp(\lambda t) = 0 \quad (29)$$

$$C_z(L,t) = -\sqrt{-\frac{\lambda}{D_L}} \sin \sqrt{-\frac{\lambda}{D_L}} L \exp(\lambda t) = 0 \quad (30)$$

$$\sin \sqrt{-\frac{\lambda}{D_L}} L = 0 \quad (31)$$

$$\sqrt{-\frac{\lambda}{D_L}} L = n\pi \quad (32)$$

$$\sqrt{-\frac{\lambda}{D_L}} = \frac{n\pi}{L} \quad (33)$$

$$\lambda = -\frac{n^2 \pi^2}{L^2} D_L \quad (34)$$

Substituting for λ into 26 gives

$$C = \pm \cos \left[\frac{n\pi}{L} z \right] \exp \left(-\frac{n^2 \pi^2}{L^2} D_L t \right) \quad (35)$$

APPENDIX E: Axial Dispersion: Equation (20) Derivation

APPENDIX E: Derivation of Equation 20

For the gas phase dispersion:

$$\mathcal{D}_G \frac{\partial^2 C_G}{\partial z^2} - \frac{U_G}{\epsilon_G} \frac{\partial C_G}{\partial z} + K_L a (HC_L - C_G) = \frac{\partial C_G}{\partial t} \quad (1)$$

For the liquid phase dispersion:

$$\mathcal{D}_L \frac{\partial^2 C_L}{\partial z^2} - K_L a \frac{\epsilon_G}{\epsilon_L} (HC_L - C_G) = \frac{\partial C_L}{\partial t} \quad (2)$$

Multiply (1) by ϵ_G and (2) by ϵ_L :

$$\epsilon_G \mathcal{D}_G \frac{\partial^2 C_G}{\partial z^2} - U_G \frac{\partial C_G}{\partial z} + K_L a \epsilon_G (HC_L - C_G) = \epsilon_G \frac{\partial C_G}{\partial t} \quad (3)$$

$$\epsilon_L \mathcal{D}_L \frac{\partial^2 C_L}{\partial z^2} - K_L a \epsilon_G (HC_L - C_G) = \epsilon_L \frac{\partial C_L}{\partial t} \quad (4)$$

The total concentration is:

$$\epsilon_G C_G + \epsilon_L C_L \quad (5)$$

$$\frac{\partial}{\partial t} (\epsilon_G C_G + \epsilon_L C_L) = \epsilon_G \frac{\partial C_G}{\partial t} + \epsilon_L \frac{\partial C_L}{\partial t} \quad (6)$$

Assume mass transfer is small; then $C_G = H \cdot C_L$. Also assume that H (Henry's Law constant) is not a function of time or location within the reactor. Then:

$$\frac{1}{H} \frac{\partial C_G}{\partial z} = \frac{\partial C_L}{\partial z} \quad (7)$$

$$\frac{1}{H} \frac{\partial C_G}{\partial t} = \frac{\partial C_L}{\partial t} \quad (8)$$

Substitute (7) and (8) into (4) and add (3) and (4) together:

$$\left(\epsilon_G \mathcal{D}_G + \frac{\epsilon_L}{H} \mathcal{D}_L \right) \frac{\partial^2 C_G}{\partial z^2} - U_G \frac{\partial C_G}{\partial z} = \left(\epsilon_G + \frac{\epsilon_L}{H} \right) \frac{\partial C_G}{\partial t} \quad (9)$$

Rearrange (9) to get:

$$\frac{\mathcal{D}_G \epsilon_G + \mathcal{D}_L \frac{\epsilon_L}{H}}{\epsilon_G + \frac{\epsilon_L}{H}} \frac{\partial^2 C_G}{\partial z^2} - \frac{U_G}{\epsilon_G + \frac{\epsilon_L}{H}} \frac{\partial C_G}{\partial z} = \frac{\partial C_G}{\partial t} \quad (10)$$

or:

$$\mathcal{D}_{EFF} \frac{\partial^2 C_G}{\partial z^2} - U_{EFF} \frac{\partial C_G}{\partial z} = \frac{\partial C_G}{\partial t} \quad (11)$$

where:

$$\mathcal{D}_{EFF} = \frac{\mathcal{D}_G + \frac{\epsilon_L}{\epsilon_G H} \mathcal{D}_L}{1 + \frac{\epsilon_L}{\epsilon_G H}} \quad (12)$$

and
$$U_{EFF} = \frac{U_G}{\epsilon_G + \epsilon_L/H} \quad (13)$$

Rearranging (13) to solve for H gives:

$$H = \frac{U_{EFF} \epsilon_G}{U_G - U_{EFF} \epsilon_G} \quad (14)$$

APPENDIX F: Derivation of Equations (23) - (28)

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APPENDIX F

Derivation of Equations (23) through (28):

From Brenner:

$$C(x,t) = 2 \exp[P(2x-t^*)] \sum_{k=1}^{\infty} \frac{P \lambda_k}{(\lambda_k^2 + P^2 + P)(\lambda_k^2 + P^2)} [\lambda_k \cos 2 \lambda_k x + P \sin 2 \lambda_k x] * \exp(-\lambda_k^2 t^*/P) \quad (1)$$

This equation is the solution for a step change problem with the same boundary conditions as for our reactor. To find the response of a delta function, differentiate Brenner's solution, $C(x,t)$, with respect to t . This will give the correct solution for the concentration, $C(x,t)$, as applied to the delta function problem.

$$C^* = -\frac{dC}{dt} = 2P \exp[P(2x-t^*)] \sum_{k=1}^{\infty} \frac{P \lambda_k}{(\lambda_k^2 + P^2 + P)(\lambda_k^2 + P^2)} [\lambda_k \cos 2 \lambda_k x + P \sin 2 \lambda_k x] * \exp(-\lambda_k^2 t^*/P) + 2 \exp[P(2x-t^*)] \sum_{k=1}^{\infty} \frac{\lambda_k^2}{P} \frac{P \lambda_k}{(\lambda_k^2 + P^2 + P)(\lambda_k^2 + P^2)} [\lambda_k \cos 2 \lambda_k x + P \sin 2 \lambda_k x] * \exp(-\lambda_k^2 t^*/P) \quad (2)$$

Simplify:

$$C^* = \frac{2}{P} \exp[P(2x-t^*)] \sum_{k=1}^{\infty} P^2 \frac{P \lambda_k}{(\lambda_k^2 + P^2 + P)(\lambda_k^2 + P^2)} [\lambda_k \cos 2 \lambda_k x + P \sin 2 \lambda_k x] * \exp(-\lambda_k^2 t^*/P) + \lambda_k^2 \frac{P \lambda_k}{(\lambda_k^2 + P^2 + P)(\lambda_k^2 + P^2)} [\lambda_k \cos 2 \lambda_k x + P \sin 2 \lambda_k x] * \exp(-\lambda_k^2 t^*/P) \quad (3)$$

Combine the two summation terms, cancel a P term, and cancel $(P^2 + \lambda_k^2)$ from the numerator and denominator.

$$C^* = 2 \exp[P(2x-t^*)] \sum_{k=1}^{\infty} \frac{\lambda_k}{(\lambda_k^2 + P^2 + P)} [\lambda_k \cos 2 \lambda_k x + P \sin 2 \lambda_k x] * \exp(-\lambda_k^2 t^*/P) \quad (4)$$

Substitute the following definitions:

$$P = \frac{Pe}{4} = \frac{UL}{4D} \quad (5)$$

$$x = z/L \quad (6)$$

$$\alpha_n = 2\lambda_k \quad (7)$$

To give:

$$C^* = 2 \exp\left[\frac{Pe(2z-t^*)}{4L}\right] \sum_{n=1}^{\infty} \frac{\alpha_n/2}{(\alpha_n^2/4 + Pe^2/16 + Pe/4)} \left[\alpha_n/2 \cos \alpha_n z/L + Pe/4 \sin \alpha_n z/L \right] * \exp(-\alpha_n^2 t^*/Pe) \quad (8)$$

Multiply numerator and denominator by 16/16 and factor a 1/2 out of the summation.

$$C^* = \exp\left[\frac{Pe(2z-t^*)}{4L}\right] \sum_{n=1}^{\infty} \frac{8\alpha_n}{4(\alpha_n^2 + Pe) + Pe^2} \left[\alpha_n \cos \alpha_n z/L + Pe/2 \sin \alpha_n z/L \right] * \exp(-\alpha_n^2 t^*/Pe) \quad (9)$$

Combine exponential terms:

$$C^* = \sum_{n=1}^{\infty} \frac{8\alpha_n}{4(\alpha_n^2 + Pe) + Pe^2} \left[\alpha_n \cos \alpha_n z/L + Pe/2 \sin \alpha_n z/L \right] * \exp\left(\frac{Pe z}{2L} - \frac{Pe t^*}{4} - \frac{\alpha_n^2 t^*}{Pe}\right) \quad (10)$$

Define

$$f_n = \frac{8\alpha_n}{4(\alpha_n^2 + Pe) + Pe^2} \left[\alpha_n \cos \alpha_n z/L + Pe/2 \sin \alpha_n z/L \right] \exp\left(\frac{Pe z}{2L}\right) \quad (11)$$

Then:

$$C^* = \sum_{n=1}^{\infty} f_n \exp\left(-\left(\frac{Pe}{4} + \frac{\alpha_n^2}{Pe}\right) t^*\right) \quad (12)$$

Define $A_n = \alpha_n^2 + Pe^2/4$

$$C^* = \sum_{n=1}^{\infty} f_n \exp\left(-\frac{A_n t^*}{Pe}\right) \quad (13)$$

Brenner's t is a dimensionless t defined as

$$t^* = t U/L \quad (14)$$

Substitute for t and the definition of the Peclet number (UL/D).

$$C^* = \sum_{n=1}^{\infty} f_n \exp\left(-\frac{A_n t D}{L^2}\right) \quad (15)$$

Brenner states that λ_k is the solution to

$$\lambda_k \tan \lambda_k - P = 0 \quad (16)$$

$$\lambda_k \cot \lambda_k + P = 0 \quad (17)$$

Substituting the definition for $\alpha_n = 2 \lambda_k$

$$\frac{\alpha_n}{2^n} \tan \frac{\alpha_n}{2^n} - \frac{Pe}{4} = 0 \quad (18)$$

$$\frac{\alpha_n}{2^n} \cot \frac{\alpha_n}{2^n} + \frac{Pe}{4} = 0 \quad (19)$$

Brenner defines his normalization factor as

$$\bar{C} = \int_0^1 C(x, t) dx \quad (20)$$

This is appropriate for a step change where the net quantity before the change or a long time after it, is not a function of time. For our system, a pulse function, the normalization factor is :

$$\bar{C} = \int_0^\infty \tilde{C}(x_0, t^*) dt^* \quad (21)$$

where x_0 is any fixed value of x for which dC/dx is zero. For our problem, L satisfies this condition. t is Brenner's dimensionless time which is defined in equation (14). By substitution of (14) into (21), the following normalization factor is obtained.

$$\bar{C} = \frac{U}{L} \int_0^\infty C(L, t) dt \quad (22)$$

APPENDIX G: Dispersion Model: Individual Detectors Best Fit Parameters

Individual Detectors - Best Fit Parameters

Detector		Slurry Mean		Norm of Residuals	Difference in Centroids (sec)	Position z (ft)	Total Height L (ft)	Reject If Norm > 0.09
		Dispersion D/(L*L) (1/sec)	Residence Time (sec)					
1	2	0.00663	69.77	0.120	2.39	25.00	18.08	yes
	3	0.00580	49.90	0.080	1.03	20.42	18.08	no
	4	0.00719	60.93	0.100	3.66	20.42	18.08	yes
	5	0.00781	59.63	0.080	2.86	20.42	18.08	no
	6	0.00791	56.89	0.080	2.82	20.42	18.08	no
	7	0.00552	49.34	0.080	0.56	19.17	18.08	no
	8	0.00683	51.13	0.070	0.63	19.17	18.08	no
	9	0.00622	52.56	0.070	0.79	19.17	18.08	no
	10	0.00648	50.60	0.060	0.38	19.17	18.08	no
	11	0.00756	36.29	0.060	0.03	12.67	18.08	no
	12	0.01662	74.65	0.300	12.69	12.67	18.08	yes
	13	0.00905	47.12	0.160	9.45	12.67	18.08	yes
	14	0.00704	38.82	0.040	0.90	12.67	18.08	no
	15	0.00758	49.90	0.170	9.35	7.17	18.08	yes
	16	0.00517	43.29	0.050	0.14	7.17	18.08	no
	17	0.00477	37.15	0.050	1.28	3.67	18.08	no
	18	0.01166	22.53	0.140	8.19	3.67	18.08	yes
	19	0.01389	25.83	0.200	22.34	3.67	18.08	yes
	20	0.00734	27.86	0.120	4.07	3.67	18.08	yes
2	2	0.00645	69.18	0.130	2.85	25.00	18.08	yes
	3	0.00547	51.66	0.110	2.40	20.42	18.08	yes
	4	0.00706	56.60	0.080	3.00	20.42	18.08	no
	5	0.00687	56.21	0.080	3.02	20.42	18.08	no
	6	0.00621	55.72	0.090	3.57	20.42	18.08	yes
	7	0.00946	48.31	0.140	2.48	19.17	18.08	yes
	8	0.00678	51.67	0.070	0.13	19.17	18.08	no
	9	0.00627	51.05	0.070	0.08	19.17	18.08	no
	10	0.00581	50.75	0.070	1.60	19.17	18.08	no
	11	0.00721	35.71	0.060	1.53	12.67	18.08	no
	12	0.01863	78.86	0.330	13.19	12.67	18.08	yes
	13	0.00984	44.42	0.180	11.35	12.67	18.08	yes
	14	0.00768	36.82	0.060	1.14	12.67	18.08	no
	15	0.00751	43.04	0.150	10.44	7.17	18.08	yes
	16	0.00555	41.28	0.060	0.37	7.17	18.08	no
	17	0.00410	35.65	0.050	2.47	3.67	18.08	no
	13	0.01163	21.00	0.180	12.57	3.67	18.08	yes
	19	0.01131	26.39	0.210	23.69	3.67	18.08	yes
	20	0.00476	31.26	0.060	1.24	3.67	18.08	no

Individual Detectors - Best Fit Parameters

Detector		Slurry Mean		Norm of Residuals	Difference in Centroids	Position z (ft)	Total Height L (ft)	Reject If Norm > 0.09
		Dispersion D/(L*L) (1/sec)	Residence Time (sec)					
3	2	0.00725	72.73	0.160	3.55	25.00	18.00	yes
	3	0.00594	51.80	0.130	2.90	20.42	18.00	yes
	4	0.00598	57.13	0.110	3.82	20.42	18.00	yes
	5	0.00694	56.74	0.100	3.11	20.42	18.00	yes
	6	0.00697	54.72	0.100	4.05	20.42	18.00	yes
	7	0.00650	51.80	0.100	1.33	19.17	18.00	yes
	8	0.00715	54.46	0.090	0.73	19.17	18.00	yes
	9	0.00608	54.35	0.090	0.81	19.17	18.00	yes
	10	0.00567	50.94	0.060	0.93	19.17	18.00	no
	11	0.00620	36.21	0.070	1.97	12.67	18.00	no
	12	0.01658	71.29	0.350	20.97	12.67	18.00	yes
	13	0.00943	44.11	0.190	12.81	12.67	18.00	yes
	14	0.00661	37.54	0.070	2.90	12.67	18.00	no
	15	0.00876	40.39	0.150	10.25	7.17	18.00	yes
	16	0.00510	42.22	0.060	0.93	7.17	18.00	no
	17	0.00375	34.84	0.100	3.17	3.67	18.00	yes
	18	0.01063	20.76	0.190	12.20	3.67	18.00	yes
	19	0.01065	26.85	0.200	20.42	3.67	18.00	yes
	20	0.00562	27.73	0.110	1.61	3.67	18.00	yes
4	2	0.00573	33.17	0.080	0.06	25.00	19.83	no
	3	0.00865	21.57	0.060	0.34	17.17	19.83	no
	4	0.01117	24.19	0.100	2.82	17.17	19.83	yes
	5	0.01163	25.83	0.130	4.33	17.17	19.83	yes
	6	0.01012	24.50	0.090	2.82	17.17	19.83	yes
	7	0.00832	25.46	0.060	0.41	20.67	19.83	no
	8	0.00814	26.90	0.060	0.27	20.67	19.83	no
	9	0.00834	26.67	0.060	0.14	20.67	19.83	no
	10	0.00786	25.94	0.060	0.41	20.67	19.83	no
	11	0.00763	22.36	0.060	0.62	12.67	19.83	no
	12	0.01123	26.80	0.160	4.16	12.67	19.83	yes
	13	0.01117	26.06	0.160	4.24	12.67	19.83	yes
	14	0.01024	24.19	0.110	3.63	12.67	19.83	yes
	15	0.00885	24.59	0.190	6.23	7.17	19.83	yes
	16	0.00623	24.14	0.060	1.25	7.17	19.83	no
	17	0.00504	21.53	0.060	0.93	3.67	19.83	no
	18	0.00887	15.94	0.160	5.08	3.67	19.83	yes
	19	0.01131	17.95	0.180	10.19	3.67	19.83	yes
	20	0.00714	17.21	0.100	1.44	3.67	19.83	yes

Individual Detectors - Best Fit Parameters

Detector		Slurry Mean		Norm of Residuals	Difference in Centroids (sec)	Position z (ft)	Total Height L (ft)	Reject If Norm > 0.09
		Dispersion D/(L*L) (1/sec)	Residence Time (sec)					
5	2	0.00719	33.57	0.080	0.58	25.00	19.75	no
	3	0.00840	21.41	0.060	0.58	17.17	19.75	no
	4	0.01024	23.82	0.080	1.83	17.17	19.75	no
	5	0.01111	24.59	0.090	2.46	17.17	19.75	yes
	6	0.01078	24.32	0.080	2.45	17.17	19.75	no
	7	0.00791	26.11	0.090	0.73	20.67	19.75	yes
	8	0.00682	27.94	0.080	0.72	20.67	19.75	no
	9	0.00730	27.56	0.070	0.03	20.67	19.75	no
	10	0.00824	26.41	0.070	0.83	20.67	19.75	no
	11	0.00942	21.39	0.100	0.37	12.67	19.75	yes
	12	0.01272	26.16	0.150	4.51	12.67	19.75	yes
	13	0.01274	26.53	0.160	4.50	12.67	19.75	yes
	14	0.00987	24.56	0.100	2.36	12.67	19.75	yes
	15	0.01055	24.79	0.160	5.73	7.17	19.75	yes
	16	0.00857	22.30	0.080	0.73	7.17	19.75	no
	17	0.00562	21.24	0.040	0.58	3.67	19.75	no
	18	0.00974	15.97	0.100	3.43	3.67	19.75	yes
	19	0.01313	17.81	0.170	8.81	3.67	19.75	yes
	20	0.00920	17.64	0.100	3.54	3.67	19.75	yes
6	2	0.00377	32.82	0.090	1.33	25.00	19.75	yes
	3	0.00375	23.25	0.210	2.53	17.17	19.75	yes
	4	0.00537	25.87	0.210	3.95	17.17	19.75	yes
	5	0.00510	25.56	0.210	3.65	17.17	19.75	yes
	6	0.00453	25.29	0.200	3.58	17.17	19.75	yes
	7	0.00394	28.87	0.160	1.04	20.67	19.75	yes
	8	0.00356	29.26	0.110	1.67	20.67	19.75	yes
	9	0.00412	28.85	0.130	1.59	20.67	19.75	yes
	10	0.00423	28.42	0.140	1.18	20.67	19.75	yes
	11	0.00364	26.27	0.260	2.67	12.67	19.75	yes
	12	0.00517	29.73	0.290	5.52	12.67	19.75	yes
	13	0.00485	28.69	0.290	6.51	12.67	19.75	yes
	14	0.00382	27.87	0.260	4.15	12.67	19.75	yes
	15	0.00390	29.96	0.410	8.13	7.17	19.75	yes
	16	0.00329	30.85	0.390	3.32	7.17	19.75	yes
	17	0.00334	23.70	0.530	5.14	3.67	19.75	yes
	18	0.00436	17.98	0.570	8.74	3.67	19.75	yes
	19	0.00512	17.94	0.570	8.36	3.67	19.75	yes
	20	0.00442	20.37	0.540	5.33	3.67	19.75	yes

Individual Detectors - Best Fit Parameters

Detector		Slurry Mean		Norm of Residuals	Difference in Centroids (sec)	Position z (ft)	Total Height L (ft)	Reject If Norm > 0.09
		Dispersion D/(L*L) (1/sec)	Residence Time (sec)					
7	2	0.00623	27.57	0.050	0.88	25.00	20.17	no
	3	0.00896	18.72	0.060	0.59	17.17	20.17	no
	4	0.01153	21.44	0.120	2.27	17.17	20.17	yes
	5	0.01186	22.12	0.130	3.90	17.17	20.17	yes
	6	0.01135	20.87	0.080	2.05	17.17	20.17	no
	7	0.00820	21.75	0.050	0.25	20.67	20.17	no
	8	0.00868	22.81	0.070	0.88	20.67	20.17	no
	9	-	-	1.000	250.49	20.67	20.17	yes
	10	0.00835	22.03	0.050	0.16	20.67	20.17	no
	11	0.00982	18.69	0.100	0.82	12.67	20.17	yes
	12	0.01224	22.76	0.150	3.50	12.67	20.17	yes
	13	-	-	0.590	59.52	12.67	20.17	yes
	14	0.01065	21.61	0.100	2.68	12.67	20.17	yes
	15	0.01253	18.78	0.180	3.90	7.17	20.17	yes
	16	0.00729	21.72	0.100	0.88	7.17	20.17	yes
	17	0.00686	18.83	0.120	0.74	3.67	20.17	yes
	18	0.01027	13.57	0.140	2.58	3.67	20.17	yes
	19	0.01121	15.96	0.210	9.33	3.67	20.17	yes
	20	0.00872	16.13	0.140	2.90	3.67	20.17	yes
8	2	0.00614	27.91	0.070	0.33	25.00	19.92	no
	3	0.01029	18.28	0.080	0.68	17.17	19.92	no
	4	0.01188	20.21	0.100	2.35	17.17	19.92	yes
	5	0.01224	21.48	0.100	2.05	17.17	19.92	yes
	6	0.01160	20.78	0.080	1.82	17.17	19.92	no
	7	0.00813	21.60	0.090	0.39	20.67	19.92	yes
	8	0.00828	21.90	0.060	0.26	20.67	19.92	no
	9	0.00802	21.34	0.090	0.47	20.67	19.92	yes
	10	0.00830	21.97	0.050	0.31	20.67	19.92	no
	11	0.00992	18.67	0.100	0.77	12.67	19.92	yes
	12	0.01300	22.62	0.190	4.79	12.67	19.92	yes
	13	-	-	1.000	258.41	12.67	19.92	yes
	14	0.01232	21.33	0.100	2.35	12.67	19.92	yes
	15	0.01166	19.52	0.260	4.43	7.17	19.92	yes
	16	0.00612	22.85	0.070	0.55	7.17	19.92	no
	17	0.00582	19.31	0.090	0.80	3.67	19.92	yes
	18	0.00692	16.49	0.130	3.45	3.67	19.92	yes
	19	0.00675	16.23	0.110	0.78	3.67	19.92	yes
	20	0.00734	17.35	0.100	2.09	3.67	19.92	yes

Individual Detectors - Best Fit Parameters

Detector		Slurry Mean		Norm of Residuals	Difference in Centroids (sec)	Position z (ft)	Total Height L (ft)	Reject if Norm > 0.09
		Dispersion D/(L*L) (1/sec)	Residence Time (sec)					
9	2	0.00533	28.73	0.090	0.95	25.00	19.92	yes
	3	0.00934	18.80	0.070	0.62	17.17	19.92	no
	4	0.01071	20.96	0.110	2.13	17.17	19.92	yes
	5	0.00995	20.97	0.110	1.79	17.17	19.92	yes
	6	0.01050	20.68	0.080	1.90	17.17	19.92	no
	7	0.00704	21.66	0.090	0.44	20.67	19.92	yes
	8	0.00731	22.40	0.060	0.13	20.67	19.92	no
	9	0.00724	21.61	0.090	0.44	20.67	19.92	yes
	10	0.00745	22.57	0.070	0.59	20.67	19.92	no
	11	0.00889	19.17	0.090	0.61	12.67	19.92	yes
	12	0.01183	22.40	0.150	3.28	12.67	19.92	yes
	13	-	-	0.760	12.43	12.67	19.92	yes
	14	0.00995	21.31	0.110	3.08	12.67	19.92	yes
	15	0.00800	22.40	1.000	578.93	7.17	19.92	yes
	16	0.00685	22.00	0.070	0.70	7.17	19.92	no
	17	0.00727	20.04	0.080	1.19	3.67	19.92	no
	18	-	-	0.730	140.01	3.67	19.92	yes
	19	0.01039	17.58	0.170	6.70	3.67	19.92	yes
	20	0.00828	17.28	0.090	2.95	3.67	19.92	yes
10	2	0.00639	28.44	0.100	0.53	25.00	19.75	yes
	3	0.00925	19.22	0.090	1.45	17.17	19.75	yes
	4	0.01137	21.51	0.130	2.46	17.17	19.75	yes
	5	0.01040	20.67	0.120	2.08	17.17	19.75	yes
	6	0.01012	20.43	0.060	0.59	17.17	19.75	no
	7	0.00734	22.96	0.090	0.25	20.67	19.75	yes
	8	0.00837	24.14	0.100	0.24	20.67	19.75	yes
	9	0.00857	23.31	0.090	0.01	20.67	19.75	yes
	10	0.00799	23.17	0.080	0.17	20.67	19.75	no
	11	0.00882	20.35	0.090	1.10	12.67	19.75	yes
	12	-	-	0.690	55.27	12.67	19.75	yes
	13	-	-	0.400	15.50	12.67	19.75	yes
	14	0.00931	21.11	0.100	1.29	12.67	19.75	yes
	15	-	-	0.710	107.65	7.17	19.75	yes
	16	0.00868	21.09	0.130	1.60	7.17	19.75	yes
	17	0.00616	21.30	0.080	1.60	3.67	19.75	no
	18	-	-	0.740	123.70	3.67	19.75	yes
	19	-	-	0.830	156.84	3.67	19.75	yes
	20	0.00780	15.69	0.120	1.09	3.67	19.75	yes

Individual Detectors - Best Fit Parameters

Detector		Slurry Mean		Norm of Residuals	Difference in Centroids (sec)	Position z (ft)	Total Height L (ft)	Reject if Norm > 0.09
		Dispersion D/(L*L) (1/sec)	Residence Time (sec)					
b1	2	0.01383	30.67	0.190	2.77	25.00	13.92	yes
	3	0.01306	15.75	0.060	0.58	11.67	13.92	no
	4	0.01996	19.05	0.170	6.70	11.67	13.92	yes
	5	0.02181	18.86	0.190	7.39	11.67	13.92	yes
	6	0.01429	16.68	0.060	1.01	11.67	13.92	no
	7	0.01443	18.46	0.050	0.44	14.67	13.92	no
	8	0.01761	21.12	0.130	4.39	14.67	13.92	yes
	9	0.01669	19.68	0.090	3.74	14.67	13.92	yes
	10	0.01560	18.96	0.060	1.09	14.67	13.92	no
	11	0.01208	16.10	0.080	1.16	8.67	13.92	no
	12	0.01891	20.23	0.230	9.71	8.67	13.92	yes
	13	0.02380	23.47	0.200	1.14	8.67	13.92	yes
	14	0.01204	17.69	0.100	3.38	8.67	13.92	yes
	15	0.01294	18.21	0.150	6.29	6.00	13.92	yes
	16	0.01235	16.44	0.130	0.72	6.00	13.92	yes
	17	0.01050	13.96	0.100	1.78	3.67	13.92	yes
	18	0.01414	10.43	0.160	0.67	3.67	13.92	yes
	19	0.01301	11.06	0.130	0.97	3.67	13.92	yes
	20	0.01077	13.19	0.080	0.97	3.67	13.92	no
b2	2	0.01560	30.22	0.170	3.21	25.00	13.92	yes
	3	0.01347	15.33	0.050	0.61	11.67	13.92	no
	4	0.01868	17.88	0.140	5.19	11.67	13.92	yes
	5	0.02119	19.86	0.190	7.56	11.67	13.92	yes
	6	0.01375	16.68	0.040	0.50	11.67	13.92	no
	7	0.01476	18.09	0.060	0.00	14.67	13.92	no
	8	0.01548	20.75	0.110	3.57	14.67	13.92	yes
	9	0.01615	19.87	0.100	3.18	14.67	13.92	yes
	10	0.01450	18.61	0.050	1.01	14.67	13.92	no
	11	0.01440	15.84	0.090	1.35	8.67	13.92	yes
	12	0.01780	19.90	0.200	8.19	8.67	13.92	yes
	13	0.01534	19.10	0.180	7.55	8.67	13.92	yes
	14	-	-	-	-	8.67	13.92	yes
	15	0.01525	16.17	0.150	5.37	6.00	13.92	yes
	16	0.00943	17.53	0.100	1.67	6.00	13.92	yes
	17	0.01227	13.68	0.110	2.33	3.67	13.92	yes
	18	0.01523	10.61	0.130	0.43	3.67	13.92	yes
	19	0.01241	12.51	0.090	0.60	3.67	13.92	yes
	20	0.01156	13.10	0.120	1.42	3.67	13.92	yes

Individual Detectors - Best Fit Parameters

Detector		Slurry Mean		Norm of Residuals	Difference in Centroids (sec)	Position z (ft)	Total Height L (ft)	Reject if Norm > 0.09
		Dispersion D/(L*L) (1/sec)	Residence Time (sec)					
b3	2	0.01448	29.74	0.170	2.69	25.00	13.83	yes
	3	0.01625	15.45	0.070	0.91	11.67	13.83	no
	4	0.02064	17.50	0.140	5.54	11.67	13.83	yes
	5	0.02441	19.35	0.200	7.78	11.67	13.83	yes
	6	0.01783	16.08	0.060	0.70	11.67	13.83	no
	7	0.01687	18.09	0.060	0.33	14.67	13.83	no
	8	0.01982	20.96	0.140	4.99	14.67	13.83	yes
	9	0.01860	20.09	0.100	3.43	14.67	13.83	yes
	10	0.01690	18.74	0.070	1.34	14.67	13.83	no
	11	0.01278	16.38	0.070	0.74	8.67	13.83	no
	12	0.01875	20.62	0.220	8.40	8.67	13.83	yes
	13	0.01740	19.10	0.200	7.46	8.67	13.83	yes
	14	0.01521	17.12	0.100	2.68	8.67	13.83	yes
	15	0.01464	18.31	0.160	5.75	6.00	13.83	yes
	16	0.01338	15.67	0.140	1.06	6.00	13.83	yes
	17	0.01070	15.16	0.070	1.31	3.67	13.83	no
	18	0.01521	11.24	0.130	0.50	3.67	13.83	yes
	19	0.01707	10.45	0.130	0.80	3.67	13.83	yes
	20	0.01118	14.06	0.060	1.01	3.67	13.83	no
b4	2	-	-	0.330	11.80	25.00	12.42	yes
	3	-	-	0.330	12.03	20.42	12.42	yes
	4	-	-	0.320	12.49	20.42	12.42	yes
	5	-	-	0.320	11.91	20.42	12.42	yes
	6	-	-	0.310	11.80	20.42	12.42	yes
	7	0.01721	34.80	0.100	3.90	13.00	12.42	yes
	8	-	-	-	-	13.00	12.42	yes
	9	0.01838	46.93	0.140	6.45	13.00	12.42	yes
	10	0.01742	39.04	0.120	3.89	13.00	12.42	yes
	11	0.01111	24.25	0.070	1.23	8.67	12.42	no
	12	-	-	-	-	8.67	12.42	yes
	13	0.01861	32.97	0.230	17.31	8.67	12.42	yes
	14	-	-	-	-	8.67	12.42	yes
	15	0.01679	24.92	0.140	7.92	6.00	12.42	yes
	16	0.01023	27.76	0.060	2.49	6.00	12.42	no
	17	0.00760	21.93	0.050	0.39	3.67	12.42	no
	18	0.01819	13.93	0.120	0.89	3.67	12.42	yes
	19	0.01677	16.12	0.090	1.20	3.67	12.42	yes
	20	0.00920	21.02	0.070	1.41	3.67	12.42	no

Individual Detectors - Best Fit Parameters

Detector	Slurry Mean		Norm of Residuals	Difference in Centroids (sec)	Position z (ft)	Total Height L (ft)	Reject if Norm > 0.09
	Dispersion D/(L*L) (1/sec)	Residence Time (sec)					
b5 2	-	-	-	-	-	-	yes
3	-	-	0.350	14.82	20.42	12.25	yes
4	-	-	0.370	14.91	20.42	12.25	yes
5	-	-	0.370	14.42	20.42	12.25	yes
6	-	-	0.390	16.23	20.42	12.25	yes
7	0.02101	38.17	0.100	2.03	13.00	12.25	yes
8	0.02187	44.49	0.130	5.98	13.00	12.25	yes
9	0.01657	48.11	0.130	4.99	13.00	12.25	yes
10	0.01853	41.71	0.110	1.18	13.00	12.25	yes
11	0.01320	23.26	0.080	1.91	8.67	12.25	no
12	0.01898	35.01	0.270	21.57	8.67	12.25	yes
13	0.01811	33.14	0.260	22.41	8.67	12.25	yes
14	0.01255	25.44	0.070	3.86	8.67	12.25	no
15	0.01572	26.98	0.160	13.72	6.00	12.25	yes
16	0.01131	24.08	0.080	3.01	6.00	12.25	no
17	0.01031	20.55	0.100	2.34	3.67	12.25	yes
18	0.01714	13.35	0.120	1.17	3.67	12.25	yes
19	0.01859	14.68	0.090	2.28	3.67	12.25	yes
20	0.01036	20.28	0.050	0.97	3.67	12.25	no
b6 2	-	-	0.340	12.54	25.00	12.25	yes
3	-	-	0.300	10.46	20.42	12.25	yes
4	-	-	0.300	12.65	20.42	12.25	yes
5	-	-	0.310	11.77	20.42	12.25	yes
6	-	-	0.310	12.52	20.42	12.25	yes
7	0.01728	35.58	0.140	5.41	13.00	12.25	yes
8	0.01950	42.81	0.180	10.27	13.00	12.25	yes
9	0.01921	42.43	0.170	10.36	13.00	12.25	yes
10	0.01661	36.57	0.110	4.06	13.00	12.25	yes
11	-	-	0.560	17.13	8.67	12.25	yes
12	0.01792	28.50	0.210	15.91	8.67	12.25	yes
13	0.01695	31.22	0.220	17.43	8.67	12.25	yes
14	0.01271	26.37	0.080	5.28	8.67	12.25	no
15	0.01459	26.92	0.160	10.20	6.00	12.25	yes
16	0.01054	27.04	0.100	8.31	6.00	12.25	yes
17	0.00918	20.59	0.060	0.52	3.67	12.25	no
18	0.01792	14.90	0.210	15.37	3.67	12.25	yes
19	0.01446	15.08	0.140	1.52	3.67	12.25	yes
20	0.01020	19.67	0.090	2.93	3.67	12.25	yes

Individual Detectors - Best Fit Parameters

Detector		Slurry Mean		Norm of Residuals	Difference in Centroids (sec)	Position z (ft)	Total Height L (ft)	Reject if Norm > 0.09
		Dispersion D/(L*L) (1/sec)	Residence Time (sec)					
b7	2	-	-	0.350	19.25	25.00	11.67	yes
	3	-	-	0.370	21.23	20.42	11.67	yes
	4	-	-	0.410	24.66	20.42	11.67	yes
	5	-	-	0.390	22.32	20.42	11.67	yes
	6	-	-	0.420	23.66	20.42	11.67	yes
	7	0.02037	59.45	0.090	2.72	12.33	11.67	yes
	8	-	-	0.350	9.21	12.33	11.67	yes
	9	0.01852	77.20	0.110	5.19	12.33	11.67	yes
	10	0.01592	70.47	0.080	1.52	12.33	11.67	no
	11	-	-	0.560	27.93	8.67	11.67	yes
	12	0.01790	41.16	0.210	23.24	8.67	11.67	yes
	13	0.01550	44.20	0.220	28.34	8.67	11.67	yes
	14	0.01107	34.15	0.060	4.81	8.67	11.67	no
	15	0.01665	33.70	0.140	17.34	6.00	11.67	yes
	16	0.01012	32.52	0.070	0.34	6.00	11.67	no
	17	0.00997	26.79	0.060	3.39	3.67	11.67	no
	18	0.02122	18.07	0.180	15.72	3.67	11.67	yes
	19	0.01905	17.80	0.140	2.07	3.67	11.67	yes
	20	0.01040	26.00	0.060	1.45	3.67	11.67	no
b8	2	-	-	0.420	26.27	25.00	11.67	yes
	3	-	-	0.390	24.27	20.42	11.67	yes
	4	-	-	0.400	24.39	20.42	11.67	yes
	5	-	-	0.430	26.10	20.42	11.67	yes
	6	-	-	0.420	26.16	20.42	11.67	yes
	7	0.02317	57.07	0.070	2.69	12.33	11.67	no
	8	-	-	0.360	6.11	12.33	11.67	yes
	9	0.02238	67.17	0.110	4.98	12.33	11.67	yes
	10	0.01708	69.06	0.090	0.21	12.33	11.67	yes
	11	-	-	0.570	24.05	8.67	11.67	yes
	12	-	-	0.450	2.55	8.67	11.67	yes
	13	0.01595	42.95	0.210	27.47	8.67	11.67	yes
	14	0.01136	33.46	0.040	3.46	8.67	11.67	no
	15	-	-	0.490	12.26	6.00	11.67	yes
	16	0.01247	30.62	0.080	1.15	6.00	11.67	no
	17	0.00863	27.86	0.080	4.66	3.67	11.67	no
	18	0.02438	16.55	0.160	14.37	3.67	11.67	yes
	19	0.02040	18.41	0.100	1.99	3.67	11.67	yes
	20	0.00970	27.15	0.050	2.51	3.67	11.67	no

Individual Detectors - Best Fit Parameters

Detector	Slurry Mean		Norm of Residuals	Difference in Centroids (sec)	Position z (ft)	Total Height L (ft)	Reject if Norm > 0.09
	Dispersion D/(L*L) (1/sec)	Residence Time (sec)					
b9 2	—	—	0.410	26.92	25.00	11.67	yes
3	—	—	0.400	24.69	20.42	11.67	yes
4	—	—	0.410	27.89	20.42	11.67	yes
5	—	—	0.420	28.49	20.42	11.67	yes
6	—	—	0.430	28.73	20.42	11.67	yes
7	0.02630	64.01	0.090	1.15	12.33	11.67	yes
8	0.02764	68.19	0.120	2.36	12.33	11.67	yes
9	0.02307	74.56	0.110	0.16	12.33	11.67	yes
10	0.01536	74.28	0.110	2.63	12.33	11.67	yes
11	—	—	0.600	33.73	8.67	11.67	yes
12	—	—	0.430	13.94	8.67	11.67	yes
13	0.01445	41.94	0.200	27.34	8.67	11.67	yes
14	0.01100	34.35	0.060	5.13	8.67	11.67	no
15	0.01938	31.68	0.150	16.45	6.00	11.67	yes
16	0.01141	33.47	0.080	0.52	6.00	11.67	no
17	0.00924	25.49	0.080	2.18	3.67	11.67	no
18	0.02520	16.32	0.240	16.71	3.67	11.67	yes
19	0.01675	19.20	0.140	1.99	3.67	11.67	yes
20	0.00837	27.53	0.070	2.88	3.67	11.67	no

APPENDIX H: Calculation of the Number of CSTR's for a Commercial Scale
Application of LPMEOH

APPENDIX H

Calculation of the Number of CSTR's for a Commerical Scale Application of LPMEOH

1. Calculate $\mathcal{D}_L$

$$\mathcal{D}_L = 0.667 (gD^4U_g)^{1/3}$$

$$D = 12.8 \text{ ft}$$

$$U_g = 0.7 \text{ ft/sec}$$

$$g = 32.2 \text{ ft/sec}^2$$

$$\mathcal{D}_L = 0.667 [(32.2)(12.8)^4(0.7)]^{1/3}$$

$$\mathcal{D}_L = 56.16 \text{ ft}^2/\text{sec}$$

2. Calculate $\mathcal{D}_G$

$$\mathcal{D}_G = 4.421 D^{1.5} U_g^{1.8}$$

$$= 4.421 (12.8)^{1.5} (0.7)^{1.8}$$

$$\mathcal{D}_G = 106.52 \text{ ft}^2/\text{sec}$$

3. Calculate U_{EFF}

$$U_{EFF} = \frac{U_g}{\epsilon_G + \frac{\epsilon_L}{H}}$$

Calculate a molar average Henry's law constant assuming outlet composition.

$$\text{Use } \bar{H} = 5.62$$

$$\epsilon_G = 0.40$$

$$\epsilon_{SL} = 0.05$$

$$\epsilon_L = (1 - \epsilon_G)(1 - \epsilon_{SL})$$

$$\epsilon_L = (0.60)(0.95) = 0.57$$

$$U_{EFF} = \frac{0.7}{0.4 + \frac{0.57}{5.62}}$$

$$U_{EFF} = 1.40 \text{ ft/sec}$$

4. Calculate $\mathcal{D}_{EFF}$

$$\mathcal{D}_{EFF} = \frac{\mathcal{D}_G + \eta \mathcal{D}_L}{(1 + \eta)}$$

$$\eta = \frac{U_G - \epsilon_G U_{EFF}}{\epsilon_G U_{EFF}}$$

$$\eta = \frac{0.7 - 0.4(1.40)}{0.40(1.40)} = 0.25$$

$$\mathcal{D}_{EFF} = \frac{106.52 + 0.250(56.16)}{(1 + 0.25)}$$

$$\mathcal{D}_{EFF} = 96.45 \text{ ft}^2/\text{sec}$$

5. Calculate Peclet number

$$Pe_{EFF} = \frac{U_{EFF} L}{S_{EFF}}$$

$$Pe_{EFF} = \frac{(1.40)(42.8)}{(96.45)}$$

$$Pe_{EFF} = \underline{0.622}$$

6. Calculate number of CSTRs

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

$$n = \underline{1.22} \text{ tanks}$$

END

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