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# EXPERIMENTAL METHODS TO CHARACTERIZE AND CONTROL LIQUID-LIQUID PROCESSES

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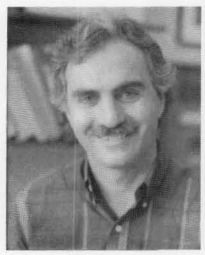

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Liquid-liquid extraction is one of the most common separation processes. It is used to separate the components of a homogeneous liquid mixture by either a solvent or a reactive liquid solution. The two liquid systems are immiscible or partially miscible, and they are introduced into contacting equipment where one of the two phases is dispersed into the other. The desired compound is then transferred from the feed to the solvent phase. The interfacial area of mass transfer is increased by mechanical agitation, and the mass transfer rate is determined by the concentration driving force, the contact area between the two phases, and the contact time. Further processing of the solvent phase is required to yield the desired component and to recover the solvent. Applications of the extraction process can be found in the petroleum industry, in hydrometallurgy,[1] in waste treatment,[2] in the nuclear industry,[3] and in biochemical separations.[4]

Industrial-scale equipment for liquid-liquid extraction includes column contactors and continuous-flow stirred tanks. A number of different types of column contactors are available, some of which perform in a comparable manner—making the selection of the equipment type a difficult problem.[5] After selection of the equipment, the next step is dimensioning of the extractor. Column height and diameter are determined in an empirical way and after a series of experiments on pilot plant units. The column diameter, for given feed-flow rates, is selected so that the continuous-phase superficial velocity is 50-60% of the maximum allowable determined at flooding.[6] The column height is determined by the summation of the theoretical height and the eddy-diffusivity height. The former is calculated for plug countercurrent flow and is a function of the column diameter, whereas the latter is estimated by axial mixing parameters. The axial-dispersion and the tank-in-series-with-backflow models have been applied to column contactors since the 1960s.[7,8] The dispersed-phase droplets are considered to have the same size by both models, and mixing parameters are considered constant throughout the column. Experiments on two or more different-diameter columns yield scale-up criteria which are used for the design of larger industrial units.

An effort to reduce expensive experimentation and overdesign problems led to a more detailed analysis of the extraction process in column contactors.[9-13] This approach is based on population balances[14-16] and considers droplet processes of breakage and coalescence. Nonuniform holdup profiles and drop size distributions along column contactors have been explained by this consideration. Population balance equations have also been applied for liquid dispersions in stirred tanks[17-18] in studies on the effect of droplet breakage and coalescence on the drop size. Simulation techniques have also been introduced[19-21] to overcome the complexity of the popu-

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lation-balance equations.

The new trends in the modeling of dispersive systems require more experimental information for model evaluation and parameter estimation. This article describes experimental techniques developed over the last few years in our laboratories for the acquisition of data such as interfacial kinetics, droplet size distributions, concentrations in both liquid phases, and volume fraction of the dispersed phase.

## EXPERIMENTS IN LIQUID DISPERSIONS

### *The Liquid Jet Recycle Reactor (LJRR)*

The LJRR has been developed[22] for evaluating interfacial kinetics for liquid-liquid systems. The basic idea of this technique is to contact the two phases in a chamber under well-known hydrodynamic flow conditions, such as the ones imposed by a laminar liquid jet, for a short period of time, and monitor the change in concentration in one of the two fluids caused by mass transfer. The jet chamber appears in Figure 1. The heavier fluid (aqueous) is introduced into the jet chamber through the nozzle, forming a liquid jet which flows concurrently with the second fluid (organic) and leads to the receiver. The organic phase is recycled, and its concentration is monitored continuously. The nozzle consists of 2mm I.D. precision-bore glass tubing. A jet of 3.54cm length is employed by this apparatus, with the flow rate varying from 70 to 130 ml/min giving a contact time in the order of 0.05s. The outer fluid flow may vary from 40 to 100 ml/min. The jet chamber has an inner diameter of 1.0cm, and the total volume of the organic phase is approximately 25ml. For a constant diameter jet whose surface velocity is proportional to the average velocity, the change in organic phase concentration with time t is given by the following relation

$$V_o \ell n\left[\frac{mC_b^a - C_b^o}{mC_b^a - C_b^o(t=0)}\right] = \frac{4\sqrt{D^a D^o Q^a \beta L}}{\sqrt{D^a} + m\sqrt{D^o}}\, t \qquad (1)$$

where

$V_o$ = volume of the organic phase

m = partition coefficient

$C_b^a$ = bulk concentration in the aqueous phase

$C_b^o$ = bulk concentration in the organic phase

$C_b^o(t=0)$ = concentration in the organic phase at zero time

$D^a$, $D^o$ = diffusivities in aqueous and organic phases

$Q^a$ = aqueous phase volumetric flow rate

***An effort to reduce expensive experimentation and overdesign problems led to a more detailed analysis of the extraction process in column contactors.***

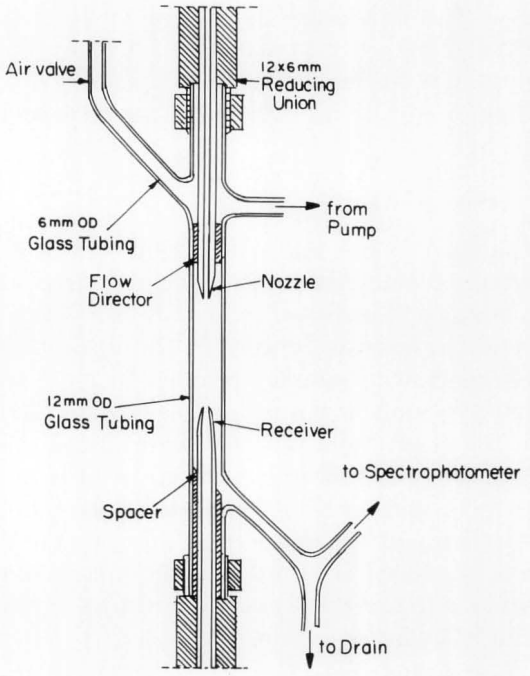


***Figure 1.*** *Jet chamber of the LJ reactor.*

L = length of the jet

β = ratio of the surface velocity to the average jet velocity

The jet surface velocity is calculated by considering a completely relaxed liquid jet, *i.e.,* no acceleration is assumed, and then solving the Navier-Stokes equations. The interfacial area between the jet and the outer fluid is determined photographically. The LJRR can be employed to obtain mass transfer coefficients and diffusivities of solutes in liquids, to study sorption phenomena, and to obtain kinetic data.[23,24] In the absence of external fields, diffusional coupling, and homogeneous reactions, the conservation equations for species j are written as follows:

*Aqueous phase:*

$$u^s \frac{\partial C_j^a}{\partial x} = D^j \frac{\partial^2 C_j^a}{\partial y^2} \qquad (2)$$

*Organic phase:*

$$u^s \frac{\partial C_j^o}{\partial x} = D^j \frac{\partial^2 C_j^o}{\partial y^2} \qquad (3)$$

subject to normal penetration theory boundary conditions

$$C_j(x,\pm\infty)=C^i_{j,b} \tag{4}$$

$$C_j(0,0)=C^i_{j,b} \tag{5}$$

where $u^s$ is the surface velocity, the subscript b refers to the bulk phase, and i refers to either the organic phase o or aqueous phase a. The x direction is parallel to the jet surface velocity, and y is perpendicular to the jet interface. The surface velocity is given by

$$u^s=\beta u_{avg} \tag{6}$$

where the proportionality constant is a function of physical, geometrical, and operating properties.[22] The power and utility of the LJRR as an experimental technique rests largely in the ability to accurately model the complex problem of mass transfer across a free surface in two-phase flow using Eqs. (2) and (3), which have received widespread attention in one-dimensional unsteady state heat or mass transfer problems. Eqs. (2) and (3) are coupled together through the interfacial fluxes by the conservation of mass. For an interfacial reaction of n components with arbitrary stoichiometry as represented by the following equation

$$\nu_1C_1+\nu_2C_2+\ldots+\nu_nC_n=0 \tag{7}$$

The conservation of mass requires that

$$\nu_iD_i\left.\frac{\partial C_i}{\partial y}\right|_{y=0}=\nu_jD_j\left.\frac{\partial C_j}{\partial y}\right|_{y=0} \tag{8}$$

One additional boundary condition required for the solution may be supplied by letting the interfacial flux of a species to be equal to the rate of interfacial reaction of the same species, or

$$D_j\left.\frac{\partial C_j}{\partial y}\right|_{y=0}=R_j \tag{9}$$

The rate of reaction $R_j$ is, in general, a function of interfacial concentrations of the reactants and products. The above problem can be solved analytically for linear kinetic rate expressions. For arbitrary kinetics, a numerical solution is required.

Results from the Liquid Jet Recycle Reactor are reproducible. The overall experimental error is less than ± 6%, providing the accuracy required to discriminate between similar models by using rigorous statistical methods. Summarizing this configuration of the LJRR permits accurate determination of the interfacial area and a simple yet satisfactory approximation of the hydrodynamics; the short contact times allow applications of the penetration theory approach. The diffusional contributions can be readily approximated or, if needed, a more rigorous numerical solution can be employed.

### The Stirred Transfer Reactor

Another experimental technique which can provide mass transfer coefficients or interfacial kinetics between two liquid phases is the stirred transfer reactor. This reactor is a modified Lewis cell which was designed by Landau and Chin[25] and further modified by Demetropoulos.[26] It consists of a cylindrical compartment divided into upper and lower sections (see Figure 2). Each section has its own agitation unit. The heavier phase is contained in the lower section and contacts the lighter phase through an annular interface. The stirrers are housed in a perforated shell in order to maintain the interface quiescent at sufficiently high rotational speeds. The fluids are pumped by the stirrers into the shell, where vertical baffles direct the flow downwards or upwards and leave the shell in a radial direction via circular perforations on the cylindrical part. All wetted parts of the reactor are made of either Teflon or glass.

The stirred transfer reactor, as well as the LJRR, provides a known interfacial area for mass transfer between the two phases. The stirred cell is valuable for low surface tension systems when the liquid jet fails. Disadvantages of the stirred transfer reactor as compared to the liquid jet recycle reactor are the complexity of the hydrodynamics and the accumulation of surface active impurities during reaction. Pure mass transfer of toluene in water and the kinetics of cobalt (II) extraction by D2EHPA (Di(2-ethylhexyl) phosphoric acid) have been studied[27] in the stirred transfer reactor.

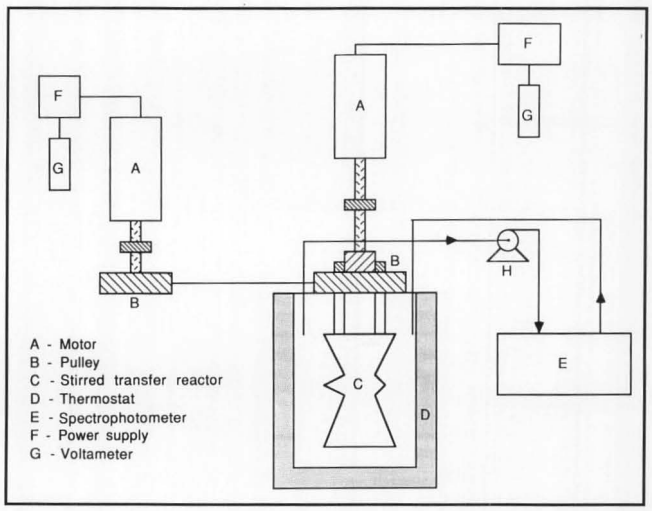


***Figure 2.*** *Flow diagram for the Stirred Transfer Reactor*

### Microphotographic Technique

Once the mass transfer coefficient or the interfacial kinetic-rate expression is obtained, the total interfacial area between the two liquid phases is required for the prediction of mass transfer or reaction rate. For the estimation of the contact area, information about the droplet size and the volume fraction of the dispersed phase is needed. A microphotographic technique for drop size measurements in liquid dispersions is described here. An optical probe[28] has been developed for drop size distribution measurements (see Figure 3). It consists of a microscope, a camera, fiber-optics, and a microflash unit. The light travels through fiber-optic light conduits to the focal point 3-5mm away from a glass window which is glued at the tip of a metal adapter. This adapter holds the objective lens of the microscope. On the other end of the microscope there exists an eyepiece lens and an adapter to hold the camera. The focal point of the microscope is located inside the dispersion, providing direct photographs of the droplets. The droplet size is measured by a semiautomatic particle analyzer (MOP-30, Carl Zeiss, Inc.) interfaced with an IBM PC. From the drop size distribution, the Sauter mean diameter, $d_{32}$, defined by

$$d_{32} = \frac{\sum_i d_i^3}{\sum_i d_i^2} \tag{10}$$

can be obtained. Then, the specific area of mass transfer, a, is estimated by

$$a = \frac{6\phi}{d_{32}} \tag{11}$$

where $\phi$ is the dispersed phase fraction. The rate of mass transfer, M, defined by

$$M = Ka\Delta C \tag{12}$$

where K is the mass transfer coefficient and $\Delta C$ the driving force, can thus be calculated.

### Laser Photometric Probe

The laser photometric probe has been developed for concentration measurements in liquid dispersions[29,30] in order to study flow properties and mass transfer coefficients. For example, one of the models used to analyze extraction in column contactors is the dispersion model which neglects the effect of drop size distribution on the mass transfer performance. For counter-current flow of both phases

$$\frac{\partial C_\alpha}{\partial t} = D_\alpha \frac{\partial^2 C_\alpha}{\partial h^2} - u_\alpha \frac{\partial C_\alpha}{\partial h} \mp K_\alpha a\Delta C \tag{13}$$

where

- $\alpha$ = continuous (c) and dispersed (d) phases
- u = superficial velocity
- C = concentration
- h = column height
- D = axial dispersion coefficient

The dispersion coefficient in both phases can be estimated by tracer experiments at which a tracer is introduced in the flow and the tracer concentration is measured at various locations. Analysis of concentration distributions yields the dispersion coefficients.

The laser probe consists of a two-loop fiber-optic setup as shown in Figure 4. The two fiber-optic bundles consist of 50μm fibers enclosed in a stainless-steel tube of 4mm outer diameter (O.D.). At the end of this tube the two bundles are separately adjusted in two small stainless-steel tubes of 0.7mm O.D., forming a forked device of 10mm in length. At the tip of each prong, a rectangular isosceles prism is located in such a way to reflect the light by 90°. The experimental setup includes a laser tube with a power supply, an electronic device, and a data-acquisition system. Laser light travels through the fiber optics and through the liquid medium between the two prisms. The intensity of the light, I, measured by an electronic device

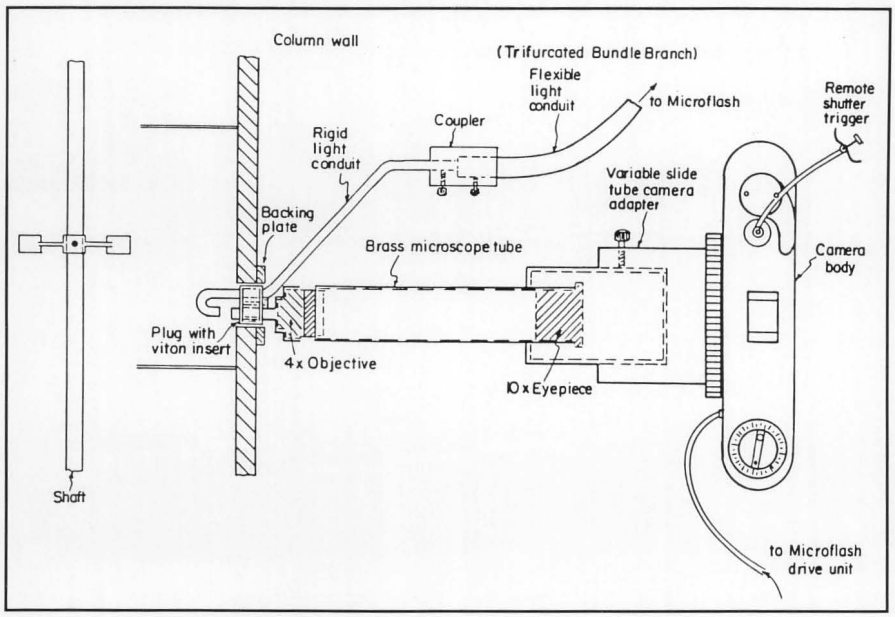


***Figure 3.*** *Microphotographic technique*

at the exit of the probe, is related to the initial intensity, $I_0$ (at zero concentration), the concentration of the investigated species in the liquid, c, and the traveling distance through the medium, x, by the Lambert-Beer law

$$I = I_0 \exp(-\varepsilon c x) \qquad (14)$$

where $\varepsilon$ is the molar absorption coefficient characteristic for each species.

The laser photometric technique can be applied for concentration measurements in liquid dispersions after the separation of the two phases. In situ separation and isokinetic withdrawal of droplets are achieved by coalescence devices supported at the tip of the fiber-optic probe.

### *Laser Capillary Spectrophotometric (LCS) Technique*

The LCS technique has been developed[31-33] for bivariate (size and concentration) distribution measurements. A bivariate drop size-concentration distribution f(v,c)dvdc represents the fraction of droplets with volume between v and v + dv and concentration between c and c + dc, and provides information about the dispersed-phase mixing. The effect of droplet mixing on reactions occurring in the dispersed phase has been studied in a number of investigations.[20,21,33-35] The basic idea of the LCS technique is to force a representative sample of drops through a glass capillary by developing a pressure difference along the tube (see Figure 5). As drops pass through the capillary, they form cylindrical slugs. The optical device is designed to measure drop size by difference of light refraction between the two phases and drop concentration by light absorbance of the solute in the drop. A laser tube of appropriate wavelength is selected as a light source. The laser beam is split into two rays by using a beam splitter and a plane mirror, and the rays pass through the center of the capillary. From the measurement of the passage time ($\Delta t_2$) of a slug

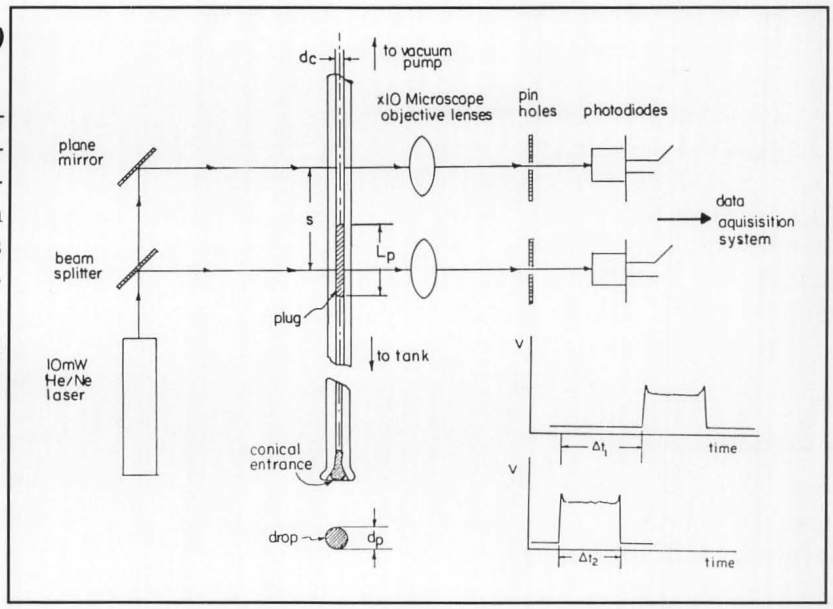


***Figure 5.*** *Optical system for the LCS technique*

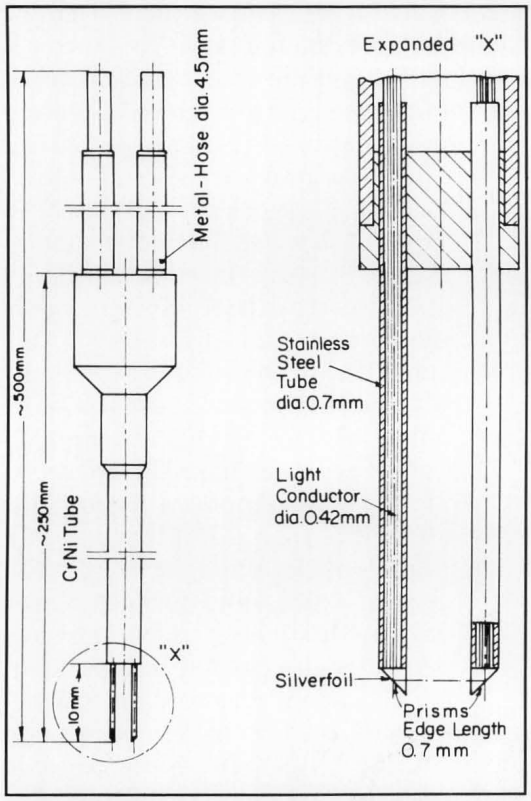


***Figure 4.*** *Laser photometric probe*

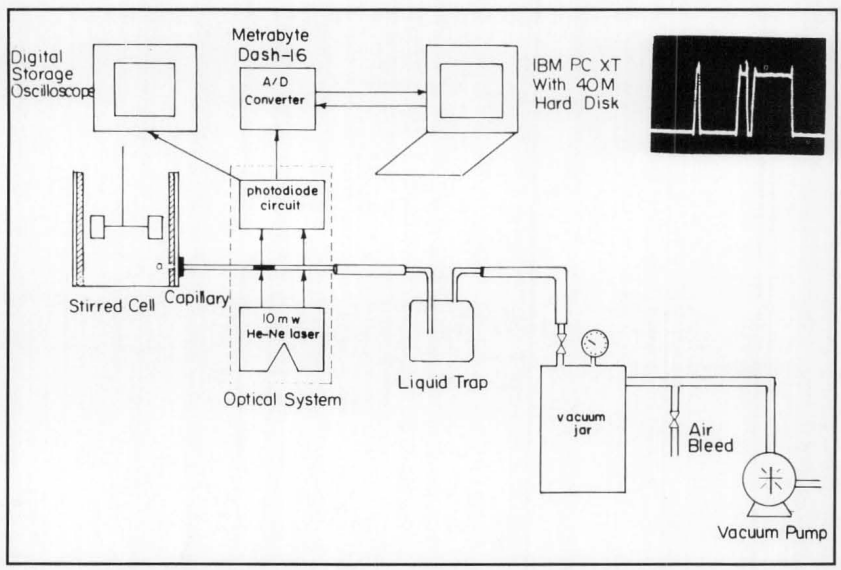


***Figure 6.*** *Experimental setup for the LCS technique*

at one detector and its travel time ($\Delta t_1$) between two detectors in Figure 5, the velocity, u, and diameter, d, of the drop can be calculated by

$$u = S / \Delta t_1 \tag{15}$$

$$L_p = u\Delta t_2 \tag{16}$$

and

$$d = \left(3/2\, d_c^2 L_p\right)^{1/3} \tag{17}$$

Here S is the distance between two detectors, $d_c$ the capillary diameter and $L_p$ the length of the slug. The width of each pulse is proportional to the drop volume and the intensity can be related to the concentration of the light absorbing species. The experimental setup is shown in Figure 6. A sample of the dispersion is withdrawn continuously through the capillary by a vacuum pump. After passing through the capillary, the two laser rays are received by photodiodes where they are translated into current. This current is changed into voltage which is sampled with a frequency of 50 KHz by and A/D converter

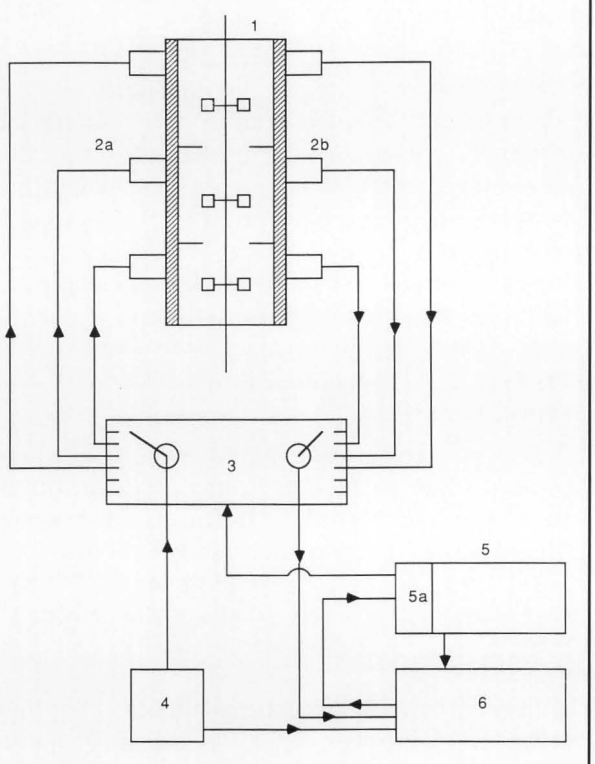


***Figure 7.*** *Ultrasonic technique*

(DASH-16, Metrabyte Co.). The LCS technique can provide steady state as well as transient information which can be processed for the description of droplet interactions and mass-transfer characteristics.

### *Ultrasonic Technique*

A noninvasive ultrasonic technique has been developed[36,37] for dispersed-phase volume fraction measurements in stirred tanks. This information is needed for the estimation of the interfacial area of mass transfer as described by Eq. (11). Also, a recently developed data-acquisition system[38] made the technique applicable for automatic on-line multipoint measurements, as shown in Figure 7, which can be used for the control of extraction columns at safe operation below flooding. A pulse generator sends a series of square pulses to a transmitting ultrasonic transducer through a dual multiplexer and to a digital oscilloscope for triggering. The transducer is activated by the electric signal and produces sound waves which pass through the liquid dispersion. The signal is received by a receiver transducer and is transmitted through the multiplexer to the oscilloscope where the travel time is calculated. The travel time through the dispersion is compared to the travel time through pure phases for the calculation of the volume fraction of the dispersed phase. By considering sound refraction and reflection on the droplet-continuous phase interface, the dispersed-phase volume fraction is calculated from the relation[39,40]

$$\phi = \frac{t^* - t_c}{g_d t_d - g_c t_c} \tag{18}$$

where $g_d$ and $g_c$ are explicit algebraic functions of the sound velocity ratio. The ultrasonic technique has been employed for process identification and control of a multistage stirred column.[41] It has also been successfully applied for low volume-fraction measurements of water in oil.

## SUMMARY

In summary, a number of experimental techniques have been developed to study some properties and parameters in liquid-liquid systems. Information obtained by these techniques significantly helps our efforts to understand and model fundamental processes occurring in liquid-liquid extraction such as droplet interactions, mass transfer phenomena, interfacial kinetics, and phase flow patterns. The Liquid Jet Recycle Reactor provides information about microscopic phenomena of mass transfer and interfacial kinetic rates between the two liquids. Similar

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use and emissions than the manufacture of a paper or plastic sack, the consumer must use the sack at least ten to twenty times before an environmental benefit is achieved.

### CONCLUSION

Assessing the total environmental impact of any product is a difficult process, involving evaluations of processing steps ranging from raw material acquisition to post-consumer waste disposal. Comparing the environmental impact of competing products is even more complex. Making comparisons between products usually involves making trade-offs between very different environmental impacts.

The purpose of this problem is to illustrate the difficulties involved in comparing the total environmental impact of different products. Paper and plastic grocery sacks were used as a case study. To compare paper and plastic grocery sacks we found that we must evaluate the trade-offs between energy use, pollutant emissions, and the depletion of natural resources. Plastic sacks appear to result in less atmospheric emissions and require less energy. On the other hand, paper sacks rely on a renewable resource for material and energy. Thus there is no clear, environmentally superior product. The consumer is left with a difficult choice, and as illustrated in the problem this choice must be made with incomplete information.

### REFERENCES


1. Hocking, M.B., "Paper versus Polystyrene," *Science,* **251**, 504 (1991)


### *Suggestions for Further Reading*


- *Resource & Environmental Profile Analysis of Polyethylene and Unbleached Paper Grocery Sacks,* Franking Associates, Ltd., Prairie View, KS (1990)
- Federal Office of the Environment, "Comparison of the Effects on the Environment from Polyethylene and Paper Carrier Bags," Bismarckplatz 1, 1000 Berlin 33, RFG, English version. August (1988)
- Riggle, D., "Recycling Plastic Grocery Bags," *Biocycle,* p 40, June (1990) ❐


## Second Law of Thermodynamics

*Continued from page 81.*

The extra cost of erasing these digits exactly cancels any energy gain elsewhere in the system.

The conundrum of Maxwell's demon has been resolved by applying the concepts of thermodynamics of irreversible computation.

In our discussions, we assumed the behavior of the demon to be completely deterministic, *i.e.,* one instruction is completed before it goes on to the next instruction. What is not so clear is what would happen if the demon could wander a little, *i.e.,* if the demon knew its instructions but was not quite sure of the order in which to carry them out. The demon would then proceed from one step to another, going forward or backward, in a somewhat random fashion. In the long run, this might allow the demon to extract some work.

There is no doubt what the outcome of the above argument is going to be, but it is a loophole which has yet to be closed.

### REFERENCES


1. Maxwell, J.C., *Theory of Heat,* 4th ed., Longmans, Green & Co., London, 328 (1875)
2. Bennet, C.H., *Sci. Am.,* **255**(11), 108 (1987)
3. Maddox, J., *Nature,* **345**, 109 (1990)
4. Peterson, I., *Sci. News,* **137**, 378 (1990)
5. Smoluchowski, M., *Z. Phys.* (1912)
6. Smoluchowski, M., Lecture Notes, Leipzig (1914)
7. Szilard, L., *Z. Phys.,* **53**, 840 (1929)
8. Bennett, C.H., *IBM J. Res. Dev.,* **17**, 525 (1973)
9. Landauer, R., *IBM J. Res. Dev.,* **3**, 183 (1961)
10. Zurek, W.H., *Nature,* **341**, 119 (1989)
11. Landauer, R., *Nature,* **335**, 779 (1988)
12. Caves, C.M., *Phy. Rev. Letters,* **64**, 2111 (1990) ❐


## Liquid-Liquid Processes

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information is obtained by the Stirred Transfer Reactor, which is a modified Lewis cell. The interfacial area between the contacted liquid phases needed for the estimation of mass transfer and reaction rates is calculated from information about the drop size distribution and the dispersed-phase volume fraction. The former is obtained by the Microphotographic Technique and/or the Laser Capillary Spectrophotometer Technique and the latter by the Ultrasonic Technique.

Tracer concentration measurements by the Laser Photometric Technique yield information about flow properties, *i.e.,* axial mixing parameters in both phases. Drop size-concentration bivariate distributions are obtained by the Laser Capillary Spectrophotometry Technique. This information is extremely valuable in model discrimination and parameter estimation of models describing droplet breakage and coalescence. It also provides information on dispersed phase mixing. Finally, the Ultrasonic Technique is also employed for the control of the dispersed-phase volume fraction in extraction columns to secure nonflooding optimum operation.

### REFERENCES


1. Flett, D.S., *The Chemical Eng.,* **32**, 1 (1981)
2. Tavlarides, L.L., J.-H. Bae, and C.K. Lee, *Sep. Sci. and*

*Tech.*, **22**, 581 (1987)
3. Naylor, A., and P.O. Wilson, in *Handbook of Solvent Extraction*, Eds, Loh, Baird, Hanson, **25**, 12, 783, John Wiley & Sons (1983)
4. Lilidis, Z., and K. Schugerl, *Chem. Eng. Sci.*, **43**, 27 (1988)
5. Ritcey, G.M., and A.W. Ashbrook, *Solvent Extraction, Part II*, Elsevier (1984)
6. Kosters, W.C.G., Chapter 13.1 in *Handbook of Solvent Extraction*, Eds., Loh, Baird, Hanson, John Wiley & Sons (1983)
7. Westertep, K.R., and P. Landsman, *Chem. Eng. Sci.*, **17**, 363 (1962)
8. Miyauchi, T., and T. Vermeulen, *Ind. and Eng. Chem. Fund.*, **2**, 304 (1963)
9. Jiricny, V., M. Kratky, and J. Prochazka, *Chem. Eng. Sci.*, **34**, 1141 (1979)
10. Cruz-Pinto, J.J.C., and W.J. Korchinsky, *Chem. Eng. Sci.*, **36**, 687 (1981)
11. Sovová, H., *Chem. Eng. Sci.*, **38**, 1863 (1983)
12. Laso, M., L. Steiner, and S. Hartland, Paper D7.8, CHISA '84, Prague, Czechoslovakia, Sept. 3-7 (1984)
13. Al Khani, S.D., C. Gourdon, and G. Cassamata, *Ind. and Eng. Chem. Res.*, **27**, 329 (1988)
14. Hulburt, H.M., and S. Katz, *Chem. Eng. Sci.*, **19**, 555 (1964)
15. Randolph, A.D., and M.A. Larson, *Theory of Particulate Processes: Analysis and Techniques of Continuous Crystallization*, Academic Press, New York, NY (1971)
16. Ramkrishna, D., *Rev. Chem. Eng.*, **3**, (1985)
17. Valentas, K.J., and N.R. Amundson, *Ind. and Eng. Chem. Fund.*, **5**, 533 (1966)
18. Valentas, K.J., O. Bilous, and N.R. Amundson, *Ind. and Eng. Chem. Fund.*, **5**, 271 (1966)
19. Spielman, L.A., and O. Levenspiel, *Chem. Eng. Sci.*, **20**, 247 (1965)
20. Hsia, M.A., and L.L. Tavlarides, *Chem. Eng. J.*, **26**, 189 (1983)
21. Bapat, P.M., and L.L. Tavlarides, *AIChE J.*, **31**, 659 (1985)
22. Freeman, R.W., and L.L. Tavlarides, *Chem. Eng. Sci.*, **35**, 559 (1980)
23. Freeman, R.W., and L.L. Tavlarides, *Chem. Eng. Sci.*, **37**, 1547 (1982)
24. Lee, C.K., and L.L. Tavlarides, *I&EC Fund.*, **25**, 97 (1986)
25. Landau, J., and M. Chin, *Can. J. of Chem. Eng.*, **55**, 161 (1977)
26. Demetropoulos, H., MS Thesis, Rutgers, The State University of New Jersey, New Brunswick, NJ (1984)
27. Lee, C.K., PhD Dissertation, Syracuse University, Syracuse, NY (1986)
28. Kirou, V.I., L.L. Tavlarides, J.C. Bonnet, and C. Tsouris, *AIChE J.*, **34**, 283 (1988)
29. Schmidt, H., C. Tsouris, E. Eggert, and L.L. Tavlarides, *AIChE J.*, **35**, 507 (1989)
30. Schmidt, H., and E. Eggert, KfK-Bericht, Nr 3630, 227 (1984)
31. Verhoff, F.H., PhD Dissertation, University of Michigan, Ann Arbor, MI (1969)
32. Verhoff, F.H., S.L. Ross, and R.L. Curl, *I&EC Fund.*, **16**, 371 (1977)
33. Bae, J.-H., and L.L. Tavlarides, *AIChE J.*, **35**, 1073 (1989)
34. Mukkavilli, S., C.K. Lee, I. Hahh, and L.L. Tavlarides, *Sep. Sci. and Tech.*, **22**(N2&3), 395 (1987)
35. Zeitlin, M.A., and L.L. Tavlarides, *AIChE J.*, **18**, 1268 (1972)
36. Sovová, H., and A. Havlicek, *Chem. Eng. Sci.*, **41**, 2579 (1986)
37. Bonnet, J.C., and L.L. Tavlarides, *I&EC Res.*, **26**, 811 (1987)
38. Tsouris, C., L.L. Tavlarides, and J.C. Bonnet, *Chem. Eng. Sci.*, **45**, 3055 (1990)
39. Yi, J., and L.L. Tavlarides, *I&EC Res.*, **29**, 475 (1990)
40. Tsouris, C., and L.L. Tavlarides, *I&EC Res.*, **29**, 2170 (1990)
41. Tsouris, C., and L.L. Tavlarides, Annual AIChE Meeting, Chicago, IL, Nov. 11-16 (1990) ❐

ChE **book review**

# COMPUTATIONAL METHODS FOR PROCESS SIMULATION

*by W. Fred Ramirez*
*Butterworths, 80 Montvale Ave., Stoneham, MA 02180; $52.95 (1991)*

***Reviewed by***
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This book provides a thorough overview of the many facets of computations in the chemical engineering curriculum. The contents of the book are ordered along the lines of a typical undergraduate curriculum. Chapters 1 through 3 present overall material and energy balances and dynamics of lumped parameter systems. Students who have mastered simple ODEs will have no problem with this material. Chapter 2 also provides an introduction to the IMSL library. Indeed, the IMSL routines are exploited throughout the book, and readers who have always wanted to learn these routines will find many excellent applications in this book.

Chapters 4 and 5 deal with applications from unit operations: the chemical reactor and reaction kinetics, and separation (*e.g.*, multicomponent distillation) operations.

Chapter 6 starts with a summary of the microscopic equations of change, using the notation and sign conventions of *Transport Phenomena* by Bird, Stewart, and Lightfoot. Some details are omitted (*e.g.*, the constitutive equation for a Newtonian fluid) but with references to *Transport Phenomena*. These set the stage of modeling of distributed parameter systems and the BVP and PDE examples of chapters 7 and 8.

By covering a wide array of chemical engineering applications (unit operations, biochemical/biomedical processes, environmental modeling are some of the areas encountered), the author has woven into this book just about every computational method of utility to the chemical engineer, with coded (Fortran/IMSL) examples for those interested in immediate application of concepts to frequently encountered chemical engineering mathematical models.

Because the book covers the entire spectrum from introductory chemical engineering courses, *e.g.*, material and energy balances, to senior-level courses on process dynamics and process design, a course based on this book would have to come somewhere near the end of the curriculum, perhaps as a senior-level elective. The book may also be of value to those who have already mastered the typical chemical engineering curriculum, *e.g.*, the chemical engineering practitioner, and are now involved in some aspect of computational or mathematical modeling of chemical engineering processes. ❐