# LETTERS TO THE EDITOR

## TO THE EDITOR: NEW RESULTS ON OXYGEN TRANSPORT IN CAPILLARY TISSUES

I am writing this letter to inform you of an error in our paper "A Digital Simulation of Transient Oxygen Transport in Capillary-Tissue Systems (Cerebral Gray Matter)," *AIChE Journal*, 15, 916 (1969).

In deriving Equation (1) for the capillary a term representing the accumulation of oxygen in red cells was left out. A more accurate representation of the capillary equation, including accumulation of oxygen in the erthrocytes, is as follows:

$$\frac{\partial P}{\partial t} = \frac{D_1}{\left[1 + \frac{N}{C_1}\frac{d\psi}{dP}\right]} \left[\frac{\partial^2 P}{\partial r^2} + \frac{1}{r}\frac{\partial P}{\partial r} + \frac{\partial^2 P}{\partial x^2}\right] - v\frac{\partial P}{\partial x}$$

The system solution using Equation (1) in our original work resulted in figure 7 (graphical demonstration of the axial reaction effect during transient changes). When the concept of axial reaction was proposed we checked our computer calculations in every way possible to ascertain if we were observing computational error. Since we were satisfied that our numerical scheme was accurate, the conclusion was drawn that a reaction front moves down the capillary faster than the convective front. This conclusion has been found to be incorrect based upon our more recent calculations.

While setting up equations for glucose transport (*1*) in the capillary-tissue system the missing term in the original oxygen model was discovered. Because of the extensive computational time necessary to solve the coupled set of nonlinear partial differential equations (10 hours for 80% convergence on an IBM-7094) a numerical technique (*2*) was developed. This method (Method of Lines) allowed model solutions about 60 times faster than with the Alternating Direction Implicit method. The results of the original and recent work are presented on Figure 1. It can be seen that there is a pronounced front moving down the capillary when the erythrocyte accumulation term is included.

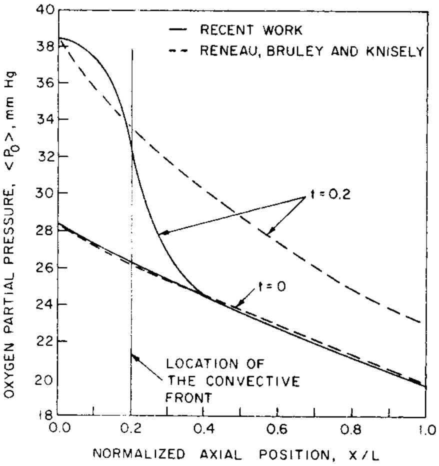

**Fig. 1. Comparison of unsteady state axial $<P_0>$ profiles in the capillary with and without accumulation of bound oxygen (no autoregulatory effects).**

The response characteristics in the tissue were found to be nearly independent of the accumulation term because the blood residence time in the capillary is only about one-half second and the tissue time constant is about one second. Therefore, the dynamic response curve at the lethal corner was essentially unaltered. All other conclusions are valid.

DUANE F. BRULEY
DEPARTMENT OF CHEMICAL ENGINEERING
CLEMSON UNIVERSITY
CLEMSON, SOUTH CAROLINA 29631

### LITERATURE CITED

1. Reneau, D. D., M. H. Knisely, H. I. Bicher, and D. F. Bruley, "Glucose Diffusion and Consumption In the Human Brain—Parts I and II," 17th National AIChE, Meeting, Atlantic City, N. J. (1971).
2. McCracken, T. A., and D. F. Bruley, "Digital Simulation of the Parallel Hybrid Computer Technique for Solving Nonlinear Parabolic PDE," 21st Can. Chem. Eng. Conf., Montreal, Canada (1971).

## TO THE EDITOR:

How refreshing to read Professor McGee's editorial (*AIChE Journal*, November, 1971). He expresses so well the thoughts of this industrial researcher who also questions the value of some of the pedestrian academic research published in the *Journal*.

A survey of the contents of the *Journal* over the past few years would almost lead one to believe that ours is not an experimentally based discipline. Indeed, the *Journal* explicity discourages photographs. It disturbs me that the journal of a profession so much concerned with fluid flow should discourage the use of this powerful experimental tool. What can possibly be more useful for the fundamental understanding of a complex fluid dynamic problem than a photograph showing stream lines, vortices, or density gradients? Can theory ever be more beautifully illustrated than this? Surely the anchoring of an elegant theory to reality by a single photograph is the stuff of which research excitement is made. Yet, the Journal's emphasis on unanchored computer problems contributes to the dullness of which Professor McGee speaks and is unrelated to the excitement of research as I know it.

No doubt it is true that the *Journal* would not prohibit the publishing of a photograph but, please, can't the Instructions for Contributors be changed to create the impression that contributions from experimentalists are actively sought? This chemical engineer wonders why those superb electron micrographs, for example, showing the crystallinity of polyethylene are published in the *Journal of Applied Physics* instead of in our journal.

J. D. CHASE
STAMFORD, CONNECTICUT

## TO THE EDITOR: ON THE REDLICH-KWONG EQUATION OF STATE

The intensive work of many people on the Redlich-Kwong equation of state (RK) has resulted in the development of many modifications. This prompted us to search for the best version of the equation for use in the prediction of vapor phase component fugacities in the Chao-Seader method which we use when computing the parameters of high-pressure vapor-liquid equilibria.

For the comparison we took two of the most impressive correlations composed by Ackerman (RKA) (*1, 2*) and by Gray et al. (RKZ) (*3*). The first was always considered to be rather good (*1, 4*). The second attracted our attention because of the article in the *Journal* (*3*) in which RKZ was described as an accurate instrument especially good in and near the critical region (exactly what we need for the phase equilibria).

Eight hydrocarbon mixtures containing methane, ethane, propane, n-butane, isobutane, n-pentane and 2-methylbutane were taken into consideration. The comparison between calculated and experimental (*5*) values of compressibility factors was undertaken

(*Continued on page 671*)

capric acid in ethylene is about $3 \times 10^{-8}$ g/dm$^3$. If the ethylene pressure is increased to about 8 MN/m$^2$, the capric acid concentration in the gas phase increases to 7 g/dm$^3$—an increase of some $2 \times 10^8$ fold! Authors Paul and Wise cite many such cases in this book to emphasize the significant increase in solubility when the gas phase is at high pressure and a low temperature, that is, near or below its critical point. In addition, they note some industrial applications, an example of which is the use of dense methane or ethylene for stripping coal tar or deasphalting. Finally, the authors explore the possibility of employing dense gas extraction in biological chemical purifications, polymer separation, desalination, chromatography, and other processes wherein high temperatures are detrimental. In pointing out the possible applications of the technique, the book is valuable, though not exhaustive, for example, no mention is made of the phenomenon's importance in cryogenic gas purification processes.

The theoretical foundation laid for understanding the phenomenon and for actually estimating the enhancement of solubility is too brief, and some of the estimation techniques are out of date. Readers unfamiliar with the area will unfortunately have to return to the original literature.

Despite its shortcomings, however, the monograph is easy to read, provocative in suggesting new applications for this phenomenon, and will be well worth the few hours spent in reading it thoroughly.

R. C. Reid
Massachusetts Institute of Technology
Cambridge, Mass. 02139

**New Energy Technology—Some Facts and Assessments,** H. C. Hottel and J. B. Howard, MIT Press, Cambridge, Mass. (1972). 364 pages. $2.95.

The authors are recognized authorities in the engineering sciences and are well qualified to present the current status of the energy crisis.

The introduction and summary are worth the price of the book. An excellent and concise presentation of the energy needs of the United States and the world is given along with the supplies available from gas, oil, coal, and nuclear power. Per capita consumption of energy in the United States if equaled by the rest of the world "will require the effective contribution of the scientist, the engineer, the economist, the industrialist, and the statesman."

Energy sources, transportation, and environmental effects are adequately covered. The effects of energy production on the environment are given from an engineering background and hence, the problems are placed in a perspective not dominated by hysteria.

The chapter on fossil fuel-to-fuel conversion is an excellent summary of the processes available at present for conversion of coal, oil, shale, and tar sands to high BTU gas and oil. Research needs for each source of energy supply are appropriately set forth and constitute a needed addition to the literature. The authors state: "a final choice of process that saves 10¢/1,000 cu. ft in manufacturing cost will, in the days when our consumption of synthetic pipeline gas is one-third that of natural gas in 1970, amount to a saving of $750 million per year." This chapter contains only a minimum amount of theory on coal gasification. Expansion of this section would be welcomed.

Sulfur-free fuels from coal that can be used in gas turbines to produce power are also recommended for consideration because of the shortcomings encountered with sulfur dioxide cleanup of power stack gases. Sixteen processes for sulfur dioxide removal from stacks are listed. The author states that sulfur dioxide pollution is a local problem and not a global problem because of the short life of sulfur dioxide in the atmosphere.

Nuclear generated electric power is expected to rise from $6 \times 10^3$ MW in 1970 to $735 \times 10^3$ MW in the year 2,000. The authors' discussion is comprehensive for the many different types of reactors, including the breeder variety. However, very little is said about nuclear fusion as a source of power. A reader will find a thorough discussion of the safety problem and disposal problems associated with spent nuclear fuel.

Finally, because of the vast amount of power consumed by the automobile and by home heating and air conditioning, the prospects of energy sources for these purposes is covered, including a comprehensive discussion of solar energy, which is not expected to contribute significantly to our energy needs. "Until new knowledge is available, studies of large-scale power from the sun via the flat-plate collector are a waste of time and money. The need is for cheaper collectors and for better photovoltaic cells." The latter appears to be "the only hope for solar power."

The book is a much needed contribution to the literature on our energy problems.

R. V. Green
E. I. du Pont de Nemours and Company
Biochemicals Department
Belle, West Virginia 25015

for 1,000 points in the temperature interval $T_r = 0.7 \div 2.6$ and pressure $P_r = 0.1 \div 5$. For the calculation the computer "Minsk-22" was used. One hundred isotherms were tested, each containing 10 points. The mean square deviation for every isotherm was taken as a measure of the correlation quality.

It was very easy to establish the striking effect of the temperature on the accuracy of all the correlations: at all pressures the RKA is the best up to $T_r = 1.4$ Above this temperature the best is the RK, but even here the RKA is not far behind.

Only for 10 isotherms was the RKZ slightly better than two others. Unfortunately for many other isotherms the deviations obtained for the RKZ are too great: 10 times and more than for the RKA and RK.

Now we consider that it might be rather sensible to use the RKA in the Chao-Seader method instead of the original RK.

### LITERATURE CITED

1. Reid, R. C., and T. K. Sherwood, The Properties of Gases and Liquids, McGraw Hill, N. Y. (1966); Russ. edit., Leningrad (1971).
2. Redlich, O., F. J. Ackerman, et al., *Ind. Eng. Chem. Fundamentals,* 4, 369 (1965).
3. Gray, R., N. H. Rent, and David Zudkevitch, *AIChE J.*, **16,** 991 (1970).
4. Rowlinson, J. S., Liquids and Liquid Mixtures, Butterworths, London (1969).
5. Tang, W. K., Assembled Tables of PVT-Data, Univ. Wisc. Madison (1956).

Boris I. Sokolov and
Anatoly A. Kharchenko
Revolution Rd 37-I-33
Leningrad 195248, U.S.S.R.

### TO THE EDITOR:

The Design Institute for Multiphase Processing (DIMP) which was discussed in the March editorial is, like many Institute activities, the product of considerable volunteer effort. Several people not currently associated with the program played key roles in advancing DIMP from inspiration to reality. In this connection we wish to acknowledge the foresight and effort of G. E. Alves and Dr. H. S. Kemp of DuPont and Dr. G. D. Towell of Shell.

W. H. Manogue
E. I. duPont de Nemours & Co.
Wilmington, Delaware 19898

E. O. Ohsol
American Cyanamid Co.
Stamford, Connecticut 06904