# LETTERS TO THE EDITOR

**TO THE EDITOR:**

The facilitated transport of an uncharged species by a charged carrier occurs in several systems, for example, in NO transfer by $Fe^{++}$ (*1*), and in CO transfer by $Cu^{+}$ (*2*) and would probably be applied to others, such as ethylene transport by $Pd^{++}$ at low temperatures in oxygen-free atmospheres.

These reactions can be modeled by

$$A + B^{n+} \underset{k_2}{\overset{k_1}{\rightleftarrows}} AB^{n+} \qquad (1)$$

reaction (1) where $A$ is the uncharged molecule and $B^{n+}$ is the charged carrier. At the high carrier salt concentration typical of physiological or industrial interest, the activity coefficient of the charged species is expected to be quite different from unity; similarly, the diffusivity of the various carrier species is also a function of ionic strength.

A recent mathematical treatment of membrane diffusion with facilitated transport in the case of NO transport in ferrous chloride formamide solutions (*1*) found that use of a constant single diffusivity and neglect of activity variations with concentration sufficed to explain the experimental data. This apparent discrepancy is shown here to arise because of two fortuitous circumstances: the free and complexed carrier have (essentially) equal diffusivities, and a reaction given by Equation (1) occurs reversibly.

The diffusivity of a charged species is

$$D = D_0\left(1 + \frac{\partial \ln \gamma}{\partial c}\right) \qquad (2)$$

If $B^{n+}$ and $AB^{n+}$ have equal diffusivities and cannot penetrate the membrane boundaries, at steady gas transport through the membrane the total ionic strength will be constant, that is, $C_{B^{n+}} + C_{AB^{n+}} =$ constant everywhere. Then $\gamma = f$ (ionic strength) $=$ constant and $\partial \ln \gamma / \partial c \equiv 0$ even though there are gradients in the individual charged species. The diffusivity is independent of ionic strength.

Reaction (1) involves a reaction between a charged and uncharged specie to form an activated complex of the same charge $(AB^{n+})^{\ddagger}$. The rate constant in concentrated solutions is given by Equation (3).

$$\ln k_1 = \ln k_1^0 + \ln\left(\frac{\gamma_A \gamma_{B^{n+}}}{\gamma_{AB^{n+}}}\right) \qquad (3)$$

The neutral molecule $A$ will experience almost no activity coefficient variation, thus $\gamma_A \simeq 1.0$. The charged species $B^{n+}$ and $AB^{n+}$, having the same charge and probably nearly identical ionic radii, will have essentially the same activity coefficients. Thus $\ln \dfrac{\gamma_A \gamma_{B^{n+}}}{\gamma_{AB^{n+}}} \sim 0$ and the forward rate constant (and, similarly, the reverse rate constant) will exhibit a constant value: the value at infinite dilution.

These two fortuitous circumstances are not expected to hold for more complex reaction systems, such as oxygen transfer by hemoglobin (*4*) and carbon dioxide absorbtion in water (*5*) where either multiple reactions are involved or where the carrier and neutral molecule reaction to give two charged species. For example

$$CO_2 + H_2O \rightleftarrows HCO_3^- + H^+ \qquad (4)$$

Thus, concentrated or nonideal systems will behave ideally only under the two restrictions discussed above, and full treatment of other systems should take cognizance of the importance of activity variations in solution.

**NOTATION**

$A, B^{n+}, AB^{n+}$ = neutral molecule charged carrier and charged carrier-neutral complex, respectively

$D\ D_0$ = diffusivity at finite concentrations and infinite dilution, respectively

$\gamma_X$ = activity coefficient of species $X$

$k_1, k_1^0$ = forward rate constant for Equation (1) and finite concentration and infinite dilution, respectively

**LITERATURE CITED**


1. Ward, W. J., *AIChE J.*, **16**, 405 (1970).
2. Ward, W. J., "Nature," to be published.
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4. Ulanowicz, R. E., and G. C. Frazier, *Math. Biosciences*, **7**, 111 (1970).
5. Astorita, G., "Mass Transfer with Chemical Reaction," p. 131, Elsevier, New York (1967).



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**TO THE EDITOR:**

The article by Vasudevan and Middleman (*1*) contains a serious error. In this note their notation has been used. Their Equation (5) should read

$$v_{r0} = N_{A0}/c \qquad (1)$$

Equations (8), (11), (15), and (26) are also changed as a result. The first term on the left-hand side of their Equations (8) and (11) should be written as follows

$$-\frac{\mathcal{D}_{AB} R_0}{(1 - x_{A0}) r} \frac{\partial x_A}{\partial r}\bigg|_{r=R_0}$$

Equation (15) becomes

$$\gamma = \frac{x_{A0} - x_{A\infty}}{\Lambda_{AB}(1 - x_{A0})} \eta_0 \frac{d\Pi_{AB}}{d\eta}\bigg|_{\eta=\eta_0} \qquad (2)$$

In place of Equation (26) they should have

$$\gamma = \frac{x_{A0}}{\Lambda_{AB}(1 - x_{A0})} \eta_0 \Pi'_{AB0} \qquad (3)$$

The definition of the parameter on the curves of Figure 10 is in error and should be replaced with $\dfrac{x_{A0}}{\Lambda_{AB}(1 - x_{A0})}$.

The example given in the paper grossly overestimated the effect of evaporation of a low vapor pressure liquid on $c_f/c_{f0}$. Using the data of the example: $\gamma \approx 0.04$ and $c_f/c_{f0} \approx 0.98$. An exact estimate is difficult to make because Figures 7 and 10 have not been extended to sufficiently low values of the parameters. The effect of evaporation is more than an order of magnitude smaller than predicted by Vasudevan and Middleman in their concluding paragraphs.

**LITERATURE CITED**


1. Vasudevan, G., and S. Middleman, *AIChE J.*, **16**, 614 (1970).



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**TO THE EDITOR:**

**THE NEW FORMAT**

The new format shown in the July issue should be very helpful to busy readers. It certainly will be helpful to indexers and literature searchers in technical libraries, who are not expert

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in every technical field. The abstracts, scopes, and summaries will be a tremendous help in having the articles properly indexed and retrieved, both in manual and automatic systems. The better the indexing, the more valuable your periodical will be in future reference work.

The only change I would like would be to put the Authors' Abstracts in the front where they won't be overlooked.

W. J. Leahy
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I believe that the new format for the *AIChE Journal* is too lengthy and not very functional. Because the scope and summary sections covered more than one page in most papers, I would prefer the older and shorter abstract format. Another possibility would be to print the scope section with the paper and the summary section, instead of the abstract, at the end of the journal.

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The proposed new journal format is an excellent improvement, and I hope you will adopt it. The reviewers of each paper should be sure to comment on the author's Scope and Summary since it is in these parts that he must clearly state the raison d'être for the paper. I'm sure the relaxed, qualitative style of the Scope will be well received by all concerned.

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# *The Journal Format for 1972*

In the July editorial we outlined briefly a few ideas for a new *Journal* format and published seven papers written in this style. The first four papers of this issue also illustrate the Scope-Summary concept.

Since the July issue, we have finalized our format requirements, which are presented in detail on the inside of the back cover of this issue. Though we encourage immediate adoption of this form, we recognize that this mandate would be unfair to many authors who are in the final stages of manuscript preparation. Therefore, use of this form will not be mandatory until January 1, 1972.

The Scope-Summary concept has been modified to emphasize the conclusions and significance of a paper. The literature citation technique has been changed to the European system, and each citation must also include the *title* of the article, patent, etc., that is referenced. In addition, emphasis has been placed on writing the main body of the article as succinctly as possible; authors are encouraged, and in many cases will be requested, to place less significant background material, extensive data, etc., in a supplement, which will be easily obtainable in microfilm or hard copy at low cost. As is the case with most journals, we receive more manuscripts that we can possibly publish. By minimizing the length of a paper, we will be able to publish more papers and to cover a wider breadth of chemical engineering research and development. We hope we are never forced to become the complete synoptic type of journal, but we do feel that a compromise is both possible and desirable.

# Instructions For Contributors

Unpublished manuscripts dealing with significant theoretical and experimental developments in chemical engineering will be considered. Manuscripts should be submitted in triplicate directly to the Editor, *AIChE Journal*, Room 12-190, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139.

Four types of manuscripts are printed in the *Journal*: Letters to the Editor, R & D Notes, Papers, and Review Papers.

### LETTERS TO THE EDITOR

Letters to the Editor are encouraged. They may, for example, concern previous *Journal* articles, comment on research trends or new developments in chemical engineering, or offer constructive suggestions toward improving the *Journal*. A letter should not exceed two double-spaced typewritten pages and should be addressed "To the Editor."

### R & D NOTES

R & D notes are limited to eight double-spaced typewritten pages *including* figures and tables. They receive one review.

These notes may, for example, elaborate on a previous *Journal* article, present new experimental data, or develop the essence of a new experimental or theoretical concept. They should briefly discuss the relevance and contribution of the work to chemical engineering problems.

Format may vary with the author's preference, but the typing, equations, figures, tables, notation, and literature citations