LETTERS TO THE EDITOR

To the Editor:

I would like to comment on the paper "System Structures for Process Simulation" by L. B. Evans, B. Joseph & W. D. Seider [*AIChE J.*, 23, 658 (1977)]. The authors make many valid points on the use of the "plex" as a computational tool for Process Simulation. The authors propose two basic solutions; the FORTRAN (or similar language) interface and the "problem-orientated language."

The FORTRAN solution has the advantages that the language is widely available, well-known and that large subroutine library facilities are available. The FORTRAN solution for this type of problem (which is by no means unique to Process Simulation) has a number of features associated with it:

1. A basic set of data management routines to handle the dynamic storage area (e.g. VAL, STOR, FREE and BRET for Evans et al.). These routines will usually be written in assembly or machine language and will be suitable for a wide class of problems.

2. A more problem-specific set of routines to perform commonly-required functions on the various data types (e.g. INPUT).

3. A complex and/or extensive set of data input format rules (see Fig. 18 in Evans et al.) containing keywords, values, user names and punctuation symbols. These will be highly problem-specific in most cases.

These features all serve to keep the engineer who actually uses the system at arms length. These restrictions are enforced because FORTRAN was not designed for this type of data manipulation. It was designed for numerical manipulations and, with some reservations, has served the scientific community well in this capacity. The essence of the problem type discussed by Evans et al. is that some of the information which the engineer wishes to manipulate is bound up in the structure of the problem. It may also be noted that, in order to allow the user to continue with a language (FORTRAN) with which he is familiar, we impose a solution on him which requires that he learn a problem-specific data input "language."

If we now consider the alternative approach also considered by Evans et al. (the "problem oriented language") we see that many of the objections above are overcome. The language features exhibited in Evans Figure 10 are designed for the problem in hand and could be implemented in a convenient and efficient manner. The penalty is of course that the user has to learn and become familiar with this new special language. This would be an acceptable route to follow if no other alternative were available.

An alternative which I would recommend for consideration is to use a more flexible language which has a sufficiently wide repertoire of data types and/or statement constructions available that special purpose packages for simulation etc. may be implemented easily and without imposition of user interfaces at arbitrary levels. A number of general-purpose procedural languages are available which, to a greater or lesser extent, exhibit much more flexible data manipulation properties than FORTRAN. The higher-level languages PASCAL and ALGOL-68 are examples orientated to batch processing. I have used an implementation of ALGOL-68 to set up data structures very similar to those suggested by Evans et al. since 1971 and found the language facilities wide enough to cater for a whole range of problems which are difficult or almost impossible in FORTRAN. In particular the so-called "plex" structure can be handled very easily (with no need for code/assembler) by the inherent list-processing capability of the language. This facility is effectively a superset of that required by Evans et al. since the garbage collection functions performed by BRET are automatically done in ALGOL-68 (see Woodward and Bond, 1971). To the engineer the real value of learning such a language is that it will be useful for a wide range of problems including any problem that can be handled using FORTRAN. The disadvantage of a more restricted program library is not particularly serious since most conventional library programs are largely irrelevant to process simulation/synthesis/flowsheeting.

Evans et al. also mention the use of such facilities in real-time computing. My own work has required extensive use of data-structures in real-time processing (see Andow and Lees, 1975). The high-level real-time language RTL/2 (see Barnes, 1976) has been found to be excellent for this purpose in addition to being a very clear and elegant language for more conventional real-time applications such as DDC, logging and sequencing. Library modules written in ALGOL-68 or RTL/2 can still be interfaced to the user at a subroutine call level or data format level if desired (we have used both approaches) but no arbitrary restrictions are placed on the level at which such an interface is pitched and the library modules can always be provided in source form if the user wishes to modify them.

P. K. ANDOW
Department of Chemical Engineering
Loughborough University of Technology
Loughborough, Leicestershire
England

LITERATURE CITED

Andow, P. K., and F. P. Lees, "Process Computer Alarm Analysis: Outline of a method based on List Processing," *Trans. I. Chem. E.*, **53**, 1 (1975).

Barnes, J. G. P., "RTL/2 Design and Philosophy," Heyden, London, 1976.

Evans L. B., B. Joseph and W. D. Seider, "Systems Structures for Process Simulation," *AIChE J.*, 23, 658 (1977).

Woodward, P. M. and S. G. Bond, "Users Guide to ALGOL-68R," Royal Radar Establishment, Ministry of Defence, Malvern, Worcs., England, 1971.

Reply:

The idea of using a higher-level language such as PASCAL, Algol-68, or PL/1 to implement plex structures for use in process simulation is attractive. We stated this in our reply to the letter by Castellano [*AIChE J.*, **24**, 752 (1978)]. Unfortunately, very few process engineers have access to these languages. We recently surveyed 16 of the major chemical and petroleum companies in the United States with IBM computers to see how many of them supported PL/1. Only 8 out of these 16 responded that they could use and maintain PL/1 programs. FORTRAN is still the language used by the vast majority of process engineers.

We are proceeding with the second alternative in our effort to build a comprehensive system called ASPEN for computer-aided simulation and design of chemical processes. Our experience indicates that it will be possible to develop a problem-oriented language with the flexibility that is required in process simulation. The advisory committee for the project, consisting of representatives from 50 companies, was unanimous in recommending FORTRAN as the programming language.

We do not see how the proposal to write simulation programs in PASCAL or Algol-68 would make the data input any less problem-specific than would the use of FORTRAN.

LAWRENCE B. EVANS
Department of Chemical Engineering
Massachusetts Institute of Technology

BABU JOSEPH
Department of Chemical Engineering
Washington University

WARREN D. SEIDER
Department of Chemical and
Biochemical Engineering
University of Pennsylvania

To the Editor:

In connection with the paper by Whiting and Ackerberg [*AIChE J.*, **24**, 341 (1978)] on the prediction of acoustic velocities in nonideal gas mixtures attention is called to my paper [*Canadian J. Chem. Eng.*, **39**, 199 (1961)] in which speeds of sound were computed by the approximate expression

$$C^2 \simeq \frac{pH}{\rho E} = zRT\,\frac{H}{H - zRT} \quad (1)$$

This is obtained from an exact expression

$$C^2 = \frac{p}{\rho}\left(\frac{\partial H}{\partial E}\right)_s = \frac{p}{\rho}\left[\frac{H}{E} + E\left(\frac{\partial H/E}{\partial E}\right)_s\right] \quad (2)$$

by neglecting the second term. The approximation was evaluated using corresponding state correlations for z and for the reduced enthalpy deviation. It was found for pure substances that the approximation compared favorably with those obtained by more exact procedures because it was not necessary to calculate derivatives such as $(\partial z/\partial p_r)_{T_r}$. It should be noted that the accuracy of a correlation for the compressibility factor does not insure a corresponding accuracy for its derivative.

By using the pseudo-critical method this procedure could easily be extended to mixtures. When experimental data for mixtures becomes available it will be interesting to see how this approximation compares with the more exact procedures.

WILLIAM SQUIRE
Department of Aerospace Engineering
West Virginia University
Morgantown, West Virginia

Reply:

Squire [*Canadian J. Chem. Eng.*, **39**, 199 (1961)] has suggested a method for predicting acoustic velocities in nonideal gases using a procedure which appears to be accurate in some cases but, as we shall see, may be highly inaccurate in others. Although Squire's method is simple and does not require the evaluation of partial derivatives of the compressibility factor $Z(P_r, T_r)$, it does involve neglecting a term of unknown magnitude and thus the accuracy of the approximation is uncertain.

To indicate the fallibility of Squire's approach, consider the equation of state

$$P(V - B) = RT,$$

which is a special form of Van der Waals equation, with the usual notation. It is not difficult to show that the exact expression for the speed of sound C_e is given by

$$C_e^2 = \frac{\gamma}{MRT}(RT + BP)^2,$$

where $\gamma = C_p/C_v$ and M is the molecular weight. If, as required by Squire's technique, we define the reference states for H and E so that they vanish simultaneously (this requires choosing $E = 0$ and $H = 0$ when $P = 0$ and $T = 0$), we find that the sound speed C_s given by Squire's method is

$$C_s^2 = C_e^2 - (BP/MRT)(BP + RT).$$

Here we have assumed constant specific heats. From this equation it is apparent that depending on the relative magnitudes of B, P, and T, the additional term could be quite large especially for high pressures, thereby introducing large errors.

Although the partial derivatives of $Z(P_r, T_r)$ are required to use the method of Whiting and Ackerberg [*AIChE J.* **24**, 341 (1978)], the recently developed corresponding states correlation of Lee and Kesler [*AIChE J.*, **21**, 510 (1975)] provides a direct method for computing these derivatives analytically. The results should be considerably more accurate than those reported by previous investigators and the resulting sound speeds should be more reliable than those predicted by Squire's method.

R. C. ACKERBERG
Department of Chemical Engineering
Polytechnic Institute of New York
Brooklyn, New York.

ERRATA

In "Slow Flow of a Non-Newtonian Fluid Past a Droplet," by M. G. Wagner and J. C. Slattery [*AIChE J.*, **17**, 1198 (1971)], the lower summation limit in Equation (71) should read $\eta = -1$. In Equation (76), there should be a negative sign preceding the first appearance of β_1 in the second line of the equation, i.e., this line should read:

$$\frac{\lambda N_{We}}{80\,N_{Re}(\kappa+1)^3}\{19\kappa^2 + 30\kappa + 16 - \beta_1(15\kappa^3 + 42\kappa^2 + 44\kappa + 24) - \ldots\ldots\ldots\ldots\}P_2(\mu)$$

In "Coal Devolatilization and Hydrogasification" by Donald B. Anthony and Jack B. Howard, *AIChE J.*, **22**, 625-656 (1976):

In Table 6 (p. 637), the H_2 and CH_4 data of Loison and Chauvin were interchanged by mistake. The columns should read

H_2	CH_4
54.3	16.9
52.8	21.8
50.3	13.1