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.

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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.

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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.

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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