

Estimation of Model Parameters Using Quasilinearization

SIR: Ramaker, Smith, and Murrill (1970) discuss the application of quasilinearization to the determination of numerical values of parameters in a dynamic model. Their efforts in studying the effect of various factors on convergence and attempts at increasing the convergence region represent a valuable contribution in the area of parameter estimation. However, a few points in the above article require clarification.

Application of the quasilinearization algorithm to the following system of nonlinear equations

$$\frac{d\bar{x}}{dt} = \bar{f}(\bar{x}, t) \quad (1)$$

results in the following system of linear equations (Lee, 1968)

$$\frac{d\bar{x}_{i+1}}{dt} = \bar{f}(\bar{x}_i, t) + \left. \frac{\partial \bar{f}}{\partial \bar{x}} \right|_{(\bar{x}_i, t)} (\bar{x}_{i+1} - \bar{x}_i) \quad (2)$$

where subscript i represents iteration number. The authors express the resulting linear equation—their Equation 6—in the form

$$\dot{\bar{x}}_{i+1} = \bar{A} \bar{x}_{i+1} + \bar{b} \quad (3)$$

where in their matrix \bar{A} corresponds to

$$\left. \frac{\partial \bar{f}}{\partial \bar{x}} \right|_{(\bar{x}_i, t)}$$

and their vector \bar{b} corresponds to

$$\bar{f}(\bar{x}_i, t) + \left. \frac{\partial \bar{f}}{\partial \bar{x}} \right|_{(\bar{x}_i, t)} \bar{x}_i$$

In applying the quasilinearization algorithm to their Equation 4, the authors have made an error in specifying \bar{b} , which is the equation above their Equation 7. The correct specification of \bar{b} is

$$\bar{b} = \begin{bmatrix} +c_i x_i + \theta_i G_i m'(t - \theta_i) \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (4)$$

The authors go on to say that the solution to Equation 3 is

$$\bar{x} = \bar{y}_p + \sum_{j=1}^k \mu_j \bar{y}_{hj} \quad (5)$$

which is their Equation 8. They then state that the coefficients μ_j would be the k initial conditions for the differential equations if they were available. This is true only for the special case in which the initial condition for the particular solution vector is the null vector and the initial condition for the matrix of homogeneous solutions is the identity matrix.

The authors state that the computational effort can be reduced by defining the state variables in terms of the change in state variables from one iteration to the next

$$\bar{\delta} = \bar{x}_{i+1} - \bar{x}_i \quad (6)$$

which is the second half of their Equation 7. They then present the differential equation

$$\dot{\bar{\delta}} = \bar{A} \bar{\delta} \quad (7)$$

which is the first half of their Equation 7, with the implication that Equation 7 is equivalent to Equation 3. Equation 3 can be written as

$$\dot{\bar{x}}_{i+1} = \bar{A}_i \bar{\delta}_{i+1} + \bar{f}_i \quad (8)$$

If

$$\bar{f}_i = \dot{\bar{x}}_i \quad (9)$$

then Equation 8 will reduce to Equation 7 and indeed Equation 7 is equivalent to Equation 3. However, from Equation 8

$$\dot{\bar{x}}_i = \bar{A}_{i-1} \bar{\delta}_i + \bar{f}_{i-1} \quad (10)$$

Thus $\bar{f}_i = \dot{\bar{x}}_i$ only when the iterative process is near convergence—that is, when $\bar{\delta}_i \approx 0$ and $\bar{f}_{i-1} \approx \bar{f}_i$. Thus the authors' Equation 7, supposedly quasilinearization in terms of state variable changes, is equivalent to the standard quasilinearization algorithm, the authors' Equation 6, only when the iterative process is near convergence.

Literature Cited

- Lee, E. S., "Quasilinearization and Invariant Imbedding," Academic Press, New York, 1968.
Ramaker, B. L., Smith, C. L., Murrill, P. W., *IND. ENG. CHEM. FUNDAM.* 9, 28 (1970).

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Vaporization of Droplets in High-Temperature Gas Streams

SIR: Frazier and Hellier (1969) have measured the vaporization of nonsupported Freon-113 droplets into heated air. They state that the correlation of Ranz and Marshall (1952) underestimates the mass transfer coefficient by a factor of 4.

To test this conclusion, we have recalculated the evaporation rate from the Ranz-Marshall correlation, corrected for transpiration effects. We find a much smaller deviation, 33%, between our predicted transfer rate and that which was observed. This is rather good agreement, in view of the uncertainties in the measurement and in our estimates of the physical properties for this system.

Our calculation procedure is an extension of that of Ranz

and Marshall, as indicated below. We use the interfacial energy balance

$$N_{A0} \Delta \bar{H}_{A0} + q_0^{(c)} + q_0^{(r)} = 0 \quad (1)$$

which holds for vaporization of pure A (here, Freon-113) from an isothermal droplet. The fluxes and interfacial states are regarded as averages over the surface of the droplet. The temperature of the gas at the interface is T_0 and the composition there is approximated as $x_{A0} = p_{A, \text{vap}}/p$.

To start the calculation, a trial value of T_0 is chosen and the resulting interfacial composition, x_{A0} , is calculated from vapor pressure data reported by Stull (1947). Then the other