LETTERS TO THE EDITOR

To the Editor:

Park and Himmelblau [*AIChE J.*, **26**, 168 (1980)] have recently demonstrated the estimation error that arises in using the usual linearized propagation-of-error formula (**LPEF**) when the function relating the dependent and independent variables is nonlinear. In particular, they analyze the relation between the equilibrium constant K and the standard free energy ΔF° given by $K = \exp(-\Delta F^\circ/RT)$, and find error of up to 50% in the **LPEF** estimations of $E(K)$ and $Var(K)$, expressed as $\hat{\mu}_K$ and $\hat{\sigma}_K$ respectively, compared to the correct values μ_K and σ_K, when assuming $\Delta F^\circ \cap N(\mu_{\Delta F^\circ}, \sigma^2_{\Delta F^\circ})$.

Although it is true that the **LPEF** does introduce error in the estimates, that error is actually rather insignificant. This will be demonstrated below for the example chosen by Park and Himmelblau.

First, it needs to be pointed out that Figure 2 and 3 in Park and Himmelblau, misrepresent the errors associated with using the **LPEF.** They show that, for a particular value of temperature (for the reaction $N_2 + 3H_2 = 2NH_3$), there is no error in the **LPEF.** This is an artifact caused by their choice of representing the error in ΔF° by various constant values of its coefficient of variation, $\sigma_{\Delta F^\circ}/\mu_{\Delta F^\circ}$. This would imply that there is no error in ΔF° when $\mu_{\Delta F^\circ} = 0$, when in fact the error is still $\sigma_{\Delta F^\circ}$. An error in ΔF° is closer to arithmetic than logarithmic and therefore a more reasonable dimensionless parameter to represent the error is $\sigma_{\Delta F^\circ}/RT$. If this is done, the ratios of the **LPEF** estimates to the correct estimates are as shown in Table 1.

We see in Table 1 that there is indeed error in the **LPEF**, as represented by the ratios $\hat{\mu}_K/\mu_K$ and $\hat{\sigma}_K/\sigma_K$. The values are similar to the largest errors shown by Park and Himmelblau, although they are not directly comparable because of the different parameter used to represent the error in ΔF° (this is related to the fact that if ΔF° is normally distributed, as assumed by **P&H**, K will be log-normally distributed, but this point will not be pursued further here). These "significant errors", nevertheless, in μ_K and σ_K are not really very significant!

Consider the worst case in Table 1, corresponding to $\sigma_{\Delta F^\circ}/RT = 1.0$. The **LPEF** estimate of μ_K, and the correct value, do differ by 39.3%. However, the correct propagated error in K is 131% of μ_K. Therefore the error in the **LPEF** estimate of μ_K is negligible compared to the error in K itself.

While it appears that the error in $\hat{\sigma}_K$ might be more significant, compared to the correct value σ_K, this error is essentially as irrelevant as that in $\hat{\mu}_K$. *Accuracy in estimating the propagated error of a variable is not very important.* We are, after all, concerned primarily with knowing whether the error is 10%, 1% or 0.1%, rather than in distinguishing between 1% and 2%. We see in Table 1 that the **LPEF** estimated and correct coefficients of variation of K actually differ, at most, by 30%. Considering that original estimates of error in ΔF° can be hardly better than that, such an error in the error is of no importance.

There is, of course, a subjective element in evaluating the significance of an error estimate. A perhaps philosophical point behind this analysis and discussion is that, when the propagated error is large, and the **LPEF** becomes inaccurate, we no longer care about the value of the error—only that it is (too) large. On the other hand, when the propagated error is small, and we do care more about the related parameter estimation, the **LPEF** is entirely adequate.

This discussion applies directly, of course, only to the specific example given by Park and Himmelblau. It is, nevertheless, the experience of this writer that there is hardly ever a practical reason to be concerned with the errors in the **LPEF** method. They may, perhaps, lead to a different conclusion on a statistical test, but then only at a significance level where the result of the test is equivocal in any case.

TABLE 1. DIVERGENCE OF THE LPEF ESTIMATES OF THE MEAN AND STANDARD DEVIATION OF K FROM THE CORRECT VALUES, AS A FUNCTION OF THE DIMENSIONLESS ERROR IN ΔF°.

$\sigma_{\Delta F^\circ}/RT$	$\sigma_{\Delta F^\circ}$ (1)	$\hat{\mu}_K/\mu_K$	$\left\lvert \frac{\hat{\mu}_K - \mu_K}{\mu_K} \right\rvert$	$\hat{\sigma}_K/\sigma_K$	σ_K/μ_K	$\hat{\sigma}_K/\hat{\mu}_K$
1.0	1,000	0.607	0.393	0.463	1.311	1.0
0.5	500	0.882	0.118	0.828	0.533	0.5
0.2	200	0.980	0.020	0.970	0.202	0.2
0.1	100	0.995	0.005	0.993	0.100	0.1

(1) cal/gmole, for T = 500°K.

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LITERATURE CITED

Park, S. W., and D. M. Himmelblau, "Error in the Propagation of Error Formula," *AIChE J.*, **26**, 168 (1980).

Reply:

The main difference between our viewpoint and that of Professor Curl lies in whether knowledge about the error in the variance of a dependent variable calculated by a first order approximation to a nonlinear function is of practical use. In particular, if the value of a variable calculated by an approximation deviates from its expected value, is the information about the error in the calculated variance of the variable useful? Suppose the error in the expected value of a variable caused by an approximation is, say, 30%. If the error in the variance can be calculated, then the variance itself of the biased mean can be calculated and used as a practical tool in statistical analysis.

We are not certain what applications Professor Curl was thinking of in stating his conclusions, but we can cite some practical examples in industrial practice where the information is indeed useful with which we are familiar, namely

(1) determination of overdesign factors (safety factors) in the design of process equipment, piping, etc.
(2) development of tolerance limits for quality control
(3) incipient malfunction detection in process equipment
(4) design of alarm systems
(5) fault tree analysis.

As a matter of clarity, we did not imply there is no "error in ΔF° when $\mu_{\Delta F^\circ} = 0$" in our note. $\mu_{\Delta F^\circ}$ is just the expected value of ΔF°, and hence $\mu_{\Delta F^\circ}$ can have a value of zero yet ΔF° can still have a large variance ("error").

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To the Editor:

With reference to the journal article "Part II: Structural Aspects and the Synthesis of Alternative Feasible Control Schemes," [*AIChE J.*, **26**, 232 (1980)], the author's conclusion (Page 238) that "simple heuristics, cause-and-effect arguments" are insufficient to draw conclusions about the feasibility of the control structure is erroneous and needs clarification. Taking their example of three interacting water tanks shown in Figure 1 (Figure 6 of the paper) the cause-and-effect graph (Govind 1978) is shown in Figure 2. This graph has been derived from the process dynamic equations. Clearly if the level in tank 1 (h_1) is to be controlled by manipulating M_3', the negative feedback loop in the graph (h_3, M_2, h_2, M_3, h_3) will control the liquid level in tank 3 (h_3), which in turn controls the flow from the tank M_3'. It is this feedback control of the level h_3, that renders the control structure shown in Figure 1 infeasible.

It is important to recognize that analyzing feasibility of control structures based on process cause-and-effects can lead to erroneous conclusions if 1) the graph is incorrect, and 2) the structure of the graph i.e., presence of feedback, feedforward loops is not considered in the analysis.

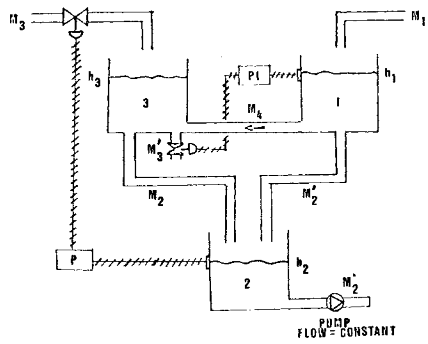

Figure 1. Three interacting watertanks—example of an infeasible control structure.

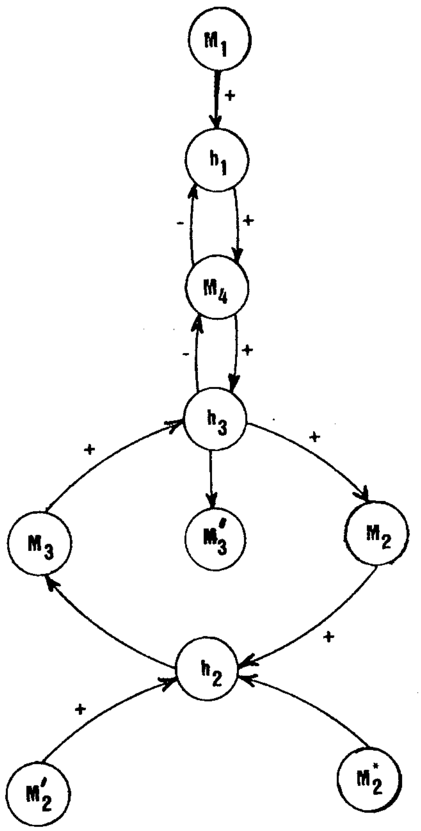

Figure 2. Cause-and-effect graph of the three interacting watertanks shown in Figure 1.

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LITERATURE CITED

Govind, R., "Control System Synthesis Strategies," PhD thesis, Carnegie-Mellon University (1978).

Reply:

We thank Dr. Govind for his interest in our article.

1) M_3' is neither determined nor influenced by h_3 as indicated in Fig. 2 of his letter, but rather h_3 is influenced by M_3'

2) Infeasibility is caused by the integral controller mode: In the steady state when h_1 is fixed by the PI controller M_2' is fixed and consequently also M_2 which in turn requires a specific height h_3. With h_3 and h_1 fixed M_4 is fixed. M_4 and M_2' fixed requires M_1 to have the specific value $M_4 + M_2'$ which is infeasible because M_1 is not manipulated. This conclusion is not apparent from the cause-and-effect graph.

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ERRATA *(Continued from page 526)*

In "Wrong-Way Behavior of Packed-Bed Reactors: I. The Pseudo-Homogeneous Model" by P. S. Mehta, W. N. Sams and D. Luss, [*AIChE J.*, **27**, 234 (1981)]. The definition of t and v_c in Equation (1) should read

$$t = \frac{\epsilon k(T_o)C_{Ao}^{n-1}\, t'}{\epsilon + (1-\epsilon)\epsilon_p + (1-\epsilon)\rho_s c_s/\rho_f c_f}$$

$$v_c = 1 + \frac{(1-\epsilon)\rho_s c_s}{\epsilon + (1-\epsilon)\epsilon_p\, \rho_f c_f}$$

In "Volatiles Loss During Atomization in Spray Drying" by Theo G. Kieckbusch and C. J. King [*AIChE J.*, **26**, 718 (1980)] the images for figures 5 and 6 were transposed. The correct versions appear below.

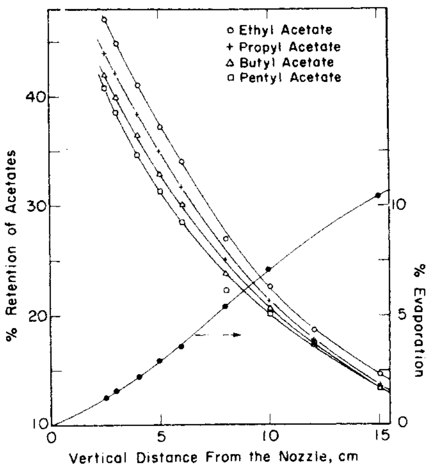

Figure 5. Retention of acetates and percent evaporation—1% sucrose solution, standard conditions; liquid flow rate = 6.4 L/h; insert 5.

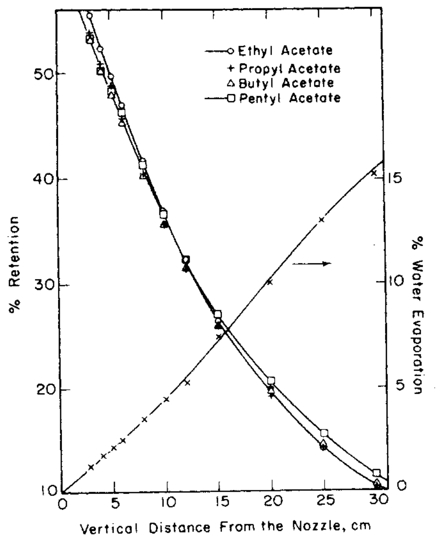

Figure 6. Retention of acetates and percent evaporation—20% sucrose solution, standard conditions; liquid flow rate = 6.75 L/h; insert J-1.