LETTERS TO THE EDITOR

To the Editor:

Mesler [*AIChE J.*, 23, 448 (1977)] has gone to ridiculous lengths to try and prove that the last 25 years of work to correlate upflow boiling in tubes was far off-target. He castigates Dengler and Addoms [CEP Symp. Ser. 52, 95 (1956)] in particular for not considering the possibility that nucleate boiling was the sole heat transfer mechanism in their tests and then goes on to "prove" that such is the case. If "proof" involves the data spread he derives from their data in Fig. 3, it is far from convincing.

He mentions the exclusion of rogue points as one of the pitfalls that Dengler and Addoms fell into. One of the two groups of rogue points involved the low coefficients observed at high vapor fractions. These corresponded to "dry wall" conditions also observed by others—these data would defy correlation by Mesler's nucleate boiling theory as well. A glance at Fig. 4 of the Dengler and Addoms paper illustrates why there were valid reasons for excluding these points from the correlation. The other set of rogue points involved unusually high coefficients encountered only at the bottom of the tube, at very low fractions vaporized. These were attributed by Dengler and Addoms to the effects of nucleate boiling and the points were indeed worked into the correlation. Another of Mesler's criticisms has to do with including the same variable in the two quantities plotted against each other. Mesler ignores the fact that the data presented were not values for the entire tube but for five separate sections of the tube. Thus for one set feed rate and overall temperature difference they obtained five different heat transfer coefficients at increasing vapor fractions up the tube. Mesler's mathematical "proof" fails to hold up under these conditions.

Mesler cites a number of other investigations which he refers to as "nucleate boiling data", including Piret and Isbin [*CEP* **50**, 305 (1954)]. Their work involved an electrically heated 1.5 m vertical tube operating with recirculation. The delta T's reported are based on the difference between the average tube wall temperature and the equilibrium temperature in the separator. The boiling point at the tube inlet would have been about 3.6°K higher than this so the delta T's reported are not true delta T's. While it is not denied that nucleate boiling may have been operating here (they considered both mechanisms and a combination of the two), it is erroneous to try and compare these data directly with those of Dengler and Addoms.

Dengler in his thesis appears to have been the first to point out that the h/h_l ratio could also be correlated against the volume fraction liquid, R_1. The correlation is simple; $h/h_l = (1/R_1)^{0.8}$, which means that one can calculate the coefficient from the conventional Dittus-Boelter equation using all-liquid properties and the actual liquid velocity in the tube. One can arrive at the same result from Chen's correlation [*IECh Proc. Des. Dev.*,] **5**, 322 (1966)]; his h/h_l ratio or F factor converts back on this basis to R_l values that agree with Dengler's and other upflow data. A simpler correlation than Martinelli's that fits the data

for water and dilute aqueous solutions is $R_l = 1/(1 + 2.5N)$, where $N = [x/1 - x)] (\rho_l/\rho_v)^{1/2}$.

Finally, Mesler seems to feel that nucleate boiling would be most likely "when evaporation occurs in annular flow where the tube is wet with a liquid film". Why, then, is heat transfer performance in the falling film evaporator, which most nearly meets this ideal, no better than in a falling film heat exchanger operating under the same conditions except that the liquid is far below its boiling point at the ambient pressure?

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Reply:

I thank F. C. Standiford for his thought provoking comments concerning the paper and wish to respond.

My paper is concerned with the data and conclusions of Dengler and Addoms and not with the last 25 years of work to correlate upflow boiling in tubes. However, since the latter work is greatly dependent upon the former it provides ample reason why the former should be re-examined to be certain it is sound. My paper advanced a new criterion to test the hypothesis of Dengler and Addoms. Using their own data the hypothesis failed the test. Thus either the hypothesis must be rejected or the criterion must be shown inconclusive or invalid.

The criterion used was predicated on Rowe's advice to avoid the inclusion of the same variable in the two quantities plotted against each other and not at all on the advice concerning exclusion of rogue points. There is no question that Dengler and Addoms were justified in their exclusion of dry wall conditions in their correlation.

The criterion advanced no more ignores the fact that the data presented were not values for the entire tube but for five separate sections of the tube than did Dengler and Addoms. After all, for each point in Dengler and Addoms' correlation in Fig. 1 there is a corresponding point in Fig. 2, and Fig. 2 provides the crux of the criterion. Since all points were considered the basis for asserting that the criterion or test fails to hold is not clear to me.

Nucleate boiling data from five investigations were shown for comparison with the data of Dengler and Addoms. Standiford feels that it was erroneous to try and compare the results of one of these investigations with those of Dengler and Addoms. Presumably he finds the other comparisons ok so let the point be based on those.

The literature casts some doubt on Standiford's notion that a falling film evaporator performs no better than a falling film heat exchanger at least for water at atmospheric pressure. Herbert and Sterns (1968) investigated heat transfer to water in falling film flow inside tubes both with and without evaporation. They noted they could find little that had been previously published. They found it necessary to correlate results for the two cases differently. An examination of their results shows the superior performance of the evaporator at their highest heat flux of .08 MW/m^2 where the effect of nucleate boiling would be greatest. They claimed that when evaporation occurred the heat transfer mechanism appeared to include contributions due to both convective and boiling mechanisms.

There are other investigations that support the importance of nucleate boiling in vertical evaporator tubes. Purcupile, Riedle and Schmidt investigated heat transfer in vertical evaporator tubes with refrigerants R-11, R-12, and R-113. They concluded that over the range of variables studied nucleate boiling was the dominant heat transfer mechanism. J. E. Backhurst in a similar study of benzene, toluene and their mixtures found that above .07 MW/m^2 nucleate boiling was the dominant mechanism.

I am grateful for this opportunity to clarify my paper and hope my efforts will now not appear quite so ridiculous to Standiford.

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To the Editor:

Huzzah to Messrs. Evans, Joseph and Seider ["System Structures for Process Simulation," *AIChE J.*, **23**, 658 (1977)]. They have addressed a long neglected facet of chemical engineering computation. The past decade has seen considerable refinement in modeling techniques for flowsheet simulation. Equally popular has been the development of algorithms for integration, convergence and the like to increase the efficiency with which solutions are obtained. Software planning and performance, on the other hand, have received little attention either in theory or in practice.

Flowsheet modeling programs deserve a special mention in this regard. Many of these packages have been in use ten years or more and it is doubtful that the original designers would recognize the present software. Coding preparation, in general, has always centered around solving the immediate vs. long range problem using only those techniques the programmer is comfortable with. By failing to recognize that systems grow as wider applications are found, software maintainers must now contend with a vagary of patches, add-ons and kludges. It is hoped that the concepts focused on in the plex approach will become a part of the blueprints for second generation simulators.

My elation in the article is partly tempered, however, by the author's continued references to FORTRAN. They are undoubtedly aware of the intrinsic advantages of PL/1 for their approach. I wish to avoid any dissertation on the relative merits of this language other than to say the dynamic storage allocation and pointer variable features alone are ideal for plex structuring. Unfortunately, the generally superior capabilities of PL/1 have been unsuccessful in loosening the traditional stronghold that FORTRAN enjoys (the "comfortability" factor again!). One finds virtually no mention of PL/1 in the academic and trade literature for the solution of engineering problems.

At a time when the computational needs of the 1980's are being outlined, the profession should also be introduced to more sophisticated programming tools. Problem oriented languages do offer clarity and convenience but necessitate special training. Surely the technical community can devote equal enthusiasm to learning a new language of almost universal application. With regard to the limited availability of the compiler for real time work, i.e., process control, the same inconvenience was shared by Fortran only a few years ago.

The cost of converting to any new programming language will be an important consideration for the moment. But at what price do we avoid a new technology that is both proven and in hand?

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Reply:

We agree that modern programming languages such as PL/1 and Pascal (ANSI, 1977; Wirth, 1973) provide improved capabilities for implementing advanced data structures for process simulation. It is also true, however, that the large majority of chemical engineers prefer FORTRAN for process calculations. We chose to illustrate the ideas of the plex data structure with FORTRAN so that it would be understandable to a larger audience. The plex data structure is a modeling concept and is independent of the language in which it is implemented.

One reason that the chemical engineering community is oriented heavily toward FORTRAN is the need for program portability. Over the years practitioners discovered that programs written in FORTRAN could be installed on a wide variety of machines, while programs in other languages often had to be reprogrammed completely. There are signs that this situation is changing. A standard (ANSI, 1977) has been issued for PL/1 and versions have been announced for UNIVAC, Honeywell and IBM computers. It is probable that in the next two years versions of PL/1 will be available on CDC computers and some of the larger minicomputers. The additional features of PL/1 such as structured programming and character string manipulation make it more attractive when compared to FORTRAN. It seems likely, therefore, that advanced process simulation systems will make greater use of PL/1 in the future for their executive programs. Since FORTRAN subroutines can be called from PL/1 programs and vice versa, existing program modules for unit operations and physical property calculations can still be used.

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To the Editor:

With reference to the R&D Note, "Process Synthesis Using Structural Parameters: A Problem with Inequality Constraints" by Jigar V. Shah and Arthur W. Westerberg, [*AIChE. J.*, 22, 378 (1977)], please be advised of earlier literature in which this problem is indicated. In Linsley (1970) and Linsley and Davis (1971), the existence of a discontinuity on the boundary of the feasible region in the space of structural parameters was illustrated. This discontinuity was not thoroughly analyzed since its presence was ancillary to the purpose of these publications. This discontinuity arose in a very simple problem without inequality constraints amongst the state variables. Of course, the structure variable inequality constraints ($0 \leq \alpha_{ij} \leq 1$)* still applied.

In the particular heat exchanger network problem of the above-mentioned R&D Note, it would appear that the ambiguity in Fig. 2 at $\alpha_{26} = 0$ results from retaining in the network the heat exchanger No. 2 with a finite area even though the cold stream flowrate through one side of the exchanger has been set to zero. Sound engineering judgement would dictate the replacement of exchanger 2 by a section of pipe when $\alpha_{26} = 0$. This would undoubtedly decrease the value of the objective function (Cost in \$/yr.). Whether subsystem 2 is a section of pipe or a shell & tube exchanger with no flow through one side, sound engineering judgement would also dictate the relaxation of the temperature approach constraint for an exchanger that is not exchanging, i.e., exchanger 2 when $\alpha_{26} = 0$ as indicated on the above-mentioned Fig. 2. This probably would not eliminate the discontinuity but it would make the objective function single-valued rather than double-valued at $\alpha_{26} = 0$ as indicated on the above-mentioned Fig. 2.

As to the structure variable approach in optimal process synthesis versus other approaches (e.g., heuristic), the beauty of the structure variable approach lies, not so much in the capability of using well-established, continuous variable, nonlinear programming techniques (e.g., dynamic programming, maximum principle, calculus), but in the thoroughness and comprehensiveness implicit in such techniques for a given process "superstructure". However, this thoroughness and the power of the continuous variable methods is usually available only in the interior of a feasible region in the space of variables (structure, decision, etc.) with respect to which one is optimizing. The boundaries of the region [Weierstrass Theorem, Courant and Hilbert (1953)] must still be considered and such consideration is, in general, a discrete activity. This does not imply that the non-comprehensive methods of process synthesis are valueless, as clearly they are sometimes computationally convenient. It would appear, however, that their principal value would be to provide insight into the "super structure" to be considered by the more certain structure variable methods of optimal process synthesis.

We would rephrase the main observation of this R&D Note thusly: When an optimization problem (process structure or other) is posed in terms of continuous variables and these variables are considered on a closed region, the boundaries of the region must also be examined and this should probably be done discretely.

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Reply:

We found the letter to you from Dr. Linsley interesting. It certainly appears to us that Dr. Linsley and we are agreeing. Our purpose in publishing the note was to counteract the rather common misunderstanding in existence in Chemical Engineering about the structural parameter method—that it is a straightforward method. This impression is readily obtained by reading the literature we referred to in our article. In each of these articles, no mention is made of potential problems at the boundaries, and unfortunately all of them illustrate their ideas with plausible but simple chemical engineering examples.

Incidentally, Dr. Linsley's discussion on the usefulness of the method is valid but perhaps one should note that many (and often most) structural parameters reside on their bounds at the optimum, in which case one has a large number of discrete tests to make. Thus, the usefulness of other synthesis methods is often very high.

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* Nomenclature is the same as that of Shah and Westerberg (1977)