Comparison of Two Methods Used in Analysis of Reactor Dynamics

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In a recent publication (*1*) Reilly and Schmitz reported results of dynamic studies of a plug flow tubular reactor with recycle. This same problem was our subject of study (*4*), but from a different point of view. Since the two approaches have a superficial resemblance rather than fundamental, the results must complement one another and not lead to contradictory conclusions. Our purpose in this paper is to make the comparisons, point out the differences, and use a numerical example to illustrate the derivation of different but consistent findings.

Reilly and Schmitz followed the changing state of a single plug as it recycled and passed repeatedly through the reactor. The result was a series of discrete points representing the reactor exit state, separated in time by the reactor residence time. A temperature-concentration phase-plane was used to plot the results. By connecting the series of discrete points a continuous curve was formed with features in some ways analogous to the trajectory of a conventional lumped-parameter analysis. The system is called *stable* to a particular disturbance, if the sequence of computed response points converges to a steady state. It is important to note, as do Reilly and Schmitz, that such a phase-plane records only behavior at the reactor exit.

In contrast, the composite phase-plane (CPP) (*2*) accounts for conditions all along the reactor by projecting temperature and concentration profiles onto a single plane. Moreover, our focus (*2*, *3*) was to find bounds on possible transients, rather than to follow specific changes in time. Because of these differences in outlook, the term stability is defined differently, with respect to allowable deviation regions at reactor inlet and exit, δ and ϵ respectively. A system is called stable (practical stability), if for a specified δ, all transients are bounded within ϵ, where the sizes of these regions have relevance to some practical design specifications.

Among the several cases studied by Reilly and Schmitz was a reactor system with a unique steady state, whose detailed study showed a series of exit states (discrete in time), that after an initial period demonstrated periodic behavior. In agreement with their definition, the steady state is identified as unstable, and the analogy is drawn to a conventional limit cycle [Figure 6 in (*1*)].

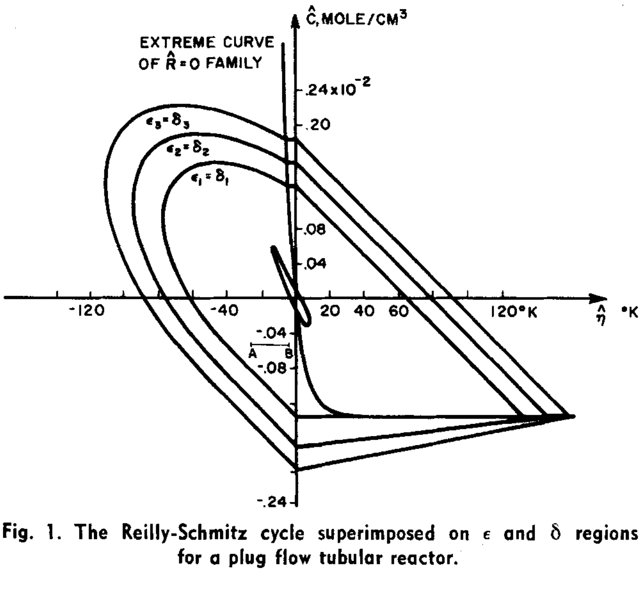

Fig. 1. The Reilly-Schmitz cycle superimposed on ϵ and δ regions for a plug flow tubular reactor.

Re-examining the same example from the viewpoint of practical stability requires the calculation of suitable δ and ϵ regions in the CPP. In this case it is most convenient to let $\delta = \epsilon$. Several such regions were computed according to the procedure detailed (*3*), and are shown in Figure 1 with the superimposed Reilly-Schmitz cycle. The superimposition is in a sense only schematic, since the position of reactor exit is only one of the infinity of positions that are represented on the CPP; nevertheless, the single figure is useful for testing consistency of results.

As illustrated in Figure 1, the computation of a $\delta = \epsilon$ region is not unique, as it provides a sufficient region but not a necessary condition. The same statement can be made for each of the three concentric contours that enclose the steady state projected as the CPP origin: transients initially within $\delta = \epsilon$ at the reactor entrance will never exceed those bounds in a single pass through the reactor. To connect the argument with the multipass recycle problem, it is necessary to stipulate that the mixing of fresh feed with the recycle stream will not produce a reactor inlet condition exceeding δ.

Because the Reilly-Schmitz cycle and their initial condition line *AB* is entirely contained within any one of the $\delta = \epsilon$ contours, no immediate questions arise that the results are indeed consistent; however, one may wonder whether still smaller $\delta = \epsilon$ contours might not raise problems by intersecting the cycle. This last doubt is dispelled by the arguments and procedures given elsewhere (*3*); no closed contour can be found that intersects the $\hat{R} = 0$ line at more than one point. Consequently, since the contour labeled $\delta_1 = \epsilon_1$ is tangent to the $\hat{R} = 0$ line, it is the smallest attainable by this technique.

This last point shows the largely conservative nature of the practical stability analysis, which is a major shortcoming. By compensating one can obtain regions of allowable combinations, rather than transients for specified initial conditions; the computations can be applied to once-through analysis as well as recycle; and there is no need for new computations when considering the effect of a fresh disturbance entering before a former disturbance has decayed. The two techniques are clearly different in outlook and goals, as well as detailed procedure. The results are complementary.

NOTATION

C = concentration of reactant
R = rate of chemical reaction
ϵ, δ = contours defining regions in the $(\hat{C}, \hat{\eta})$ plane
$\wedge$ = superscript for deviation from steady state
η = reduced temperature, defined in (*2*)

LITERATURE CITED

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3. *Ibid.*, **14**, 000 (1968).
4. ———, *Proc. Joint Autom. Control Conf.*, 107, Philadelphia, Pa. (June 1967).