A.I.Ch.E. JOURNAL

Computing Machines and the Patterns of Research

Certainly one of the most important developments of recent times is the computing machine that can accomplish detailed calculations of enormous intricacy in a very short time. These machines are now becoming available in such a wide variety of places and at such reasonable cost that they are bound to have a great influence on chemical engineering generally and on research in particular. One aspect of this consequence seems very much worth considering. A computing machine, at least at present, cannot examine experimental results for the fundamental parameters or constants of the problem. It cannot analyze; it can only synthesize. If the appropriate equations and known values of the basic parameters are fed to the machine, it can put them all together and present us quickly with results to be expected in an experiment or for a given set of design conditions. It is important to recognize this distinction between analysis and synthesis because it will have a vital bearing on future trends in research programs.

The simplified experiment, the clean-cut determination of one dependent variable or one measurable quantity, may be coming back into prominence. In the relatively recent past the simplified experiment has been somewhat discredited because it did not closely approximate a real application with which an engineer might be faced. Since this application was often of paramount importance, experiments have been developing into closer and closer approaches to the exact problem at hand until the difference between experiment and design is essentially only that of size.

As an example, one may cite the study of mass transfer phenomena in fixed beds. We have always recognized that the mechanism of this process involves both solid and fluid diffusion, and it is becoming more and more apparent that axial diffusion, as well, plays a big part. Yet, despite this recognition, there have been very few attempts to measure separately these fundamental quantities. We have preferred, in the past, to set up and solve (with many simplifying assumptions) the appropriate differential equations, to devise an elaborate experiment which closely resembles the ultimate application, and to determine the fundamental parameters by careful and detailed studies of the experimental results, in this case the "break-through" curves. This procedure has proved to be very difficult, and there have been many areas of disagreement in methods and results. It is also noteworthy that the addition of axial diffusion complicates the problems so much that the appropriate differential equations have not been solved, at least for finite bed lengths, and this approach becomes impossible. While the fixed-bed problems are particularly good examples of this difficulty, there are certainly several more which come to mind such as the treatment of consecutive and simultaneous reactions and of nonisothermal reactions, the analysis of shock-tube results, and heat and mass transfer in catalytic converters.

Perhaps it is time to abandon this analytical experimental approach and return to the simplest possible experiments. Equipment and procedure should be devised to permit the measurement of solid diffusivities alone, fluid-phase transfer coefficients or even "film" thicknesses under simplified circumstances, axial diffusion coefficients without transfer and without any other effects. The last approach, incidentally, has been begun by several research groups and is proving interesting indeed.

These simplified experiments should yield values of the basic constants and their dependence on such operating variables as flow rates, temperature, and pressure. For a given set of operating conditions, one has only to evaluate the parameters and "plug them into" the machine. The machine can tell us what results are to be expected probably as accurately as we could measure them and certainly a great deal more quickly.

H.B.