Consider modeling transient state reactions with spreadsheets

New techniques streamline analyzing process control variables

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A newly developed mathematical model can simulate transient state chemical reactions in a continuous stirred tank reactor (CSTR) with an Excel spreadsheet program. This model simulates the dynamic behavior of a first-order chemical reaction with a decay constant in a continuous flow stirred-tank reactor.

Analytical and numerical solutions of the dynamic model were done using the spreadsheet and the Fortran programs. The results from these methods had good agreement, justified using the Excel spreadsheet program as an integral part of a reactor-control system. The following example demonstrates the benefits from this method.

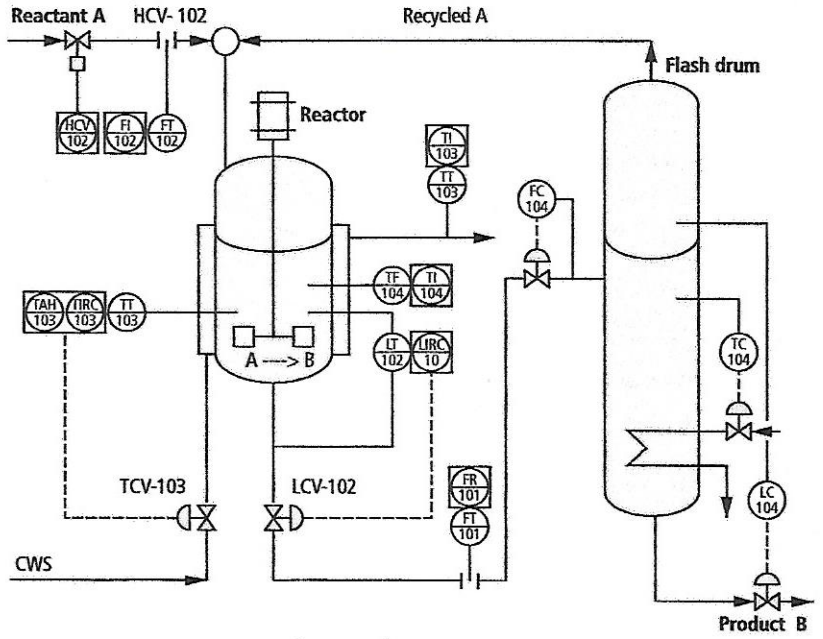

FIG. 1 Plantwide control system for a CFSTR, flash tank, and recycle stream.

Background. In the very competitive world, engineers and designers have very demanding work schedules and deadlines. These activities vary from routine process calculations (e.g., pipe pressure drop analysis, equipment and instrument sizing, material and energy balances, etc.) to rigorous computations involving the use of either developed programs or commercial simulation packages. Recent equation-solving programs have facilitated solving complex problems previously handled by high-level languages such as the FORTRAN language.[1,2,3] These equation-solving programs vary in degree of effectiveness and usage.[4] Their common advantage is in displaying the solutions in a variety of tabular and graphical forms.

An inexpensive equation-solving program is the spreadsheet. The matrix-like structure of the spreadsheet is ideal for solving both simple and, to some extent, complicated problems. These may involve a system of coupled linear algebraic equations, nonlinear equations to numerical methods of both ordinary and partial differential equations. Chemical and petroleum engineers are familiar with flowsheets that present large quantities of information in an understandable form. Spreadsheet flowsheets have enabled engineers to investigate the effects of many variations and instantly observe the results.[5] Its use has also been a valuable tool in process modeling.[6]

In one example, the spreadsheet (LOTUS 1,2,3) is used in both mass balance and equipment design of a sewage treatment. The novel process uses fine magnetite particles, a naturally occurring iron oxide and a flocculant such as alum to absorb the impurities in the raw material of physico-chemical sewage purification. Both the magnetite and alum can be chemically cleaned and regenerated to reduce costs and environmental impact.[7,8]

The Excel spreadsheet is readily available on most PCs. Its limited power and speed are compensated for by ease of programming and immediate presentation of results. Recently, the Excel spreadsheet was used to document and size relief-system for multiple process batch reactors. This method enabled engineers to continuously update files and review the relief system design basis under management of change procedures.[9]

In the following example, the modeling of a first-order chemical reaction with a decay parameter demonstrates the power of the Excel spreadsheet to simulate a concentration profile over time in a system undergoing a chemical reaction during a transient state