Using Spreadsheets in Chemical Engineering Problems

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General

The row and column format of spreadsheets fits beautifully into the type of calculations which Chemical Engineers often make. In this chapter we will show that many spreadsheet functions can be used in Chemical Engineering. As a vehicle for this demonstration we will use the simple process flow diagram shown in Fig. 1, but the techniques used in this example have much wider applicability than just flowsheeting. In addition to simply drawing and converging the flowsheet, we will consider:

- Two methods of equation solving
- Table lookup procedures
- Linear and logarithmic interpolation
- Linear regression of data
- Flash calculations
- Damage Control
- Graphing
- Spreadsheet documentation

The examples in this chapter were created using Microsoft Excel, Version 7.0 (for Windows95). Readers still using earlier versions will notice slight though usually self-explanatory differences. With the exception of the code used in macros, anything shown in this chapter can be performed on any of the major spreadsheets with very little modification. Beginning in version 5.0, Excel altered its macro language to Visual Basic for Applications (VBA), making it entirely different from its own previous macro code and that of other spreadsheets. The code for two useful macros is shown in this chapter, but the rest of the examples can be performed perfectly well without using macros at all.

A reader who is interested in general Chemical Engineering can easily follow the steps outlined in this chapter to produce the final flowsheet and thereby use all its associated equation solvers, table lookups and interpolators. Whoever wishes to do so should start with a blank workbook containing seven worksheets. He can then follow the steps in this chapter exactly. A reader only interested in some of the procedures (for example, equation solving) can begin at that step and reproduce only the relevant portion of the spreadsheet. In some cases, where input val-
ues come from another part of the spreadsheet, the selective reader may have to create artificial input values.

The complete spreadsheet containing all the examples detailed in this chapter is included on the disk and named ChemEng.XLS

**Flowsheeting**

Let us suppose that a chemist at our company research facility has invented a marvelous new product which we will call “P”. It is made from two raw materials, “R1” and “R2” in the gas phase according to this stoichiometry:

\[ R1 + 2R2 \rightarrow 2P \]

Our job is to develop a flowsheet and material balance for this process. Apart from the chemistry, all we know is that we can expect 70% of the R1 fed to the Reactor to be converted to P. There is no excess R2. The Separator (we will assume for now) is a perfect separator which produces pure P in one stream and pure R1 for recycle to the Reactor in another.

Actual drawing of the flowsheet in Fig. 1 is done by clicking on the drawing button (circle, triangle and square icon) and putting the arrows and rectangles together to give the proper diagram. We will not dwell on the details of how this