## Identifying and Thinking Through <br> Reaction Progress Problems

Identifying Reaction Progress Problems: In this course, other than in Unit 1, reaction progress problems will not occur as stand-alone problems. Instead, you will need to solve them during the course of solving different kinds of kinetics and reaction engineering problems. Most commonly you will know what chemical reactions are taking place and you will know or be given the initial (or inlet) amounts of all chemical species. You will additionally know one or more final (or outlet) amounts or reaction progress variables. Either you will need to calculate the amounts of other chemical species or reaction progress variables, or you will need an expression for the amount one chemical species in terms of the amount of another or in terms of a reaction progress variable.

Thinking Through Reaction Progress Problems: Once you have identified a problem (or some smaller part of a problem) as a reaction progress problem, you need to think through the solution to the problem. The following is a series of questions that may prove helpful as you develop your ability to do so. This isn't a magic recipe for solving all problems, and it may require adaptation for a particular problem. This series of questions is provided here to help you understand how to think through reaction progress problems the first few times you are called upon to solve them. As you practice and gain experience, these thought processes should become automatic and you shouldn't need this handout.

What quantities are known? To answer this, read through the problem statement and each time you encounter a quantity, assign an appropriate symbol to it.

What quantities are being sought? To answer this, read through the problem statement and each time it asks for a quantity, assign an appropriate symbol to it.

Is it permissible to assume a basis? To answer this, examine the known and sought quantities. If any one of them is an extensive quantity you may not assume a basis. If none of the quantities are extensive, choose a value for one extensive quantity as a basis and assign an appropriate symbol to it.

In the context of this problem, what equations relate the known quantities and the sought quantities to each other? To answer this, if the known and sought quantities are directly related to each other, for example by definition, write the corresponding equations.

Otherwise, identify those known and sought quantities that, in the context of this problem, would change if the final molar amounts of the chemical species changed, and write defining equations for them in terms of the final molar amounts of the chemical species. Then re-write those defining equations substituting expressions for the molar amounts of the chemical species in terms of the extents of reaction. In order to do this, you will need to ask yourself which of the chemical reactions taking place can be eliminated because they are not mathematically independent? To answer this, you need to determine the number of mathematically independent reactions and eliminate reactions that are not mathematically independent (see Supplemental Unit S1 if you don't know how to do this). Once all of this is done, the unknowns will consist of the extents of the independent reactions and the sought quantities.

What kind of equations are these? For reaction progress problems, the resulting equations will virtually always be algebraic equations.

How can these equations be solved? For reaction progress problems, these equations can almost always be solved manually.

What is needed in order to do so? To solve algebraic equations manually one only needs to identify N independent equations that contain N unknowns.

Do I have everything that is needed to solve the equations, and if not, how can I get the missing items? In most reaction progress problems, at this point the number of equations will equal the number of unknowns, and everything needed to solve the equations is available.

What will I get from solving the equations? In most reaction progress problems the sought quantities will be among the unknowns found by solving the equations.

Does that answer the question, and if not, what additional calculations are needed? In most reaction progress problems, no additional calculations will be needed.

