A First Course on Kinetics and Reaction Engineering

Example 5.2

Problem Purpose

This example illustrates the analysis of a chemical reaction to determine whether it *could* be elementary.

Problem Statement

Do you believe reaction (1) or reaction (2) below *could* be an elementary reaction?

$$C_2H_6 + 3½\ O_2 \rightarrow 2\ CO_2 + 3\ H_2O \quad (1)$$

$$2\ C_2H_6 + 7\ O_2 \rightarrow 4\ CO_2 + 6\ H_2O \quad (2)$$

Problem Analysis

We've already learned that you can't tell whether a reaction ***is elementary*** just by looking at the equation for it. However, knowing that an elementary reaction must be an exact description of what occurs in a singular molecular event, it is often possible to determine that a reaction ***is not elementary***. That is the approach we will take here.

Problem Solution

Reaction (1) is the standard combustion reaction for ethane. Notice that it specifies three and a half O_2 molecules as reactants. If you were able to observe this system at the molecular level, you would not see half molecules; there is no such thing. Therefore reaction (1) is not an elementary reaction.

Reaction (2) is the same reaction, but written using stoichiometric coefficients that are all integers. When the reaction is written in this way, it does not involve any fractional molecules. As such, one might suspect that this *could* be an elementary reaction. However, if reaction (2) is an elementary reaction, that means that in order for the reaction to occur, nine molecules of the proper type must simultaneously collide, every single bond in the nine reactant molecules must simultaneously break, and all the bonds in the products must simultaneously form. Quite simply, this will never happen. Recall, even for a termolecular reaction it becomes necessary to drop the requirement of simultaneous contact between all three reactants and replace it with a requirement that their centers all lie within some arbitrary, small distance of each other.

In fact, if reaction (2) were elementary, it would require the simultaneous collision of ten molecules, not nine. The reason for this is the principle of microscopic reversibility which says that any reaction that occurs in the forward direction must also occur in the reverse direction. The reverse of reaction (2) involves 10 species.

As a general rule of thumb, any reaction that involves four or more reactants ***or*** four or more products is not elementary. We conclude that neither reaction (1) nor reaction (2) could be an elementary reaction.