1 Introduction

Chemical reaction stoichiometry (CRS) is a branch of chemical stoichiometry dealing with the constraints, in the form of chemical equations, placed on changes in the composition of a closed reacting system by the requirement for conservation of the amount of each atomic species and of the total charge. This simple conservation concept has far-reaching consequences for all of chemistry and chemical engineering, including reaction kinetics and reactor design, reaction equilibrium, and reaction "book-keeping" in general. If chemical equations are to be used to express this concept, it is important to have a universal, systematic method for generating a proper set for *any* system under consideration. However, many methods currently in use, particularly in introductory teaching, do not properly or fully exploit the concept, and may give incomplete or misleading results; their scope is very limited, rendering them obsolete for general use.

To understand the role played by CRS, we believe that it is desirable to study it in its own right, "uncontaminated" by implications stemming from such things as reaction networks, reaction mechanisms, and equilibrium. Conversely, CRS does not contribute to intrinsic predictive information for kinetics or equilibrium, but only provides constraints on any predictions.

The universal, systematic method we describe in this paper and implement on the web site is not new, and has been described extensively elsewhere (Smith and Missen, 1979; 1982, 1991). As an aid to the efficiency of learning about CRS, it builds on a student's existing knowledge of very basic material (in addition to the concept of atomic conservation): the representation of a chemical species by a molecular formula, and the solution of sets of linear algebraic equations. Since it uses elementary matrix operations for the latter, we call it the *matrix reduction method* (MRM); we remark that it employs only such basic matrix manipulations as those involved in the solution of sets of linear equations, and essentially uses a matrix only as a convenient tabular way of organizing the calculations. MRM can be implemented by hand-calculation, and, for convenience in complex cases, can be programmed for implementation by computer. A new Java applet for the latter is introduced in this tutorial, and is accessible for use interactively on the web site located at http://www.chemical-stoichiometry.net

In spite of a long history of the use of an algebraic method for the simplest situation in CRS, that of balancing a single specified reaction (method of Bottomley, 1878), there appears to be considerable resistance on the part

of instructors to the use of such a method in CRS. The reasons given are: (1) that it emphasizes mathematics and not chemistry, (2) that, as a result, students don't learn about chemistry in the form of "oxidation numbers" and "half-reactions", and (3) that, if implemented by computer, it uses a "sledgehammer" to "crack the egg" of (in many cases) a relatively simple problem. In response, it can be argued that (1) students learn precisely what part of chemistry is involved in CRS (see also Olson, 1997), (2) other parts are extraneous to, and unnecessary for, CRS, and (3) use of computers and computer software is simply a matter of convenience to eliminate tedium for large-scale systems, but is not a necessity.

To overcome our suspicion of resistance on the part of many instructors, we are taking advantage of two advances in technology which may act as a catalyst to achieve adoption of MRM: ease of accessibility afforded by a web site on a global basis, and the interactive capability of a Java applet for implementation of the method.

The purpose of this tutorial is to provide a treatment of CRS as the basis for MRM. The tutorial first describes the nature and importance of CRS, and provides some historical background. It then shows the genesis of chemical equations from algebraic atom-balance equations. This is followed by a simple algorithm for the procedure used in MRM. Implementation of MRM by various means, including use of the Java applet, is illustrated with examples. The new Java applet itself, JSTOICH, is also described, with sections on "Getting Started", "Capabilities", and "Help." JSTOICH is intended to be both a teaching/learning tool and a user tool, and can be used interactively on the web site. Exercises are provided for the reader to gain experience in using MRM, particularly by implementation with JSTOICH. They also explore further aspects of CRS, including some examples of apparent confusion in the literature.