Cellular Automata Modeling of Chemical Systems

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A textbook and laboratory manual

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Preface

Over the past two decades there has been a significant growth in the use of computer-generated models to study dynamic phenomena in the nature. These studies have ranged over many of the fields of human endeavor. For example, insect behavior is a target for dynamic models; automobile traffic is another. The sociologists have picked up on the possibilities afforded by computer models to study dynamic systems. In the physical and biological sciences, dynamic computer models have been used to study a variety of phenomena. Some studies in chemistry have appeared in the literature, but the field is so vast that only a small area has been considered for computer modeling. In our view chemistry is ripe for studies utilizing this paradigm. The study of chemistry is usually focused on changes; we establish a structure, a form, but it is of real interest when we consider how and to what it is transformed. Laboratory studies in schools introduce the student to simple processes that always work. More complex transformations are difficult to set up as experiments; they often do not "work" and so the didactic value of such experiences is marginal.

It is our purpose in this book to explore and reveal how some computer models might enrich the practical experiences, traditionally carried out in "wet" labs. We pursue this goal using one of the modeling schemes that was developed a half century ago: cellular automata. The record of cellular automata as a modeling paradigm is revealed in the literature. We have used cellular automata in our research for a decade, modeling solution and kinetic phenomena of chemical systems. We feel that this approach can bring new meaning to experimental chemistry in the form of *in silico* experiments. This book is dedicated to that objective.

The book is organized into three sections. In the first section we introduce the student to some of the concepts that are fundamental to an understanding

of chemical phenomena. These include a look at the subject of complexity. Imbedded in these concepts are general chemical phenomena such as self-organization, emergent properties, and local interactions. This section sets the stage for a look at some of the modeling techniques used to explore complex systems.

In the second section we present a brief overview of some currently used dynamic modeling methods before introducing cellular automata. After a brief history of this method we describe the ingredients that drive the dynamics exhibited by cellular automata. These include the platform on which cellular automata plays out its modeling, the state variables that define the ingredients, and the rules of movement that develop the dynamics. Each step in this section is accompanied by computer simulation programs carried on the CD in the back of the book.

With this background the student is then equipped to witness what has been done in chemistry using cellular automata models. These studies are accompanied by unfinished studies and challenges, "what if" ideas for the student. The laboratory in a general chemistry course is an ideal place to use this approach since it brings to the student views of many phenomena, previously difficult to visualize. As an adjunct to experimental work in the lab, it opens up a new level of understanding. It may even pique interest in pursuing new theoretical investigations in chemistry.

At a near final stage of writing this book, we had a golden opportunity to test the modeling exercises. Seven students in the Integrated Life Sciences graduate program at the Virginia Commonwealth University were asked to read the text and to perform many of the examples and studies. Their experiences were of immense value to us in finalizing the manuscript. We want to acknowledge them and thank them for their efforts. They are Xiangrong Kong, Julie Naumann, Jean Nelson, Antoine Nicolas, Elizabeth Prom, Alexander Tulchinsky, and Carl Zimmerman. We also want to thank Yingjin Cui for her help in creating some of the figures. The authors thank Marco Tomassini for early, helpful reviews of the manuscript. We thank Enguang Zhao for his help in preparing the Java version of the CA program. Finally we acknowledge the scholarly climate and encouragement given to us at the Center for the Study of Biological Complexity at the Virginia Commonwealth University.

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