CHAPTER 11
CHEMICAL ORGANISATION THEORY

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Abstract: Complex dynamical reaction networks consisting of many molecular species are difficult to understand, especially, when new species may appear and present species may vanish completely. This chapter outlines a technique to deal with such systems. The first part introduces the concept of a chemical organisation as a closed and self-maintaining set of molecular species. This concept allows to map a complex (reaction) network to its set of organisations, providing a new view on the system’s structure. The second part connects dynamics with the set of organisations, which allows to map a movement of the system in state space to a movement in the set of organisations. The relevancy of this approach is underlined by a theorem that says that given a differential equation describing the chemical dynamics of the network, then every stationary state is an instance of an organisation. Finally, the relation between pathways and chemical organisations is sketched

Keywords: reaction networks, constraint based network analysis, hierarchical decomposition, constructive dynamical systems

1. INTRODUCTION

The rapidly increasing size and complexity of reaction system models requires novel mathematical and computational techniques in order to cope with their complexity.9 This chapter describes a technique that allows to identify for a given reaction network important sub-structures, called chemical organisations.10,38 These

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organisations allow to explain the (potential) behaviour of the reaction system from a global and more abstract perspective.

The theory aims at those systems where different combinations of molecular species (compounds) are present at different points in time. These systems are characterised by the fact that they are changing not only quantitatively, that is, by a change in the concentration of a molecular species, but also qualitatively when new molecular species appear or a present species completely vanish. Fontana and Buss\textsuperscript{20} called systems that display the production of novelty constructive (dynamical) systems.

Classical approaches describe the dynamics of a reaction system as a “quantitative” movement in a fixed state space,\textsuperscript{22} where a state is usually described by a concentration vector.\textsuperscript{16} Here, we will operate on a higher level of abstraction and consider qualitative movements from a set of molecular species to another set of molecular species. We can interpret this qualitative change as a movement that goes from state space to state space, as new molecular species appear and old species disappear.

The lack of a theory for such constructive dynamical systems has been presented, identified, and discussed in detail by Fontana and Buss\textsuperscript{20} in the context of a theory for biological organisation. As a partial solution, they suggest the important concept of a (biological) organisation as a set of molecules that are algebraically closed and dynamically self-maintaining.

Closure means that no new molecular species can be generated by reactions among molecules inside the organisation (Section 3.1). As such no novelty can spontaneously appear. Note that closure, as a property of a set of molecules, should not be confused with the thermodynamical closure of a system, which are two different and separated concepts.

Self-maintaining roughly means that every consumed molecule of the organisation has a way to be generated within the organisation such that it does not disappear from the system (Section 3.3).

Although closure and self-maintenance do not assure that a set of species will remain unchanged in time, the lack of them does imply that the system will eventually qualitatively move to a different set of molecules (Section 4.2). In a vast class of systems, which we call consistent (Section 3.5), it is possible to define a generator operator such that for any set of molecules an organisation is uniquely defined. The organisation generated by a set $A$ represents the largest possible set of molecules that can stably exists when starting with $A$.

This implies that organisations partition the set of all possible sets of molecules, where a partition consists of all combinations of molecular species that generate the same organisation. Thus, as the system qualitatively progress from one set to another we can follow it on the more tractable set of all possible organisations (Section 4.3, Figure 4). The study of this movement together with a theorem relating fixed points to organisations will be the core concepts of the dynamical part of chemical organisation theory (Section 4).