Special Anniversary Issue

MODELS IN CHEMISTRY

(3) 'Modeling Complex Systems'

Editorial

It seems to be a general rule that the less scientific objects are subject to experimental preparation and simplification the more scientists depend on conceptual idealization, model building, and reflections thereon. Experimental simplifications are particularly restricted if chemists leave their well-defined laboratory systems in order to use their concepts for 'real world systems'. However, the same also applies to laboratory and artificial objects if it is just the nonsimplified version or the dynamics that matters. Suddenly, everything appears to be complex – with regard to one or the other notion of complexity.

The third and final series of papers as part of our special topic 'Models in Chemistry' are devoted to such complex dynamical systems. As an editor depending on what is submitted after a public call for papers, I am more than happy that we have such a broad scope of approaches. Not only do the four papers represent four different chemical subdisciplines with four different kinds of systems to be modeled (chemical engineering, environmental chemistry, biochemistry, and physical organic chemistry), they also discuss quite different modeling approaches of general importance, such as dimensional analysis, dynamical and self-organizing systems approaches, neural network modeling, and fuzzy and possibilistic reasoning. Moreover, from their particular methodological analyses the authors draw general philosophical conclusion concerning the boundaries of scientific knowledge as well as social and ethical implications of model building.

Among the nonlaboratory systems, those of the technological sphere are frequently overlooked by philosophers because they tend to believe that artificial systems are well-understood – a widespread misunderstanding of the *verum factum* principle. Belgium philosopher of chemistry Jaap van Brakel analyzes how chemical engineers mathematically model their processing devices at the 'simplest' level of dimensional analysis, which among others allows dealing with scale-up problems. Though this approach originated from 19th century physics as a way to grasp similarity in mathematical terms, philosophers of physics have been reluctant to cope with such depths of 'real

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world' problems. By pointing out the various assumptions, idealizations, and *ceteris paribus* conditions of that 'simplest' modeling approach, van Brakel argues that the system to be mathematically modeled is already a model and that all we have in science is "a world of interrelated models".

The two German biogeochemists Daniel Haag and Martin Kaupenjohann deal with another kind of nonlaboratory systems, the natural environment. From an epistemological point of view, they critically analyze various assumptions of the dynamic system approach, which generally aims at mathematical models for simulating and predicting the behavior of biogeochemical systems. Moreover, as compared to the self-organizing system approach, the former neglects particularly openness, self-modification, and historicity of systems. Since these assumptions and neglects make, according to the authors, non-trivial and reliable predictions impossible, the role of simulation models is restricted to heuristics. In addition, they argue that such modeling processes actually help communication and mutual learning among various disciplinary groups involved in the process.

Once the quantum paradigm of theoreticity was left behind, theoretical biochemistry emerged as one of the most fascinating scientific fields. British biochemist Sylvia Nagl leads us to the forefront of biochemical model building. Protein domains, the relatively stable and independently fold parts of proteins, are conceived as self-organizing subsystems subject to evolutionary development. The peculiar way she models this process is by using a neural network approach. Since biomolecular modeling is strongly related to possibly technical or medical interventions of moral significance, she argues that the choice of models should responsibly be made in the awareness of these moral issues. In particular, insofar biomolecular engineering assists medicine the classical bioethical principles of beneficence and nonmaleficence apply already at the state of model building.

Finally, British philosopher of chemistry Michael Akeroyd reminds us that also classical chemists are confronted with complexity in apparently simple organic reactions. Referring to the early days of physical organic chemistry, he argues that Hugh and Ingold were forced to adopt fuzzy principles and possibilistic reasoning when establishing the first models of reaction mechanism, because of 'fuzzy data'. This modeling step as well as later modifications is paralleled by earlier developments of fuzzy logic controller devices. By analogy he argues that, unlike classical approaches, the success of fuzzy modeling is partly due to is ability to incorporate human experience into a formal model.

Enjoy reading!

Joachim Schummer, Editor