Abstract

Both the short-term and long-term performance of a cement-based material largely depend on its microstructure. The microstructure determines the interaction of the material, and even of the structure as a whole, with its environment. This paper deals with models for simulation and prediction of microstructural development. Due attention is paid to modelling of the interaction between microstructural development and hydration kinetics. The potentialities of numerical simulation models for both fundamental research and engineering applications are discussed. Some of these potentialities will be elucidated with examples. The question of how available models can be helpful in enhancing the durability of real structures is briefly addressed.

1. Introduction

From the materials science point of view, hydration and microstructural development of polynuclear and polysize cement-based systems represent a very complex world (Fig. 1). This world comprises a number of disciplines, such as chemistry, physics, colloid chemistry, crystallography, and stereology. In each of these disciplines, cement-based systems are studied more or less intensively. A huge amount of experimental data has been generated and interesting ideas have been put forward concerning particular aspects of hydration processes and microstructural development. Intra-disciplinary models have been developed with the aim of describing or explaining particular phenomena which occur during
hardening. Although these intra-disciplinary models and concepts have led to a better understanding of many aspects of hardening in cement-based systems, they finally turn out to suffer from the reductionist approach that was adopted. Most of the models are "one-dimensional" and only cover a small segment of reality. If we want to make further progress in mathematical modelling of complex systems in the future, we have to bridge the gaps between the different disciplines and tear down existing "cultural and language barriers" between them. For the development of mature and comprehensive models, a multi-disciplinary approach is a prerequisite. In such comprehensive models, the ideas, concepts, and laws developed within individual disciplines have to be considered and implemented in a consistent way.

![Diagram](image)

"real world"

"reductionistic scientific approach"

**Figure 1.** The "real world" of cement-based materials and the reductionist approach adopted in science.

### 2. Models And Modelling: What Do We Mean?

In science the words model and modelling are used for different things. Here we will restrict ourself to so-called "subjective models", i.e. models which are found or chosen by man [1]. According to their function we can further distinguish between *Models for Knowledge* and *Models for Manufacturing*. Models for knowledge are applied for investigating and describing the law, the order, or the structure that holds in reality. They help us to understand why a certain phenomenon manifests itself in the way it does. The hydration concepts of Le Chatelier and Mechaelis and the models for C-S-H gel proposed by Taylor [2], by Feldman and Sereda [3], and the Munich model proposed by Wittmann [4] are examples of models for knowledge. Models for manufacturing are developed on