

## **Fundamental materials research in view of predicting the performance of concrete structures**

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### **Summary**

For advanced civil engineering structures a service life of hundred up to hundred fifty and even two hundred years is sometimes required. The prediction of the performance of concrete structures over such a long period requires accurate and reliable predictive models. Most of the presently used, mostly experience based models don't have the quality and reliability that is required for reliable long-term predictions. The models designers are searching for should be based on an accurate description of the relevant degradation mechanisms. The starting point of such models is a realistic description of the microstructure of the concrete. In this presentation the need and the role of fundamental microstructural models for predicting the performance of concrete structures will be presented. An example will be given of a microstructural model with a proven potential for long-term predictions. Besides this also the role of models in general, i.e. in the whole design and execution process of concrete structures, will be dealt with. Finally recent trends in concrete research will be presented, like the research on self-healing cement-bases systems.

### **1. INTRODUCTION**

Mankind pays a lot for lack of durability. Figures are impressive. The direct cost for reconstruction of bridges in the USA has been estimated between \$ 20 billion and \$ 200 billion. The average annual maintenance cost for bridges in that country is estimated at \$ 5.2 billion. Comprehensive life cycle analysis indicate that the indirect costs due to traffic delays and associated lost productivity are more than 10 times the direct cost of maintenance and repair [1]. In The Netherlands the one third of the annual budget for large civil engineering works is spent on inspection, monitoring, maintenance, upgrading and repair.

These high costs are a big concern for society. Comprehensive life cycle cost analyses demonstrate an urgent need for another approach in the engineering profession, or may be even a complete paradigm shift [2]. The increasing awareness of the environmental impact of industrial activities, including the building industry, has generated incentives for studies aiming at a reduction of energy consumption and reduction of the use of scarce raw materials. One of the possible ways to save energy and raw materials consists of the increase of the service life of

concrete structures [3]. The cradle-to-grave approach, or holistic approach, has been launched by a couple of researchers and reflects their concern about our globe. However, even though these researchers are convinced of the need of a new paradigm, i.e. structural designs in which not primarily strength and stiffness are the decisive parameters but where the structure's whole life cycle is judged in terms of environmental impact, they all are aware of the constraints accompanied by such a paradigm shift. Recently Woudhuysen et al. [4] wrote a book with the challenging title "Why is construction so backward". In that book he listed a number of reasons why this is the case. The building industry is very complex, tradition plays an important role and concrete structures are often one-of-a-kind products. Even if the building process is sub-divided in smaller parts, these parts still exhibit a high degree of complexity. This high degree of complexity has stimulated efforts to simplify the situation in order to make it manageable. Simplifications, resulting in simple models, may have their right of existence. However, for a more comprehensive modelling of reality more advanced models are required.

This paper deals with the role numerical models could have for producing durable structures and for predicting structural performance during the structure's lifetime. Emphasis is on the need to develop these models on a fundamental basis, i.e. by going down to the micro- or even nano-scale where the deterioration processes actually occur. First some key issues in view of durability are discussed.

## **2 PERFORMANCE OF CONCRETE STRUCTURES - KEY ISSUES**

### **2.1 Deterioration factors**

An analysis of failures of concrete structures shows that about 40 percent of them can be attributed to the natural or man-made environment. Another 40 percent of the failures must be attributed to inadequate cover depth, poor quality of the concrete, poor detailing and poor workmanship [5]. Another way of listing failures shows that the majority of durability problems are carbonation- or chloride-induced corrosion of reinforcing steel. Factors which promote corrosion are a high permeability of the concrete, small cover depth, (micro)cracking and high temperatures [6]. Reliable predictions of the probability and rate of corrosion requires correct input of the (micro)climate, the initial state of stress and/or cracks in the structure, the kinematic boundary conditions and the materials properties.

### **2.2 Durability and cracking**

The majority of failures of reinforced concrete structures are attributable to rebar corrosion. The quality of the concrete cover plays a key role in the probability of corrosion and in the rate of corrosion once it has started. This quality depends on a variety of influencing factors. The dominant parameter in this respect is the permeability of the concrete. The permeability is determined by the pore structure, more in particular the pore size distribution and the connectivity of the pores. The main factors determining the permeability are the water/cement ratio, the type of cement, amount and type of fillers and the curing regime. The presence of cracks is often considered as a factor that impairs the quality of the concrete, but this is still a point of much debate. In a review article on autogenous healing of cracks Neville [7] quotes three authors, who found that cracks would not be harmful if they would not exceed a width of 0.2 mm, 0.3 mm and 0.4, respectively. In other reports, however, it is stated that the presence of microcracks could

jeopardize the structure's durability significantly. Without further commentary these reports seem contradictory and are not very helpful in supporting engineers in designing durable structures. Observations of the correlation between corrosion and crack width should be accompanied by information on the microclimate the concrete had been exposed to. Microcracks, if present, might promote corrosion when they enhance the permeability of the concrete cover. In that case microcracks should form a continuous network of cracks. To which extent the small cracks may close due to self-healing is another point of discussion. In spite of statements that cracks may be not that harmful as some people try to make us believe, there is no doubt that in view of durability cracks are potentially weak points [8].

### 2.3 Preventing early-age cracking

In the past prevention of early-age cracking of concrete structures has been a matter of controlling temperature differentials between old and newly cast concrete elements or within a concrete cross section. Particularly for judging the risk of cracking of structures made with low water-binder ratio mixtures, however, these temperature criteria are generally not reliable. In those mixture self-desiccation may generate large shrinkage strains, which make temperature-based criteria inappropriate. Moreover, temperature criteria by no means reflect the actual degree of restraint. What in fact counts are the induced stresses, or strains, and these in relation to the generated tensile strength and strain capacity of the concrete. Meanwhile a couple of computer packages exist with which temperature distributions in hardening concrete structures can be predicted quite accurately [9]. Stress predictions are possible as well, albeit that they are less accurate than temperature predictions. What complicates the stress predictions is the role of relaxation and accurate prediction of autogenous deformations. In a more fundamental procedure the development of stresses is modelled explicitly as a function of the evolution of the microstructure [10]. In those models the degree of hydration is the key parameter for the description of the microstructure. As will be emphasised further in this contribution, microstructural models are the basis for future numerical models for integral assessment of the quality and durability of concrete structures.

## 3 PREDICTIVE MODELS FOR DEGRADATION PROCESSES

### 3.1 Deterministic and probabilistic models

For degradation processes, like carbonation, rebar corrosion, sulphate attack and alkali-silicate reaction, a variety of *deterministic* models have been proposed [11,12]. Even though much is known about the individual deterioration mechanisms, many of these predictive models are rather simple. For example, the rate of carbonation is often described as a square root of time, whereby coefficients allow for the type of cement and the w/c ratio or, even more crude, only the compressive strength of the concrete. For the rate of chloride ingress Fick's second law of diffusion is commonly used, even though it is known that in most cases both the migration of chloride ions in the pore system is not simply a matter of diffusion. The actual complexity is then hidden in model parameters derived from compliance tests. The amount and quality of the experimental data used for the determination of the parameter values determine the reliability of these predictions.

The *probabilistic* concept is the basis for most of the currently used structural codes and more recently this concept is also used for quantitative serviceability assessments [13]. For a

probabilistic assessment of the moment that a structure fails to meet the required performance criteria both the actions ( $S(t)$ ) and the resistance ( $R(t)$ ) can be considered variables with a normal distribution. Schematically the concept is shown in Fig. 1. Both the resistance and the loading may change with time. The resistance may increase due to continuing hydration and densification of the microstructure, but may decrease due to carbonation, corrosion or cracking. The load, i.e. the input for the degradation model, may change as well, for example due to changes in the local or global climate. These predictive models can be either phenomenological or fundamental. It is believed that in the future the more fundamental models, with which the degradation processes are modelled explicitly, will become increasingly important. Firstly, because the knowledge about degradation processes has reached the stage that modelling of them on the micro level, or even the nano-level, is possible. Secondly, the power of the present generation computers allows developing these models on the indicated levels. For transferring the results of microscale simulations to the macroscale will require multi-scale modelling. In fact many durability problems are multi-scale problems, which can only be dealt with appropriately with a multi-scale approach [8].

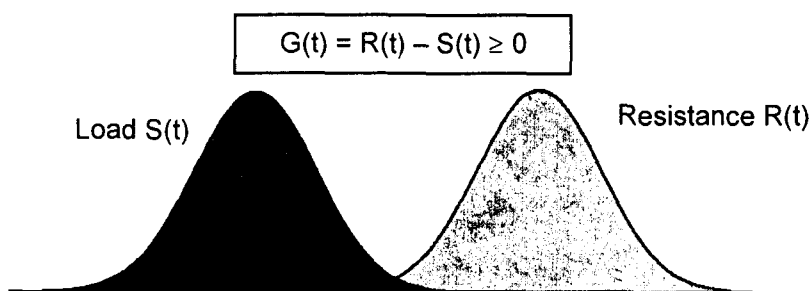


Figure 1 Schematic representation of probabilistic durability design

### 3.2 Advanced models for hydration and microstructure development

The starting point for modelling degradation processes is the microstructure of the material and the state and composition of the water in the pore structure. This initial state is the result of the hydration process and is determined by the raw materials from which the concrete is made. A few models have been proposed with which the evolution of the hydration process and of the microstructure can be predicted as a function of the mixture composition and curing conditions. The four most frequently discussed microstructural models are the NIST model [14], Navi's model [15], the Ducom model [16] and the HYMOSTRUC model [17]. In the NIST model the cement particles are considered to consist of pixels,  $1 \mu\text{m}^3$ , each particle representing a certain type of solid. The cement particles dissolve pixel-wise, each pixel making random walks through the paste until fusion with other pixels may result in reaction products that precipitate on the surface of dissolving cement grains or in water-rich areas. This process results a 3D-network. The pore structure is an inherent by-product of the simulation process and is the starting point for quantitative transport simulations and degradation processes. In the HYMOSTRUC model, like in Navi's model, cement particles are considered as spheres. Due to the formation of reaction products these spheres "grow" concentric-wise. During this process contacts are made with adjacent particles. The way in which the formation of interparticle contacts are formed differs,

but in all cases a 3D-network of connected particles is formed. Also in these models the pore structure is an inherent by-product of the simulation. The physical interaction between hydrating cement particles is assumed to affect the rate of hydration. The interaction between the rate of hydration and the formation of interparticle contacts has been termed “integrated kinetics” [17].

The HYMOSTRUC concept is shown schematically in Fig. 2. In the middle a central particle of a cubic cell is shown in an arbitrary state of growth. All growing particles together make up a 3D virtual microstructure shown in the right part of the figure.

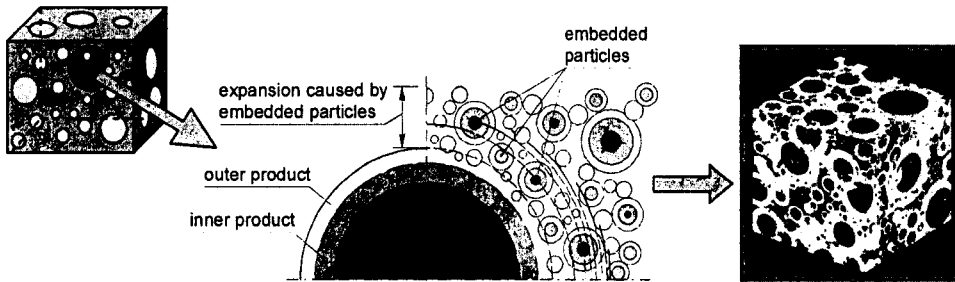


Figure 2. Schematic view of HYMOSTRUC concept: Growth mechanism of individual particles resulting in a 3D-microstructure [8,18,20]

### 3.3 Validation of advanced microstructural models

The HYMOSTRUC model has been developed for predicting the evolution of heat of hydration and the formation of microstructure as a function of the particle size distribution of the cement, the water-cement ratio, the reaction temperature and the type of cement. In order to validate the model different types of experiments were carried out on young (hardening) systems [19,20,21]:

- Adiabatic temperature rise for validating the kinetic module of the model
- Measurements of the amount of non-evaporable water for determination the degree of hydration for validating the kinetic module.
- Ultrasonic pulse velocity measurements for validating microstructure development
- MIP-tests for validation trends in changes of the pore structure
- ESEM studies for validating trends in changes of the pore structure
- Strength and stiffness tests for validating the proposed relationship between microstructural feature and microscopic properties
- Volume changes of low water-cement ratio pastes for validating moisture-structure interactions
- Permeability tests for validating permeability parameters of virtual microstructures.

In all these tests a fairly good agreement between experimental results and model predictions was found. As an example figure 3 shows the correlation between the measured resonance modulus of hardening cements pastes and the increase in the calculated contact area between hardening cement paste [19].

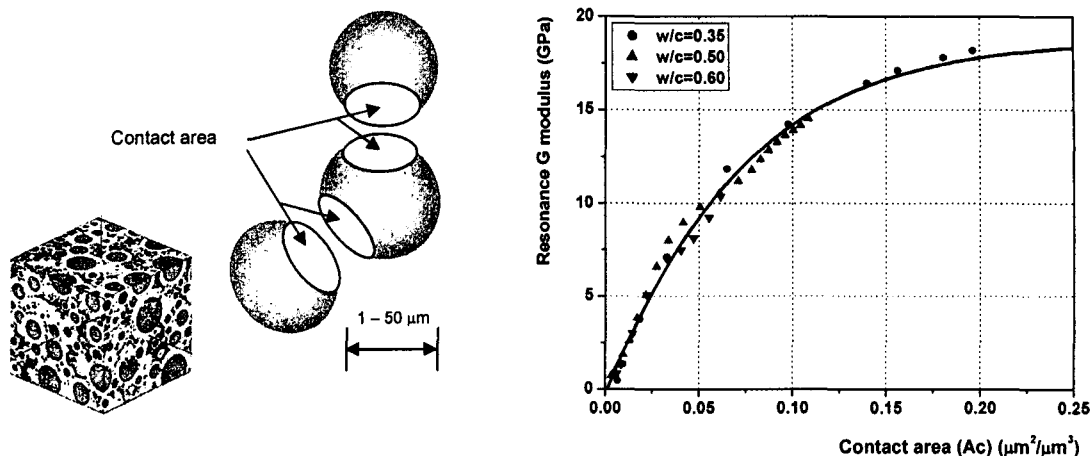


Figure 3. Concept of interparticle contact area (middle) and relationship between calculated contact area of a virtual microstructure (left) and resonance G modulus (right) [19]. Typical radius of 'building blocks' ranges from 1 - 50 μm.

### 3.4 Transport properties: Predicting durability

Durability is a multi-disciplinary and multi-scale issue. Fig. 4 illustrates the multi-scale character of durability aspects of a concrete wall. In so far the permeability of the concrete and the presence of cracks determine the durability of a concrete structure, numerical models can support decision-making processes as regards the effect of the mixture composition, the execution procedures and curing regimes, detailing and structural design on the quality of the structure.

Microstructural models can deal with the reaction process and formation of the microstructure. With these models the effect of particles size distribution of the cement and fillers, their chemical composition, water-powder ratio, reaction temperature and external supply or premature evaporation of water on the progress of the reaction process can be quantified. The progress of the reaction process can be expressed in parameters like maturity and/or degree of hydration. For a particular mixture the evolution of the materials properties can be described as function of the degree of hydration. Volume changes associated with the hydration process, particularly autogenous volume changes in low water-powder ratio concretes, are still difficult to predict, but also here a lot of progress has been made. The evolution of materials properties and of volume changes forms the input for meso-scale analyses. With meso-structural models the stresses in the matrix caused by stiff aggregates and the probability of microcracking can be quantified. In macro-structural models temperature and moisture distributions in hardening concrete structure are analysed. Subsequently macroscopic stress fields and probability of cracking can be predicted. With regard to the stress predictions it is noticed that quantitative data on creep and relaxation of hardening concrete is still scarce and modelling of these properties needs further in-depth research.

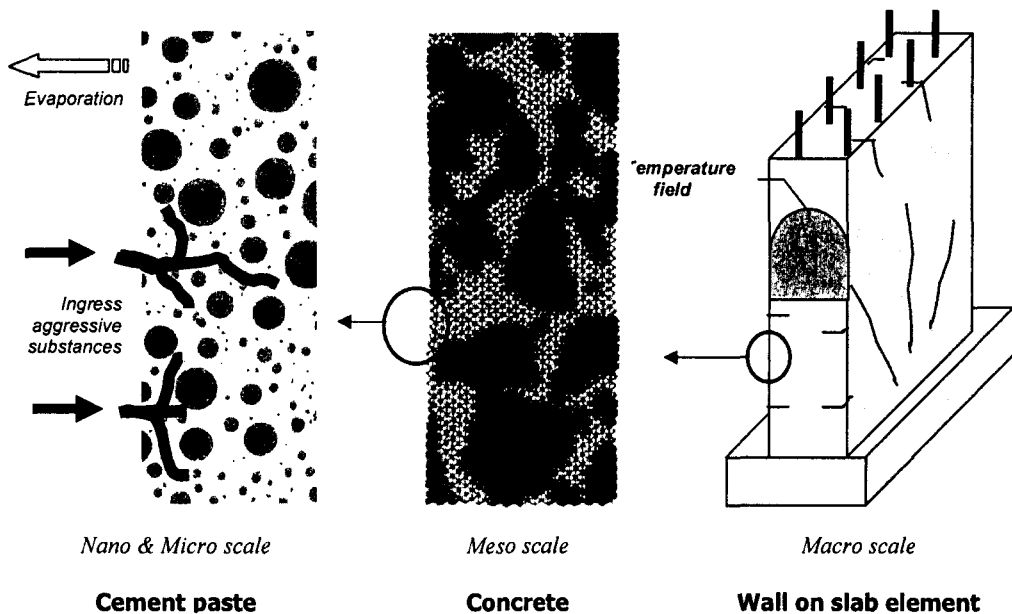


Figure 4. Scheme of multi-scale nature of the durability issue

#### 4. PRODUCING DURABLE CONCRETE STRUCTURES.

##### 4.1 A DREAM CODE as a tool for promoting an integral quality culture

For “producing” durability it is of utmost importance that the cover concrete is of good quality and that the thickness of the concrete cover is not smaller than specified. Realizing this is not a matter of materials science, advanced modeling or sophisticated simulations. What is needed for achieving durable structures is compliance with what has been called a “DREAM CODE” for durability [22]. The acronym DREAM CODE stands for a number of components of an integral quality concept, viz. Dedication, Responsibility, Expertise, Awareness and Alertness, Materials, Modelling and Management, Communication, Codes and Certificates, Organisation, Discipline and Education. In figure 5 the DREAM CODE is presented as a chain of which all links are connected in series. The weakest link determines the strength of the chain and hence the quality of the product, i.e. the concrete structure.

A first condition for achieving good quality concerns the *dedication*, and motivation, of the all parties involved in the realization of the structure. To keep people motivated and dedicated becomes more difficult with increasing distance of the workers to the final product. Quality management should focus, therefore, on restoring and maintaining the relation craftsman-product.

In most cases the knowledge to make a good product is available, but poor management and negligence can easily undo the craftsman’s potential to deliver a good product. For managers there is a world to win if they realise that 99% of quality-related costs are due to carelessness of designers and workers and poor site management [23].

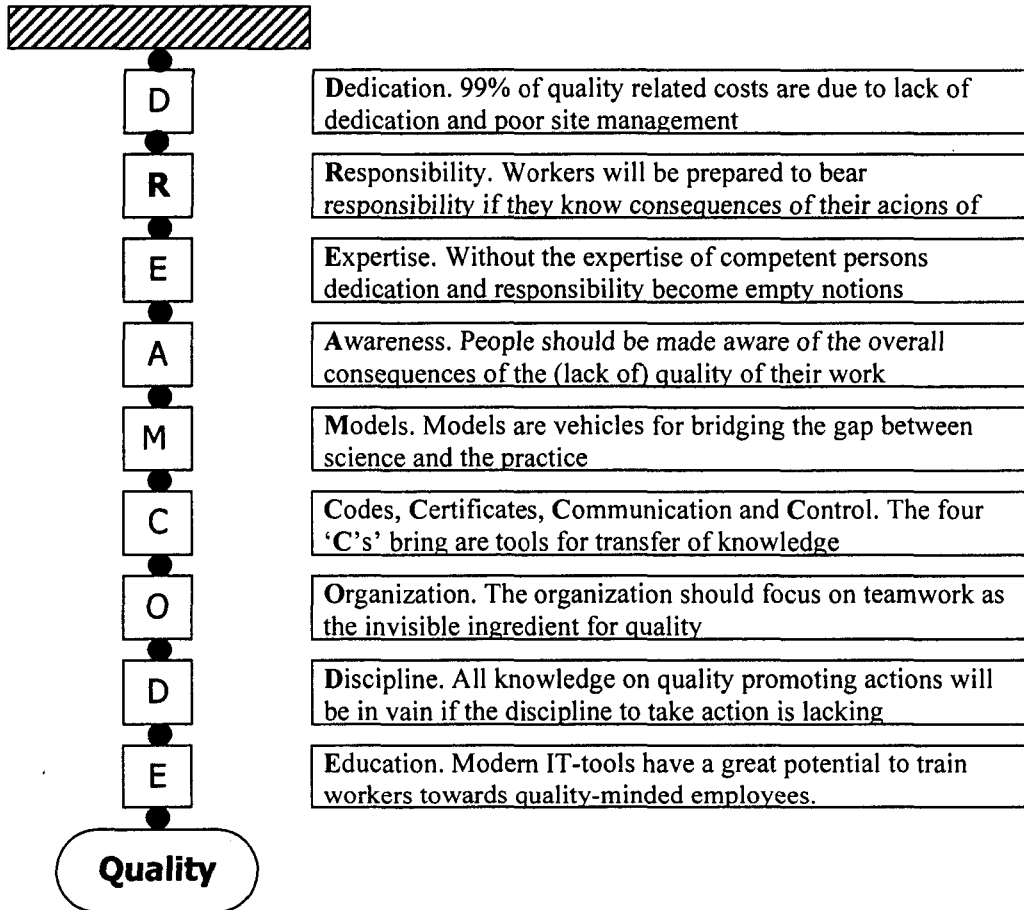


Figure 5. "DREAM CODE" for producing durable concrete structures (after [22])

Workers will be more inclined to take *responsibility* for their work if they know how important their part in the whole building process is in view of achieving durable concrete structures. In this respect it is important that they always get feed back in different stages of the building process so that they have the possibility to reflect on the consequences of their own work.

Dedicated people who know their responsibility, but *don't* have the required *expertise* and knowledge, will not be able produce good quality. However, it will be just their dedication and sense of responsibility that will make them realising that they might miss specific expertise and that they have to borrow this from elsewhere. The required expertise presupposes training of workers and knowledge of the consequences of their specific role in the process in view of the quality of the structure.

In the different states of the building process, and not in the least in the initiation phase, all parties should be *aware* of the consequences of their decisions and actions for the quality of the work. Workers should be aware of the consequences of poor curing and of unstable



reinforcement cages. This will result in a bad quality of the concrete cover and a big scatter in the thickness of the concrete cover, both increasing the probability of corrosion.

In fact *materials* do not seem to cause big quality problems. This is true for traditional materials with which a lot of experience exists. It is not true, however, for the variety of new materials and if we have to make predictions of long-term performance of these materials and of the structures made with these materials. We do not know much about these materials yet, and that makes it difficult to predict their behaviour under a variety of exposure conditions. This lack of knowledge can be considered as a predictability gap. Fundamental models, which describe the relevant (degradation) mechanisms and processes on a fundamental level, will be the appropriate vehicles that bridge the gap between research and science on one hand and practice on the other hand [24].

Failing *communication* will almost unavoidably lead to poor quality. Communication channels should be clear and unambiguous. *Codes* and *certificates* can be considered as communication tools in which huge amounts of knowledge and expertise have been put together and made digestible. Both are vehicles for transfer of knowledge. Codes give descriptions of materials behaviour, detailing and execution. Certificates guarantee the quality of a material, a procedure or a service. However, neither codes nor certificates can replace the designer's responsibility for the choices he or she will make.

A prerequisite for achieving quality is the understanding that the building process is well-*organised* teamwork. This teamwork presupposes that experts from different disciplines are prepared to invest beyond the border of their own territory. Investing in other disciplines and communication with other experts is not only the basis for quality, but in many cases it has also proved to be the basis for innovation. The reverse is true as well. Poor communication is often the cause of premature failure.

Quality requires the right material on the right place at the right time and processed by the right people with the right working attitude. Without *discipline* and commitment of all parties involved in the building process the risk of one or more weak links is real. When a lack of discipline causes failures the costs will generally be much higher than the extra costs for maintaining discipline. For increasing the awareness of workers predictive models and simulation models can be of great help. These models can clearly identify the role of each partner in the building process in a quantitative way. Thus the effect of any failure or delay can be demonstrated. In this way the model serves as a tool that teaches us that working in a disciplined way pays off!

For all the foregoing aspects it holds that *education* is crucial. Education and training concern all stages and levels of the building process. In a discussion about the introduction of design life into the design process Beeby [25] even recommends to concentrate on workmanship and education in favour of the use of sophisticated predictive models. The importance of education and workmanship for achieving quality can hardly be overestimated. In this respect the role of predictive models is certainly challenging, is not indispensable.

#### **4.2 The role of fundamental models in integral quality management**

Even though models represent only one of the links in a long chain of aspects, which together constitute an integral quality concept, the role of models is, or can be, of utmost importance. Like other aspects also models interfere with other quality components. Schematically this is shown in Fig. 6. Models can be used to develop *educative* software. This software can serve a wide variety of goals. Software that sheds light on how a building project is *organised* clarifies the position of

all parties in the entire building process. From that information their *responsibility* for the end product can be deduced. Advanced *material* models can be used to demonstrate the effect of poor curing on the risk of early age cracking and the long-term performance of a concrete structure. Such software can also illustrate what kind of *expertise* is needed for producing a good quality. Software that visualises the consequences of poor workmanship for the quality of the end product will make workers aware of their role in the building process and may contribute to the worker's *dedication*.

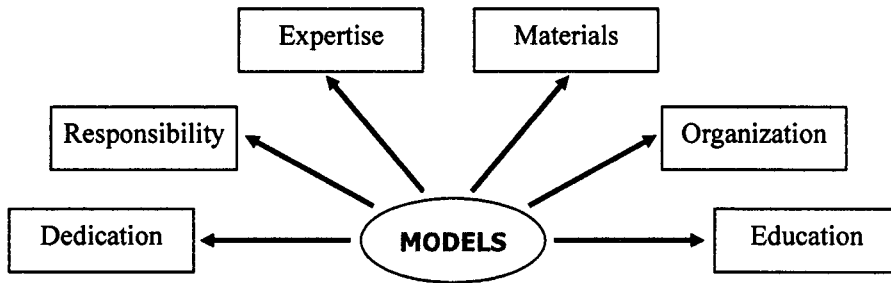


Figure 6. Position of fundamental models with focus on different aspects of integral quality management

## 5 CONCLUSIONS

For many infrastructural works a design lifetime of 100 to 150 years becomes a rule rather than an exception. To ensure that a structure will last that long without huge maintenance and repair costs is not an easy task. With the knowledge of today it is too big a claim to say that we can rely completely on predictive durability models. The reliability of model-based predictions depends on the completeness and consistency of the models and on the quality of the input, i.e. the assumed boundary conditions, loadings and exposure conditions (micro-climate). With increasing 'maturity' of predictive models the length of the period over which reliable predictions are possible will increase.

We can say that today the potential of predictive durability models to forecast a structure's lifetime in absolute terms is gradually increasing and will certainly increase further. The role of these models, however, is wider than generating absolute numbers. Of utmost importance is their potential to perform parameter studies, in which the impact of mix design, execution procedures, curing, structural boundary conditions and detailing on the structure's expected lifetime can be quantified already in the design stage of the project. In that way these models can be extremely helpful in discussions between owners, concrete technologists, designers and contractors about durability issues and in decision-making processes concerning optimal execution processes, curing regime and maintenance strategies. Further to the latter point: predictive durability models should be used in combination with well-considered short- and long-term monitoring and maintenance programs. Unforeseen circumstances, or simply lack of information or knowledge in the design stage of a project, can then be 'repaired'. The input of the models, or the models themselves, can be improved, which will enhance the reliability of the predictions for the remainder of the structure's lifetime.

A major challenge is the development of self-repairing modifications of traditional concrete. Such materials might extend the service life of concrete structures and hence reduce the costs of monitoring, maintenance and repair. Since self-repair by definition always starts at the atomic and molecular level, the development of these smart materials requires fundamental research and, if it comes of modelling, fundamental models. Research has started already several years ago and it is not easy to make big steps in short time. However, results are believed to be imminent.

Even though the power of predictive models has increased enormously in recent decades, it is still true that their predictive power is limited by the quality of the input and by the nature of the model itself. Moreover, what finally counts in view of the service life of concrete structures is not the *predicted* quality of the concrete, but the *produced* quality. Producing quality requires a series of skills, competences and attitudes, which can never be replaced by the use of models. The relevance of models should be judged in relation to other technical and non-technical factors affecting the quality of the structure. The balance between all influencing factors, in this contribution brought together under the title 'DREAM CODE', is considered the key for successful quality management and for achieving concrete structure that meet required specifications. In this integral quality management concept the role of advanced fundamental models is believed to increase in importance. Sharing knowledge and expertise and implementation of this knowledge in elegant and advanced simulation models will provide the designer with a tool that enables him to optimise the building process in both economic and environmental terms.

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