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# **Computer Codes for Material Science and Structural Engineering**

Codes de calcul pour la science des matériaux et la construction Programmeinheite für Werkstoffwissenschaften und Baustatik

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#### SUMMARY

A system of finite element modules has been developed to study and characterize the material behaviour of concrete and, at the same time, to provide realistic material laws for structural analysis. Some of the most important modules are briefly described. Several modules are combined for the prediction of the deflexions of a large span prestressed bridge during and after construction.

## RÉSUMÉ

Un ensemble de logiciels, basés sur la méthode des éléments finis, a été développé pour étudier et caractériser le comportement du béton, et permettant en même temps de fournir des lois des matériaux réalistes utilisables dans les calculs de structure. Les programmes les plus importants sont brièvement décrits dans la présente contribution. Plusieurs modules ont été combinés pour prédire les flèches d'un pontpoutre précontraint de longue portée pendant et après la construction de celui-ci.

## ZUSAMMENFASSUNG

Ein System von modularen Programmeinheiten wurde entwickelt, um einerseits das Verhalten des Betons zu studieren und zu charakterisieren und andererseits um realistische Werkstoffgesetze für die Baustatik zu formulieren. Einige der wichtigsten Programmeinheiten werden kurz beschrieben. In einem Beispiel wird gezeigt, wie mehrere Programmeinheiten kombiniert werden können, um damit die Durchbiegungen einer vorgespannten Brücke im Bauzustand und nach Fertigstellung zu berechnen.



Traditionally simplified material laws are used in structural engineering. Before the introduction of powerful computers there were no means to take the complex behaviour of a material such as concrete into consideration in an approximately realistic way. Nowadays the possibility exists to use more complicated material laws in computerized structural analysis. It has soon been realized that pure experimental studies cannot provide us with a better understanding of the materials behaviour. Numerical analysis and simulation of the different processes allows us to develop realistic material laws in a systematic way.

First it will be pointed out in this contribution in which way finite element analysis can be applied in materials science. Heat and moisture transfer are chosen as examples. Specific modules have been developed within a wider system called FEMMASSE to deal with these problems. For a more rigorous study of the behaviour of the composite material concrete the 3L-Approach has been developed [1-3]. As an example it will be explained how the obtained results can be used directly in a comprehensive numerical structural analysis of a prestressed concrete bridge.

Big computer are not available everywhere and their use is certainly not justified for structural analysis of simple structures under usual conditions. But even with a PC material laws more realistic than those given by normal codes can be used. One aim of building materials science today is to develop realistic but simple material laws to be used directly in structural analysis. In this way many of the contraversial points which can still be found in modern codes can be overcome. Numerical methods can be looked upon to be the major link between advanced materials research and structural analysis. At the end of this contribution this statement will be illustrated with an example.

## 2. DEVELOPMENT OF A SYSTEM OF SOFTWARE MODULES

## 2.1. The aim

When young concrete is exposed to an arbitrary climatic environment it has usually to be considered to be a drying and aging material. During hydration of cement heat of hydration is liberated in a concrete element. That means that during service life of most concrete structures pore humidity H, temperature T and degree of hydration  $\alpha$  vary as function of time. In order to be able to determine point properties under these conditions the following three basic equations have to be solved :

 $C_{\rm H} \dot{\mathbf{h}} + \mathbf{p} \dot{\alpha} = \operatorname{div} \lambda_{\rm HH} \operatorname{grad} H + \operatorname{div} \lambda_{\rm HT} \operatorname{grad} T$  (1)

$$C_{T} \dot{T} - q \dot{\alpha} = div \lambda_{TH} grad H + div \lambda_{TT} grad T$$
 (2)

$$\dot{\alpha} = f_1(\alpha) f_2(T) f_3(H)$$
(3)

In these equations  $C_H$  and  $C_T$  stand for hygral and thermal capacity, p and q are material parameters which depend essentially on the type of cement,  $\alpha$  is the degree of hydration,  $\lambda_{HH}$  and  $\lambda_{TT}$  are the hygral and thermal permeability coefficients whereas  $\lambda_{HT}$  and  $\lambda_{TH}$  are the cross coefficients; in equation (3)  $f_1(\alpha)$  takes the influence of degree of hydration and the concrete composition into consideration,  $f_2(T)$  stands for the well-known Arrhenius equation, and  $f_3(H)$  finally describes the influence of pore humidity on rate of hydration. Further details of this set of differential equations can be found in Ref. [4].



Equations (1) to (3) are solved in order to obtain pore humidity, temperature and degree of hydration in any point of a given concrete element. These equations can be simplified if for instance the temperature distribution under sealed conditions or the moisture distribution under isothermal conditions is of interest.

The moisture and temperature distributions can be used directly. Furthermore these distributions can serve as a basis in rate-type constitutive equations. In this case the overall material behaviour is determined as the resultant of all point properties.

## 2.2. Brief description of some existing modules

A series of modules has been developed. Although they have primarily been produced for use in research projects and to solve practical problems some are at the same time used in teaching. An overview of the so far existing modules of FEMMASSE is given in Ref. [5]. Here only a brief description of the most important modules can be given :

#### - Heat/1

Time-dependent temperature distribution (2D) in a concrete element can be calculated. Heat of hydration as well as external heating can be taken into consideration. The influence of cooling pipes and formwork on the temperature gradient is predicted. For further details see Ref. [6].

#### - Moist/l

In using a humidity-dependent diffusion coefficient the time-dependent moisture distribution of a drying concrete element is calculated [7].

#### - Fracture/1

Based on the concept of the fictitious crack [8] crack propagation in notched bars, beams, CT-specimens, ring-beams and cubes can be simulated [9].

#### - Softfit/1

Tensile strain softening of a material is determined from the measured load-displacement diagram [10].

#### - CCB/1

It is possible to simulate different stages during the construction of a large span prestressed concrete bridge. Tendon paths of prestressing elements are calculated and stress losses due to friction and relaxation are determined. Inhomogeneous shrinkage and creep in the cross sections are taken into account. Time-dependent deformations and stresses during and after the construction are calculated. This module can also be used to determine the so-called excess heights of the shuttering necessary to compensate for subsequent time-dependent deflexions. This module is an extended version of an earlier published program [13].

#### - HMG/1

This module is developed for the analysis of non-stationary coupled flow of moisture and heat in 2D in a gravity field [12].

These modules can be used separately or they can be combined in a more comprehensive analysis. In the next paragraph two examples for the use of individual modules are given, and in paragraph 5 combination of modules is demonstrated in form of a practical application. 3. TWO EXAMPLES FOR THE APPLICATION OF FEMMASSE MODULES

3.1. Heat/1

This module together with the theoretical background is described in detail in Ref. [6]. Let us consider a cross section of a girder. The web of the girder is supposed to be casted two weeks before the deck. The deck plate is furthermore supposed to have a thickness of 150 mm and a 400 kg/m<sup>3</sup> of a rapid hardening cement is used.

For the sake of simplicity the temperature distribution 12 hours after placing the fresh concrete is shown exclusively in Fig. 1. Isotherms are shown by solid lines. The thermal conductivity of the hardened web is much higher than the one of the formwork of the deck plate therefore the maximum temperature of  $45,4^{\circ}$ C is not obtained above the web.



Fig. 1 Calculated temperature distribution 12 hours after concreting.

If we admit daily temperature changes due to solar radiation for instance we can introduce at the border a temperature-time relation for the top  $T_t$  and for the bottom  $T_b$  as follows (if t is counted in hours) :

Τt	=	25 +	10 sin	(0.26 t + 5.0)	(4)
Th	=	18 -	5 sin	(0.26 t + 5.0)	(5)

The resulting temperature functions in points along an arbitrarely chosen cross section are shown in Fig. 2. It can be seen that the heating of the young concrete due to the heat of hydration fades away very quickly. Thus can be explained by the dimensions of the plate and the fact that a rapid hardening cement has been used.



Fig. 2 Calculated development of nodal temperatures.

## 3.2. Moist/1

The drying of a cross section of a box girder bridge is chosen as an example to demonstrate the applicability of module Moist/1. A typical cross section is shown in Fig. 3. In this case it is assumed that the surface is covered with a moisture barrier. The relative humidity of the surrounding air varies in yearly cycles (if t is given in days) :

$$H = 70 + 10 \sin(0.02 t)$$

(6)

In the box the relative humidity remains higher for a long time and it does not vary as much as outside. For this reason a constant value of RH = 80 % has been chosen.

The moisture distribution calculated under these conditions is shown in Fig. 3 by means of isohygres (lines of equal pore humidity) for a drying time of 1000 days. It is obvious from this result that even after three years the construction is still far from hygral equilibrium.

The nodal moisture development along an arbitrarely chosen line in the cross section is shown in Fig. 4. The layer close to the outer surface follows after a drying time of little more than a year the reasonal humidity changes. At deeper layers the amplitude of the humidity-time function is changes and a phase shift is observed. The inner surface layer reaches hygral equilibrium after about two years, while the center part is still wet after three years.



Fig. 3 Calculated moisture distribution 1000 days after demoulding.

## 4. APPLICATION OF MODULE CCB/1

## 4.1. Description of the problem

At this moment a bridge over the Rhone near Riddes (Valais, Switzerland) is in construction. The general situation, cross sections, longitudinal sections and side views of this bridge are shown in Fig. 5. The main span of 143 meters and the side spans each of 55 meters are erected by means of the cantilever method. A problem to solve was the prediction of the excess heights of the shuttering in every construction stage, needed to compensate the time-dependent deflexions. Therefore a very accurate prediction of the time-dependent behaviour is needed.



Fig. 4 Calculated development of nodal moisture.



Fig. 5 General situation, cross sections and a longitudinal section of the bridge in construction near Riddes.

Update creep and shrinkage laws of CEB-FIP model code 1978 were implemented in an earlier version of module CCB/1 and the time-dependent behaviour of about 9 large span bridges have been predicted successfully [13]. This purely empirical approach may be sufficient for usual applications but from a materials science point of view it is unsatisfactory and more important it cannot be applied in a generalized way. Therefore, in the context of a research project, a more realistic analysis based on a point property approach was carried out at EPFL.

## 4.2. Analysis

The first step in the analysis was the determination of the moisture and temperature distributions as function of time in some characteristic cross sections of the bridge. The drying process was simulated with module Moist/1 and the calculated moisture distributions were stored on disc files. It was assumed that there were no temperature gradients in the structure and that the temperature of the bridge followed the temperature of the surrounding air. The creep deformations have been calculated with an aging Maxwell chain model as proposed by Bazant [14]. The calculated moisture distributions were used to determine the shrinkage and the so called effective time "te" in a number of points of the

cross sections. Creep and shrinkage experiments have been carried out on cylinders prepared with the concrete on the site to determine the materials parameters used in this analysis.

## 4.3. Results

All most all relevant results of module CCB/1 are given in a graphical form. In Fig. 6 details of one of the composite elements is shown. All practical and useful information is indicated in this computer plot and helps to check if the input data was correct. A calculated tendon path of the prestressing elements and the determined prestressing forces are shown in Fig. 7. In addition the elongation at both ends of the tendon as well as the slip length are indicated in this figure. A large computer plot is made of the side view together with all calculated deflexions of the bridge during and after completion of the construction. A detail of this computer plot is shown in Fig. 8. From the data of the desired alignement at a given time and the calculated deflexions of the bridge the excess heights of the shuttering in every construction stage is determined. Some results of this analysis are shown in Fig. 9. In Fig. 10 the evolution of the stresses in the uppermost and lowermost fibre of an element during and after completion of the construction is plotted.



Fig. 6 General information of a composite element in order to check on input data errors.



Fig. 7 Tendon layout, calculated prestressing forces, and elongations of the tendon.





Fig. 8 Detail of a larger computer plot concerning the geometry, tendon layout and calculated deflexion lines.



Fig. 9 Calculated evolution of the stresses in the upper and lowermost fibre of a composite element.



Fig. 10 Calculated deflexion lines of the bridge at different construction stages, from which excess heights of the shuttering can be determined.

At this moment the construction of the main span is half way but it is still too early to draw final conclusions on the comparison between the predicted and measured deformations. So far, however, the observed differences were very small. Conclusions of the final comparison will be published elsewhere.

## 5. REALISTIC SIMULATION OF DRYING SHRINKAGE WITH A PC

From what is presented in the preceeding paragraphs one might get the impression that realistic materials laws can be introduced in structural analysis with the help of very powerful computers only. We will demonstrate here, however, that this also can be realized approximately but with sufficient accuracy for many practical situations with a small PC.

The example we choose is the analysis of the drying process of a cross section of the before mentioned bridge at Riddes, in order to determine an effective axial and rotation shrinkage strain. The cross section and its devision in subsections is shown in Fig. 11. It was assumed that the drying process could be described by a uniaxial nonlinear diffusion equation. A relatively small computer code has been developed on a PC which can solve this uniaxial (and also axi-symmetric) nonlinear diffusion equation with variable boundary conditions. The parameters of the nonlinear diffusion equation were determined from shrinkage measurements performed on cylinders with a diameter of 160 mm stored at a constant temperature of  $18^{\circ}$ C and a constant RH of 65 %. The dependence of the diffusion coefficient on the relative humidity was described by a mathematical expression proposed by Bazant and Najjar [15]. This function originally has been determined by data fitting. More recently a physical explanation has been given and thus a basis for more general applications [16]. The influence of temperature on the diffusion coefficient was, for the expected conditions (relatively small variations), supposed to be linear.

The nonlinear diffusion equation and the boundary conditions used for subsection 5 are shown in Fig. 12. The temperature and relative humidity of the surrounding air as function of time are based on meteorological observations in situ. In Fig. 13 measured shrinkage values of concrete cylinders are compared with the calculated shrinkage curve. This function is considered to be the standard shrinkage of the type of concrete used. The calculated shrinkage based on this predetermined material law is shown in Fig. 13 as function of time of all subsections. As can be seen in Fig. 13 the shrinkage curve of subsection 4 intersects the shrinkage curves of subsection 2 and 5. This is caused by the effect of paving with asphalt on the top of subsection 4, which is taken into account in the analysis.



Fig. 11 Division of a cross section in elements.



Fig. 12 Diffusion equation and boundary conditions used in the drying analysis of element 5 of the cross section.



Fig. 13 Calculated evolution of the average relative humidity in the different elements of the cross section.

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