

Fig. 1-Environmental penetrations into concrete



Fig. 2-Percentage reference made to various mechanisms



Fig. 3—Simplified model representing corrosion mechanism



Fig. 5—Freeze-thaw (salt attack)-permeability interaction model

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Fig. 6-Sulphate attack-permeability interaction model



Fig. 7----Influence of acid attack on permeability



Fig. 8-Alkali attack-permeability interaction model



Fig. 9-Alkali-silica reaction-permeability interaction model



Fig. 10—Tree of cracking



Fig. 11---Number of references made to factors influencing durability



Fig. 12-Causes of deterioration-permeability interaction model

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# Mathematical Modeling of Concrete Durability: The Use of Thermodynamics of Irreversible Processes

## by J.P. Bournazel and M. Moranville-Regourd

<u>Synopsis</u>: Physico-chemical processes, such as thermal effects, fluid transfer and alkali-aggregate reaction can induce expansion and damage and cracking of concrete structures. Maintenance and repair are costly on one hand and the prediction of service life is still difficult on the other.

A mechanical model (for characterising the degradation of concrete) using the thermodynamics of irreversible processes is presented. The state of concrete as a material is described by different variables such as D (damage), MT (mass transfer), A (alkali), T (temperature). The choice of variables depends on the physico-chemical process and on the volume of the concrete structure considered. To justify the modelling major hypotheses must be discussed. This model has already been applied to a dam, and a good relationship between predicted and actual damage induced by thermal effects in a gravity dam has been obtained.

<u>Keywords</u>: Alkali aggregate reactions; <u>concrete durability</u>; creep properties; damage; heat generation; <u>mathematical models</u>; microstructure; shrinkage; temperature; <u>thermodynamics</u>.

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#### Introduction

Modern computers permit now the calculation of concrete structures under severe loading. The classical mechanical approach is not sufficient anymore because designers must introduce in their computations new parameters associated to physico-chemical phenomena.

To solve these problems, researchers must develop mathematical models capable of describing the major phenomena responsible for the mechanical effects, such as cracking and damage of concrete structures. The use of thermodynamics of irreversible processes appears to be a good framework to formulate theoretical modeling of differents types of materials (1). Application of this theoretical approach to three problems of durability of concrete structures is discussed in this paper.

#### Thermodynamic State Variables

The starting postulate is that the thermodynamic state of a material in a concrete structure, at a given meso level and a given time, is completely defined by the knowledge of the values of the state variables. This postulate implies that phenomena can be described with a precision which depends on the choice of the nature and number of thermodynamic state variables.

Strain, temperature and humidity are the state variables which can be observed. On the contrary, plastic strain and damage, which are the internal variables, are not directly measurable. Introduced in the constitutive equations both internal and observable variables describe the actual state of the medium and automatically adapt the behavior of the material to this state.

From a general point of view, we define the thermodynamic potential by the free energy of the material. All state variables and their associated thermodynamic loads are summarized in Table 1.

The potential depends on state variables and it can be defined by the relation [a].

[a]

$$\rho \psi = \rho \psi(\varepsilon, T, V_k)$$

where  $\varepsilon$  is the strain, T is the temperature and V<sub>k</sub> internal state variables

The first state law gives the expression of the stress,  $\sigma$ , which is the associated variable of strain,  $\varepsilon$ , and which be deduced from the free energy, by the relation [b]:

$$\sigma = \rho \frac{\partial \psi}{\partial \varepsilon}$$
 [b]

The theoretical modeling is correct if the second principle of thermodynamics is respected, as shown by [c] :

$$\sigma \cdot \vec{\varepsilon} - \rho(\vec{\psi} + ST) - \frac{\vec{q}gradT}{T} \ge 0$$
 [c]

where S is the entropy and q is the thermal flow.

We present hereafter the description of three major physico-chemical processes acting on concrete structures, and their consequences on the mechanical behavior of concrete.

#### Setting, hardening and mechanical behavior of concrete in a structure

There is a considerable amount of information on chemical processes of hydration (2). Three stages can be distinguished in the evolution of the microstructure of concrete (3). They are : the suspension period, the setting period and the hardening period. At t<sub>o</sub>, the time corresponding to the beginning of the setting period, the Poisson's ratio, which was 0.5 during the suspension period, begins to decrease and the Young's modulus, which was negligible, starts to increase. Simultaneously, strains appear due to self-desiccation, thermal gradient, environnemental effects (humidity, wind, temperature), and concrete composition.

In the case of mass concrete, we can consider that an elementary volume in the mass is an isolated system in which the shrinkage is only autogeneous and in which restrained strains induce stresses and risk of damage.

Through the concept of state variables and associated thermodynamic loads, two major state variables are introduced into the model :

1. the evolution of the microstructure is described by a state variable called maturity,  $\boldsymbol{M}$ 

2. the state of damage is described by a scalar state variable called damage, D. The free energy can be expressed as the potential in equation [d].

$$\rho \psi = \frac{1}{2} \Lambda(M)(1-D)(\varepsilon - (\varepsilon^{th} + \varepsilon^{sh} + \varepsilon^{cm})):(\varepsilon - (\varepsilon^{th} + \varepsilon^{sh} + \varepsilon^{cm}))$$
  
+ $\rho \psi_M + \rho \psi_{TU}$  [d]

where

-  $\rho \psi$  is the free energy,

-  $\rho\psi_{\scriptscriptstyle M}$  is the free energy due to maturation,

-  $\rho \psi_{TH}$  is the free energy due to thermal effects,

-  $\Lambda$  is the tensor of elastic characteristics.

Equation [e] expresses the hypothesis of strains partition

$$\varepsilon = \varepsilon'^h + \varepsilon^{sh} + \varepsilon^{cm} + \varepsilon^c \qquad [e]$$

-  $\epsilon^{th}$  +  $\epsilon^{sh}$  are the volumic strains due to thermal variations and autogeneous shrinkage

- $\epsilon^{cm}$  is the maturation creep strain
- $\epsilon^e$  is the elastic strain.

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It is possible to deduce the expression of stress from the free energy according to the sate law defined by equation[f]:

$$\sigma = \rho \frac{\partial \psi}{\partial \varepsilon^{e}} = (1 - D) \Lambda(M) (\varepsilon - (\varepsilon^{th} + \varepsilon^{sh} + \varepsilon^{cm}))$$
[f]

### 1. Maturity

Based on previous works by Carino (4), Regourd, Gautier (5) and Malhotra (6), we choose for the maturity variable the following equation [g]

$$M = \frac{e^{-\frac{E}{RT}} \langle t - to \rangle_{+}}{1 + e^{-\frac{E}{RT}} \langle t - to \rangle_{+}}$$
[g]

where

- E represents the activation energy

- T is the temperature (Kelvin)
- t is time

- to the setting time

to can be determined by an experimental method (7) as shown in Fig. 1.

Maturity is directly related to the Young's modulus and can be expressed by the relation [h]

 $E = E_{\infty}M$  [h] In this relation  $E_{\infty}$  is the Young's modulus for M=1.

## 2. Damage

In a uniaxial isotropic case, the damage variable D is related to the Young's modulus by the following equation [i] given by Mazars (8):

$$E = Eo(1-D)$$
[i]

One can consider that there is a partition between tension  $(D_t)$  and compression  $(D_c)$ . The evolution law of D is thus given by the relation [j] :  $D = \alpha_c D_c + \alpha_1 D_t$  [j]

Di is either Dt in tension or Dc in compression, as shown by the equation [k]