

Modeling of thermohydration, the drying and the shrinking of the concrete

Summary

One describes two types of phenomena here occurring at periods distinct from the life of a concrete:

- on the one hand a reaction of thermohydration generating a withdrawal known as endogenous, appearing with the young age of the concrete (the first 100 days),
- in addition an evaporation of part of the water not used in the process of hydration, phenomenon called drying and involving a withdrawal of desiccation. This phenomenon can last, according to dimensions of the structure of concrete implemented, of a few months to several years.

These phenomena are modelled in *Code_Aster* in the form of equations of diffusion whose solution is represented by new variables making it possible to directly calculate the deformations of the endogenous withdrawal (of with the hydration) and of the withdrawal of desiccation (of with drying).

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1 Introduction

The behavior of the concrete, fragile in extension, heterogeneous and porous material is governed by the many ones and complex physicochemical phenomena. The losses of prestressings induced by the behavior differed from the concrete (withdrawal and creep) reduce in the course of time the field of loading which the structure can support. These differed deformations which appear in the concrete during the life of this one, are composed by the withdrawal with the young age (endogenous withdrawal specific to the hydration and thermal withdrawal), by the withdrawal of desiccation with the modeling of drying, and as soon as it undergoes constraints, by clean creep and the creep of desiccation.

In the rules of dimensioning, the deformations differed from the concrete are based generally on empirical rules fixed on a large number of results resulting from the literature, fascinating of account the principal parameters, like the temperature, moisture, the content of aggregate, the proportion water/cement. The kinetics of the phenomena uses the equivalent times calculated using a law of Arrhenius to take into account ageing and the temperature.

A fine analysis of the physicochemical phenomena which are at the origin of the various deformations differed from the concrete makes it possible to propose a modeling on the basis of model of type continuous medium are equivalent [bib2], which was introduced into *Code_Aster* (clean creep and the creep of desiccation are not treated here).

1.1 Phenomenologic aspects of the behavior of the concrete to the young age: thermohydration

One defines the young age as the first 100 days of the life of the concrete. Endogenous withdrawal or withdrawal of hydration, and the thermal withdrawal intervene as of the first moments of the catch (with the young age), for one duration going from a few hours to a few days, for the thermal withdrawal, and of a few months to one year, for the withdrawal of hydration, in general finished at the time of the setting in prestressing. Phenomena of prevented withdrawals or withdrawals differential, under formwork, can be at the origin of constraints or cracks which should be evaluated. In liquid phase, the concrete is a viscous fluid in which the solid matter constituents are in suspension in the hydraulic binder containing of the solid particles (cements...). Following the formation of the first hydrates, the catch of the concrete intervenes, about ten hours after its manufacturing, which corresponds to the establishment of related bridges hydrates between the cement grains in the totality of material. With the whole beginning, the grains are relatively dispersed in mixing water. In the course of time, the hydration of the cement grains is accompanied by a consumption of this mixing water. In experiments, it is noted that the voluminal assessment of the reaction is negative; it is the contraction of Chatelier. Known as simply, the total volume of the hydrates is lower of almost 10% than the total volume of these components. Mechanically, at the level of cement grains, the phenomenon stops when the bridges of hydrates formed between the grains are sufficiently rigid to prevent a possible relative bringing together of the grains. The macroscopic effects on the works are practically non-existent since in all the duration of this phase, the concrete is still deformable, and that any contraction is compensated by a granular readjustment of material against the walls of the formwork. Although of relatively weak width, and insufficient mechanical effect to generate a real cracking of the concrete, the constraints generated with the interface of two consecutive liftings can start of 50% the margin of resistance in traction of material.

The catch of the concrete accompanied by the hydration of cement involves an exothermic reaction. In massive structures the temperature can then rise with more $50^{\circ}C$. The hydration is an thermo-activated reaction, i.e. the speed of hydration increases with the temperature. When the speed of hydration decrease, the temperature decreases, involving a thermal withdrawal. Moreover mechanical properties of the concrete vary according to its degree of hydration, and finally the water consumption occurring during the hydration involves a capillary withdrawal. The various withdrawals can cause constraints much higher than resistance (weak) in traction of the concrete and bring to a cracking of material.

The calculation of the fields of temperature and degree of hydration is available with the order `THER_NON_LINE` (cf [U4.30.02]). The calculation of the mechanical fields taking of account the endogenous withdrawal is carried out with the order `STAT_NON_LINE`.

1.2 Drying and withdrawal of desiccation

To model drying is important owing to the fact that the physicochemical and mechanical properties of material are strongly dependent on moisture inside this last. The objective is to propose a macroscopic modeling of the drying of the concrete starting from a restricted number of parameters, easily measurable in experiments, starting from a law of transitory diffusion nonlinear of the moisture, chained at the temperature, while being freed from the complex mechanical, physical and chemical couplings, at the level of material.

With the dismantling, the concrete is plunged in an external environment which in general presents a percentage of moisture of about 60 to 80% HR (relative humidity = report of the steam pressure on the steam pressure saturating for a given temperature). It undergoes a true hydrous shock then (by analogy with a thermal shock). The concrete is then in thermodynamic imbalance with the atmosphere. Drying will enable him to find a hydrous balance with the external medium. Physically, drying brings into play complex phenomena closely coupled the ones with the others, depend on the heterogeneous and granular structure of the concrete. On a macroscopic scale, it is possible [bib2] to model drying like a nonlinear phenomenon of diffusion, with diffusion in liquid phase of type **Darcy**, as long as there is continuity of the liquid phase, and with diffusion in gas phase of type **Fick**, for the steam.

The withdrawal of desiccation is the macroscopic consequence first of the drying of the concrete. It is the direct prolongation of the phenomena of capillary tension which are at the origin of the endogenous withdrawal. By its intensity, deformations being about $400 \cdot 10^{-6}$ to $800 \cdot 10^{-6}$ for 50% of hygroscopy and current concretes, it is of one to three times the more important than the elastic strain for a loading close to 10 MPa .

One initially presents the modeling of thermohydration in the nonlinear operator of thermics of *Code_Aster*, then the modeling of drying, and finally, the introduction of the endogenous withdrawal and the withdrawal of desiccation into the nonlinear operator of mechanics.

2 Formalization of thermohydration

2.1 Equation of thermohydration

As mentioned in the introduction, the hydration of the concrete is a strongly exothermic reaction. Its taking into account in the equation of heat as **source term** is thus necessary (see [R5.02.02]). The second member who contains the internal sources of heat can then be enriched in the following way¹:

$$\left. \begin{aligned} \rho C_p \frac{dT}{dt} + \operatorname{div} \mathbf{q} &= Q \frac{d\xi}{dt} + s \\ \mathbf{q} &= -\lambda \operatorname{grad} T \end{aligned} \right\} \quad \text{éq 2.1-1}$$

where:

- \mathbf{q} is the heat flow,
- s is an internal source of heat (in $J/s \cdot m^3$),
- ρC_p is voluminal heat with constant pressure (in $J/m^3 \cdot K$),
- λ is thermal conductivity ($W/m^2 \cdot K$),

and specifically with the hydration:

- ξ is the degree of hydration, by definition $\xi \in [0; 1]$;
- Q is the heat of hydration (in J/m^3), that is to say the heat produced by the hydration of a voluminal unit of concrete.

The evolution of the hydration depends on the composition of the concrete and of the temperature, a high temperature accelerates the reaction of hydration.

The equation [2.1-1] can be solved if the function $\xi(t, T)$, and thus $\frac{d\xi}{dt}(t, T)$, is known.

In *Code_Aster* parameter is preferred $d\xi/dt$ compared to the hydration itself, and time thus is eliminated t . The corresponding function is called **affinity** in *Code_Aster* :

$$\frac{d\xi}{dt} := \text{AFF}(\xi, T) \quad \text{éq 2.1-2}$$

In *Code_Aster*, heat of hydration Q and the function $\text{AFF}(\xi, T)$ must be well informed by the user under the keyword `THER_HYDR` of `DEFI_MATERIAU` (see [U4.43.01]). Their experimental determination is shown using an adiabatic test ([§2.2]).

2.2 Exploitation of the adiabatic test for the determination of the function affinity and the heat of hydration.

In an adiabatic test, a sample of freshly-mixed concrete and thermically isolated is plunged in a calorimeter and one measures the change of the temperature $T^{ad}(t)$ in the course of time until hardening.

1. **Notice** : in the framework of nonlinear thermics [R5.02.02], the first of the equations 2.1-1 is often written in the equivalent form:
 $\frac{d\beta(T)}{dt} + \operatorname{div} \mathbf{q} = Q \frac{d\xi(T)}{dt} + s$, β being voluminal enthalpy. Indeed, in the command file *Code_Aster* it is necessary to inform the enthalpy and not voluminal heat, to see [R5.02.02].

This test can be used to determine the heat of hydration as well as the function affinity. Indeed, in adiabatic [2.1-1] is simplified because $\text{div } \mathbf{q} = 0$. Moreover, $s = 0$ because it is considered that the only source of heat is the hydration of the concrete. The integration of [2.2-1] beginning ($\xi = 0$) with the degree of hydration ξ give the expression then:

$$Q\xi(T^{ad}(t)) = \rho C_p (T^{ad}(t) - T_0) \quad \text{éq 2.2-1}$$

So in [2.2-1], one makes the assumption that $\xi = 1$ (end of the test), one obtains the heat of hydration:

$$Q = \rho C_p (T_\infty^{ad} - T_0) \quad \text{éq 2.2-2}$$

where T_0, T_∞^{ad} are the temperatures measured at the beginning and the adiabatic test.

While replacing in [2.2-1] the expression of the heat of hydration [2.2-2], one obtains the evolution of the hydration (and thus of his derivative $d\xi/dt$), in the form:

$$\xi(T^{ad}(t)) = \frac{T^{ad}(t) - T_0}{T_\infty^{ad} - T_0} \quad \text{éq 2.2-3}$$

The adiabatic test thus provides the functions $\xi(T^{ad})$ and $T^{ad}(t)$. Parameters of the function affinity $AFF(T, \xi)$ can be identified starting from the points of measurements obtained during the adiabatic test, $AFF(T^{ad}, \xi^{ad})$.

An expression of $AFF(T, \xi)$ was suggested by [Bib.2] in the form of exponential of the temperature:

$$\frac{d\xi}{dt} = AFF(\xi, T) = A(\xi) \exp\left(-\frac{E_a}{RT}\right) \quad \text{éq 2.2-4}$$

where E_a/R is the constant of Arrhenius (variable rather empirical parameter enters $4000^\circ K$ and $7000^\circ K$, and regarded as being equal to $4000^\circ K$ in the absence of extra information). For the adiabatic test one has then:

$$A(T^{ad}(\xi)) = \frac{1}{T_\infty^{ad} - T_0} \frac{dT^{ad}}{dt}(T^{ad}(\xi)) \cdot \exp\left(\frac{E_a}{RT^{ad}(\xi)}\right) \quad \text{éq 2.2-5}$$

where the functions opposite ξ^{-1} , $(T^{ad})^{-1}$ were used to eliminate the parameter time t .

Notice : [2.2-3] can also be written in the following way:

$$\xi(t) = \frac{T^{ad}(t) - T_0}{T_\infty^{ad} - T_0} = \frac{Q(T(t))}{Q(T_\infty)} \quad \text{éq 2.2-6}$$

In fact, one can define generally the degree of hydration at every moment t as being the report of the quantity of heat released until the moment t on the quantity of total heat released at the end of the process of hydration.

3 Discretization of the problem of thermohydration

3.1 Choice of the method of resolution

The selected method consists in solving the nonlinear equation overall [2.1-1] by making profitable the algorithm of nonlinear thermics of *Code_Aster* and to solve the equation locally [2.2-4] which represents the law of evolution of a kind of internal variable representing the degree of hydration, this law expressing itself by a function of the thermal state of the system. Indeed, there is no differential operator spaces some for the variable ξ in the equations and thus not need for finite element. The relation [2.2-4] a local law as in plasticity represents. One then preserves the same number of degrees of freedom as for classical thermics. Such an uncoupled process involves nevertheless the calculation of the same quantities several times. Indeed, let us suppose that ξ that is to say discretized with the nodes of the elements. Let us consider the example schematized by [Figure 3.1-1].

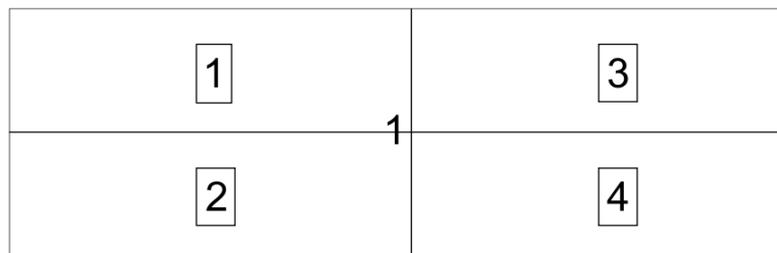


Figure 3.1-1

On the node 1, the equation of evolution [2.2-4] four times will be integrated. A possible solution would have been that local calculations can be done on fields with the nodes (concept Aster `CHAM_NO`) and not on fields of nodes by element (concept Aster `CHAM_ELEM`, option `ELNO`), which is currently impossible.

The solution which was finally adopted, consists in calculating ξ at the points of Gauss of the element, which is all the more natural as for mechanical calculation the Young modulus depends explicitly on ξ . This generates nevertheless much local calculations except strongly under-integrating the finite element. For example, if a comprising grid is considered N hexahedral elements with 20 nodes, there exists about $4N$ nodes and $27N$ points of Gauss.

3.2 Algorithm of resolution

The weak formulation of the equation [2.1-1] is written in the following way:

$$\int_{\Omega} \dot{\beta}(T) \cdot T^* d\Omega + \int_{\Omega} \lambda(T) \nabla T \cdot \nabla T^* d\Omega = \int_{\Omega} s \cdot T^* d\Omega + \int_{\Omega} Q A(\xi) e^{-\frac{E_a}{RT}} \cdot T^* d\Omega + \int_{\Gamma} \Phi \cdot T^* d\Gamma \quad \text{éq 3.2-1}$$

$$\forall T^*$$

The development of thermohydration within the algorithm general of nonlinear thermics in *Code_Aster* thus consist in discretizing in an explicit way in the second member the term

$$\int_{\Omega} Q A(\xi) e^{-\frac{E_a}{RT}} \cdot T^* d\Omega \cdot$$

While noting respectively ξ^-, T^-, ξ^+, T^+ , the variables of hydration and temperature at the beginning and the step of time, one calculates in each point of Gauss the quantity:

$$QA(\xi^-)e^{-\frac{E_a}{RT^-}}$$

who is integrated directly in the second member. After each resolution of the current step, the variables are reactualized ($\xi^+ = \xi^-$, $T^+ = T^-$). The test of convergence is active only on the temperature, the variable ξ not entering the iterative process of Newton used in nonlinear thermics. The taking into account of the hydration is in fact only the taking into account of a source of heat known at the beginning of the step of time. This purely explicit discretization thus requires to use steps of sufficiently small times.

4 Formalization of drying

This part refers to the document of specification of the development of drying in *Code_Aster* [Bib.3] , like with the thesis of L. Granger [Bib.2] .

4.1 Modeling and equations of drying

Modelings of thermics or thermohydration and drying are uncoupled at the time of the resolution. Drying is then presented like an operation chained to thermics. As the equations making it possible to solve drying and thermal nonlinear are similar for it except for the coefficients, this decoupling makes it possible to integrate the resolution of the calculation of drying in *Code_Aster*, by directly using the module of resolution of nonlinear thermics, without adding new phenomena, new types of elements nor new options of calculation, and by thus minimizing the volume of added and duplicated code.

Concentration or water content C , variable of calculation in the modeling of drying, is comparable, in term of the type of variable, at a temperature (standard `TEMP`). The transitory field of temperature, intervening in the equation of drying, is only one auxiliary parameter whose possibly the coefficient depends on diffusion.

The phenomena of thermics and drying, within the framework of a modeling uncoupled between thermics and drying, are governed by the following equations:

- equation of "classical" thermics:

$$\left. \begin{aligned} \rho C_p \frac{dT}{dt} + \text{div } \mathbf{q} &= Q \frac{d\xi(T)}{dt} + s(T) \\ \mathbf{q} &= -\lambda(T) \text{grad } T \end{aligned} \right\} \quad \text{éq 4.1-1}$$

(ρC_p voluminal heat with constant pressure, λ , thermal conductivity, Q heat of hydration and s the internal source).

- equation characterizing drying:

$$\frac{\partial C}{\partial t} - \text{Div} [D(C, T) \nabla C] = 0 \quad \text{éq 4.1-2}$$

where C (m^3/m^3 or l/m^3) is the variable of calculation (concentration or water content voluminal),

T is the variable of entry of calculation (the temperature), variable auxiliary of the resolution of drying,

D (m^2/s) is a coefficient of diffusion, characterizing to it not linearity of the equation, and depending at the same time on the variable of calculation, C , and of the auxiliary variable, T . This law of diffusion is given in various forms, according to the model selected, (law of **Bazant**, law of **Granger**, law of **Mensi**, cf [§4.3] and [bib2]).

The equations [éq 4.1-1] and [éq 4.1-2] correspond to a thermal chained calculation/drying. One can thus calculate T without knowing the water concentration, then to calculate the latter, for which T is then a parameter, (by making the assumption that thermal conductivity λ does not depend water concentration C). Also let us note that the phenomenon of drying is uncoupled from the mechanical evolutions of the concrete.

4.2 Coefficient of diffusion

The material is described by the coefficient of diffusion D , characteristic of material, depending at the same time on the temperature T and of the water concentration C . The equation of the migration of moisture in the concrete is resulting from those of the mechanics of the porous environments. One will refer to [bib2] for more precision. Classically, a law of diffusion expresses a flow like the product of a size characteristic of material by the gradient of an intensive size. The various sizes considered are defined by an average on representative ground volume, in so far as one can define this average for material considered, so that the operators of derivation have a direction. One thus makes in general the assumption which consists in supposing that the phases liquid and gas are related:

- for the diffusion of the vapor, one leaves the positivity of dissipation associated with transport with the gas phase, by differentiating two phenomena, a phenomenon of standard permeation (**Darcy**), related to gradients of pressure, and a phenomenon of standard diffusion (**Fick**), related to the gradients of concentration,
- for the diffusion of liquid water, the positivity of dissipation associated with transport with liquid water, and the law of **Darcy**, allows to express the flow of liquid according to the pressure of the liquid. The law of **Kelvin** describing the coexistence of the two phases liquid and gas by the writing of the equality of the mass free enthalpy leads to the expression of flow according to the gradient of the percentage of moisture.

From the two preceding results, one obtains the expression of total flow according to the gradient of degree of the water concentration. The classical experimental methods in the problems of drying generally give access to the water concentration, and very seldom with the relative humidity. It is thus preferable to express flow according to the water content, by classically using the isotherm of desorption of the concrete, which connects the water content, C , and relative humidity, h . The relative humidity is the relationship between steam pressure and saturating steam pressure.

The postulate of the local state stipulates that the actual position of a homogeneous system in unspecified evolution can be characterized by the same variables as with balance, and than it is independent speeds of evolution. In other words, water content C , and relative humidity h , are well connected by the same relation as to balance. What leads to the classical equation of the diffusion:

$$\frac{\partial C}{\partial t} - \text{Div}[D(C, T)\nabla C] = 0 \quad \text{éq 4.2-1}$$

This equation highlights the nonlinear character of the diffusion of moisture in the concrete. In the industrial cases, the temperature is in general not uniform in the structure. It is thus necessary to take into account a coefficient of diffusion of the moisture which depends on the temperature. In practice, in the literature, the authors most known (**Bazant** cf [bib2]) propose an expression of the coefficient of diffusion of the type:

$$D(C, T) = D(C, T_0) \left(\frac{T}{T_0} \right)^{\left(\frac{-Q_s}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right)} \quad \text{éq 4.2-2}$$

with $Q_s/R = 4700 \text{ K}^{-1}$ and T in $^\circ\text{K}$

Note:

Way in which the things are presented, it would seem that one did not use the fact that drying is a phenomenon coupled with mechanics, (i.e. he is the cause of a withdrawal of

2 The temperature entered in degree Celsius in the setting in data. Conversion into degree Kelvin is made in the sources.

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desiccation). Actually, we made the assumption of a decoupling of the phenomena, when we used the curve of sorption/desorption. In fact, during the measurement of the loss in weight to balance according to H , the body of test carries out one withdrawal. At the microscopic level, all occurs like if the withdrawal, modifying porosity, were going to interact on the relative hygroscoy inside the sample, since the steam pressure and H increase. This withdrawal of desiccation being very weak, it is usual to neglect it in calculations of the water content. There is thus only one chaining between the calculation of the water content and the mechanical calculation of withdrawal of desiccation.

4.3 Usual laws of diffusion

The law of diffusion, function of the two parameters, C and T , can be freely defined by the user in the form of a tablecloth. However, usual expressions of the law of diffusion, which one finds in the literature are the following ones:

Law suggested by Granger:

$$D(C, T) = A \cdot e^{(B \cdot C)} \left(\frac{T}{T_0} \right) e^{\left(\frac{-Q_s}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right)} \quad \text{éq 4.3-1}$$

A (m^2/s), B , T_0 , Q_s , and R (Q_s/R in $^\circ K$) are coefficients chosen by the user. D is function of the temperature and water concentration.

Law of Mensi:

$$D(C) = A \cdot e^{(B \cdot C)} \quad \text{éq 4.3-2}$$

A and B are coefficients chosen by the user. D is function only of the water concentration.

Law of Bazant:

The law of Bazant is expressed starting from the percentage of moisture h , which is connected to the water concentration by the curve of sorption/desorption. The form of this law is the following one:

$$D(h) = D_1 \left(\alpha + \frac{1 - \alpha}{1 + \left(\frac{1 - h(C)}{1 - 0.75} \right)^n} \right) \quad \text{éq 4.3-3}$$

Usually,

$$D_1 = 3 \cdot 10^{-10} m^2/s$$

α is understood enters 0.025 and 0.1 ,

n is about 6 .

$h(C)$ is the percentage of moisture, which is expressed according to the water concentration using the curve of sorption/desorption.

The curve of sorption/desorption can be introduced in the form of a tabulée standard function, knowing that actually, this curve has a hysteresis, but can be regarded as being invertible, if one takes account only of one direction of course.

4.4 Modeling of the boundary conditions

The boundary conditions are expressed in general by a nonlinear relation between flow of the water concentration ($l/m^3 \times ms^{-1}$) w^f and water concentration. These conditions are thus similar to the conditions known as of exchange in thermics. One will be able for example to use the formula suggested by L. Granger [bib2] page 181:

Its expression is the following one:

$$w^fl = \frac{0.5\beta}{(C_0 - C_{eq})^2} [C - (2 \cdot C_0 - C_{eq})] (C - C_{eq}) \quad \text{éq 4.4-1}$$

where
re C_{eq} is the water concentration for a moisture of 50%HR,
 C_0 is the water concentration for a moisture of 100%HR,
 β ($l/m^3 \times m/s$) is a coefficient, which can be defined in experiments and can evolve according to the cracking of the heat-transferring surface ([bib2]),
and C is the current concentration (unknown) on the heat-transferring surfaces.

5 Integration of drying in Code_Aster

These developments relate to the axisymmetric elements 2D and elements, as well as the elements 3D isoparametric, of many nodes unspecified, linear and quadratic.

5.1 Introduction of the concept of behavior into the nonlinear operator of thermics

The operator `THER_NON_LINE` was reserved exclusively for the nonlinear thermics, which will remain **the option of calculation by default**. But one uses the same module of resolution to solve the problems of drying and hydration, because of analogy of the equations.

The concept of behavior was added in the nonlinear operator of thermics, with a nomenclature and a syntax analogues with those of the operator of nonlinear mechanics. It implies for drying a concept of entity topological, to which this behavior is applied. This can be useful, when there are several types of possible laws of diffusion, or when one wants to do a purely thermal calculation on part of the grid, whereas on another part one does a calculation of thermohydration (on the other hand, the simultaneous use on the same grid of behaviors of type drying, and behaviours of the thermal type or hydration would not have a direction).

A behavior 'drying' is associated with each law of diffusion, such as one can find them in the literature, just as a specific material is associated with each law of diffusion, to define the characteristic coefficients of them. The resolution of drying is identical, except for the coefficients, with that of nonlinear thermics, and no modification was made to the algorithm of resolution.

For drying, four distinct behaviors are defined under the keyword '`SECH_GRANGER`', '`SECH_BAZANT`', '`SECH_MENSI`', or '`SECH_NAPPE`', to characterize each law of possible diffusion. They can be allotted to parts complementary to the grid, during the same calculation. The simultaneous definition several behaviors 'drying' associated with different topological entities requires several occurrences of the keyword '`BEHAVIOR`'. Then, the topological entity will have to be identified by informing one of the keyword `GROUP_MA` or `MESH`.

In parallel of the four behaviors 'drying', in the operator `DEFI_MATERIAU`, four materials initially make it possible to define the values of the coefficients of the laws of diffusion, nonlinear functions of the water content and the temperature. The user can choose to it (or them) law (S) of his choice, and defines the value which it wishes for each one of these coefficients.

The keyword `SECH_GRANGER` allows to define the law of diffusion of liquid and gas water in its most classical form among the expressions of the literature. Four coefficients as well as a temperature of reference T_0 characterize this law.

Keywords `SECH_MENSI` and `SECH_BAZANT` allow to define the laws of **Mensi** and **Bazant**, using the coefficients which are appropriate. The law of **Bazant**, expressing itself starting from the percentage of moisture, requires to define a curve of desorption allowing to convert the water content into percentage of moisture within the framework of this modeling.

Lastly, the keyword `SECH_NAPPE` allows to use a law of diffusion, starting from a tabulée function of two variables, which will be interpolated in calculations starting from the values of the water concentration and the temperature. This last possibility presents the disadvantage of not raising ambiguity between these two variables associated with an identical type, 'TEMP'.

It is necessary, for drying, to introduce as starter calculation a concept of the type `[evol_ther]`, representing the evolution of the field of temperature of the concrete structure, within the framework of a thermal chained calculation/drying. Indeed, the calculation of drying requires the preliminary calculation of the temperature and possibly of the hydration, because the coefficient of diffusion $D(C, T)$ depends on the temperature.

5.2 Implementation of the boundary conditions for drying

5.2.1 Expression of the boundary conditions

The boundary conditions are expressed in the form of flow of moisture on surfaces in contact with the external medium according to the expression [éq 4.4-1].

5.2.2 Delimitation of the calculation of drying using the boundary conditions

The calculation of drying is defined on the totality of the grid where finite elements are affected. To make effective the calculation of drying only on one portion of the grid (this with an aim of preserving the same model for calculations of drying and mechanical calculations and of facilitating the "continuations" of calculation Aster [bib4]), one will use the boundary conditions. Indeed, drying does not take place that if there is exchange with outside. It is thus the attribution of the boundary conditions which makes it possible "to locate" calculation. The absence of drying on a portion of the structure will be expressed by the absence of boundary conditions on the heat-transferring surfaces concerned.

5.2.3 Implementation in Aster

The boundary conditions can be defined, as in thermics, in the form of normal flow not linear formulated starting from a function tabulée of the variable of calculation, and interpolated at the time as of calculations. That makes it possible to avoid creating new options of calculation, similar to the options of nonlinear thermics `char_ther_fluxnl` and `resi_ther_fluxnl` who calculate the first and the second member, and who can be used directly for drying. It is then enough to choose a tabulée function corresponding to the expression of flow, given by the equation [éq 4.4-1].

Using a preset function (`FORMULA`), the expression of flow, given in polynomial form and function of the variable of calculation, is transformed into tabulée curve, via the operators Aster (`CALC_FONC_INTERP`). One thus does not create a new option of calculation for the treatment of the boundary conditions.

The calculation of new options would have the advantage of being optimal in term of result (because of absence of interpolations and "exact" calculations of derivative), but would require to develop two new options of calculation, similar to the options `char_ther_fluxnl` and `resi_ther_fluxnl`.

5.2.4 Example of working of the boundary conditions

The sequence of orders, described in the example which follows (resulting from the test `HSNA100` [V7.20.100]) the creation of a boundary condition implements `CHARSE05` on a group of meshes `L_INT`.

Note:

'`FORMULA`' Aster is the digital expression of flow of the normal water concentration which takes again the equation [éq 4.4-1].

```
BETA=3.41557E-08  
C_0=105.7  
C_EQ_I05=69.1
```

```
C_EQ_E05=69.1
C_EQ_I10=51.6
C_EQ_E10=69.1
```

```
FL_INT05 = FORMULA (NOM_PARA=' TEMP',
VALE= '' (0.5*BETA/((C_0 - C_EQ_I05) ** 2)
* (TEMP - (2.*C_0 - C_EQ_I05))* (TEMP - C_EQ_I05))''')
```

```
LIST0=DEFI_LISTE_REEL (DEBUT=0., INTERVALLE= (_F (JUSQU_A = 200. , NOT =
10.)))
```

```
HU_INT05=CALC_FONC_INTERP ( FONCTION=FL_INT05,
LIST_PARA=LISTE0, NOM_PARA = 'TEMP', NOM_RESU=' FL_INT05',
PROL_GAUCHE=' LINEAIRE', PROL_DROITE=' LINEAIRE',
INTERPOL=' LIN', TITRE=' FLOW D HUMIDITE' )
```

```
CHARSE05=AFFE_CHAR_THER_F (MODELE=MOTH,
FLUX_NL=_F ( GROUP_MA = 'L_INT', FLUN = HU_INT05))
```

Note:

It is important that the interpreted function and the tabulée function do not bear the same name, so that the interpolations on the right and on the left are suitably defined, because exclusions on the right and on the left “do not overload” not the prolongations of an interpreted function, transformed using the operator CALC_FONC_INTERP.

5.3 Digital integration of drying

The equation of heat $\rho C_p \frac{dT}{dt} - \text{Div}(\lambda \text{grad } T) = s(T)$ or $\dot{\beta} - \text{Div}[\lambda(T) \nabla T] = s(T)$ conduit, in the case of a boundary condition in normal flow on the border Γ with the variational formulation:

$$\int_{\Omega} \frac{\partial \beta}{\partial t}(T) v \cdot d\Omega + \int_{\Omega} \lambda(T) \nabla T \cdot \nabla v \cdot d\Omega = \int_{\Omega} s(T) \cdot v \cdot d\Omega + \int_G \lambda(T) \frac{\partial T}{\partial n} \cdot v \cdot dG \quad \text{éq 5.3-1}$$

In a similar way, the equation governing drying $\frac{\partial C}{\partial t} - \text{Div}[D(C, T) \nabla C] = 0$ conduit, in the case of a boundary condition in normal flow on the border Γ with the variational formulation:

$$\int_{\Omega} \frac{\partial C}{\partial t} v \cdot d\Omega + \int_{\Omega} D(C, T) \nabla C \cdot \nabla v \cdot d\Omega = 0 + \int_G D(C, T) \frac{\partial C}{\partial n} \cdot v \cdot dG \quad \text{éq 5.3-2}$$

The resolution of drying is integrated into the operator THER_NON_LINE, while replacing ρC_p by the constant function equalizes with the identity, and conductivity by the diffusion $D(C, T)$, the temperature intervening like a constant in calculations (auxiliary variable). According to the law of diffusion chosen, it is necessary to calculate the value of the coefficient of diffusion like its derivative, according to temperature and the water concentration at the moment running, at the current point.

One will refer to the documentation of the nonlinear operator of thermics [R5.02.02] for further details on the digital integration of nonlinear thermics.

Within the framework of drying, the boundary conditions are given in term of normal flow, and lead, as in thermics, with a term in the first member, associated with the option of calculation rigi_ther_fluxnl, and in the term in the second member, associated with the option char_ther_fluxnl.

6 Formalization of the endogenous withdrawal and desiccation

6.1 Withdrawal in Code_Aster

Within the framework of a formalization of the withdrawal in term of deformation, the total increment of deformation can break up thermal component all in all, of a component representing the endogenous withdrawal, and of a component representing the withdrawal of desiccation, added to the mechanical component (elasticity, creep,...).

One can model the withdrawal of desiccation in the form:

$$\Delta \varepsilon_{\text{desiccation}} = \left[-\kappa (C^+) (C_0 - C^+) + \kappa (C^-) (C_0 - C^-) \right] \cdot I^d \quad \text{éq 6.1-1}$$

where C is the water concentration, C_0 initial water concentration.

and κ a coefficient characterizing the withdrawal, depending mainly on the water concentration.

One can model the endogenous withdrawal in the form:

$$\Delta \varepsilon_{\text{endogène}} = -\beta \cdot \Delta \xi \cdot I^d \quad \text{éq 6.1-2}$$

where ξ is the hydration, and β a coefficient characteristic of the material whose dependences are badly known.

The withdrawals of desiccation and endogenous can thus intervene a law of behavior by replacing the usual terms there $\Delta \varepsilon - \Delta \varepsilon_{\text{thermique}}$ by $\Delta \varepsilon - \Delta \varepsilon_{\text{thermique}} - \Delta \varepsilon_{\text{desiccation}} - \Delta \varepsilon_{\text{endogène}}$. In Code_Aster, these terms are taken into account for the elastoplastic behaviors of type Von Mises and for the concrete models. One has then for example in **elasticity 1D** :

$$\Delta \varepsilon = \frac{1}{E(\xi)} \Delta \sigma + \left(\Delta \varepsilon_{\text{thermique}} + \Delta \varepsilon_{\text{endogène}} + \Delta \varepsilon_{\text{desiccation}} \right) \quad \text{éq 6.1-3}$$

The mechanical parameter E (Young modulus) depends mainly of the variable of hydration ξ .

This formulation of the withdrawal of desiccation and the endogenous withdrawal has the advantage of using the water content directly C , that one can connect to the weight loss by simple integration on volume. If the relative humidity were used h , it would have to be retranslated in term of water content by the means of the isotherm of desorption of each various concrete.

For Code_Aster, these parameters can be defined within a framework relatively general, like functions of the various variables of calculation and auxiliary variables (temperature, hydration, concentration out of water, or constants) to leave the choice to the user to define the dependences of the parameters freely. It remains with the load of the user to use the functions of Code_Aster to reproduce the expression of the Young modulus given in the equation [éq 6.1-3].

For more detail on these formulations, and the means of calculating the coefficients κ and β , one will refer to the thesis of L. Granger, [bib2], on pages 99 and following, and pages 210 and following.

For mechanical calculation variables ξ (the hydration) and C (water concentration) are data, like the east the temperature during a thermomechanical calculation.

6.2 Integration of the withdrawal in the law of behavior mechanics

Thermics and drying are uncoupled from the mechanical resolution, just like drying is an operation chained with thermics and the hydration. This decoupling makes it possible to integrate the withdrawal in the operator of resolution of nonlinear mechanics, without adding new phenomena, behaviors, types of elements and options of calculation. Moreover, it makes it possible to introduce the simple withdrawal of way into all the nonlinear laws of behavior. The syntax of the operators of mechanics `STAT_NON_LINE` and `MECA_STATIQUE` is not modified.

In the current version of the nonlinear operator of mechanics, the withdrawal was integrated into the elastic behavior (`ELAS`), with the elastoplastic behavior of Von Mises (`VMIS_ISOT_*`) and with the models specific to the concretes: `MAZARS`, `ENDO_ISOT_BETON`, `BETON_DOUBLE_DP`, `GRANGER*`, `BETON_UMLV_FP`. It consists in removing the terms of withdrawal to the total deflection, before the resolution of the equilibrium equations at the points of Gauss, in the same way which is taken into account thermal dilation.

Coefficients κ and β characterizing the withdrawals endogenous and of desiccation are defined under the keyword '`ELAS_FO`' (operands `K_DESSIC` and `B_ENDOGE` respectively), like constants. Other mechanical characteristics, Poisson's ratio and modulus Young can also be defined like functions of the new variables `HYDR` and `SECH`, which was added to the catalogues of the two operators `DEFI_FONCTION` and `DEFI_NAPPE`.

Results, of type [`evol_ther`], resulting from a nonlinear calculation of thermics, or thermohydration, and a calculation of drying, and corresponding respectively to the fields thermo-hydrous of type '`TEMP/HYDR`', or with the field drying of the type '`TEMP`', are transmitted to mechanical calculation via the operator `AFFE_MATERIAU` (keyword `AFFE_VARC`). Mechanical calculations associating these fields allow:

- to calculate the withdrawals endogenous and of desiccation, if the associated characteristics material are before defined in `DEFI_MATERIAU`,
- to interpolate the Young modulus and the Poisson's ratio when those are functions of the variables hydration or drying.

Notice 1:

*In the presence of a field of drying, it is necessary to inform the keyword `VALE_REF` in the order `AFFE_MATERIAU`. This value defines the value of `SECH` for which the withdrawal of desiccation is null.
It is thus necessary to take care to be coherent with the values `SECH` used (in particular at the initial moment!).*

Notice 2:

Drying and the hydration are not taken into account for the elements of structure. For this kind of elements, it will be necessary to define coefficients κ and β worthless, if not calculation will stop in fatal error.

6.3 Tangent matrix

The calculation of the tangent matrices of the various laws of nonlinear behavior is not affected by the addition of the endogenous withdrawal and the withdrawal of desiccation, because one neglects the derivative compared to the variables of hydration and drying, of the terms of the equilibrium equations, just as are usually neglected the derivative compared to the temperature of these same terms. These derivative intervene with the second order.

7 Bibliography

- [Bib.1] C. DURAND: Nonlinear thermics. Manuel de Référence de *Code_Aster*. Document [R5.02.02]
[Bib.2] L. GRANGER: Behavior differed from the concrete in the enclosures of nuclear power plant: analysis and modeling. Doctorate of the ENPC (February 1995).

[Bib.3] B. CIREE: Specifications of the development of the drying of the concrete in *Code_Aster*. Report CS IF DSN/128EE1/RAP/98.044 Version 1.1

[Bib.4] B. CIREE: Specifications of the development of the endogenous withdrawal and the withdrawal of desiccation in *Code_Aster*. Report CS IF DSN/128HJ1/RAP/98.088. Version 1.0

Description of the versions of the document

Version Aster	Author (S) Organization (S)	Description of the modifications
5	G.DEBRUJNE EDF- R&D/AMA	Initial text
09/04/09	G.DEBRUJNE EDF-R&D/AMA	Modification due to the variables of orders
11	MR. BOTTONI EDF-R&D/AMA	Generalization of the function affinity