Modelization of thermohydration, the drying and the shrinking of the Summarized

concrete

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 shrinkage known as endogenous, appearing with the young age of the concrete (the first 100 days),
•on the other hand an evaporation of part of the water not used in the process of hydration, phenomenon called drying and involving a shrinkage of desiccation. This phenomenon can last, according to dimensions of 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 strains of the endogenous shrinkage (of with the hydration) and of the shrinkage of desiccation (of with drying).

Contents

1 Introduction

the behavior of the concrete, brittle 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 (shrinkage and creep) reduce in the course of time the field of loading which the structure can support. These differed strains which appear in the concrete during the life of this one, are composed by the shrinkage with the young age (endogenous shrinkage specific to the hydration and thermal shrinkage), by the shrinkage of desiccation with the modelization of drying, and as soon as it undergoes stresses, by clean creep and the creep of desiccation.

In the rules of design, the strains differed from the concrete are generally based on empirical rules fixed on a large number of results resulting from the literature, taking into 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 model of Arrhenius to take into account the aging and the temperature.

A fine analysis of the physicochemical phenomena which are at the origin of the various strains differed from the concrete makes it possible to propose a modelization on the basis of model of type equivalent continuum [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 shrinkage or shrinkage of hydration, and the thermal shrinkage intervene as of the first times of the catch (with the young age), for a period going from a few hours to a few days, for the thermal shrinkage, and of a few months to one year, for the shrinkage of hydration, in general finished at the time of the setting in prestressing. Phenomena of prevented shrinkages or shrinkages differential, under formwork, can be at the origin of stresses 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 training of the first hydrates, the catch of the concrete intervenes, about ten hours after its fabrication, which corresponds to the establishment of related bridges hydrates between the cement grains in the totality of the 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 period of this phase, the concrete is still deformable, and that any contraction is compensated by a granular readjustment of the 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 stresses generated with the interface of two consecutive liftings can start of 50% the margin of strength in tension of the 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 $50\,°C$. The hydration is an thermo-activated reaction, i.e. the velocity of hydration increases with the temperature. When the velocity of hydration decrease, the temperature decreases, involving a thermal shrinkage. 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 shrinkage. The various shrinkages can cause stresses much higher than strength (weak) in tension of the concrete and bring to a cracking of the material.

The computation fields of temperature and degree of hydration is available with command THER_NON_LINE (cf [U4.30.02]). The computation mechanical fields taking into account the endogenous shrinkage is carried out with command STAT_NON_LINE.

1.2 Drying and shrinkage desiccation

Modelize drying is important owing to the fact that the physicochemical and mechanical properties of the material are strongly dependant on moisture inside this last. The purpose is to propose a macroscopic modelization of the drying of the concrete from a restricted number of parameters, easily measurable in experiments, from a model of transitory diffusion nonlinear of the moisture, chained with 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 = ratio 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 as a thermodynamic unbalance with the atmosphere. Drying will enable him to find a hydrous equilibrium with the external medium.
Physically, drying brings into play complex phenomena closely coupled the ones with the others, depend on 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 Darcy **type**, as long as there is continuity of the liquid phase, and with diffusion in gas phase of Fick **type**, for the steam.

The shrinkage of desiccation is the macroscopic consequence first of the drying of the concrete. It is the direct elongation of the phenomena of capillary tension which are at the origin of the endogenous shrinkage. By its intensity, the strains being about 400.10-6 to 800.10-6 per 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 modelization of thermohydration in the nonlinear operator of thermal of *Code_Aster,* then the modelization of drying, and finally, the introduction of the endogenous shrinkage and the shrinkage 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 **a source term** is thus necessary (see [R5.02.02]). The second member who contains the internal sources of heat can then be enriched 1 [1] :

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

where:

- $\mathbf{q}$ is the heat flux,
- 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 [éq 2.1-1] can be solved if the function $\xi(t,T)$, and thus $\frac{d\xi}{dt}(t,T)$, are known.

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

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

In *Code_Aster*, the heat of hydration Q and the function $AFF(\xi,T)$ must be indicated by the user under key word THER_HYDR of DEFI_MATERIAU (see [U4.43.01]). Their experimental determination is done using an adiabatic test (see [§2.25]).

2.2 Operating 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. ***Note:*** *in the frame of the nonlinear thermal [R5.02.02], the first of the equations éq 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 adiabat [éq 2.1-1] is simplified because $\operatorname{div}\mathbf{q}=0$. Moreover, $s=0$ because it is considered that the only heat source is the hydration of the concrete. The integration of [So 2.2-1] of the beginning ($\xi=0$) to the degree of hydration ξ gives the statement then:

$$Q\xi\left(T^{ad}(t)\right)=\rho C_p\left(T^{ad}(t)-T_0\right) \qquad \text{So 2.2-1}$$

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

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

where $T_{0,}T_\infty^{ad}$ are the temperatures measured at the beginning and the adiabatic test .

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

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

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

A statement of $AFF\left(T,\xi\right)$ was suggested by 15 in the form of exponential of the temperature:

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

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

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

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

Note: [*éq 2.2-3] can also be written in the following way:*

$$\xi(t)=\frac{T^{ad}(t)-T_0}{T_\infty^{ad}-T_0}=\frac{Q\left(T(t)\right)}{Q\left(T_\infty\right)} \qquad \textit{éq 2.2-6}$$

In fact, one can at every moment define generally the degree of hydration t as being the ratio of the quantity of heat released until time 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 to solve overall the nonlinear equation [éq 2.1-1] by making profitable the algorithm of nonlinear thermal of *Code_Aster* and to locally solve the equation [éq 2.2-4] which represents the law of evolution of a kind of local variable representing the degree of hydration, this model 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 [éq 2.2-4] represents a local law as in plasticity. One then preserves the same number of degrees of freedom as for the classical thermal. Such a decoupled process involves nevertheless the computation of the same quantities several times. Indeed, let us suppose that ξ is discretized with the nodes of the elements. Let us consider the example schematized by [Figure 3.1-1].

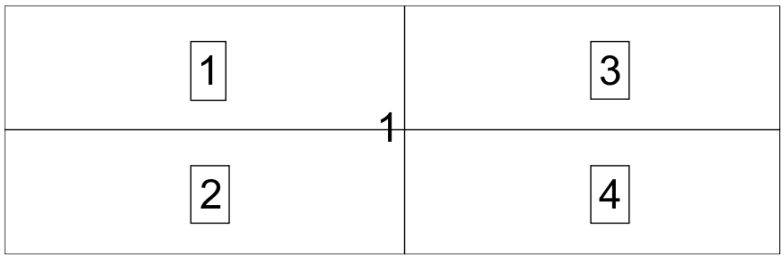

Figure 3.1-1

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On node **1**, the equation of evolution [éq 2.2-4] will be integrated four times. A possible solution would have been that local computations can be done on fields at nodes (Aster concept CHAM_NO) and not on fields of nodes by element (Aster concept 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 computation the Young's modulus depends explicitly on ξ. This generates nevertheless much local computations except strongly under-integrating the finite element. For example, if one considers a mesh comprising N hexahedral elements with 20 nodes, there exist about $4\mathrm{N}$ nodes and $27\mathrm{N}$ Gauss points.

3.2 Algorithm of resolution

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

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

$$\forall T^*$$

the development of thermohydration within the general algorithm of the nonlinear thermal in *Code_Aster* thus consists 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 at the end of time step, one calculates in each Gauss point the quantity:

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

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 the nonlinear thermal. The taking into account of the hydration is in fact only the taking into account of a heat source known at the beginning of time step. This purely explicit discretization thus requires to use time step the sufficiently small ones.

4 Formalization of drying

This part refers to the document of specification of the development of drying in *Code_Aster* 15, like with the thesis of L. Granger 15.

4.1 Modelization and equations of drying

the modelizations of the thermal or thermohydration and drying are decoupled during the resolution. Drying is then presented like an operation chained to the thermal. As the equations making it possible to solve drying and the nonlinear thermal are similar except for the coefficients, this decoupling makes it possible to integrate the resolution of the computation of drying in *Code_Aster*, by means of directly the modulus of resolution of the nonlinear thermal, without adding new phenomena, new element types nor new computation options, and by thus minimizing the volume of added and duplicated code.

The concentration or water content C, variable computation in the modelization of drying, is comparable, in term of the type of variable, with 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 thermal and drying, in the frame of a decoupled modelization between the thermal and drying, are governed by the following equations:

- equation of the “classical” thermal:

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

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

- equation characterizing drying:

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

  where C (ou) m^3/m^3 l/m^3 is the variable of computation (concentration or water content voluminal),
  T is the variable of entry of computation (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 computation C, and the auxiliary variable T. This model of diffusion is given in various forms, according to the model retained, (model of **Bazant**, model of **Granger,** model of **Mensi**, cf [§4.3] and [bib2]).

The equations [éq 4.1-1] and [éq 4.1-2] correspond to a thermal chained computation/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 on the

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 the material, depending at the same time on the temperature T and the water concentration C . The equation of the migration of moisture in the concrete is resulting from those from mechanics of porous media. One will refer to [bib2] for more accuracy. Classically, a model of diffusion expresses a flux like the product of a quantity characteristic of the material by the gradient of an intensive quantity. The various quantities considered are defined by an average on representative ground volume, in so far as one can define this average for the material considered, so that the derivative operators have a meaning. 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 model of **Darcy**, makes it possible to express fluid flux according to the pressure of the fluid. The model of **Kelvin** describing the coexistence of the two phases liquid and gas by the writing of the equality of the mass free enthali leads to the form of flux according to the gradient of the percentage of moisture.

From the two preceding results, one obtains the form of total flux 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 flux according to the water content, by means of classically the isotherm of desorption of the concrete, which connects the water content C , and the 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 the equilibrium, and than it is independent the velocities of evolution. In other words, water content C , and the relative humidity h , are well connected by the same relation as to the equilibrium. What leads to the classical equation of the diffusion:

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

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 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 most known authors (**Bazant** cf [bib2]) propose a statement of the coefficient of diffusion of the type:

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

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

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 the mechanics, (i.e. he is the cause of a shrinkage of 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 the equilibrium according to H, the body of test carries out a shrinkage. At the microscopic level, all occurs like if the shrinkage, modifying porosity, were going to interact on the relative hygroscopy inside the sample, since the steam pressure and H increase. This shrinkage of

desiccation being very weak, it is usual to neglect it in computations of the water content. There is thus only one sequence between the computation of the water content and the mechanical computation of shrinkage of desiccation.

4.3 Usual models of diffusion

the model of diffusion, function of the two parameters, C and T , can be freely defined by the user in the form of a three-dimensions function. However, usual statements of the model of diffusion, which one finds in the literature are the following ones:

Model suggested by Granger:

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

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

Model of Mensi:

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

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

Model of Bazant:

The model 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 model is the following one:

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

Usually, $D_1=3.10^{-10}m^2/s$
α lies between 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 tabulated standard function, knowing that actually, this curve has a hysteresis, but can be regarded as being invertible, if one takes account only of one meaning of path.

4.4 Modelization of the boundary conditions

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

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

where 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 the elements, as well as the elements 3D isoparametric, of many nodes unspecified, linear and quadratic.

5.1 Introduction of the notion of behavior into the nonlinear operator of thermal

operator THER_NON_LINE was reserved exclusively to the nonlinear thermal, which will remain **the computation option by default**. But one uses the same modulus of resolution to solve the problems of drying and hydration, because of analogy of the equations.

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

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

For drying, four distinct behaviors are defined under key word "SECH_GRANGER", "SECH_BAZANT", "SECH_MENSI", or "SECH_NAPPE", to characterize each model of possible diffusion. They can be allotted to parts complementary to the mesh, during the same computation. The simultaneous definition several behaviors “drying” associated with different topological entities requires several occurrences of the key word "BEHAVIOR". Then, the topological entity will have to be identified by informing one of key word 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 models of diffusion, nonlinear functions of the water content and the temperature. The user can choose to it (or them) model (S) of his choice, and defines the value which it wishes for each one of these coefficients.
Key word SECH_GRANGER makes it possible to define the model of diffusion of liquid and gas water in its most classical form among the statements of the literature. Four coefficients as well as a reference temperature T_0 characterize this model.
Key keys SECH_MENSI and SECH_BAZANT make it possible to define the models of **Mensi** and **Bazant**, using the coefficients which are appropriate. The model of **Bazant**, being expressed starting from the percentage of moisture, requires to define a curve of desorption making it possible to convert the water content into percentage of moisture in the frame of this modelization.
Lastly, key word SECH_NAPPE makes it possible to use a model of diffusion, from a tabulated function of two variables, which will be interpolated in computations 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 computation a concept of the type [evol_ther], representing the evolution of the field of temperature of concrete structure, in the frame of a thermal chained computation/drying. Indeed, the computation of drying requires the preliminary computation of the temperature and possibly of the hydration, because the coefficient of diffusion $D(C,T)$ depends on the temperature.

5.2 Put in work of the boundary conditions for drying

5.2.1 Statement of the boundary conditions

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

5.2.2 Delimitation of the computation of drying using the boundary conditions

The computation of drying is defined on the totality of the mesh where are affected of the finite elements. To make effective the computation of drying only on one portion of the mesh (this with an aim of preserving the same model for computations of drying and mechanical computations and of facilitating the "poursuites" of Aster computation [bib4]), the boundary conditions will be used. 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" computation. The absence of drying on a portion of 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 thermal, in the form of normal flux nonlinear formulated from a tabulated function of the variable of computation, and interpolated during computations. That makes it possible to avoid creating new computation options, similar to the options of nonlinear thermal char_ther_flunl and resi_ther_fluxnl which calculates the first and the second member, and which can be used directly for drying. It is then enough to choose a tabulated function corresponding to the form of flux, given by the equation [éq 4.4-1].
Using a preset function (FORMULA), the form of flux, given in polynomial form and function of the variable of computation, is transformed into tabulated curve, via the operators Aster (CALC_FONC_INTERP). One thus does not create a new computation option for the processing of the boundary conditions.

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

5.2.4 Example of working of the boundary conditions

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

Note:

The "FORMULA" Aster is the numerical statement of flux of 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', TITER=' FLUX 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 tabulated 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 operator `CALC_FONC_INTERP`.

5.3 Numerical integration of drying

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

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

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

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

the resolution of drying is integrated into operator `THER_NON_LINE`, while replacing ρC_p by the constant function equal to the identity, and conductivity by the diffusion $D(C,T)$, the temperature intervening like a constant in computations (auxiliary variable). According to the model of diffusion chosen, it is necessary to calculate the value of the coefficient of diffusion like its derivatives, according to temperature and the water concentration at time running, at the current point.

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

In the frame of drying, the boundary conditions are given in term of normal flux, and lead, as in thermal, with a term in the first member, associated with the computation option `rigi_ther_fluxnl`, and the term in the second member, associated with the option `char_ther_fluxnl`.

6 Formalization of the endogenous shrinkage and desiccation

6.1 Shrinkage in *Code_Aster*

In the frame of a formalization of the shrinkage in term of strain, the total increment of strain can break up thermal component all in all, of a component representing the endogenous shrinkage, and of a component representing the shrinkage of desiccation, added to the mechanical component (elasticity, creep,…).

One can model the shrinkage of desiccation in the form:

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

where C is the water concentration, C_0 initial water concentration.
and κ a coefficient characterizing the shrinkage, depending mainly on the water concentration.

One can model the endogenous shrinkage in the form:

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

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

The shrinkages of desiccation and endogenous can thus intervene a constitutive law by replacing the habituelspar terms there $\Delta \varepsilon - \Delta \varepsilon_{thermique}$ $\Delta \varepsilon - \Delta \varepsilon_{thermique} - \Delta \varepsilon_{dessiccation} - \Delta \varepsilon_{endogène}$. 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** :

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

mechanical parameters E (Young modulus) and α thermal thermal expansion) depend mainly on the variable of hydration ξ .

This formulation of the shrinkage of desiccation and the endogenous shrinkage has the advantage of directly using the water content C , which 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 *the Code_Aster*, these parameters can be defined in a relatively general frame, like functions of the various variables of computation 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 *the Code_Aster* to reproduce the statement of the Young modulus given in the equation [éq 6.1-3].

For more detail on these formulations, and the layers to calculate 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 computation the variables ξ (the hydration) and C (water concentration) are data, like the east the temperature during a thermomechanical computation.

6.2 Integration of the shrinkage in the constitutive law mechanics

the thermal and drying are uncoupled from the mechanical resolution, just like drying is an operation chained with the thermal and the hydration. This decoupling makes it possible to integrate the

shrinkage in the operator of resolution of the nonlinear mechanics, without adding new phenomena, behaviors, element types and computation options. Moreover, it makes it possible to introduce the simple shrinkage of way into all the nonlinear constitutive laws. 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 shrinkage was integrated into the elastic behavior (ELAS), the elastoplastic behavior of Von Mises (VMIS_ISOT_*) and into the models specific to the concretes: MAZARS, ENDO_ISOT_BETON, BETON_DOUBLE_DP, GRANGER*, BETON_UMLV_FP. It consists in removing the terms of shrinkage to the total deflection, before the resolution of the balance equations to Gauss points, in the same way which is taken into account thermal thermal expansion.

The coefficients κ and β characterizing the shrinkages endogenous and of desiccation are defined under key word "ELAS_FO", like constants. The other mechanical characteristics, Poisson's ratio, modulus Young, thermal coefficient of thermal expansion can also be defined like functions of new variables HYDR and SECH, which were added to the catalogs of two operators DEFI_FONCTION and DEFI_NAPPE.

Results, of type [evol_ther], resulting from a nonlinear computation of thermal, or thermohydration, and a computation of drying, and corresponding respectively to the fields thermo-hydrous of type "TEMP/HYDR", or to the field drying of the type "TEMP", are transmitted to mechanical computation via operator AFFE_MATERIAU (key word AFFE_VARC). Mechanical computations associating these fields allow:

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

Note:

> *In the presence of a field of drying, it is necessary to inform key word VALE_REF in command AFFE_MATERIAU. This value defines the value of SECH for which the shrinkage of desiccation is null.*
> *It is thus necessary to take care to be coherent with values SECH used (in particular at initial time!).*

6.3 The computation stamp

tangent tangent matrixes of the various constitutive laws nonlinear is not affected by the addition of the endogenous shrinkage and the shrinkage of desiccation, because one neglects derivatives compared to the variables of hydration and drying, of the terms of the balance equations, just as usually the derivatives are neglected compared to the temperature of these same terms. These derivatives intervene with the second order.

7 Bibliography

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[Bib.3] B. CIREE: Specifications of the development of the drying of the concrete in *the Code_Aster*. Ratio CS IF DSFN/128EE1/RAP/98.044 Version 1.1
[Bib.4] B. CIREE: Specifications of the development of the endogenous shrinkage and the shrinkage of desiccation in *the Code_Aster*. Ratio CS IF DSFN/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.DEBRUYNE EDF-R&D/AMA	initial Text
04/09/09	G.DEBRUYNE EDF-R&D/AMA	Modification due to command variables
11	Mr. BOTTONI EDF-R&D/AMA	Generalization of the function affinity