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PHENOMENOLOGICAL MODELLING OF IMPACT OF TEMPERATURE ON SORPTION ISOTHERMS AND INDUCED EFFECTS ON TENSILE STRENGTH

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Abstract. A modelling of water retention curves and hysteresis based on the amount of C-S-H contained in the cement paste (data from a hydration model) is thus proposed and the temperature effect is investigated from experimental results and modelled based on these microstructure consideration. Secondly, in a sake of applicability to simulation at structural scale, a simplified model (neglecting hysteresis) is proposed, and the water retention model based on hydration development is used to identified the parameters of this "structural scale" law.

1 INTRODUCTION

In French nuclear power plants, the prestressed reinforced concrete containment vessel plays a major role to limit the radionuclide dispersion in the environment in case of failure of the first two barriers. It is thus of primary importance to ensure the containment building tightness during all the duration of a severe accident. In the scenario of a severe accident, the internal pressure and temperature on the inner face of the concrete containment structure are maintained constant during two weeks.

During this accident scenario, the evolution of temperature and relative humidity in the concrete wall is going to affect the mechanical behaviour of concrete and steel. Recent researches have shown in particular that tensile strength is affected by the water content of the concrete, through the effect of capillary pressure induced by drying, but that this effect is attenuated at temperature.

The work presented here focuses on the modelling of adsorption and desorption isotherms at different temperatures, since it is a key element in the development of capillary depressions and vapour and liquid water transfers that lead to variations in physical and mechanical properties of concrete.

We chose to use a model to obtain the sorption isotherms from, among other things, the Van Genucthen equation and the composition of the material. It is a semi-empirical model that allows to determine the sorption isotherms from the amount of CSH gel present in the material and that can be evaluated using an hydration model [1, 2].

2 Semi-empirical model for water retention curve based on microstructure considerations

The semi-empirical model proposed for the prediction of water retention curve and hysteresis is based on the knowledge of paste microstructure and more especially on the quantity and nature of C-S-H (given by an hydration model [1,2]).

Indeed, the results of the literature show that below a certain relative humidity (corresponding to the saturation of C-S-H and identified at 76%), the sorption isotherms are only due to the filling of the pores of C-S-H [3]. We therefore propose to model the sorption curves according to the diagram shown in figure 1.

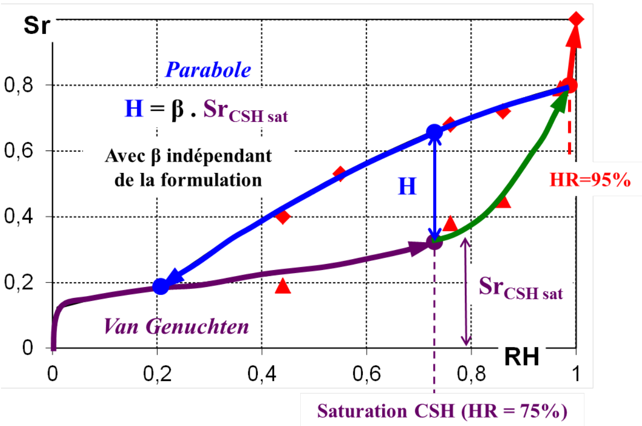

Figure 1: Schematical representation of water retention curve modeling (experimental points form [4])

HR	Sl ads	Sl des	
0	0		No Hysteresis
20%	$Sl_{ads}(20\%)$		
76%	Sl_{CSHsat}	$\beta.Sl_{CSHsat}$	Issued from hydration model
95%	Sl_{hygro}		No Hystérisis
100%	1		

Figure 2: Key points of the water retention curve moelling

In the modelling approach, 4 points are used to determine the expression of the water retention curves:

- RH=20%: Below this value, no hysteresis is considered
- RH=76%: saturation of C-S-H on the adsorption curve (and effect of hysteresis on desorption curve);
- RH=95%: Beyond this value, the behaviour of the concrete is no longer considered hygroscopic (red part on figure 1). This part is associated with capillary filling of the largest pores or defects [4] and corresponds to a degree of saturation noted Sl_{hygro} which depends mainly on the ratio E/C and on the size of the specimen.

For the adsorption curve, the fact that below 76% of relative humidity, the water is only contained in the C-S-H allows to determine the purple part of the curve only using an hydration model to determine the C-S-H porosity for the material tested. A Van Genuchten's type law is fitted to reach this point at RH=76%.

$$Sl_{a_{0-76}} = \frac{m_{CSH}(\alpha)\left(1 + (K(\alpha) \cdot Pc)^{\frac{1}{1-m}}\right)^{-m}}{\phi(\alpha)} \quad (1)$$

Where:

- P_c is the capillary pressure;
- m is a material parameter;
- m_{CSH} is the mass of C-S-H in the paste (issued from hydration model [1,2];
- ϕ is the porosity (issued from hydration model [1,2];
- $K(\alpha)$ is evaluated from the results of hydration model to ensure that the equation gives the saturation of C-S-H porosity for RH=76% (at 20 ° C).

The adsorption curve is finalized using a parabolic law that connect Van Genuchten's inspired law respecting the gradient at RH=76% (green part of the curve).

The hysteresis on sorption and desorption phenomena is taken into account for relative humidities between 20% and 95% [3,5]. The desorption curve is thus modelled by a parabola on this range of relative humidity, and the amplitude of the hysteresis by the parameter β.

The phenomenon of hysteresis is associated to the presence of small pores, its intensity will depend on the quantity of C-S-H (because they are associated to the pore distribution modes with small pore radius).

It is proposed to take this into account by considering that the degree of desorption saturation for a humidity of 76% will therefore be increased compared to the saturation of C-S-H alone (water trapped in capillary pores not directly connected to the surface because of the smaller pores). This increase will be taken proportionately to the amount of C-S-H (and therefore to $H = \beta \cdot Sl_{CSH,sat}$ on figure 1).

3 Effect of temperature on isotherms

In the literature it can be found that temperature leads to a decrease in the phenomenon of hysteresis as well as a shift in desorption curves towards lower saturations (fig. 3).

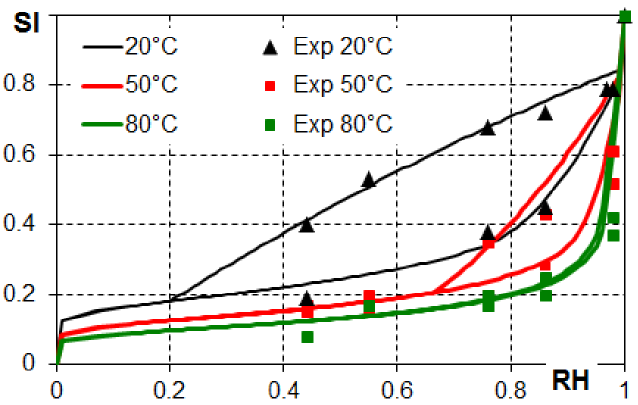

Figure 3: Water retention curves for different temperatures (experimental points issued from [4])

Since the temperature (for these studied temperatures below 100 ° C) does not affect the structure of the C-S-H [6], a shift in the desorption curves towards lower saturations actually corresponds to an increase in the relative humidity value allowing saturation of the C-S-H (saturation point of the C-S-H at 76% RH at 20 ° C and at higher RH if T increases).

This effect can be reproduced into the water retention curve model by modifying only β (which controls the amplitude of the hysteresis) and $RH_{CSH,sat}$. The parameters identified by inverse analysis on the [4] tests are presented in the table 1. .

Table 1: Model parameter identifed for different temperatures

T	20 ° C	50 ° C	80 ° C
Sl_{hygro}	0.85	0.85	0.855
$RH_{CSH,sat}$	76%	90%	95%
β	1	0.8	0.1

Evolution curves can then be proposed in this temperature range (20-100 ° C) to extrapolate this temperature effect.

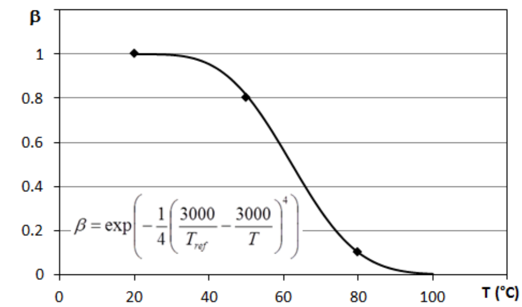

Figure 4: Effect of T on β

Figure 5 shows that taking into account Kelvin-Laplace's law to model the effect of temperature on C-S-H saturation is not sufficient, which tends to show that capillarity is not the only cause. We therefore propose to use a polynomial empirical law.

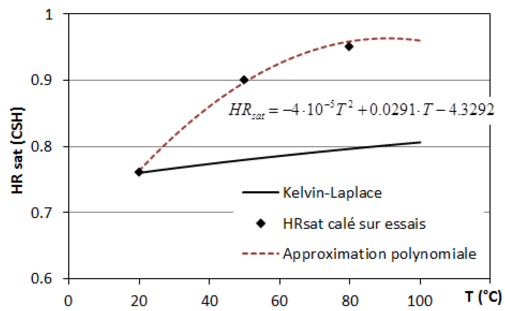

Figure 5: Effect of T on $RH_{CSH,sat}$

4 Macroscopic modelling for simulation of massive concrete structures

When modelling the hygromechanical behaviour of a concrete structure subjected to variations in temperature and relative humidity, it is necessary to have a law to represent the water retention curves that can be implemented numerically in a simple way. Hysteresis is therefore a limitation on the use of laws developed from the microstructure for simulations at structural scale. These semi-empirical laws obtained from the hydration model are therefore used here as reference curves to identify a more classical Van Genuchten law (unique in adsorption and desorption, see Eq. 2).

$$Sl = \left(1 + \left(\frac{P_c}{M_{shr}(T)}\right)^{\frac{1}{1-m_{vg}}}\right)^{-m_{vg}} \qquad (2)$$

Since desorption is the most frequent case, we choose to identify the M_{shr} and m_{vg} parameters on the desorption curves obtained in temperatures by the previous model (see figure 3). The mvg parameter is chosen constant with the temperature (identified equal to 0.4) and only M_{shr} is identified for the 3 temperatures (20, 50 and 80°C).

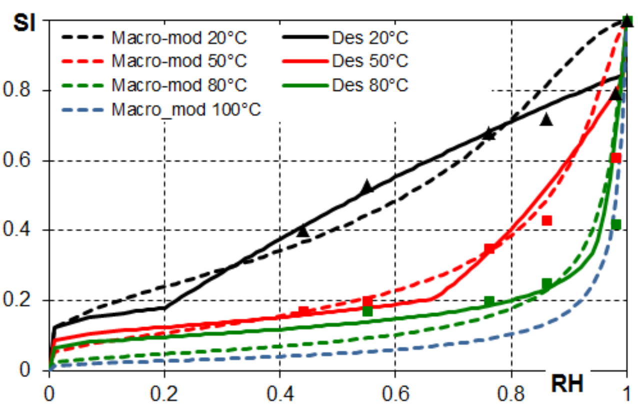

Figure 6: Desorption isotherms at $\neq$ T$^\circ$C

The values obtained are plotted on figure 7 and are used to fit an activation law of according to temperature (Eq. 3 with $T_{k,vg} = 45^\circ C$ and $M_{shrref} = 26$MPa).

$$\frac{M_{shr}(T)}{M_{shrref}} = \exp\left(-\frac{T - T_{ref}}{T_{k,vg} - T_{ref}}\right) \qquad (3)$$

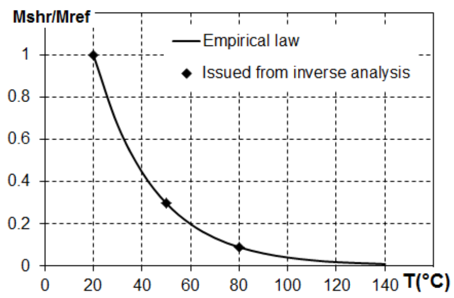

Figure 7: Evolution of M_{shr} according to temperature

5 Effect of capillary pressure and temperature on Rt

During drying, the loss of the paste water can lead to micro-cracking by strain incompatibility between paste and aggregates, this effect having been observed experimentally on model materials for example in [7], and confirmed by X-ray tomography analyses as part of the ANR Mosaic project. This would therefore lead to a loss of mechanical properties that could be translated into damage. However, recent results obtained in the project ANR Mosaic [8] show an increase in tensile strength as the degree of saturation decreases (see figure 8, blue curve). This increase in strength is explained by the fact that the application of capillary depression to the skeleton prestresses the paste [9].The results shows that this effect is predominant over the loss of properties induced by microcracking.

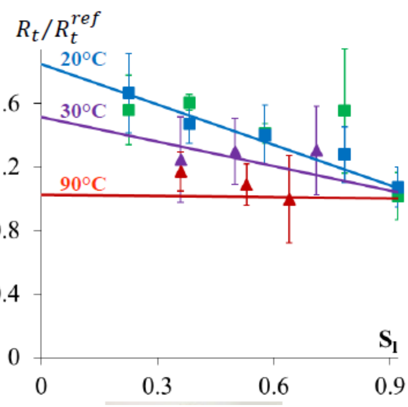

Figure 8: Evolution of tensile strength according to saturation degree and temperature (experimental results from **[?]**

The tests conducted at SIAME as part of Macena project [10] on concretes subjected to varying (but controlled) temperatures and saturations confirm this increase in resistance. But it was observed that the effect decreases with temperature (see figure 8 green and red curves). These tests also showed that the effect of the degree of saturation on the Young's modulus (macroscopic indicator of damage) was quite limited, so it seems consistent to neglect the macroscopic effect of microcracking induced by aggregates. The consolidation effect of the material by the degree of saturation is therefore only considered, by proposing a law of evolution of the tensile strength as a function of the degree of saturation (Eq. 4).

The decrease in the effect of saturation degree when the temperature increases is attributed to the effect of temperature on the desorption isotherm. Indeed, if the temperature increases, the capillary depression will be reduced for the same degree of saturation. This effect is therefore modelled in the equation 4 by the term $\frac{M_{shr}(T)}{M_{shrref}}$ which has been previously defined to take into account the effect of temperature on desorption isotherms (Eq. 3).

$$\frac{R_t}{R_{tref}} = 1 - K^w \cdot \frac{M_{shr}(T)}{M_{shrref}} \cdot (Sl - Sl_{ref}) \quad (4)$$

Where:

- R_{tref} is the reference tensile strength measured for the reference temperature and saturation degree (usually T=20° and Sl=90% (endogenous conditions));
- K^w is a material parameter identified at the reference temperature (0.85 pour 20°) ;
- $\frac{M_{shr}(T)}{M_{shrref}}$ is the law proposed in Eq. 3 to modeled the effect of T on the desorption isotherm.

6 Conclusion

The paper presented an approach based on knowledge of the microstructure of cement paste to model sorption isotherms and the hysteresis effect. This approach is based in particular on the prediction of the quantity of water contained in C-S-H by a multiphase hydration model. The modelling is then extended in a semi-empirical way to model the effect of temperature on these isotherms.

These approaches remain a first step, and the fact that the laws of evolution cannot be phenomenological here, due to the lack of knowledge of physical phenomena for the moment, shows that there are many perspectives on these aspects. The evolutions highlighted here are not valid beyond the range of studies, if only because the structure of C-S-H can be affected by higher temperatures.

In order to be used in a finite element structural computation code, a simplified approach is proposed with the modelling of a single isothermal curve (desorption and neglected hysteresis) whose temperature dependence is identified on the previous model and extrapolated beyond 80°C.

This temperature effect on the development of capillary pressures is also used to reproduce the experimentally observed effect on the evolution of the tensile strength of concrete under varying saturation and temperature conditions.

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