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Application of a hygrothermal model to predict temperature and humidity development in the VeRCoRs benchmark case

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ABSTRACT

This study presents a multiphysics model developed to predict the internal temperature and moisture development in a concrete reactor containment at an early age. The work is a part of the benchmark study, VeRCoR, provided by EDF. The model was applied on an experimental reactor containment mock-up erected in the vicinity of Paris. The 3D geometry was provided from VeRCoRs. The model includes concrete hydration, heat release, chemical moisture binding, and a moisture transport model with relative humidity as a driving potential. Results from the simulation was compared with temperature sensors located in the mock-up. The model was found to be able to predict the temperature development at early age. There was no possibility to compare the relative humidity because of lack of humidity sensors.

INTRODUCTION

Swedish power industry has initiated several studies with the objective to provide guidance on the use of advanced calculation tools for the analysis of mechanics and transport mechanisms of hydropower and nuclear power concrete structures. The mechanics part includes concrete strain, deformation, strength, fracture and cracking, and the transport mechanism part includes moisture binding, mass and heat flux in the concrete.

The present work has been carried out by Vattenfall, Lund University and the Royal University of Technology with funding from the Swedish energy research centre Energiforsk with support from the Swedish nuclear fuel and waste management company SKB. Energiforsk is an industrially owned body dedicated to meeting the common energy challenges faced by industries, authorities and society.

THE BENCHMARK CASE

An experimental reactor containment mock-up at 1/3 scale that EDF erected in the vicinity of Paris has provided a platform for benchmark work carried out under the framework of VeRCoRs. The containment structure is pre-stressed by non-grouted tendons and holds no liner. The last parts of the construction works (inner vessel and stretching of tendons) was completed in September 2015. An extensive set of installed sensors makes it possible to follow its behaviour from early stage and over time.

The overall objectives of VeRCoRs are:
- Study of the reactor containment’s early age behaviour
- Study of the leak-tightness behaviour over time (aging affects)
- Study of the behaviour under severe accident conditions
The first benchmark covered by this paper will be followed by an assessment of the impact of two successive identical loadings while taking into account aging (2017), and a prediction of the behavior under severe accident conditions (2021).

The physical dimensions of the 463 m³ concrete mock-up are roughly 22 m height and 15 m external diameter. Its design was given to the benchmark participants by a down-loadable CAD-model.

The theme 1 report presented results to be compared to temperature measurements from four monitored positions at the gusset (F1, F2, G1 and G2).

The concreting works of the mock-up was cast in 16 successive lifts over a 15 months period (April 2014 to July 2015). The formworks were of 36 mm wood material (removed about one day after casting). The period air-temperature varied from -6°C to 36°C, with the mean temperature being 12.4°C. The casting of the gusset was supported by air heaters.

**METHODS**

The project VeRCoR provided 3D geometries of the reactor container. They were all provided in IGES-file format. Three files were supplied which represented the concrete parts, the pre-stressed steel and the hatches and holes. In this study the 3D geometry file for the concrete parts was used for temperature and moisture development simulation.

In this study the concrete geometry IGES-file was imported into the software COMSOL Multiphysics with a CAD Import Module. COMSOL Multiphysics is a software that can be used to simulate any multi physics-based system. Multi physics simulations involve multiple physical models or multiple simultaneous physical phenomena.

The original model contained more than 2000 domains. However, these domains were merged to only seven different domains in order to simplify the geometry. The seven different geometries consisted of the foundation disc at the bottom the first pedestal, the second pedestal, the wall, and finally the dome, see Figure 1. The approximate location of the sensors determining the temperature are shown in Figure 2.

**MODEL OF CONCRETE HYDRATION**

There are number of different models available to describe the hydration kinetics of concrete with respect to time. In this study we used the mathematical expression by Byfors [1] to describe the hydration of concrete, \( \alpha(t) \):

\[
\alpha(t) = e^{A \log(t) B}
\]  

(1)
where $A$ and $B$ are curve fitting parameters, in this study the parameters values were $A=-7$ and $B=-2.7$. These parameters were determined by using the provided temperature development from VeRCoR at adiabatic conditions from the actual used concrete together with the maximum heat release from hydration. The cement used in the actual concrete mixture, CEM I 52,5 N CE CP2 NF Gaurain, has a maximum heat release of 376 [kJ/kg].

The hydration kinetics in early age concrete are described by adopting a model presented by Norling Mjörnell [2]. The mathematical formulation of hydration of concrete $\frac{d\alpha(t)}{dt}$ is shown in equation 2

$$\frac{d\alpha(t)}{dt} = \beta_{WC}\beta_{T}\beta_{\varphi}\left(\frac{d\alpha(t,e)}{dt}\right)_{ref}$$

where $\beta_{WC}, \beta_{T}, \beta_{\varphi}$, are rate factors for the water cement ratio, the temperature and the relative humidity respectively and $\left(\frac{d\alpha(t,e)}{dt}\right)_{ref}$ is the hydration rate in a reference climate 20 °C and at fully saturated conditions.

The equation to calculate the water cement ratio rate factor is shown in equation (3)

$$\beta_{WC} = \left(\frac{\alpha_{max}-\alpha}{\alpha_{max}}\right)^{A_{betaWC}}$$

where $\alpha_{max}$, here 0.98, is equal to the maximum possible hydration degree and $A_{betaWC}$, here 1.9, which is a parameter used to fit the current hydration development to a reference hydration development on a concrete with a reference water cement ratio.

The temperature dependency on hydration rate is based on the Arrhenius equation for thermal activation and is described by the maturity function shown in eq (4)

$$\beta_{T} = e^{\left(\frac{1}{T_{ref}}-\frac{1}{T}\right)\theta}$$

where $T_{ref}$ is the reference temperature, in our case 298.15 [K], $T$ is the actual temperature in [K], and $\theta$ is the temperature dependency of the activation temperature. This temperature dependency is described by equation (5)

$$\theta = \theta_{ref}\left(\frac{30}{7+10^{-273.15}}\right)^{\kappa_3}$$

where $\theta_{ref}$, here 4700 and $\kappa_3$, here 0.54 are empirical constants derived from experimental adaptations.

Finally $\beta_{\varphi}$, is a function determined by the proportion of capillary pores filled with water, as it is mainly the water that contributes to the formation of hydration products. The capillary pore volume $P_{cap\_p}$ is determined by using equation (6)

$$P_{cap\_p} = \frac{W_{\alpha} - 39\cdot\alpha(t)}{0.324\cdot\frac{W_{\alpha}}{C}}$$

where $\frac{W_{\alpha}}{C}$ is the water cement ratio in [kg/kg]. And the factor $\beta_{\varphi}$ is then described by equation (7)

$$\beta_{\varphi} = \frac{\frac{W_{\alpha\_\varphi}}{C} - P_{cap\_p\_\varphi}\cdot\alpha(t)}{\frac{W_{\alpha\_\varphi}}{C} - 19\cdot\alpha(t) - P_{cap\_p\_\varphi}\cdot\alpha(t)}$$
TEMPERATURE DEVELOPMENT MODEL

The temperature conditions inside the RC concrete wall were determined by solving the conventional energy-balance equation (8),

\[ \rho \cdot C_p \cdot \frac{\partial T}{\partial t} = \nabla (k \nabla T) + Q \quad (8) \]

where \( \rho \) represents the density \( 2350 \ [\text{kg/m}^3] \), \( C_p \) the specific heat capacity \( 880 \ [\text{J/kgK}] \), \( T \) the temperature in K and \( k \) the heat conductivity \( 1.8 \ [\text{W/mK}] \). The heat released from the hydration reaction \( Q \), was also included as a function of the hydration rate see equation (9),

\[ Q = \frac{\partial a(t)}{\partial t} \cdot q_{\text{hu}} \cdot C \quad (9) \]

where \( q_{\text{hu}} \) represents the maximum heat released by hydration and \( C \) represents the cement content in the concrete mixture, \( 320 \ [\text{kg/m}^3] \). The initial concrete temperature of each lift was provided by the VeRCoRs project.

MOISTURE TRANSPORT MODEL WITH AIR RELATIVE HUMIDITY AS DRIVING POTENTIAL

Moisture transport may be modelled by using a number of different transport potentials, such as air vapour content, air vapour pressure and capillary pressure. The selected model used relative humidity as a driving potential and was developed in the Nugenia-Acceppt project [3]. Results from the simulations were verified qualitatively with measurements from Swedish nuclear reactor Ringhals 4 performed in another study [4]. Moisture transport, \( J \), is modelled by using the relative humidity as the driving potential, see equation (10)

\[ J = -\delta \frac{\partial \varphi}{\partial x} \quad (10) \]

where \( \varphi \) [kg/kg], ratio between actual and saturation vapour content, is the RH in the pores of the material and \( \delta \) [m²kg/(s²m³)] is the moisture dependent moisture transport coefficient with RH as the transport potential.

The moisture transport in the proposed model [3], is based on the mass conservation equation, Fick’s second law, equation (11),

\[ \frac{\partial W_e}{\partial t} = \frac{\partial W_e}{\partial \varphi} \frac{\partial \varphi}{\partial t} = V (\delta \varphi \nabla \varphi) + Q_2 \quad (11) \]

where \( \frac{\partial W_e}{\partial \varphi} \) represents the moisture capacity deduced from the sorption isotherm, \( \delta \) represents the moisture transport coefficient with relative humidity as a driving potential, \( \varphi \) is the relative humidity, and \( Q_2 \) represents the self-desiccation of concrete. The self desiccation was evaluated by using equation (12)

\[ Q_2 = \frac{\partial a(t)}{\partial t} \cdot C \cdot 0.25 \quad (12) \]

where \( \frac{\partial a(t)}{\partial t} \) represents the hydration rate, \( C \), represents the cement content [kg/m³] in the concrete mixture and 0.25, which represents an assumed maximum possible amount of water chemically bounded by the cement.

BOUNDARY CONDITIONS

Climatic conditions used in the model was partly provided from the VeRCoRs project. The air temperature was determined with one sensor and logged continuously throughout the erection of the reactor containment. This air temperature was provided from the VeRCoRs project and served as the boundary condition for the performed simulation of the heat transfer. For special parts of the simulation other boundary conditions were used. One such example is for instance the first wall lift, Gusset, as air heaters were used to increase the surrounding air temperature.

A convective heat flux was used at the vertical concrete surfaces, which for an initial 24 hours
incorporated the wood used as formwork material. In addition, the ground was assumed to have a constant temperature of 12° C.

It was decided to use a simple sinusoidal variation of the air relative humidity with 80 ± 10 % RH. Climatic data for Paris was used as a reference.

The surface mass transfer resistance with RH as a driving potential, $k_{RH}$, was modelled by using Lewis relation [5], see equation (13),

$$k_{RH} = \frac{h v_s}{\rho_{air} C_p(air)}$$

where, $h_v$ is the convection heat transfer coefficient [W/(m²K)], $v_s$ is the saturation vapour content [kg/m³], $\rho_{air}$ is the air density [kg/m³], and $C_p(air)$ is the heat capacity of air [J/kgK]. This model is an estimation of the surface mass transfer resistance.

**RESULTS**

Results from calculations performed by using the presented model, regarding temperature development, is shown in Figure 3. The calculated temperature in point G1 and G2, increases rapidly the first 24 hours. This increase in temperature is, apart from the energy release caused by cement hydration, affected by the air heaters used after pouring the concrete. As air heaters and formwork are removed the temperature decreases. These results may be compared with Figure 4, which show the temperature development determined by sensors (green curve) and the simulations performed by EDF at point G1 [6].

![Graph of temperature development at Point G1 and G2](image1)

**Figure 3. Temperature development at Point G1 and G2.**

![Graph of temperature development at Point G1 results from experimental (temperature sensor) green curve and calculations (red curve) [6].](image2)

**Figure 4. Temperature development at point G1 results from experimental (temperature sensor) green curve and calculations (red curve) [6].**

Furthermore, the calculated relative humidity at points G1 and G2 is shown in Fel! Hittar inte referenskälla. The relative humidity is 98% RH initially and then decreases significantly during the first 24 hours. This rapid decrease may be explained as chemical drying as a major part of hydration occurs at this early stage. At a later stage after some 24 hours and beyond, the humidity at this shallow depth about 20 mm from the concrete surface, will be more affected by the exterior humidity conditions.

In addition the calculated relative humidity distribution through a cross section of the 400 mm thick containment wall is shown in Figure 6. The cross section is located at the same height as point G1, z=0.21 m. The different lines represents times from the start until 72 hours with intermediate results every 6th hours. This results shows that there is a difference between the center and the superficial parts of the reactor containment walls.

![Graph of relative humidity distribution through a cross section](image3)
CONCLUSIONS

In this study a multiphysics model was developed which is able to predict interior temperature and moisture development of a concrete structure of significant size at early age. The simulated temperature development was validated at a number of points where temperature sensors were located. The humidity development was not possible to validate since there was no humidity sensor installed in the concrete structure.

The provided 3D IGES-geometry file was difficult to adopt in Comsol Multiphysics. The number of domains could be reduced. Furthermore the 3D geometry could also be adjusted to fit to the actual concreting sequence especially regarding the actual altitude, $z \ [\text{m}]$.

In order to better simulate the internal relative humidity development it would be of great importance to measure the relative humidity at the construction site. As this data was missing the moisture boundary conditions were roughly estimated.

Apart from the temperature development, the internal moisture development is of great importance in order to predict hydration of concrete. These two physical quantities may be used to simulate the development of other concrete properties at early age. Given the history of these physical quantities of a concrete structure it is also possible to model the development of for instance, modulus of elasticity and strength. The present work will continue in order to also model shrinkage (induced by drying), creep and displacement of the concrete structure.

REFERENCES

[6] Preliminary analysis reportV0.pdf, distributed by EDF, VeRCorRs, EDF, 2015.