Supplementary material in addition to SR-Site modeling report TR-10-11 as requested by SSM

1.3. Description of how the CRT-model was used and how THM and TH models differ in terms of analyzing the hydration process

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2 Introduction

The Swedish Radiation Safety Authority (SSM) requests a description of how the "CRT-model" was used in the study described in Åkesson et al. (2010), chapter 3.4 and how thermo-hydraulic (TH) models and thermo-hydro-mechanical (THM) models differ in terms of the water saturation process (SSM2011-2426-81).

These notes first briefly describe general differences that may affect the water saturation process between TH and THM models expressed in the "Code_Bright formulation". There after follows a description of the "CRT-model" which also serves as a specific case describing how responses of TH and THM models differ.

3 Differences in water saturation process using a TH and THM formulation

Describing the hydraulics' dependency on mechanics in general, for the Code_Bright formulation used in Åkesson et al. (2010), chapter 3.4, following statements, taken from the Code_Bright user's manual (UPC, 2012), are instructive:

- Water storage: Changes in porosity affect the available volume for water.
- Liquid water transport: Changes in porosity affect the hydraulic conductivity.
- Gaseous water (vapour) transport: Changes in porosity affect the vapour diffusion coefficient.

Furthermore, if using a possibility present in Code_Bright, letting the function expressing the water retention properties, here denoted by $\tilde{S}_l$, include a dependency on porosity, n, i.e.

$$S_l = \tilde{S}_l\left(P_g - P_l, n\right),$$

additional mechanical dependencies to the ones listed above become activated. This feature was, however, not utilized in Åkesson et al. (2010), chapter 3.4, but is never the less considered highly relevant for our systems and therefore here discussed. So, with $\tilde{S}_l$ dependent on porosity, changes in porosity of course affect the degree of water saturation directly. In addition, the degree of water saturation is also included in the water storage capacity and vapour diffusion coefficient which then will be affected indirectly by changes in porosity through the presence of degree of water saturation.

4 Description of the usage of the "CRT-model"

Turning towards describing the "CRT-model", it should be mentioned that CRT is an abbreviation of Canister Retrieval Test, an experiment realized at the Äspö Hard Rock Laboratory in Sweden. In chapter 5.4 of Åkesson et al. (2010), regarding "Buffer homogenisation", CRT was used as a case for which the homogenization process was studied by performing plane axisymmetrical THM simulations. The model regarded most representative was denoted CRT 6b.

In chapter 3.4 of Åkesson et al. (2010) model CRT 6b was recycled, but in an attempt to facilitate readability somewhat, it was now called THM CRT, since TH versions (TH CRT I and TH CRT H) without the mechanics also were used, as described below. This information, about the connection between CRT 6b and THM CRT, was unfortunately missing in Åkesson et al. (2010). Detailed information about model THM CRT can be found in Åkesson et al. (2010), chapter 5.4.

With that said, we turn to describing the actual purpose for using the THM model of CRT in chapter 3.4 of Åkesson et al. (2010). The analysis in Åkesson et al. (2010), chapter 3.4, where the CRT-model was utilized, served as motivation for being able to use two global TH-models with different "immobile mechanical representations", i.e. different density distributions, rather than performing one full global THM-simulation, and still being able to consider effects from the homogenization process. Performing detailed coupled THM-simulations on a global scale can be very challenging in terms of computational demand and numerical stability and that is why it was desirable to use two TH-models with different immobile mechanical representations at the global scale to circumvent these issues.

The strength of the coupling between TH and M in the buffer materials cannot be said to be insignificant, most parameters have some dependency on density (porosity), and therefore, the pair of two extreme immobile mechanical representations are used to account for this dependency. As mentioned, the immobile mechanical representations are represented by two extreme density fields, either equal to the *Initial* state as obtained at installation or a fully *Homogenized* state, i.e. the pellet slot density equals that of the buffer block.

The conceptual idea behind the model setup in the study within chapter 3.4 of Åkesson et al. 2010 is schematically described in Figure 1. In a deposition hole buffer, present at a *global* scale, THM-processes in a disc at canister mid-height (visualized to the left of the hatched vertical line in Figure 1) are considered to be sufficiently accurate represented by a plane axisymmetric model at a *local* scale (visualized to the right of the hatched vertical line in Figure 1). For this to be true the boundary conditions prescribed on the local model have to be representative for the processes on the global scale.

The most general of the three local representations used in the analysis is the THM CRT model where the homogenization process is simulated, as indicated in Figure 1. TH parameters/variables may thereby vary with the mechanical process and this may significantly affect the TH-process.

The two TH-models, indicated by the top and bottom schematic geometries in Figure 1, are obtained from either using the initial state density field, as in model TH CRT I, or a density field where full homogenization of the buffer has been assumed, as in model TH CRT H. Note that the fully homogenized state most likely differs from the final state obtained at full saturation as indicated in Figure 1. Thus, full homogenization cannot generally be assumed for a fully water saturated state.

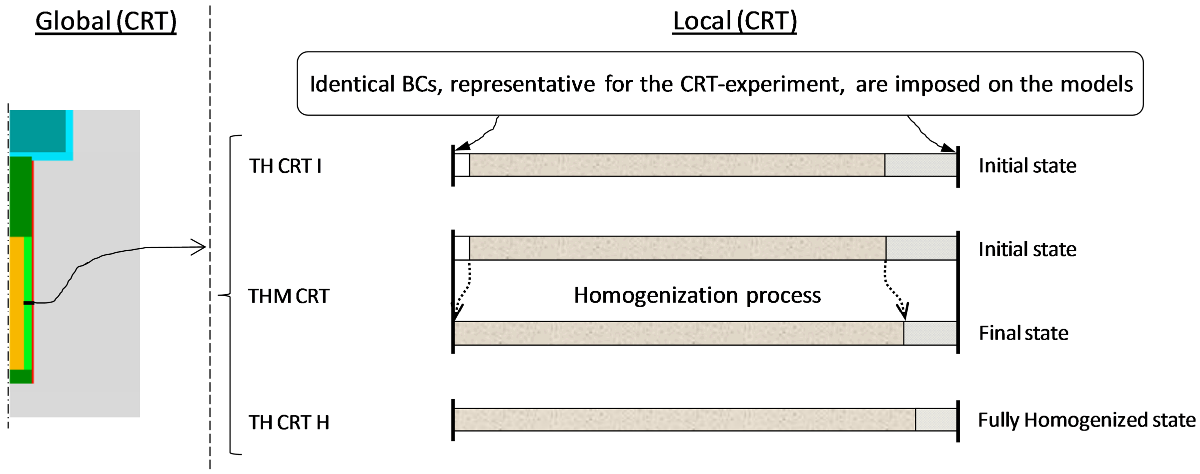

Figure 1. *Schematic description of the relation between models used in chapter 3.4 of (Åkesson et al, 2010). An imagined global model of the CRT-experiment is visualized to the left. To the right three local models, representing an axisymmetric disc at canister mid-height of the global model, are visualized. The local models are, from top to bottom, TH CRT I(nitial), THM CRT, and TH CRT H(omogenized). To the right of the schematic geometries of the local models the states considered are indicated. When using the THM-model the effect from the homogenization process is considered directly. When using the pair of TH-models and evaluating their responses together, an indirect consideration of the homogenization is possible.*

Figure 3-9 in Åkesson et al. (2010) is repeated below in Figure 2. It shows water saturation histories at three radial positions (r = 585, 685 and 785 mm) for the THM-model and the two TH-models. As can be seen, in the studied example, the THM responses are "bounded" by the responses of the TH-simulations. There is a significant difference between the THM and the TH-models, in this special case most so for the TH-model with the homogenized mechanical assumption. With the notation used in the legends in Figure 2 the relation between the saturation times, t_{sat}, of the models can be expressed,

$$t_{sat}(\text{TH CRT Initial}) \quad < t_{sat}(\text{THM CRT}) < \quad t_{sat}(\text{TH CRT Homogenized}),$$

which in (Åkesson et al, 2010) were taken as motivation for being able to use two global TH-models with different immobile mechanical representations, with saturation times bounding the THM-model's saturation time.

It should also be mentioned that the comparison of the three CRT models described above was not considered totally fair towards the homogenized TH-model. In chapter 3.4.2 in Åkesson et al. (2010) the CRT models were altered somewhat to make them more comparable and as a result, both TH-models' saturation times became closer to what the THM-model produced.

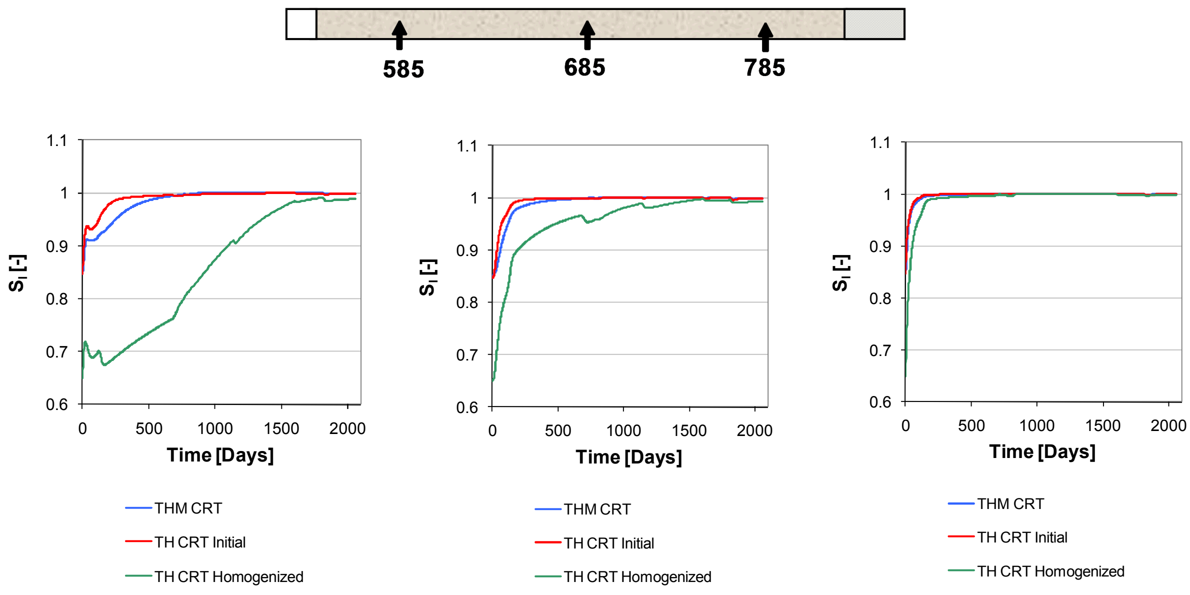

Figure 2. *Water saturation evolution at three different radii (585, 685 and 785 mm), Figure 3-9 in Åkesson et al.(2010).*

5 References

Åkesson M, Kristensson O, Börgesson L, Dueck A, Hernelind J, 2010. THM modelling of buffer, backfill and other system components. Critical processes and scenarios. SKB TR-10-11, Svensk Kärnbränslehantering AB.

UPC, 2012. CODE_BRIGHT, User's Guide, https://www.etcg.upc.edu/recerca/webs/code_bright/code_bright.