

Development of a Special COMSOL® Interface Based on an Alternative Model for Bentonite Re-Saturation

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Abstract

Bentonite is a versatile material that is, among other things, envisaged in most countries worldwide for use in radioactive waste repositories to protect the waste canisters against groundwater. The saturation process of bentonite is commonly described with thermo-hydro-mechanically (THM) coupled models. As an alternative to the formulations in these THM models, a thermo-hydraulically coupled saturation model for confined conditions has been developed and realized for 1D-problems in the FORTRAN code VIPER. To enhance the possible range of applications of code VIPER, a new interface has been developed using the COMSOL® Physics Builder. The resulting VIPER interface can be used like a native COMSOL® interface. At first, a COMSOL® model based solely on the VIPER interface has been set up that matches an isothermal water uptake test performed at GRS. After successfully completing this step, further terms in the balance equation as well as equations of state were added which are required for calculating non-isothermal water transport in the bentonite. Furthermore, a full coupling of the VIPER interface with the native Heat Transfer in Porous Media interface has been realized. The new coupling has been checked based on temperature and humidity measurements from the FEBEX in-situ experiment performed at the Grimsel Test Site in Switzerland. The FEBEX experiment was intended to represent the initial phase of storage of heat-producing nuclear waste where canister-like heaters were installed inside compacted bentonite blocks and emplaced in a tunnel in the granitic rock. Wetting of the bentonite buffer was provided by the quite strongly water conducting host rock. Measured and simulated temperature evolution as well as wetting dynamics in the buffer were found to match satisfyingly well. The work presented here allows for the application of the alternative re-saturation concept to a wide range of three-dimensional problems not applicable to the original code VIPER. Also, the process of creating, testing, and implementing an own COMSOL® interface using the Physics Builder is illustrated in this context.

Keywords: Bentonite, thermo-hydraulically coupled saturation model, Physics Builder

Introduction

In the search for a possible repository for radioactive waste, many questions need to be answered. In particular, the hazardous waste must be sustainably isolated from the biosphere. Therefore, worldwide, so-called deep geological repositories (DGR) are favoured, which means storage underground at depths of several hundred meters.

In general, a multi-barrier concept is followed to prevent the potential release of radionuclides from the repository by different means. The technical barrier involves the immediate containment of waste in containers. Since these waste containers are susceptible to corrosion to some extent, it is the main task of the two additional barriers to effectively prevent groundwater access to the containers and, in the event of a leakage, the spread of radionuclides into the geosphere and biosphere. The technical barrier is followed by the geotechnical barrier, which surrounds the technical barrier with natural materials that impede flow. The third barrier is formed by the host rock in which the repository is constructed. This is also called the "geological barrier" because only formations with low water permeability are suitable as a host rock.

The materials eligible for the geotechnical barrier depend on the host rock. In the case of granite or claystone, the natural material bentonite is used to protect the waste containers against groundwater. Bentonite is a type of rock that consists predominantly of clay minerals, is mined worldwide, and has versatile applications. It forms a porous medium that, due to its unique water absorption behavior, is attractive as a geotechnical barrier for a repository. When it comes into contact with water, it immediately starts absorbing water, resulting in swelling of the bentonite into the surrounding free space. If the bentonite has no room to expand, high pressures, known as swelling pressures, can build up, concurrently reducing water permeability. Bentonite exhibits its sealing effect "automatically" only when the problem of water ingress arises.

The hydraulic and mechanical processes involved may additionally depend on temperature. Due to these characteristics, bentonite has been investigated in laboratory and in in-situ experiments for several decades to determine its suitability as a geotechnical barrier in a repository. Since these tests only provide insight into bentonite behavior during the immediate period after repository closure, long-term predictions

about the development of the geotechnical barrier are only possible by simulation calculations based on them.

In the field of repository research, an approach for this type of modeling is established where thermal, hydraulic, and mechanical (THM) processes that can influence bentonite saturation are considered and simulated simultaneously. These models are referred to as "THM models" although conceptually they define more than just the coupling.

The solution approach implemented in this work, hereinafter referred to as the "VIPER approach", differs from the established approach in several aspects. It is assumed here that mechanical effects play only a minor role when bentonite is mechanically confined [1]. An isothermal bentonite saturation model based on the VIPER approach has already been realized as an equation-based model in COMSOL including a comparison with measured data [2].

To simplify the application of the VIPER equations in COMSOL, a dedicated interface was created using the COMSOL Physics Builder in the framework of COMSOL version 6.1. In a first step, an isothermal version of the VIPER interface was created and checked by a comparison with the results from the equation-based model [2]. Then further terms and equations of state were added to solve non-isothermal problems. Subsequently, the new implementation was checked against a laboratory and an in-situ test.

COMSOL Physics builder

The Physics Builder is a COMSOL proprietary tool that is available in the basic version of the simulation software COMSOL Multiphysics and allows for the creation of custom designed interfaces for COMSOL. This capability is utilized in this work to create a custom VIPER interface, which could then be coupled with a Heat Transfer Interface. The key components of the Physics Builder are described in the following.

Variables

All parameters contained in the equations must be declared and defined as variables or alternatively be specified as values directly in the equation. The declaration assigns a name and a unit to the variable. The unit of the variable can be selected either from the existing COMSOL definitions or defined within the Physics Builder. Within the variable declaration, also a user input can be defined which later assigns a value chosen by the user to the variable.

In the definition of the variable, the value is set as well as the type of the variable which could be a single value, a vector, or a matrix.

The dependent variable, i.e., the variable that the problem should be solved for, is differently treated compared to the other variables. For VIPER, this variable is the vapor density ρ_v , which must be defined in a special way in the Physics Builder. All

other variables are defined and declared as described above.

Equations

To implement the VIPER balance equation (see Appendix) in the Physics Builder, it first needs to be transformed into the weak form. Then, all parameters of the equation must be declared and defined as variables as described above. The equation can then be included in the interface using the declared variables under the weak form equation menu entry.

Solver

For solving a conservation equation, COMSOL offers a wide range of different solvers, which can be classified into the categories of direct and iterative solvers. When using the interfaces offered by COMSOL, the user usually does not need to change the solver settings, as a good solver with corresponding parameter settings is already proposed as the default setting. For the VIPER interface, a similar default setting can be created and stored in the Physics Builder to make the interface more user-friendly.

Multiphysics coupling

The Physics Builder offers the possibility to prepare a coupling with another interface. However, it is necessary to define such a coupling in both interfaces to be coupled. Since the common COMSOL user is not allowed to modify the native COMSOL interfaces, this option is only of interest if exclusively self-developed interfaces are to be coupled. This is not the case for the problem at hand which is solved here by preparing the necessary coupling parameters in the VIPER interface. Therefore, an input is created in the VIPER interface, to which the user later assigns the temperature calculated in the Heat Transfer interface. The water content distribution has an influence on the thermal conductivity as well as the heat capacity which are calculated within the VIPER interface. For a full coupling these two parameters must be assigned manually to the corresponding porous medium in the Heat Transfer interface.

Implementation of the VIPER interface

To use a self-created interface in COMSOL, it must first be compiled and then inserted into the program directory of COMSOL. To do this, the Physics Builder Manager is used within the Physics Builder. Within it, the .mphphb file of the interface is added as a Builder File under the Development Files menu entry. Then, a storage location for the compiled files is defined under the Archives menu. Afterwards, the interface can be exported as a plug-in and should be stored in the installation directory of COMSOL in the subdirectory `\\COMSOL\\COMSOL61\\Multiphysics\\plugins`. After restarting COMSOL, the custom interface can now be used in the Model Builder, just like any other COMSOL interface.

Simulation Results and Discussion

General remarks

With the newly developed VIPER interface, two model calculations are carried out to validate the interface. In a first test, the isothermal bentonite saturation measured in the laboratory [3] is successfully modeled, which was already the basis for the previous work [2]. The second test case is based on a thermally-hydraulically coupled system, which replicates the in-situ experiment FEBEX, e.g., [4].

Isothermal model

For a first test, an isothermal and one-dimensional problem was selected for which both modeling results and experimental results are available [3]. In the experiment, a series of cylindrical bentonite samples were under confined conditions with water contact on one side. After different periods of time, the individual tests were terminated, and the water content distribution along the sample axis was determined. This experiment was already recreated equation-based using the VIPER approach in COMSOL [2]. The simulation results matched the previous results as shown in Figure 1.

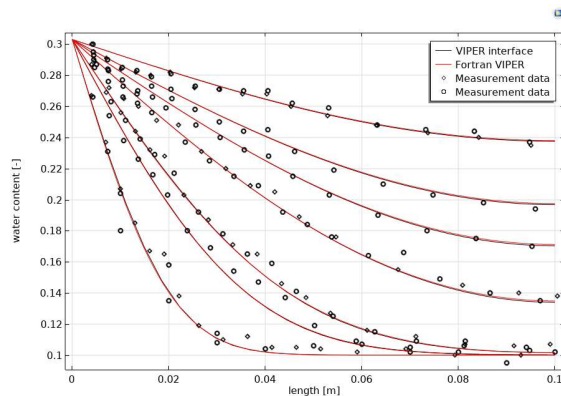


Figure 1. Comparison of measured data and simulation results for an isothermal laboratory water uptake test.

FEBEX in-situ test

Non-isothermal model FEBEX

The FEBEX experiment was an in-situ experiment that was conducted in the underground laboratory Grimsel in the Swiss Alps from 09/95 to 07/15, with the aim of simulating the disposal of heat-generating waste on a 1:1 scale. To do this, a tunnel was excavated and then instrumented with temperature, pressure, and humidity sensors. According to the disposal concept at that time, a liner made of pre-compacted bentonite blocks was then installed, as

shown in Figure 2. To simulate the heat-generating waste, two electric heaters were used in the liner.

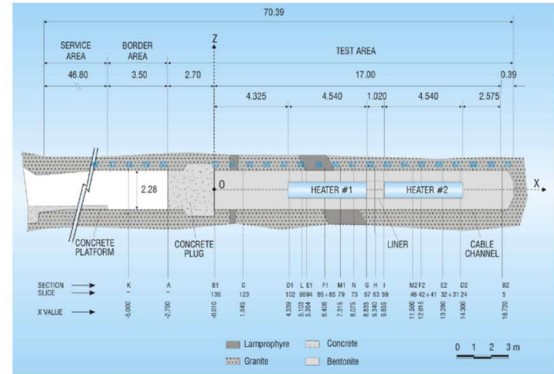


Figure 2. FEBEX test layout [4].

At the beginning of the experiment, the heaters were heated with a power of 1200 W each. When it was observed that the planned target temperature of 100 °C could not be reached at the surface of the heaters, the heater power was increased to 2000 W after 20 days. When the target temperature of 100 °C was reached after 55 days, the heater's power supply was switched to a temperature control mode based on sensor data from the canister surfaces to maintain the temperature for the remaining time of the experiment. At the same time, the power consumption of both heaters was measured. The first heater was shut down and removed from the test after 1827 days, marking the end of the first phase of the experiment. In the second phase of the experiment, only the second heater was in operation, which was then shut down after 6626 days [4].

Using the VIPER interface, coupled with the proprietary Heat Transfer in Porous Media interface, the first phase of the FEBEX experiment was simulated. To limit computational effort, the geometry is simplified using a 2D axisymmetric model. This model will be referred to as the "COMSOL-VIPER model".

Geometry

The geometry of the experimental space in the model is an exact replica of the experimental layout depicted in Figure 3. The size of the rock mass considered in the model is determined by the condition that the heat introduced through the heaters should not leave the model area. This condition is necessary to use a classic no-flow boundary at the outer boundary.

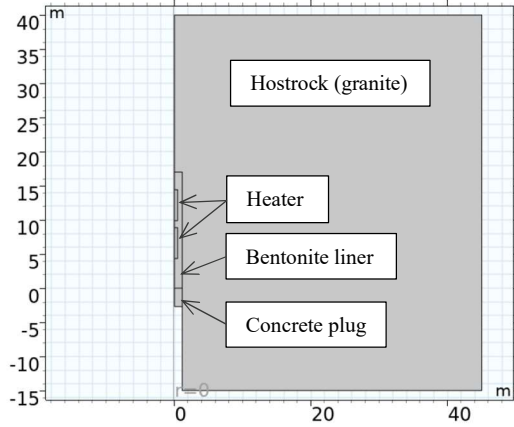


Figure 3. Model geometry.

More precisely, this boundary represents a natural boundary condition for heat flow. Therefore, the size of the model area must be optimized so that the model area does not become too large, to limit the computational effort, but also large enough to avoid heat accumulation at the closed boundary. For this reason, an optimal size for the model area is empirically determined by varying the size of the domain using an observation point at the model boundary. At the chosen radial distance of 45 m, an increase in temperature from 12 °C to 12.24 °C can be observed at the boundary after 2000 days of model time. The resulting distorting influence on the results appears to be negligible.

Material

The material properties for the liner (bentonite) as well as for the tunnel closure (concrete) need to be defined, while those for the heaters (AISI 4340 steel) and the surrounding host rock (granite) could be taken from the material library in COMSOL. The assumed parameters for the bentonite are taken from [4] and are listed in Table 1. The required parameters for the concrete are assumed according to [5] and are listed in Table 2.

Table 1: Material properties of bentonite; from [4]

Parameter	Value	Explanation
T	$ht.T$	Temperature (Heat transfer interface)
$\rho_{v,sat}$	0.0165 kg/m ³	Saturation vapor density
ϕ	0.231	Porosity
τ	0.65	Tortuosity of the pore space
ρ_d	1600 kg/m ³	Dry density
ρ_s	2780 kg/m ³	Grain density
τ'	0.3	Tortuosity of the interlayer
w_0	0.1	Initial water content
D'	$4 \cdot 10^{-10}$ m ² /s	Coefficient of the interlayer diffusion
ρ_w	1000 kg/m ³	Water density
D_{mol}	$2.16 \cdot 10^{-5}$ m ² /s	Molecular diffusion coefficient

Table 2: Material properties of concrete; after [5]

Parameter	Value	Explanation
λ	1.8 W/(m K)	Thermal conductivity
c_s	880 J/(kg K)	Heat capacity
ρ	2300 kg/m ³	Density

VIPER interface

Since solely the liner consists of bentonite, the VIPER interface is only applied to the liner. Because the surrounding granite is water-conducting, a Dirichlet boundary condition for vapor density is set at the contact between the liner and the granite, corresponding to the defined vapor saturation density of 0.0165 kg/m³. This means that the water supply for the bentonite is not restricted by limited flow from the rock. The rate of saturation is also dependent on factors such as temperature. This dependency is realized in the model by using the dependent variable $ht.T$ of the Heat Transfer Interface as a temperature input in the VIPER interface. An impermeable boundary for water flow is defined at the contact areas between the liner and the heaters, as well as at the contact between the liner and the concrete plug. While water uptake by the heaters was not possible in the experiment, water uptake by the concrete cannot be ruled out. However, due to its minimal influence on the model and the significant effort required for implementation, this effect is not taken into account.

Heat transfer interface

The Heat Transfer in Porous Media interface is applied to the entire model domain to allow heat to spread freely. The liner is defined as a porous medium while the heater, closure structure, and surrounding rock are defined as solids. The required values for thermal conductivity, density, and heat capacity for the solids can be directly obtained from the material definitions. For the liner, both the definition of the porous matrix as well as the definition of the fluid are necessary. The porosity and dry density are already defined within the VIPER interface and are linked to the porous medium in the Heat Transfer in Porous Media interface, using $id.phi$ and $id.rhod$. In case of a porous medium, two different materials are present in one area. Since COMSOL only allows one material to be assigned to a model domain, the material data for the fluid must be assigned manually from the material list using the call $mat6.def.variable$. The two heaters are defined as heat sources, which are controlled through variables using the Events interface as described below. Furthermore, the temperature in the free section behind the closure structure is set to 12 °C through a Dirichlet boundary condition. This is a realistic value due to the ventilation in the mine shaft.

Events interface

The control of the heaters was realized using the Events interface. This allows control variables for the heaters to be defined, which can change either depending on the model time or depending on another model parameter. These events are called explicit or implicit events. By using these options, a thermostat control with a delay of 0.01 days is implemented [6]. When reaching the target temperature at an observation point, this thermostat control reduces the heater power by 20 % until the temperature at the heating surface drops below 98 °C, and then reheats the model with full heater power. The control parameters for this temperature control are determined empirically for the model. The goal had been to achieve a minimal calculation time with a low temperature deviation.

Meshing

The different size of the model zones makes an adaptive meshing necessary to reduce the computational effort. While the mesh generator in COMSOL already shows some adaptivity in the standard meshing, manual intervention is required. The mesh used here requires strong local refinement in the area of the experiment.

Plausibility check

To verify the plausibility of the results, the temperature across the entire model area and the water content in the liner are plotted for 100 and 1800 days of testing time. The temperature distribution in the model area is depicted using isosurfaces in 2 degree increments within a range of 12 to 100 °C. This temperature range is determined by the difference between the initial system temperature of 12 °C and the target temperature of 100 °C on the surface of the heater. Over time, the spatial propagation of heat originating from the heaters can be observed, like shown in Figure 4. The humidity evolution within the liner plotted in Figure 5 shows a spread of the moisture front, starting from the contact zone with the granite.

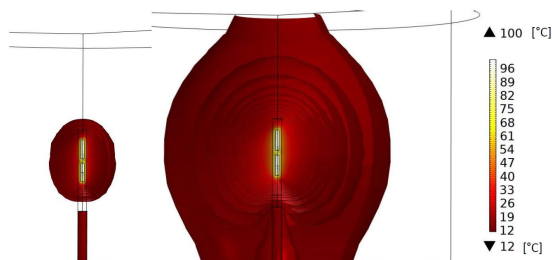


Figure 4. Temperature propagation, left: after 100 days; right: after 1800 days.

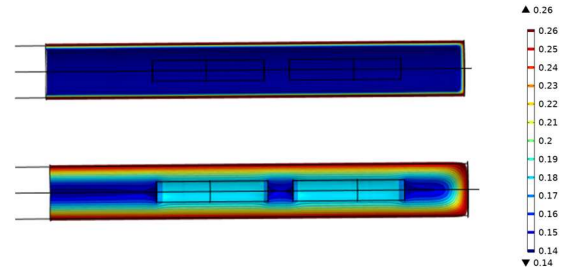


Figure 5. Humidity evolution in the liner; up: after 100 days; below: after 1800 days.

Comparison with measurement data

The FEBEX experiment was monitored with many sensors, so there are many control points available for model validation. This mainly included humidity and temperature data, which represent a local development. Additionally, as mentioned before, the power consumption of the heaters was recorded.

Four data sets have been selected from the multitude of time series' and cross-sections for this work to demonstrate the functionality of the VIPER interface. These consist of the humidity evolution over time at control points P2 (see Figure 6) and P3 on cross-section C (cp. Figure 2), the temperature profile along cross-section AS1 at different times (see Figure 7), and the power uptake of the electrical heaters.

The temperature profile demonstrates the proper simulation of heat propagation, and the humidity evolution proves the successful operation of the VIPER interface. The feedback of the water absorption of the bentonite on the heat propagation, which could not be considered with the experimental code VIPER, is indirectly reflected in the development of power consumption of the heaters. As the water content in the bentonite increases, the effective thermal conductivity also increases, resulting in faster heat dissipation from the liner. Therefore, an increasing amount of electrical power is required to maintain a temperature of 100 °C at the heater surface, as shown in Figure 8.

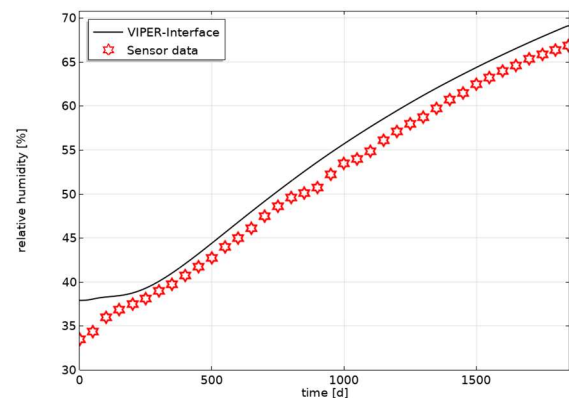


Figure 6. Humidity evolution at comparison point P2 over 1800 days.

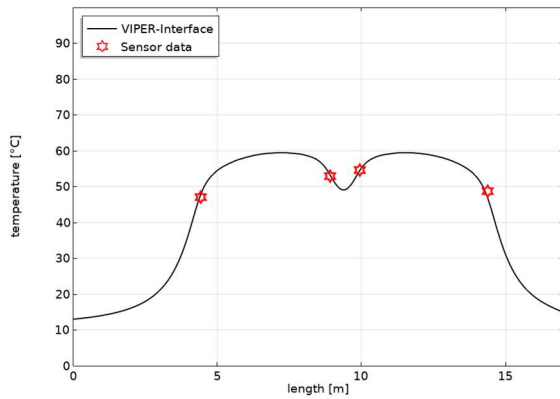


Figure 7. Temperature after 90 days along cross section AS1.

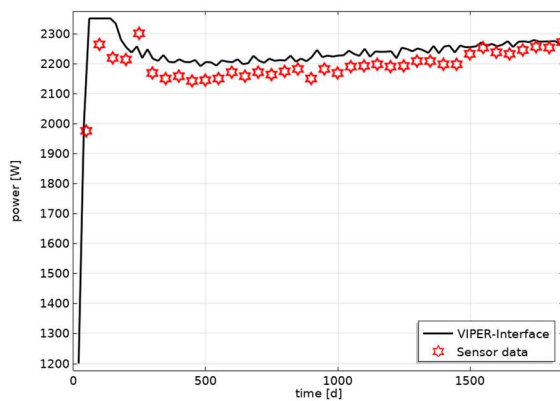


Figure 8. Evolution of heater power uptake over 1800 days.

Conclusions

Due to the range of data against which the results from the VIPER interface have been successfully compared, it becomes clear that the non-isothermal VIPER approach for bentonite saturation has been successfully ported to COMSOL. This represents another milestone in the model-based development and implementation of the VIPER approach. By creating the VIPER interface for modeling non-isothermal bentonite saturation, the range of processible problems for models based on the VIPER approach is significantly expanded. In addition to the ability to comfortably create multi-dimensional models in COMSOL, full coupling with a Heat Transfer interface is now available. This creates a COMSOL-VIPER model that can be widely applied in practice.

Further modeling tasks related to isothermal or non-isothermal bentonite saturation will show whether adjustments or further developments will be necessary or even required in the future. One possible topic could be the swelling of pre-compacted bentonite into a free space, where the space could either be completely free or perhaps

have a limited volume. In such cases, it may be useful to expand the existing thermal-hydraulic coupling according to the VIPER approach in COMSOL with a mechanical component if a simpler approach by means of an empirical relationship is not available.

For applications involving models with a large number of nodes and elements, further investigation may also prove useful to systematically examine the suitability of the solvers implemented in COMSOL for such COMSOL-VIPER models, which was beyond in the scope of this work. Referring investigations would also need to include the optimization of parameters for preconditioners and solvers.

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Appendix

VIPER equation

$$\begin{aligned}
& \rho_d \frac{\partial w}{\partial r_h} \frac{1}{\rho_{v,sat}} \frac{\partial \rho_v}{\partial t} \\
& + \left(\rho_d \frac{\partial w}{\partial T} \right) \frac{\partial T}{\partial t} \\
& + \left(-D_a - \rho_d D'_a \frac{\partial w}{\partial r_h} \frac{1}{\rho_{v,sat}} \right) \Delta \rho_v \\
& + \left(-\frac{\partial D_a}{\partial T} \nabla T - \rho_d D'_a \left[\nabla \left(\frac{\partial w}{\partial r_h} \right) \right] \frac{1}{\rho_{v,sat}} - \rho_d D'_a \frac{\partial w}{\partial r_h} \left[\nabla \left(\frac{1}{\rho_{v,sat}} \right) \right] - \rho_d \frac{\partial D'_a}{\partial T} \nabla T \frac{\partial w}{\partial r_h} \frac{1}{\rho_{v,sat}} \right) \cdot \nabla \rho_v \\
& + \left(-\rho_d \frac{\partial w}{\partial r_h} \frac{1}{(\rho_{v,sat})^2} \frac{\partial \rho_{v,sat}}{\partial T} \frac{\partial T}{\partial t} + \rho_d D'_a \left[\nabla \left(\frac{\partial w}{\partial r_h} \right) \right] \frac{1}{(\rho_{v,sat})^2} \frac{\partial \rho_{v,sat}}{\partial T} \cdot \nabla T + \rho_d D'_a \frac{\partial w}{\partial r_h} \nabla \left(\frac{1}{(\rho_{v,sat})^2} \frac{\partial \rho_{v,sat}}{\partial T} \right) \cdot \nabla T \dots \right. \\
& \quad \left. \dots + \rho_d \frac{\partial D'_a}{\partial T} \nabla T \frac{\partial w}{\partial r_h} \frac{1}{(\rho_{v,sat})^2} \frac{\partial \rho_{v,sat}}{\partial T} \cdot \nabla T + \rho_d D'_a \frac{\partial w}{\partial r_h} \frac{1}{(\rho_{v,sat})^2} \frac{\partial \rho_{v,sat}}{\partial T} \Delta T \right) \rho_v \\
& + \left(-\rho_d D'_a \left[\nabla \left(\frac{\partial w}{\partial T} \right) \right] - \rho_d \frac{\partial D'_a}{\partial T} \nabla T \frac{\partial w}{\partial T} \right) \cdot \nabla T \\
& + \left(-\rho_d D'_a \frac{\partial w}{\partial T} \right) \Delta T = 0
\end{aligned}$$

$$D_a = D_{mol} \phi \tau$$

$$D'_a = \tau' D'$$

ρ_d	dry density
w	water content
r_h	relative humidity
ρ_v	vapour density
$\rho_{v,sat}$	saturation vapor density
t	time
T	temperature
D_a	vapour diffusion coefficient
D'_a	coefficient of the interlayer diffusion