STUDYING THE INTERACTION BETWEEN LIQUID, GAS AND HEAT FLOWS IN A SOIL UNDER EVAPORATION CONDITIONS BY MEANS OF NUMERICAL MODELING

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Simulation of an evaporation test in a soil column have been carried out to characterize the properties of the topsoil of the El Cabril Radioactive Waste Disposal Facility and the evaporation process. The conceptual model considers unsaturated liquid flow, vapour flows and heat flows of a sample of 14 cm. of the vegetal soil. Vapour fluxes become the main water flow mechanism under very dry condition. Water leaves the column as vapour only at the top of the column, due to the difference of relative humidity and temperature between the column and the laboratory. Very dry conditions necessitate the modification of the retention curve to represent oven dry condition and it has been calculated considering the experimental values obtained by CIEMAT (Villar et al. 2012). The model has been calibrated with the experimental data obtaining the values of the parameters of the constitutive laws and of the boundary conditions, suggesting that it can be used to assess the behavior of the soil under evaporation conditions. Finally, an abnormal behavior of the sample during the test has been displayed due to a bigger value of β.
1 - INTRODUCTION

Most of the radioactive wastes generated in Spain are of the low and intermediate level type and are produced at hospitals, research centers, industries and nuclear power plants. Spain has solved the issue of managing these wastes through the El Cabril centralized disposal facility in Hornachuelos (Córdoba).

The waste is placed in cells of concrete that will be covered by a capillary barrier. The requirement of this barrier is to guarantee isolation of the waste until radiation has decayed to permissible level in 300 years. It will prevent the infiltration of water to avoid that the water is in contact with the underlying waste determining water contamination and deterioration of the concrete that contains the waste. The third chapter of this thesis show the different kind of barriers with their different layers and properties in order to understand the advantages and disadvantages of each one.

This work focuses on the evaporation test of a sample of the topsoil of the capillary barrier in El Cabril.

In the literature there are similar works where evaporation tests have been studied in order to obtain the water retention curve and the other parameters of the samples. For instance, Chaparro et al. (2011) determined the water retention curve of the concrete of the cells of El Cabril from evaporation tests on columns of concrete carried out in the laboratory. Inside the column of concrete there were sensors that measured the temperature and the relative humidity. Moreover Chaparro et al. analyzed the results of these evaporation tests with one-dimensional numerical models to obtain the water retention curve and calibrating the permeability and the tortuosity.

Understanding evaporation is necessary in many fields of earth system sciences. In fact, soil evaporation is crucial in controlling the balance of water and energy in arid and semiarid areas (Saito et al. 2006). The actual mechanisms controlling evaporation are intricate. Soil evaporation may be controlled by the soil-atmosphere boundary layer when the soil is moist or by hydraulic conditions when it is dry (Schneider-Zapp et al., 2010). In the latter case, evaporation causes the soil to dry and heat up causing liquid, vapour and heat fluxes to interact. The presence of solutes increases the complexity of the system and exacerbates the consequences, leading to salinization.

A number of researchers have analyzed this problem from an experimental prospective (Wheeting, 1925; Scotter, 1974; Nassar and Horton, 1989; Scanlon, 1992). They conclude that water flux in dry and salinized soils is controlled by
salinity and temperature gradient. Evaporation depends also on temperature and absorbs energy. Thereby, evaporation is affected by water flow and energy and solutes transport. The interaction of matric potential, temperature and salinity gradients under very dry conditions was studied by Gran et al. (2011), who observed salinity to decrease below the evaporation front, which they attributed to condensation of downward vapor flux. Unfortunately, experimental studies do not yield direct measurements of flow and phase change processes, which must be indirectly inferred from state variable measurements. Therefore, quantitative understanding of the above processes requires mathematical modeling.

Most models of evaporation focus on the interactions between water and heat flow and it has been noticed that the vapour flux is dominant near the surface where the soil is dry, and that water flows in the liquid phase below the evaporation front. The width of this front is subject to debate. Under hot and/or dry conditions, the residual saturation of water in soil can no longer be considered a lower bound for saturation (Milly and Eagleson, 1982; Rossi and Nimmo, 1994; Prunty, 2003). A modification of the retention curve must therefore be considered to represent water contents under oven dry conditions.

The aim of the thesis focuses on the analysis of the superficial layer of the capillary barrier of El Cabril that is the most critical one due to the contact with the atmosphere. There are some data measured in the laboratory by CIEMAT (Villar et al. 2012) on a soil sample of 14cm of the vegetal layer and with them the calibration of the parameters of the constitutive laws and of the boundary conditions has been obtained by modeling this sample in Code Bright and comparing modeling’s results with the data measured. The numerical modeling shows the interaction between liquid, gas and heat flows in a soil under evaporation conditions without considering the presence of solutes. The evaporation test has been simulated in order to have a better knowledge of the properties of the layer and of the evaporation process.

The next chapter shows the disposal facility of El Cabril focusing on the design and monitoring system of two pilot covers (Gran et al.). These covers, with no waste beneath them, are multilayer covers based on capillary barrier concepts and are disposed to study the behavior of the barrier. From this pilot cover, CIEMAT (Villar et al. 2012) picked up the sample of topsoil that has been studied. The evaporation test with the experimental results obtained by CIEMAT (Villar et al. 2012) have been shown in the fourth chapter. These data have been used to obtain the water retention curve and to calibrate the tortuosity
and the other parameters that characterizes the constitutive laws and the boundary conditions of the column (chapter 5). The sixth chapter shows the calibrated graphs of suction, relative humidity, temperature, loss of water and degree of saturation. The experimental results have been reproduced by the model in order to evaluate also the magnitude and direction of the fluxes (liquid, vapour and heat fluxes). In the last chapter an abnormal behavior of the sample during the test has been displayed due to a bigger value of \( \beta \). In this way we are able to have a characterization of the vegetal soil during an evaporation process to develop and study the behavior of the barrier during all the time that we need and to check if it guarantees the requirements.
2 - THE DISPOSAL FACILITY OF EL CABRIL

2.1 INTRODUCTION

The Spanish facility for disposal of low and intermediate-level radioactive waste is located at El Cabril (Cordoba, in southern Spain) and is administered by ENRESA. Low and intermediate level wastes are materials contaminated with radioactive isotopes whose radioactivity will be reduced by half in less than 30 years. They may be tools, working apparel, medical instruments and other materials used in certain industries and at hospitals, research laboratories and nuclear power plants. The group of low and intermediate level wastes also includes what are known as very low level wastes, which in view of their low radioactivity content entail less demanding requirements for their management. Most of these wastes arise from the dismantling of nuclear power plants and represent a very high volume within the overall category of low and intermediate level wastes.

The facility, located in the hills of the Sierra Albarrana, has two platforms for the disposal of low and intermediate level radioactive waste and another with specific structures for very low level wastes. In addition, the facility has the resources required for the treatment and conditioning of wastes requiring such processes.

Figure 2.1: El Cabril facility for disposal of low and intermediate level radioactive waste
The disposal system is based fundamentally on the incorporation of natural and engineered barriers safely isolating the materials disposed for the time necessary for them to be converted into harmless substances.

The basic objectives of the El Cabril Disposal Facility are to guarantee the protection of persons and the environment against ionising radiations and to allow use to be made of the site 300 years after its has ceased to operate.

In order to achieve this, the following is necessary:

- Effective isolation of the radioactive wastes and preventing their possible dispersion. To achieve this, three barriers are placed between the wastes and the environment: a first barrier, made up of the conditioned waste and the container; a second barrier, consisting of the engineered structures housing the wastes and a third and final barrier, formed by the natural soil of the site at which the facility is located.

- Limitation of the activity of the wastes: to achieve this objective the El Cabril facility accepts only radioactive wastes with a half life of less than 30 years or wastes with very low levels of long-lived radioactive substances.

The El Cabril centralized disposal facility has two functionally differentiated areas: the buildings area and the disposal area. This separation allows for the efficient performance of the activities of the centre, facilitating their monitoring and control and differentiating the radiologically regulated zones.

**Buildings area**

The buildings area has two laboratories for verification of the quality of the wastes. Also located here are the conditioning buildings, in which the waste treatment activities are performed, and the control room, where all the information on operation of the facility is centralized. The auxiliary installations include administration, industrial safety, technical services, general services, temporary storage installations, manufacturing of containers, the maintenance workshop, the canteen, etc.

**Low and intermediate level waste disposal zone**

The low and intermediate level waste disposal zone is formed by two platforms: the north platform, which includes 16 disposal cells, and the south platform, which has 12 such cells.

**Very low level waste disposal zone**
The very low level waste disposal zone is formed by a platform made up of four structures that will be constructed as they are needed.

The El Cabril installations are characterized by the following:

- Automatism: the capacity to be operated from a control room, thus minimizing the exposure of the workers.
- Seismic resistance: the capacity to withstand the earthquakes foreseeable in the area.
- Solidification: the capacity to dispose of all the wastes in solid form.

The low and intermediate level wastes generated at any location in Spain arrive at El Cabril and are unloaded at a conditioning building or one of the temporary storage facilities. Most of these wastes, generated at the nuclear power plants, are already conditioned on arrival, while those coming from hospitals, research centers or industries are treated and conditioned at El Cabril installations. The waste drums received are placed in concrete containers with a capacity for 18,220-litre drums. When a container is full, its drums are immobilized by means of injected mortar. The compact block is placed in the disposal cell, which is a structure of reinforced concrete. Once the disposal cell is filled with 320 containers, the upper reinforced concrete closure slab is constructed and weatherproofed. Each of the 28 disposal cells has a sump connected to the seepage control network located beneath the platforms. This allows that possible in-leakages of water will be detected and, if they occur, repaired. As from this moment, a 300-year site surveillance and control phase will begin.

Very low level wastes are solid materials, generally scrap and rubble, that are minimally contaminated with radioactive isotopes. They may arrive at the facility in sacks, drums or containers and may be disposed of directly in the specific disposal structure or first be taken to the area set aside for their treatment, if necessary.

Once the capacity of the platforms has been depleted, these will be covered with a final coverage consisting of a complete system of barrier, the last of which will be of topsoil, allowing for integration into the environment. It will cover the platforms for a long time and it will be made of some layers of geological materials (gravel, sand, clay soil and topsoil) and geotextile which thickness will be of about 0.1-0.5 m.

The purpose of this cover is to reduce the erosion, remove the surface water, protect against the biointrusion, minimization of the permeability to reduce the infiltrated water and the drainage of the seepage. Moreover, nowadays, the
characterization of the geological materials is useful to plan the new cover layers and to improve safety studies that are systematically required by the Nuclear Safety Council.

2.2 PILOT COVERS

A cover has been planned for the final confinement of disposal cells, which contain radioactive waste.

Two pilot covers have been designed at the facility, with no waste beneath them, to evaluate and analyze the behavior of this kind of cover. They are multilayer covers based on capillary barrier concepts and the requirement is that they guarantee isolation of the waste until radiation has decayed to permissive level in 300 years. The purpose of the pilot is to test the cover with respect to surface erosion and runoff, infiltration and biointrusion and determine the final design. The objective is to establish the definitive design for the confinement of the waste in order to avoid any root or animal entry and minimize water infiltration, in liquid or vapour phase, so that the final design can guarantee the isolation of nuclear waste and avoid the contamination of the water and the deterioration of the cells of concrete.

There is a monitoring system with more than 200 sensors to measure temperature, water content, suction, surface runoff and infiltration.

A capillary barrier is a combination of an unsaturated fine-grained soil overlaying unsaturated coarse-grained soil along a sloping contact. Under appropriate conditions the arrangement diverts infiltrating water away from the coarser material. The mechanism relies on the properties of hydraulic conductivity as a function of pressure potential (Ross, 1990). The relative permeability is significantly reduced when lowering the water content. The textural resistance impedes the descendent water flow and tends to maintain the lower layer dry until breakthrough occurs. That happens at the point along the interface where the matric suction in the fine layer becomes equal to the water entry pressure of the coarse layer (Pease and Stormont, 1996). If the layers are sloped, water can be diverted descending along the interface between the two layers. The diversion capacity is a linear function of the inclination of the system (Kampf et al., 2003) and if a layer's disposition is horizontal water will accumulate in the fine-grained layer, constituting a water reserve available for evaporation or evapotranspiration through the roots of the plants.

The textural contrast between two layers is also a determinant factor (Smesrud and Selker, 2001). It has been demonstrated that in 80% of the studied cases, the
maximum deviation is reached at a 2.5 ratio between coarse and fine materials. That means that high contrasts are not necessary to reach an 80% deviation of the water but it could promote particles passing through the coarse layer, breaking the capillary barrier effect and allowing the descendent water flow (Smesrud and Selker, 2001; Tidwell et al., 2003).

The gravel-soil mixture increases the surface resistance to erosion, but could diminish the evapotranspiration (Albright, 2002). Gravel-soil mixtures with 22% and 33% gravel turn out to be equally effective in reducing erosion without affecting the growth of vegetation or the evaporation (Waugh et al., 1994).

It has been observed that a gravel layer (0.5-1.5cm diameter) above a pebble layer (10-20cm) is effective to prevent animal and root entry (Anderson and Forman, 2002; Albright 2002). A pebble layer at a width of 30cm placed between two sand layers that are 10cm in width is successful in deflecting the entry of excavation ants (Gaglio et al., 2001).

The pursuit of an adequate cover design has led to the development of numerous pilot covers combining a variety of materials, widths, organizations and slopes. Scanlon et al., (2005) performed three different types of covers in arid and semiarid regions. Two of them were based on the mechanism of evapotranspiration (ET) and a third was based on the capillary barrier concept (CB). They observed that the vegetation controls water balance in the ET covers, making them less robust, and they emphasize the success achieved with the CB cover. Waugh et al. (2004) carried out lysimeter test to see the result of using different soil types and compaction degrees. They concluded that the outcomes were very different, particularly in the wet season. The more compacted and less granular soils show a lower retention capacity, hindering vegetation growth and reducing evapotranspiration, leading to higher infiltration. Dwyer (2003) performed six cover test on a large scale. Three involved very low saturated hydraulic conductivities (resistive type) to prevent water flux, two involved a CB cover and the last ET cover. The one that showed the best results (a low infiltration rate) was the ET cover. They observed that the resistive type exhibit a lower water retention capacity, less evaporation, bigger infiltration rates and were affected by erosion, frosts and biointrusion. The CB covers suffered from an excess of compaction and consequently poor vegetation. They were also ineffective as biointrusion barriers.

At present an effective cover design that is able to comply with the entire set of requirements for guaranteeing the preservation of the nuclear waste does not exist yet. The two pilot cover tested have a new design based on the capillary
barrier concept and with a set of layers that combined could be effective in satisfying all the requirements that the preservation of these residues entails. Basically, the design aims to achieve lateral deviation of the infiltrated water, high evaporation rate and preservation of the materials against biointrusion. This cover need also a durability of hundreds of years until radiation has decayed to permissible level. The geometry of the cover present a 40% slope that will strongly determine the conditions of flow within the cover and will hinder the tasks of reduction of erosion and restoration of the vegetation.

A complete system of monitoring and infiltrated water collection has been designed for the pilot to obtain an optimal flux balance and avoid the previous work’s problems in calculating evapotranspiration (Dwyer, 2003). The monitoring system will allow to quantify the heat and water flows. The instrumentation data has been used to interpret the fluxes and validate the modeling results.

This devices are used to study the multiphase flow processes improving the understanding of the behavior of liquid, vapour and heat flow and studying the effects of different hydraulic properties, capillary pressure and degrees of saturation of the materials on the magnitude and direction of these flows.

2.3 COVER DESIGN

The pilot tests are made up of two multilayer covers divided by a concrete gallery that contains the data collection system.

Two different cover designs, called Test I and Test II, have been performed to compare the results of the different combinations of materials that have been applied in each cover. The two covers have equal dimensions (22m long by 11m width) and the upper zone of each cover has a 2% slope and the lower zone has a 40% (Fig. 2.2). They are multi-layer adjacent covers based on the capillary barrier concept and a sand layer superimposing a clay layer forms each one. In the case of Test I the sequence is repeated, with one capillary barrier above another. A diagram showing the layers in the two covers can be seen in Figure 2.3.
Figure 2.2: view of the pilot cover. Test I lies on the left hand side of the gallery and Test II on the right.

Figure 2.3: section view of the layers in the Test I, top picture, and Test II, bottom picture.
In the two diagrams above, it is possible to see the number and order of the layers that comprise each cover. Total thickness of the layer ensemble is 3.15m for Test I and 2.95m for Test II and every layer or set of layers has a particular purpose:

- **Vegetal soil (0.4m width):** to promote the growth of vegetation preventing the erosion from wind and run-off; to favour evapotranspiration by plants, capturing a high percentage of seepage; integration into the landscape.

- **Soil (0.4m width):** to retain enough water to allow vegetation establishment, promoting evapotranspiration, and favouring the growth of short-root plants.

- **Sand and Gravel (0.15m width, each one):** jointly they perform a filter function, preventing the contamination between materials since they prevent fine materials mixing with lower coarse materials. These layers also represent one first capillary barrier. Moreover the lower layer of the filter (gravel) together with the pebble layer acts as a barrier against biointrusion. Furthermore, the sand layer beneath the clay layer acts as a capillary barrier and works as a drainage in case of breakthrough.

- **Pebble (0.4m width):** together with the gravel layer, this layer works as a biointrusion barrier. As a non-retentive material, it forms a drainage layer for the removal of whatever water might have seeped into the upper layers. It also prevents the root growth and the animal entry by combining different grain sizes. For example, the largest sizes cannot be carried by small size species and they also show poor stability, collapsing when larger species excavate. Furthermore, ants and small mammals can't dig out preferential paths, allowing water to enter and reducing the cohesion of the materials.

- **Clay (0.45m width in Test I and 1m in Test II):** with the sand below, it acts as a capillary barrier. Thus, its greater capacity of water retention and its greater permeability promote the deviation of water in a horizontal direction, near the base of the clay layer, hindering its entry into the sand.

The base of both covers is made up of a PEAD geomembrane (it's a completely impermeable sheet designed to prevent the entrance of water) between two anti-punching sheets of geotextile (a sheet woven with polyester threads that prevents the mixing of layers while allowing water to pass through). Also, the geotextile has been used to separate the materials between different layers during the cover's construction.
2.4 MONITORING SYSTEM

A complete monitoring system involving more than 200 sensors has been developed in the two pilot covers. Each of the two covers is divided in four sections (Fig. 2.4). The division is a result of the different flow conditions expected in every zone of the cover. With respect to the different slopes and the amount of water stored, there is a low volume of water (limited to the precipitation from above it) in the upper zone (section 1) and it is expected to have a medium water volume in the section 2. In sections 3 and 4 there is a steep slope with an increasing volume of water in descendent direction, generating high soil humidity conditions. The water content, the temperature and the suction have been measured at different depths in the centre of each section. Data for surface run-off and water infiltrated volume are collected at the frontal zone of the tests.

![Figure 2.4: general view of the pilot cover where it is possible to see the four sections. In the center of each section has been installed a full complete set of sensors](image)

The flow conditions with the different properties of the cover's materials and the limitations of the instrumentation result in a complex combination of sensors in each layer. The aim of the sensors is to obtain the maximum information possible without interference between them (as there are a lot of sensors in a reduced space). There are sensors for thermal, water content and suctions measurements. Regarding the temperature measurement there are thermocouples, soil thermal properties sensors (which measures conductivity,
diffusivity and heat capacity of the soil) and the plate, which measures the heat flow in the soil.

With respect to the water content data there are the TDR.

To measure suctions they use the tensiometer (for low suction values), the psychrometer and matric potential sensors (for medium suction values) and the hygrometer (for the higher suctions).

At the same time, a complete meteorological station record meteorological data such as wind direction and velocity, short-wave radiation, temperature and relative humidity.

Moreover, installation of extensometers in the slope change (in the middle of each test, between section 2 and 3) allows us to take deformation data of the PEAD geomembrane. There are also inclinometers along the changing slope, but inside the clay layer, in order to measure possible differential settlement between the 2% and 40% slope areas.

All wiring has been laid horizontally, parallel to the base and ceiling of the layers, avoiding connections among the materials. The wires run from the sensors to the gallery where the data-loggers have been installed. The gallery gives a separation between the two tests and also a place to set up all the data-loggers and the monitoring systems that control the frequency of the data measurements. The gallery also contains the system to measure the infiltrated water volume. The infiltrated water is collected by a gutter displayed all along the front of the cover, underneath the materials, where the layers finish. They contain tilted pipes that favour the diversion of the water to the gallery (Fig. 2.5).

![Figure 2.5](image)

**Figure 2.5:** section of one of the gutters that collect the infiltrated water from the bottom of the layers and divert it to the gallery to be quantified

Inside the gallery, a quantification system, which is based on the tipping bucket concept, has been placed together with an automatic water sampler. The reason for taking water samples is that they have set out some tracers in the clay layers
of each test and in soil and vegetal soil layers of Test II. The tracer experiment is looking for the correlation of the slope of the breakthrough tail with the distribution of soil connectivity. To carry out the experiment and control the amount of water infiltrated in each layer, a system of channels has been performed. Six drain lines in Test I and five drain lines in Test II are in charge of collecting the water of certain layers or combination of layers and channelling it to the gallery to be measured and sampled. The drain lines finish in the front wall where pipes have been placed to collect the water and carry it to the gallery. Nowadays the cover construction is recently finished and the data from the sensors is being collected. In this work M. Gran et al. are starting to get the data while they are working on the 2D model. The model is a non-isothermal multiphase flow model using the coupling of Retraso-CodeBright codes. The model is the last key element to improve the knowledge of the processes in the cover and it will enable the verification of the cover's effectiveness and contribute to the definitive design for the confinement of the waste.
3 - CAPILLARY BARRIERS

3.1 BARRIER LAYERS

Surface covers are a component of all waste-containment facilities. Their primary purpose is to isolate the waste from the environment, prevent infiltration, improve the aesthetic value of the landfill, and prevent biointrusion and gas emanation. Reducing the volume of percolating water reduces the rate of leachate generation and the risk of groundwater contamination.

Cover designs range from simple compacted soil layers to multi-component, engineered systems. Materials used for surface barriers commonly include soils of various grain sizes, geosynthetics, and compacted soil. The barrier layer minimizes infiltration through the cover due to its greatly reduced hydraulic conductivity. The surface barrier promotes storage in the overlying layers until the moisture may be removed by evapotranspiration or internal drainage.

At most sites, regulations prescribe a final cover design based on resistive principles, i.e., layers having low saturated hydraulic conductivity (compacted clay barriers, geosynthetic clay liners, and/or geomembranes). These covers are referred as "conventional covers".

Alternative cover designs are also permitted provided that the alternative cover is equivalent to the prescriptive cover. Equivalency generally requires that percolation from the alternative cover be less than or equal to percolation from the prescriptive cover.

Alternative covers (e.g. the capillary barriers) based on water balance principles are currently being considered for closing many waste containment facilities, particularly in semi-arid and arid regions. These covers limit the amount of water entering the waste by exploiting the water storage capacity of finer textured soils and the water removal capability of vegetation. This natural approach to isolating waste is different from the approach employed by prescriptive covers, and is more likely to be effective over the long-term because it is congruent with nature. An additional benefit is that alternative covers typically are less costly than prescriptive covers. Alternative designs and methods should be investigated to find the most reliable and economical cover design.
3.2 CONVENTIONAL COVERS

The conventional cover design for waste containment facilities employs the resistive barrier as a final cover for a landfill. It includes a hydraulic barrier layer to control drainage into the underlying waste. Depending on the type of base liner underlying the waste at the landfill, the barrier layer in a conventional cover may consist of a fine-grained soil having low saturated hydraulic conductivity (compacted fine-textured soil) or a composite barrier consisting of a geomembrane underlain by fine-grained soil. The layer of fine-grained soil (typically 450 mm thick) is compacted to achieve sufficiently low saturated hydraulic conductivity ($<10^{-5}$ or $10^{-7}$ cm/s, depending on the properties of the base liner in the landfill).

Geomembranes are thin sheets of plastic (i.e., polyvinyl chloride or polyethylene, 1-2 mm thick) used to limit infiltration into (cover) or out of (liner) subsurface waste. Geomembranes are not as affected by differential settlement as other materials. They have a high ductility and will deform to some extent without tearing. The main concern with geomembranes is installing them without compromising their integrity by puncture holes or defects in the seams. The seams must be welded together to prevent moisture from penetrating into the underlying layers. Holes or seam defects will increase the effective hydraulic conductivity through the cover.

Alternatively, a geosynthetic clay liner (GCL) may be substituted for the compacted fine-grained soil. It is a thin layer of bentonite (approximately 5 mm) supported by geotextiles and/or geomembranes. GCLs are convenient since they are rolled out at the project site. Overlapping of the seams allows them to be self-sealing upon hydration through expansion of the bentonite clay. A principal concern with GCLs is their long-term stability due to their low interfacial shear strength. The angle of internal friction of bentonite clay is significantly reduced from dry to wet conditions.

In most cases, conventional covers are required to meet material specifications (e.g., a maximum saturated hydraulic conductivity for the barrier layer), but are not subjected to a performance criterion such as a maximum percolation rate.

An important consideration for all of these materials is their long-term ability to limit infiltration into the underlying waste.

Conventional covers that rely solely on a fine-textured soil barrier layer are typically used at sites with a similar liner beneath the waste. The soil barrier layer generally is compacted under conditions that yield low saturated hydraulic conductivity, i.e., with higher compaction water content and compactive effort.
Covers that rely solely on fine-textured soil for the barrier are referred to as compacted, low permeability soil layers. They offer the advantages of low cost, familiarity and material availability. The addition of bentonite to local soil allows these layers to achieve the low saturated hydraulic conductivity that may be required by regulatory agencies.

A variety of studies have suggested that the low hydraulic conductivity of the clay barrier in compacted clay covers can be compromised by wet/dry cycling, freeze/thaw cycling, differential subsidence, and/or biota intrusion. For example, laboratory studies have shown that compacted fine-grained soils crack under volumetric strain caused by desiccation and root development into the layer. This can cause channels of preferential flow that greatly increase the saturated hydraulic conductivity and the drainage rate through the cover. Desiccation cracking of clay barrier layers has been observed in the field, and several studies have attributed changes in drainage from compacted clay covers to preferential flow and changes in the hydraulic conductivity of the clay barrier caused by cracking. For example Montgomery and Parsons (1989) tested two clay covers over four years of monitoring of drainage. They concluded that cracks in the clay barrier layers were responsible for the increase in drainage rate, that the cracks persisted regardless of soil water status of the clay layer, and that the thickness of the surface layer did not affect the drainage rate.

Laboratory studies have shown that the change in the layers follows a drought period during which time the soil water storage decreased monotonically. The amount of drainage, relative to precipitation, increased following the drought, and at the same time, a change in temporal response of drainage to individual precipitation events has been shown. The pattern of the drainage changed from a steady flow, relatively independent of the timing of precipitation prior to the drought, to rapid and intermittent flow closely related to precipitation events after the drought that shows the preferential flow. The influence of drought is also evident in the quantity of drainage resulting from individual precipitation events, in terms of the average daily drainage rate for precipitation events of different size before and after the drought. Greater drainage occurs after the drought for almost all precipitation events and the difference between drainage before and after the drought increased with increasing size of the precipitation event. The sensitivity of the difference in drainage rates before and after the drought may be due to the amount of infiltration stored in the surface layer due to a precipitation event. For small precipitation events, nearly all of the infiltration is
stored in the surface layer, preventing flow into the barrier layer; in contrast, infiltration from larger storms is sufficient to initiate flow into the barrier layer. The post-drought observation suggest also that preferential flow and the increase of the rate of drainage occurs through the barrier layer regardless of the soil water content.

The temporal variation in water content in response to precipitation is more rapid after the drought than before. Post-drought precipitation typically results in an abrupt increase in water content (it suggests that the hydraulic conductivity of the barrier layer increases appreciably post-drought and that it is caused by a dense network of cracks), whereas pre-drought changes in water content were more gradual. Patterns in surface runoff suggest that changes in the soil barrier layer had little effect on the occurrence or quantity of surface flow.

Hydraulic conductivities that have been recorded in some tests show that the hydraulic conductivity of the barrier layer increases a lot, most likely because of the network of cracks in the soil barrier. Therefore desiccation, or weathering in general, causes relatively rapid degradation of soil barriers, and the effectiveness of soil barrier covers as hydraulic barriers can be compromised over a relatively short period of time. Thus, in applications where clay layers are used as hydraulic barrier layers in landfill covers, the design should include features (e.g., an overlying geomembrane) to ensure that the barrier layer will not be adversely affected by weathering.

### 3.3 ALTERNATIVE COVERS

The alternative covers limit the amount of water entering the waste by exploiting the water storage capacity of finer textured soils and the water removal capability of vegetation. Finer textured soil layers are designed to store infiltrating water with minimal drainage during periods of vegetative dormancy or excessive precipitation.

In some cases, layers with contrasting particle size (i.e., coarse vs. fine soil) are used to create a capillary break that enhances the water storage capacity of the finer textured storage layer.

Two kinds of alternative covers are the monolithic barriers and the capillary barriers.

Monolithic barriers are covers comprised primarily of a thick layer of finer textured soil.
Capillary barriers are covers that rely on a capillary break to enhance water storage. Although great emphasis is placed on the soil in alternative covers, the vegetation plays an equally vital role because the plants remove the stored water and return it to the atmosphere. All available soil water should be removed by the end of the growing season so that the reservoir for soil water storage has sufficient capacity to store infiltration during the subsequent period of vegetative dormancy.

3.4 CAPILLARY BARRIERS

The cover that has been planned for the final confinement of disposal cells in El Cabril and the two pilot covers are multilayer covers based on the capillary barrier concepts. Traditionally, capillary barriers have been studied for covers of urban and industrial landfills, with the aim of diverting water flows and isolating the materials (Stormont and Morris, 1998). Also they have been studied to investigate the effects of heterogeneity and anisotropy (Stormont, 1995; Ho and Webb, 1998) and to see the influence of geometry on their effectiveness. Earthen covers employing capillary barriers can be effective in minimizing percolation into underlying waste or contaminated soil in semiarid and arid regions due to the high evaporation rate. They can be constructed in various forms, ranging from a simple design consisting of two layers of contrasting particle size to more complex design with multiple layers of fine-grained and coarser-grained soils (Stormont 1995). In its basic form a capillary barrier consist of an unsaturated finer-grained layer overlaying unsaturated coarser-grained layer. The contrast in unsaturated hydraulic properties between the finer and coarser-grained layers restricts movement of water across the interface between the layers and forms the hydraulic impedance that limits downward water movement. Data in Stormont and Anderson (1999) show that significant amounts of water will enter the coarser soil only when the matric suction at the surface of the coarser layer decreases to the value near the bend in the soil water characteristic curve near residual water content (noted as $B_c$ in Fig 3.1). This value is the water entry pressure of the coarse layer where the corresponding matric suction is $\Psi_b$ and the volumetric water content in the coarser layer is $\theta_{BC}$. 
Continuity in the pore water pressure requires that the matric suction in the two layers must be equal at their interface. As a result, the matric suction in the finer layer at the interface is $\Psi_b$ before that the water will enter the coarser layer. The water content in the finer layer at $\Psi_b$ is noted as $\theta_{BF}$ (Fig. 3.1) and it corresponds to point $B_F$ on the soil water characteristic curve for the finer layer. Even when $B_F$ is reached, water still enters the coarser-grained layer slowly because the hydraulic conductivity of the coarser-grained layer is still low at $B_c$ (Fig. 3.2).

**Figure 3.1**: Soil Water Characteristic Curves (SWCC)

**Figure 3.2**: Unsaturated Hydraulic Conductivity functions for finer- and coarser- grained soils
The hydraulic impedance provided by the capillary interface causes the finer surface layer to act as a buffer that stores infiltrated water as soil water storage ($S_w$) until $\theta_{BF}$ is reached.

The soil water characteristic curves (SWCCs) and the hydraulic conductivity curves [Figs. 3.1, 3.2 respectively] are described in terms of the van Genuchten and van Genuchten-Mualem functions (Mualem 1976; van Genuchten 1980). The Figures 3.1 and 3.2 show that the matric suction in soil is a function of moisture content and that at most values of matric suction, the hydraulic conductivity of the coarse soil is negligible compared to that of the fine soil.

If the matric suction is large enough, (i.e., water content less than saturation) the moisture in the fine layer will be limited from entering the coarse layer.

Much of the stored water in the finer-grained layer is later released back to the atmosphere via evapotranspiration (ET). Alternatively, the water may be diverted via lateral drainage (L) in capillary barriers employing drainage layers. If the storage capacity of the finer-grained layer is adequate and sufficient evapotranspiration or lateral drainage exists to remove the stored water, percolation into the underlying waste can be reduced to a small quantity (Ward and Gee 1997).

When relying only on soil water storage to design a two-layer capillary barrier, layer thicknesses and unsaturated hydraulic properties are manipulated to obtain a design that has adequate soil water storage capacity so that an acceptable percolation rate is obtained.

Water balance simulation were conducted to assess how layer thicknesses, unsaturated hydraulic properties, and climate affect the performance of capillary barriers (Milind V. Khire, Craig H. Benson, and Peter J. Bosscher(2000)). The thickness, the hydraulic properties of the surface layer and the climate significantly affect the water balance of capillary barriers.

The critical meteorological conditions for a capillary barrier are site dependent; they generally occur when precipitation ($P_r$) is more frequent during periods of low potential evapotranspiration (ET). Flow into the coarser layer occurs after a sustained period when $P_r$ equaled or exceeded ET (i.e., $ET - P_r \leq 0$).

In many cases, the critical period is in winter, when potential evapotranspiration is low and more frequent and less intense storms occur. Such storms generate less runoff and more infiltration into the surface layer. These conditions generally result in accumulation of water in the surface layer and breakthrough across the interface between the finer and coarser layers if the soil water storage capacity of the surface layer is exceeded.
Snowfall also occurs during winter, and inundation by snowmelt during winter can overwhelm the soil water storage capacity of the finer-grained layer, resulting in percolation (e.g., Khire et al. 1999). Field studies (Hakonson et al. 1994, Gee et al. 1993, Ward and Gee 1997, Khire et al. 1999) have illustrated the importance of snowmelt and it has been shown that large snowmelt events resulted in substantial infiltration, higher than expected soil water storage, and greater than anticipated percolation.

Greater soil water storage capacity is required at sites where the season with more frequent and less intense precipitation does not coincide with the season having highest evapotranspiration.

Water balance predictions have been conducted for capillary barriers at Wenatchee having finer-grained surface layers (SM: silty sand) 15, 30, 45, and 60 cm thick and an underlying coarser-grained layer (SP: uniformly graded medium sand) 75 cm thick (Milind V. Khire, Craig H. Benson, and Peter J. Bosscher, 2000). Percolation decreases as the thickness of the surface layer increases because the soil-water storage capacity of the surface layer becomes larger, which allows the surface layer to store more water for a longer period of time without drainage to the underlying layer. Increasing the surface layer thickness from 15 to 30 cm results in a reduction in percolation from the base of the cover from. Increasing the surface layer to 45 or 60 cm reduces percolation to a very small quantity. When the surface layer is thicker, the soil water storage curve has a higher peak and greater breadth. The larger and more prolonged soil water storage provided by the thicker finer-grained surface layer also permits a greater quantity of water to be removed by evapotranspiration (increasing the thickness of the finer layer increase the evapotranspiration). An adequate surface layer thicknesses should be checked using suitable long-term simulations performed with meteorological data representing the most stressful conditions that the cover is likely to endure. In addition, surface layers must not be made too thick, or long-term accumulation of water and percolation may occur if deep rooted vegetation is not present.

Moreover percolation increases when the thickness of the coarser-grained layer decreases, but the increase in percolation is small. Also the onset of percolation occurs slightly earlier when the coarser layer is thinner. Decreasing the thickness of the coarser layer has a much smaller effect than reducing the thickness of the finer-grained layer because coarser materials drain readily, and thus a thicker coarser layer provides little additional storage capacity.
Other important element that influences the percolation in the capillary barrier are the hydraulic properties.

Percolation decrease reducing the saturated hydraulic conductivity of the finer-grained surface layer. Consequently, the infiltration capacity is smaller and more runoff occurs; soil water storage fluctuates less which is consistent with the increase in runoff associated and the evaporation is also smaller, because less water is available. Because less water enters these soils, there is also additional unused soil water storage capacity in the finer layer. Consequently, more severe precipitation conditions (e.g., heavier storms or more prolonged periods of rainfall or snowmelt) can be handled without percolation when these soils are employed. Preferential flow may occur during heavy rains or during snowmelt due to desiccation cracking of the finer layer.

The saturated hydraulic conductivity of the finer layer increases after it undergoes several wetting and drying cycles.

The formation of cracks and the corresponding increase in saturated hydraulic conductivity would probably outweigh the advantages of using a surface layer with a very low saturated hydraulic conductivity (like CL: lean clay). Better performance is likely to be obtained with soil that is resistant to desiccation cracking, such as the SM (silty sand), SMML (non plastic sandy silt), or ML (low plasticity silt). In addition, even without cracking of the CL soil, the ML and SM-ML soils yield nearly the same low percolation. These soils are also more suitable for vegetation, but can be more susceptible to erosion.

Care must be used when selecting surface layer soils. Soils should be selected that are resistant to desiccation cracking and erosion and are suitable for vegetation. Silts, silty sands, sandy silts, and clayey sands are likely to be suitable surface layer soils.

As we have already seen, the thickness of the coarser layer is less important than that of the finer layer, but the hydraulic properties of the coarser layer affect the storage capacity of the finer layer and percolation from the cover. Clean sands and gravels are suitable soils for the coarser-grained layer, and in most cases a 30 cm thick coarser layer should be adequate.

Vegetation has also an important role in the performance of capillary barriers, because vegetation is largely responsible for water removal from the barrier. Alternatively, the water may be diverted via lateral drainage (L) in capillary barriers employing drainage layers.

Lateral drainage may occur if the fine/coarse interface is sloped since an unsloped barrier does not divert water. This inclination introduces a gravity
force on the moisture which will help drive it in the down dip direction of the slope. The moisture content increases in the down dip direction, which keeps the soil in the up-dip portion of the interface far from reaching the saturation. The diversion length is defined as the length of interface in the down-dip direction until breakthrough occurs and it depends on the infiltration rate and the material properties. For capillary barriers to be effective at laterally diverting water over distances needed for many cover applications, designs are needed to increase diversion lengths. The diversion length of a capillary barrier is increased with the introduction of an hydraulic transport layer which is a well-sorted sand layer immediately above the fine/coarse interface. It may give to the capillary barrier an acceptable diversion length required to cover a subsurface waste containment facility. The transport layer has a greater hydraulic conductivity than the fine layer at near saturation conditions and when the moisture accumulates in the fine layer, the increased hydraulic conductivity of the transport layer helps to laterally divert the moisture in the down-dip direction.
4 - EVAPORATION TESTS ON THE TOPSOIL OF THE COVER

4.1 INTRODUCTION

A specific knowledge of the thermal, hydraulic and mechanical properties of all the materials of the pilot covers is useful to interpret and model adequately the results of the monitored parameters. The aim of the thesis focuses on the analysis of the superficial layer, the topsoil, that is the most critical layer. There are some parameters of this layer that are unknown and so in this thesis there is a modeling, in Code Bright, of a sample of the topsoil used for the pilot cover. In order to calibrate this parameters the results of the model have been compared with some data that have been measured by CIEMAT (M.V. Villar & F.J. Romero, 2012) in the laboratory on a soil sample of 14cm of the vegetal layer. Comparing these results we will be able to obtain the unknown parameters and have a characterization of the vegetal soil to model the entire cover during all the time that we need, checking if it guarantees the requirements.

In order to have a characterization of the materials of the cover, CIEMAT (M.V. Villar et al. 2012) realized some evaporation tests with these materials that have been prepared with initial conditions similar of those of the cover of the pilot tests of El Cabril. The evaporation tests are useful to obtain the relative permeability of the material if you know his retention curve. With this purpose an evaporation test with a column of compacted topsoil (vegetal layer) of the pilot cover of El Cabril has been realized.

4.2 THE MATERIAL

The material known as "vegetal soil with gravel" is a mixture of soil and gravel with a ratio of 60/40. The soil comes from the excavation realized in the cell 29 and the gravel is with a diameter between 50 and 150mm, with less than 25% of diameter which is lower than 125mm. For the installation of the cover, the mixture has been compacted with the 95% of the Modified Proctor Test, the dry density measured in situ is 1,7-1,9 g/cm³ and the humidity is between 5 and 8%. In March 2010 CIEMAT picked up 13 Kg of the topsoil of the material stored in El Cabril and they used this material for the laboratory tests. Before using this material in the laboratory, they removed, by sieving, the part with a dimension greater than 2 mm which is the 53 % of the material.
The mineralogical components of the topsoil are quartz (75%), phyllosilicates (15%), plagioclase (9%) and dolomite/ankerite (1%).

CIEMAT realized the characterization of the material and some of the results that they reached (Tab. 4.1) are the hygroscopic humidity (w), the particle size and the specific weight of the solid part (Gs).

<table>
<thead>
<tr>
<th>w (%)</th>
<th>Gs (a)</th>
<th>Gs (b)</th>
<th>Sand (%)</th>
<th>Silt (%)</th>
<th>Clay (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,3</td>
<td>2,68</td>
<td>2,67</td>
<td>56</td>
<td>36</td>
<td>7</td>
</tr>
</tbody>
</table>

**Tab 4.1:** Properties of the vegetal soil (a) Norma UNE 103-302-94, (b) helium pycnometer

According to the Unified Soil Classification System of the ASTM (American Section of the International Association for Testing Materials), which considers the data of the particle size distribution with the plasticity tests of the fine fraction, the topsoil of the evaporation test in the laboratory is a silty sand (SM).

![Figure 4.1: Particle size distribution of the vegetal soil before of its preparation for the laboratory test (pilot cover) and after that the fraction greater than 2mm is eliminated (laboratory)](image)

The saturated permeability of the vegetal soil of the pilot tests is \(3,5\times10^{-8}\) m/s (so the intrinsic permeability of the vegetal soil of the pilot is \(K_{\text{int}}=10^{-7}\times K_{\text{sat}}=3,5\times10^{-15}\) m²) and the water retention curve (WRC) obtained with different methods is shown in Fig. 4.2.

Instead in Fig. 4.3 there are the results of the relation between the suction and the saturation grade with its fit to the expression of Van Genuchten (1980):
Where:

- \( S_e \): is the effective degree of saturation \((0 \leq S_e \leq 1)\);
- \( P \): is a parameter of the material which is in related with the air entry value (MPa);
- \( \lambda \): is a parameter that controls the shape of the Water Retention Curve;
- \( P_g - P_l \): is the suction (MPa);
- \( S_{rl} \): is the residual degree of saturation;
- \( S_{ls} \): is the maximum degree of saturation.

In order to fit the curve M.V. Villar et al. have considered that the \( S_{rl} = 0 \) and \( S_{ls} = 1 \). The parameters that they have obtained are shown in Tab. 4.2.

\[
S_e = \frac{S_l - S_{rl}}{S_{ls} - S_{rl}} = \left(1 + \left(\frac{P_g - P_l}{P}\right)^{\frac{1}{1-\lambda}}\right)^{-\lambda}
\]  

\( (4.1) \)

Figure 4.2: Water Retention Curve (WRC) of the compacted soil with an initial \( \rho_d = 1.8 \) g/cm³. Matric suction for the points obtained in membrane cells (following the paths) and with filter paper, total suction for the sample in laboratory condition (Villar 2011)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Wet</th>
<th>Drying</th>
</tr>
</thead>
<tbody>
<tr>
<td>( P ) (MPa)</td>
<td>0.01</td>
<td>0.29</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>0.17</td>
<td>0.29</td>
</tr>
</tbody>
</table>

Tab. 4.2: Parameters for the Van Genuchten’s expression of the retention curve of the vegetal soil
4.3 THE EVAPORATION TEST AND HIS RESULTS

An evaporation test has been realized with the compacted topsoil of the cover. For the column of the test of evaporation, the vegetal soil was mixed with deionized water in order to obtain a gravimetric humidity of 4% and it was left to stabilize for 40 days (the humidity should have been greater to be like that of the pilot cover). The mixture was compacted in a cylinder of methacrylate with an inner diameter of 7.9 cm in 3 tiers resulting in an height of 14 cm (Fig 4.4). Previously at the wall of the cylinder of methacrylate have been realized 5 perforations with the diameter of 1 cm at different heights. After that the soil was compacted it was perforated through the perforations of the cylinder to insert the sensors, that penetrated the clay for 3.9 cm. The contact between the sensors and the methacrylate was sealed with silicone.

They used five sensors Sensirion SHT75 of relative humidity (HR) and temperature (T). These sensors have an accuracy of 2% for the HR in the rank between 20 and 80 %. There was also a sensor at 12 cm on the top of the column to record the changes in the environmental conditions. The upper part of the column was in contact with the atmosphere in order to have the evaporation of the water. The column was placed on a balance to record the mass changes during the evaporation process (Fig 4.5).
Periodically the measurement of the sensors and of the balance were recorded with an automatic system of data acquisition.

At the beginning of the test the dry density and the humidity of the column were 1.82 g/cm$^3$ and 4%. The average relative humidity recorded, with the sensors inside the column, before the beginning of the evaporation was 96.6±0.1%, corresponding to a suction of 4.7±0.1 MPa. The values of the relative humidity recorded for the sensors during the test are shown in Fig. 4.6 and it is shown a
gradual decrease that is greater at the beginning in the sensors closest to the surface. This sensors (1 and 2) are the most affected by the oscillations of the relative humidity and the temperature of the laboratory, instead the sensors at the bottom (4 and 5) show an evolution of the relative humidity that is not affected by the atmospheric changes.

![Graph showing the evolution of relative humidity](image)

**Fig. 4.6:** Evolution of the HR in the column during the evaporation test (HR1 at 1cm from the surface of the column, HR2 at 3cm, HR3 at 6cm, HR4 at 9cm, HR5 at 12cm, HRamb above the column)

The measurements of the relative humidity and temperature obtained by the sensors were converted to suction (Fig. 4.7) by the psychrometric law:

\[
HR = \exp \left( \frac{-M^w \ast (P_g - P_l)}{R \ast T \ast \rho_l} \right) \quad (4.2)
\]

where:
- \(M^w\): molecular weight of water (0.018 kg/mol);
- \(R\): ideal gas constant (8.3143 J/(mol*K));
- \(P_g, P_l\): gas and liquid pressure (Pa);
- \(T\): temperature in K;
- \(\rho_l\): liquid density (= 1000 Kg/m^3)

At the end of the test all the sensors (unless the 4) recorded values of the relative humidity which are like the values of the environment; it shows that nearly all the water had evaporated.
Fig. 4.7: Evolution of the suction in the column during the evaporation test (s1 at 1cm from the surface of the column, s2 at 3cm, s3 at 6cm, s4 at 9cm, s5 at 12cm, samb above the column)

Fig. 4.8: Evolution of the rate of evaporation during the test

In the Fig.4.8 M.V. Villar et al. represented the values of the suction along the column for different times during the evaporation test.
They have also recorded the changes of mass of the column during the evaporation test and it is greater in the first 3500 hours and then it changes more slowly coinciding with a period of oscillation of the temperature in the
laboratory (Fig.4.9). At the end of the evaporation test in the laboratory there is a loss of water (change of the weight of the column) of 33.2 g.

![Graph](Image)

**Fig. 4.9:** Change of the mass of the column (blue line) and evolution of the temperature of the laboratory during the evaporation test

The test started the 9th of June 2011 (but the evaporation started three days later) and lasted 312 days. At the end of the test the sensors and the column have been removed from the cylinder (Fig. 4.10). When the column was out it was cut in five parts with 2.8 cm of thickness and in each part the dry density (though immersion in mercury) and the gravimetric humidity (drying by heater at 110°C for 24h) has been calculated. The gravimetric humidity is: \( \frac{W_w - W_d}{W_d} \times 100 \); where \( W_w \) is the weight of the sample wet and \( W_d \) is the weight of the sample dry.

The values obtained are indicated in the Tab 4.3 and in the Fig 4.11 with the final values of relative humidity recorded by the sensors.

The final average humidity along the column was 1.3±0.1%, the average dry density 1.82±0.02 g/cm\(^3\) and the final HR measured by the sensors was 39±7%, corrsponding to a suction of 127±23 MPa. Even if the gravimetric and relative humidity increase slightly at the bottom, all the values are in a very small range.

The average dry density at the end of the test is the same of the beginning (after that the column was compacted) because during the test there wasn't changes of dimensions (dry density=\( \rho_d = \gamma_d / g = W_d (V \times g) \)).
Fig. 4.10: Column at the end of the test

The dry density of the sample number 4 is greater than that of the other parts of the column and greater than the average dry density at the beginning of the test; instead the gravimetric humidity of the part 4 is like that of the other parts. This section corresponds to the area of contact between the first two tiers of fabrication and the greater density could be due to the greater energy of compaction that could have been applied at the surface of the first level (Fig.4.4). The greater value of the dry density and the normal value of the gravimetric humidity in the part 4 could explain the abnormal greater value of the relative humidity recorded in the sensor 4 at the end of the test, considering that the degree of saturation is greater in this part.
Fig. 4.11: Gravimetric humidity and dry density measured in the five parts at the end of the evaporation test and the last values of HR recorded by the sensors.

Fig. 4.12: WRC shown in Fig. 4.2 modified with the initial and final values obtained in the evaporation test.

At the end of the test the gravimetric humidity is similar to the hygroscopic humidity measured before for the loose material and it is similar to the final humidity after a drying process of a block compacted like the pilot cover in contact with the atmosphere until the stabilization. It confirms that the maximum evaporation was reached during the test.

With the measurements of the sensors at the beginning and at the end of the evaporation test M.V. Villar et al. obtained the total suction that can be related...
with the initial and final average humidity. In this way there are other two point
in the WRC (Fig 4.12).
CIEMAT obtained in the laboratory also the volume of void that is 215 cm$^3$ and
so the porosity of the sample is 0.32 (considering that the volume of the column
is 686 cm$^3$).
During the evaporation process the water leaves the column as vapour only at
the top of the column due to the difference of the relative humidity and
temperature between the sample and the laboratory.
The values and the graphs obtained in the evaporation test and with the other
methods are useful to improve the characterization of the sample and to start the
modeling of the sample in Code Bright.
5 - MODELING OF THE SAMPLE

5.1 CODE BRIGHT

The aim of the thesis focuses on the analysis of the topsoil of the pilot cover. Simulation of evaporation tests have been carried out in order to characterize better the properties of the vegetal soil of the El Cabril Radioactive Waste Disposal Facility and the evaporation process. The results of the laboratory (obtained by CIEMAT, Villar et al. 2012) are useful to obtain a good model of the sample that has been analyzed with a one-dimensional numerical modeling. The sample of 14 cm of topsoil (the same that has been studied in the laboratory by CIEMAT) has been modeled by Code Bright and a calibration of the parameters of the constitutive laws and of the boundary conditions has been obtained. The numerical modeling shows the interaction between liquid, gas and heat flows in a soil under evaporation conditions.

Code Bright, which stands for COupled DEformation, BRIne, Gas and Heat Transport problems, is a tool designed to handle coupled problems in geological media. In porous media, subjected to thermal, hydraulic and mechanical conditions relevant thermo-hydro-mechanical (THM) phenomena takes place. In fact, there exist a number of mutual interactions that must be taken simultaneously into account in analyses. The program has been created for modeling THM processes in a coupled way in a geological media. In this thesis there is a modeling of the sample considering only the thermo-hydraulic problem (we are not considering the displacement and the solute phase).

The program CODE_BRIGHT uses the finite element method to solve the coupled equations presented above. The main features of the numerical approach are:

- Linear interpolation functions on segments, triangles, quadrilaterals, tetrahedrons, triangular prisms and quadrilateral prisms. Analytical integration is used for segments, triangles and tetrahedrons. Numerical integration is used for quadrilateral, arbitrary triangular prisms and quadrilateral prisms;
- Finite differences and implicit scheme are used for time integration;
• Newton-Raphson method for solution of the non-linear system of algebraic equations that results once the space and time discretizations are applied;
• LU decomposition and backsubstitution (non-symmetric matrix) or conjugate gradients squared to solve the system of linear equations that result from the Newton-Raphson application (in this thesis has been used the first one);
• Automatic discretization of time. Increase or reduction of time increment according to convergence conditions or output requirements.

5.2 CONCEPTUAL MODEL

The theoretical approach consists of a set of governing equations, a set of constitutive laws and a special computational approach.

The equations that govern this problem can be categorized into four main groups. These are: balance equations, constitutive equations, equilibrium relationships and definition constraints.

The balance equations that have been considered in this modeling are:

• balance of water mass for the variable liquid pressure $P_l$,
• balance of air mass for the variable gas pressure $P_g$,
• balance of internal energy for the variable temperature $T$,

In the mass and energy balance equations the following terms may be distinguished:

• storage terms (represent the variation of mass or energy content);
• advective fluxes (caused by motion of fluids computed using Darcy's law);
• non advective fluxes (computed through Fick's law, are proportional to gradients of mass fractions which do not belong to the set of unknowns);
• sink/source terms

The conceptual model is based on considering the column of topsoil as a unsaturated porous medium formed for 3 phases. The solid phase has only the soil component, the gas phase is formed by two components, dry air and air vapor, and the liquid phase consists of water and dissolved air.

The other information about the model are about the constitutive laws and the boundary conditions that characterize the sample.
The model is one-dimensional in a vertical direction, without axisymmetry and the sample is composed of only one material. The simulated time of the evaporation test lasts 309 days and the values obtained by the modeling are the evolution of some parameters along the sample and during all the time of the experiment. These parameters are:

- $P_g$: gas pressure (MPa);
- $P_l$: liquid pressure (MPa);
- $T$: temperature ($^\circ$C);
- $\rho_g$: gas density (kg/m$^3$);
- $\rho_l$: liquid density (kg/m$^3$);
- $\omega_l^a$: air mass fraction in liquid phase (considering that $\omega_l^w + \omega_l^a = 1$, but $\omega_l^a$ is neglected and so $\omega_l^w = 1$);
- $\omega_g^w$: water mass fraction in gas phase;
- $q_g$: advective gas flux of the vapour (m/s)
- $q_l$: advective liquid flux of water (m/s)
- $i_c$: conductive heat flux (J/s)
- boundary flows

### 5.2.1 MASS BALANCE OF WATER

The thermohydraulic model focuses on the mass balance of water (liquid water and vapour) and air (dissolved in water and in the gas phase) in terms of pressure, and the energy balance in terms of temperature. Water is present in liquid and gas phase. The mass balance of water in liquid and in the gas phase is expressed as:

$$\frac{\partial}{\partial t} (\omega_g^w \ast \rho_g \ast S_g \ast \phi) + \nabla (j_g^w) = f_{\text{evaporation}} + f^w \quad (5.1)$$

$$\frac{\partial}{\partial t} (\omega_l^w \ast \rho_l \ast S_l \ast \phi) + \nabla (j_l^w) = f_{\text{condensation}} + f^w \quad (5.2)$$

where $f^w$ is an external supply of water and the internal source terms that represent phase change are:

$$f_{\text{evaporation}} + f_{\text{condensation}} = 0 \quad (5.3)$$

Adding the two mass balance equation leads to the equation of the total mass balance of water that Code Bright solves:
\[
\frac{\partial}{\partial t} \left( \omega_l^w \rho_l S_l \phi + \omega_g^w \rho_g S_g \phi \right) + \nabla \left( j_l^w + j_g^w \right) = f^w \quad (5.4)
\]

where subscripts \( l \) and \( g \) refer to liquid and gas phase and superscript \( w \) to water.

- \( \omega \) is the mass fraction \((\text{kg/kg}^{-1})\) of a component in a phase;
- \( \rho \) is the density \((\text{kg/m}^3)\) of a phase;
- \( S_l \) is the hydraulic saturation of water in liquid phase \((\text{m}^3\text{m}^{-3})\);
- \( S_g \) is the hydraulic saturation of water in gas phase \((\text{m}^3\text{m}^{-3})\) \((S_g = 1 - S_l)\);
- \( \phi \) is the porosity \((\text{m}^3\text{m}^{-3})\);
- \( j \) \((\text{kg m}^{-2} \text{s}^{-1})\) is the total flux (advective, diffusive and dispersive);
- \( f^w \) is an external source/sink term \((\text{kg m}^{-3} \text{s}^{-1})\).

The first two terms in the equation represent the change of mass of water (during the 309 days of the experiment) in the liquid and gas phase respectively and the third and fourth terms represent the fluxes of water in liquid and gas phase respectively.

A state variable is associated with each mass balance and in the water mass balance it is the liquid pressure \( P_l \).

The final objective is to find the state variable from the governing equations. Therefore, the dependent variables will have to be related to the unknowns in some way.

Constitutive laws must be used to express the mass balance equation as a function of the state variables.

### 5.2.2 ENERGY MASS BALANCE

The thermohydraulic model focuses on the mass balance of water (liquid water and vapour) and air (dissolved in water and in the gas phase) in terms of pressure, and the energy balance in terms of temperature.

The equation for internal energy balance for the porous medium is established taking into account the internal energy in each phase \((E_l, E_g, E_s)\). The equation of energy mass balance that Code Bright solves is written as:

\[
\frac{\partial}{\partial t} \left( E_l \rho_l S_l \phi + E_g \rho_g S_g \phi + E_s \rho_s (1 - \phi) \right) + \nabla \left( i_c + j_{adv,l} + j_{adv,g} \right) = f^Q \quad (5.5)
\]
where subscripts \( l, g, \) and \( s \) refer to liquid, gas and solid phase and superscript \( w \) to water:

The internal energy in each phase can be calculated as a function of internal energy of each component. About the liquid phase \( \omega_l^a \) (air fraction in liquid phase) is neglected and so \( \omega_l^w = 1 \).

- \( E_l = C_w^*T \) where \( C_w \) is the specific heat of liquid water (J/kg/°C) and \( E_l \) is the specific internal energy of liquid water (J/kg);
- \( E_g = E_g^w * \omega_g^w + E_g^a * \omega_g^a \) considering that \( \omega_g^w + \omega_g^a = 1 \);
- \( E_s = C_s^*T \), where \( C_s \) is the specific heat of the soil (J/kg/°C) and \( E_s \) is the specific internal energy of the soil (J/kg);
- \( i_c \) is the energy flux (J*m\(^{-2}\)*s\(^{-1}\)) owing to conduction through the porous medium;
- \( j_{adv, l} \) and \( j_{adv, g} \) (J*m\(^{-2}\)*s\(^{-1}\)) are the advective heat fluxes of energy caused by mass motion of every species in the medium;
- \( f^O \) is an internal and external supply (J*m\(^{-3}\)*s\(^{-1}\)) that accounts for boundary condition at the top (e.g. heat entry from a lamp) and at the laterals (i.e. heat entrance through column walls).

The firsts three terms in the equation represent the change in energy (during the 309 days of the experiment) in the liquid, gas and solid phase respectively and the fourth and fifth terms represent the fluxes of heat.

The advective heat flux (\( j_{adv, l} \)) caused by liquid water motion is expressed by this law:

\[
j_{adv, l} = C_w * j_{liq} * T \quad [J/m^2/s] \quad (5.6)
\]

where:

- \( C_w \) is the specific heat of the liquid water (4180 J/(kg*°C));
- \( T \) is the temperature in °C;
- \( j_{liq} \) is the liquid flux: \( \rho_l^*q_l \) (kg/(m\(^2\)*s))

The advective heat flux (\( j_{adv, g} \)) caused by advective and diffusive vapour motion is expressed by this law:

\[
j_{adv, g} = \left( q_g * \rho_g * \omega_g^w + j_g^w \right) * E_g^w \quad [J/m^2/s] \quad (5.7)
\]

where:
• $q_g * p_g * \omega_g^w$ is the advective vapour flux (kg/m$^2$/s);
• $i_g^w$ is the diffusive vapour flux (kg/m$^2$/s);
• $E_g^w$ is the specific internal energy of water in gas phase per unit mass of water:

$$E_g^w = L + C_v * T \quad (5.8)$$

where:

• L is the vaporization latent heat (2.5*10$^6$ J/kg);
• $C_v$ is the specific heat of water in gas phase

$$C_v = (1900 - (R/M^w)) \quad (5.9)$$

• $M^w$: molecular mass of water (0.018 kg/mol);
• R: ideal gas constant (8.3143 J/(mol*K));

Associated to each mass balance there is a variable, i.e. the unknown that is obtained by solving the corresponding equation and in the energy mass balance it is the temperature T.

**5.2.3 HYDRAULIC CONSTITUTIVE LAWS**

The constitutive equations establish the link between the independent variables (or unknowns) and the dependent variables.

The fig 5.1 displays all the parameters of the constitutive laws of the material. The Water Retention Curve that has been used is the modified equation of Van Genuchten which represents in a good way the behavior of the sample considering also the saturation below the residual saturation. The assumption is that the soil can reach full drying, i.e. if evaporation takes place near the surface under a dry or hot atmosphere (Ross et al., 1991).

This equation is a modification of the expression of Van Genuchten (eq. 4.1) where:

$$S_e = \frac{(S_l - S_i)}{(1 - S_i)} \quad (5.10)$$

In order to extend this curve for high suctions (i.e. conditions of drying by evaporation) and to represent the oven dry branch that goes from the residual saturation to the oven dryness, the minimum degree of saturation is expressed as follow:
where there are three parameters: \( \alpha, S^0 \) and \( P_{c,dry} \).

The latter can be identified with the capillary pressure for the dry material and can be considered equal to \( P_{c,dry} = 1000 \text{MPa} \). However, lower values may be considered if dryness is induced by atmospheric condition that are less extreme than oven dryness \( (P_{c,dry} = 400 \text{MPa}) \).

\( S^0 \) is the residual saturation for which liquid water becomes discontinuous so that liquid permeability is zero.

Parameter \( \alpha \) scales the transition from the Van Genuchten branch to the oven dry branch of the proposed retention curve. Its value may be chosen as:

\[
\alpha = \frac{1}{\ln\left(\frac{P_{c,dry}}{P_c^o}\right)} \quad (5.12)
\]

where \( P_c^o \) is the capillary pressure for which the oven dry branch crosses \( S^0 \) (i.e. \( S^0 = S_i \)). It shouldn't be chosen smaller than \( P_o \) and not very large. It has been adopted \( P_c^o = 0.8 \text{ MPa} \), for which \( \alpha = 0.16 \).

Another constitutive law is about the intrinsic permeability:

\[
(K_i = \frac{\mu_l}{(g * \rho_l)} * K_{sat} = 10^{-7} K_{sat}) \quad (5.13)
\]

The intrinsic permeability \((\text{m}^2)\) is different from the relative permeability \((\text{m/s})\) because depends only on the dimension and position of the pores; instead the relative permeability depends on the degree of saturation of the soil.

The advective flux of a phase \((\alpha)\) (liquid \((l)\) or gas \((g)\)) is calculated with the Darcy's law \((\text{m/s})\):

\[
q_\alpha = -\frac{k_i * k_{r\alpha}}{\mu_\alpha} (\nabla \rho_\alpha - \rho_\alpha * g) \quad (5.14)
\]

where:

- \( \mu_\alpha \) is the viscosity of the phase
- \( k_{r\alpha} \) is the relative permeability of the phase.

The porosity of the sample is constant during the evaporation test and so the intrinsic permeability doesn't change:

\[
K_i = K_0 = \text{const.} \quad (5.15)
\]
The molecular diffusion of the vapour has been expressed by the Fick's law and the value of the coefficient of tortuosity ($\tau_o$) that has been calibrated is 0.7:

$$i_{g}^w = -\left(\tau \phi \rho_g S_g D_m^w * 1\right) \nabla \omega_g^w$$  \hspace{1cm} (5.16)

where:

- $D_m^w = \tau D \left(\frac{273.15 + T}{P_g}\right)^n$ is the molecular diffusion coefficient of vapour (m$^2$/s$^{-1}$);
- $\tau = \tau_o (S_g)^m$;
- $D$= diffusion coefficient (m$^2$s$^{-1}$K$^{-n}$Pa);
- $n$ is a parameter of the molecular diffusion;
- $m$ is the power for tortuosity function of saturation;
- $S_g$ is the degree of saturation of the gas phase (1-$S_l$);
- $\omega_g^w$ is the water mass fraction in gas phase;
- $\tau$ is the tortuosity, a constant that takes into account that in a porous medium the path of diffusion is longer than that in a pure gas.

The non-adveective flux of a species in a phase is composed by molecular diffusion and mechanical dispersion.

Mechanical dispersion mass flux is computed by means Fick's law written as:

$$i_t^a = -\left(\rho_a D'_{\alpha} \right) \nabla \omega_t^a$$  \hspace{1cm} (5.17)

where the mechanical dispersion tensor $D'_{\alpha}$ is in function of the longitudinal and transversal dispersivity ($D'_{\alpha} = v_{\alpha} *$dispersivity)

For the liquid phase relative permeability we assume that the distribution of liquid phase only depends on saturation. Therefore it is expressed with the model of Mualem-Van Genuchten:

$$k_{rl} = \sqrt{S_e \left(1 - \left(1 - S_e^{1/\lambda}\right)^\lambda\right)^2} \quad \text{if } S_l > S^o$$

and  $k_{rl} = 0$ if $S_l \leq S^o$  \hspace{1cm} (5.18)

where $S_e = (S_l - S^o)/(1 - S^o)$

and:

- $k_{rl}$ is the relative permeability of the liquid phase;
- $S_e$ is the effective degree of saturation for permeability.
The water mass fraction in gas phase is:

\[ \omega_g^w = \frac{P_{v,sat} \cdot M_w \cdot HR}{R \cdot \rho_g \cdot (T + 273.15)} \]  \hspace{1cm} (5.19)

where:

- \( M_w \): molecular weight of water (0.018 kg/mol);
- \( R \): ideal gas constant (8.3143 J/(mol*K));
- \( T \): temperature in °C;
- \( \rho_g \): gas density (1.12 Kg/m³);
- \( HR \) is the relative humidity measured in the laboratory
- \( P_{v,sat} \) is the vapour pressure at saturation (\( HR = P_v/P_{v,sat} \)) obtained considering the Psychrometric law:

\[ P_{v,sat} = 136075 \cdot \exp\left(\frac{-5239.7}{273.15 + T}\right) \]  \hspace{1cm} (5.20)

Note that a change in the temperature (T), at constant values of relative humidity, causes a change in the vapour pressure at saturation (\( P_{v,sat} \)) and so also in the water mass fraction (\( \omega_g^w \)) and in the diffusive vapour flux (\( i_g^w \)).

5.2.4 THERMAL CONSTITUTIVE LAWS

In heat transfer, conduction (or heat conduction) is the transfer of heat energy by microscopic diffusion and collisions of particles or quasi-particles within a body due to a temperature gradient. They transfer microscopically disorganized kinetic and potential energy, which are jointly known as internal energy. Conduction can only take place within an object or material, or between two objects that are in direct or indirect contact with each other. Conduction takes place in all forms of ponderable matter, such as solids, liquids and gases.

The conductive heat determines a spontaneously flows from a body at a higher temperature to a body at a lower temperature. In the absence of external drivers, temperature differences decay over time, and the bodies approach thermal equilibrium. This thermal equilibrium has been shown in the paragraph 6.4 (evolution of the temperature) where the temperature in all the sample reaches the same temperature of the laboratory.

The law of heat conduction, also known as Fourier's law, states that the time rate of heat transfer through a material is proportional to the negative gradient in the temperature.
The conductive flux of heat \( (i_c) \), expressed by the Fourier's law, is:

\[
    i_c = -\lambda \nabla T \quad (5.21)
\]

The equation is solved assigning the conductivity of the phases of the soil. In this case the \( \lambda_{dry} \) (thermal conductivity of the dry porous medium, W/(K*m)) and \( \lambda_{sat} \) (thermal conductivity of the water saturated porous medium, W/(K*m)) depend on porosity and are calculated in this way:

\[
    \lambda_{dry} = \lambda_{solid}^{(1-\phi)} \cdot \lambda_{gas}^{\phi} \quad (5.22)
\]

\[
    \lambda_{sat} = \lambda_{solid}^{(1-\phi)} \cdot \lambda_{liq}^{\phi} \quad (5.23)
\]

\[
    \lambda_{solid} = (\lambda_{solid})_0 + a_1 \cdot T + a_2 \cdot T^2 + a_3 \cdot T^3 \quad (5.24)
\]

\[
    \lambda = \sqrt{S_t} \cdot \lambda_{sat} + (1 - \sqrt{S_t}) \cdot \lambda_{dry} \quad (5.25)
\]

Mechanical dispersion heat flux is computed by means Fourier's law written as:

\[
    i_h = -(c_\alpha \cdot \rho_\alpha \cdot D'_\alpha) \nabla T \quad (5.26)
\]

where \( c_\alpha \) is the specific heat of the \( \alpha \) phase, and the mechanical dispersion tensor is defined in the same way as before but using the corresponding dispersivities for heat dispersion.

### 5.2.5 BOUNDARY CONDITION

Application of the Green's theorem to the divergence term (both in the balance or equilibrium of stresses equations) produces terms which represent fluxes or stresses across or on the boundaries. These terms are substituted by nodal flow rates or forces in the discretized form of the equations.

The boundary condition for vapour and heat were chosen to reproduce the laboratory conditions. In the model there aren't prescribed force/displacement boundary condition but there are only flux boundary condition on the top and at the side of the sample. The boundary condition is incorporated by adding a flux or flow rate. The mass flux or flow rate of species \( i=w \) (water) as a component of phase \( \alpha=g \) (gas), i.e. the inflow or outflow of vapour, is calculated as:

\[
    j_g^w = (\omega_g^w) \gamma_g (P_g^0 - P_g) + \beta_g \left( (\rho_g \omega_g^w)^0 - (\rho_g \omega_g^w) \right) \left[ \frac{Kg}{s \cdot m^2} \right] \quad (5.27)
\]

where:
• $\gamma_g$ and $\beta_g$ are two parameters of the boundary condition.

Positive values of mass flow rate indicate injection to the medium.

This general form of boundary condition, includes two terms:

• The first term is the mass inflow or outflow that takes place when a phase pressure is prescribed at a node. The coefficient $\gamma_g$ is a leakage coefficient, that is, a constant that allows to prescribe a pressure with more or less strength. If $\gamma_g$ is large pressure will tend to reach the prescribed value. $P_g^0$ is the prescribed gas pressure and $(\omega_g^w)^0$ is the prescribed vapour mass fraction of the laboratory. $P_g$ is the gas pressure at the top of the column that is unknown.

• The third term is the mass inflow or outflow that takes place when species mass fraction is prescribed at a node (vapour flux due to the difference of vapour density between the environment and the top of the column).

For energy the boundary condition has the general form:

$$j_e = \gamma_e (T_0^0 - T) + E_g^w (j_g^w) \left[ \frac{1}{s \cdot m^2} \right] (5.28)$$

where:

• in this case there isn’t a prescribed heat flow;

• $T_0^0$ is the prescribed temperature of the laboratory, $T$ is the temperature of the sample at its boundary and $\gamma_e$ is a parameter of the heat that increasing causes an increase in the heat flow.

• the lasts terms imply that mass inflow and outflow through the boundary induces energy transfer (advective heat flux due to mass motion).

5.3 PARAMETERS OF THE MODEL

The discretization of the sample is made up by a mesh of 50 nodes with 49 elements which is more refined at the top. The elements have a length of 0,005 m. in the lower part and 0,002 m. at the top.

All the parameters of the constitutive laws and of the boundary conditions have been obtained by manual calibration adjusting the numerical model using the laboratory data (Villar et al. 2012).
The graphs of the values measured in the laboratory (Villar et al. 2012) that have been used for the calibration of the model are:

- evolution of the suction in the five sensors during the evaporation test;
- evolution of the relative humidity in the five sensors and outside the sample during the evaporation test;
- evolution of the temperature in the five sensors and outside the sample during the evaporation test;
- the profile of the temperature along the sample after 30, 60, 90, 120, 190, 250 and 309 days;
- the values of the degree of saturation in the five sensors at the end of the test;
- the loss of water;

Moreover, as we can see in the Tab. 4.3 the average final suction of the sample is 127 MPa and the average final degree of saturation is 0.072.

The initial average value of suction is 4.7 MPa and considering that the loss of water that has been measured is 33.2 g, the initial average value of the degree of saturation is 0.226. The other values shown in the figure 5.1 (s1,s2,s3,s5) have been measured by CIEMAT (Villar et al. 2012, Tab. 4.3) at the end of the evaporation process in the sensors 1,2,3,5. We are not considering the sensors 4 because there is an abnormal value as we have already seen in chapter 4.

Using this laboratory values (the points in the Fig. 5.1) and with the calibration of the other graphs the parameters of the water retention curve have been estimated.

At the end of the calibration \( \text{P} \) (measured pressure of air entry at 20 °C) is 0.016 MPa and \( \lambda \) (the shape function of the water retention curve) is 0.24. These values belong also to the range of values calculated in the laboratory (CIEMAT, Villar et at. 2011, Tab.4.2). All the parameters of the modified equation of Van Genuchten are shown in the table 5.1.
Fig. 5.1: Water Retention Curve (WRC) - Modified Van Genuchten Model and initial and final values of the laboratory by CIEMAT

The molecular diffusion of the vapour has been expressed by the Fick's law (5.16) and the value of the coefficient of tortuosity ($\tau_o$) that has been calibrated is 0,7.

The other values of the Fick's law (5.16) are literature values (M. Gran, J. Carrera et al. (2011)):

- $D= 5,9*10^{-6}$ (m$^2$s$^{-1}$K$^{-9}$Pa);
- $n=2,3$;
- $m=3$;

In the equation of the relative permeability (5.18) the values of $\lambda$, the residual saturation and the maximum saturation are the same values of the WRC. However, different values can be used to define these parameters.

Note that for saturations below $S^o$ the capillary pressure can be calculated from the retention curve, but the relative permeability is zero. This allows representing water isolated in the meniscus that cannot flow as a liquid phase but can still evaporate.

The conductivity of the phases of the soil (in the Fourier's law (5.21) of the constitutive flux of heat ($i_c$)) are literature values (M. Gran, J. Carrera et al. (2011)):

- $(\lambda_{\text{solid}})_o$: solid thermal conductivity $= 2$ W/(K*m);
- $\lambda_{\text{liquid}}$: liquid thermal conductivity $= 0,025$ W/(K*m);
• $\lambda_{\text{gas}}$: gas thermal conductivity$= 0,6 \text{ W/(K}\cdot\text{m})$.

$K_0$ is an intrinsic permeability and the calibrated value is $1,45*10^{-15} \text{ m}^2$. This value of intrinsic permeability ($K_0$) has been chosen with the calibration of the graphs and considering that the $K_{\text{sat}}$ of the soil of the pilot cover is $3,5*10^{-8} \text{ m/s}$. $\phi_0 (=V/V_{\text{tot}}*100)$ is the reference porosity at $K_0$ and, like we have already seen it is 0,32.

<table>
<thead>
<tr>
<th>Water Retention Curve (WRC) (eq. 5.10 to 5.12)</th>
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<tbody>
<tr>
<td>Measured pressure of air entry at $20^\circ\text{C}$ ($P$)</td>
</tr>
<tr>
<td>Surface tension at temperature in which $P$ was measured ($\sigma_0$)</td>
</tr>
<tr>
<td>Shape function for the WRC ($\lambda$)</td>
</tr>
<tr>
<td>Residual saturation ($S^*$)</td>
</tr>
<tr>
<td>Maximum saturation</td>
</tr>
<tr>
<td>$P_{c,\text{dry}}$</td>
</tr>
<tr>
<td>$\alpha$</td>
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<table>
<thead>
<tr>
<th>Intrinsic permeability ($K_i$) ($\text{m}^2$)</th>
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</thead>
<tbody>
<tr>
<td>Intrinsic permeability ($K_0$)</td>
</tr>
<tr>
<td>Reference porosity ($\phi_0$)</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Dispersive fluxes of mass and energy (eq. 5.17, 5.26)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Longitudinal dispersivity for heat</td>
</tr>
<tr>
<td>Longitudinal dispersivity for vapour</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Conductive flux of heat (W/m$^2$) (eq. 5.21 to 5.25)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solid phase thermal conductivity</td>
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<tr>
<td>Liquid phase thermal conductivity</td>
</tr>
<tr>
<td>Gas phase thermal conductivity</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Molecular diffusive fluxes of vapour (eq. 5.16)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion coefficient ($D$)</td>
</tr>
<tr>
<td>Parameter ($n$)</td>
</tr>
<tr>
<td>Power for tortuosity function of saturation ($m$)</td>
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<tr>
<td>Coefficient of tortuosity ($\tau$)</td>
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<table>
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<tr>
<th>Liquid phase relative permeability (eq. 5.18)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power ($\lambda$)</td>
</tr>
<tr>
<td>Residual saturation ($S^*$)</td>
</tr>
<tr>
<td>Maximum saturation</td>
</tr>
</tbody>
</table>

**Tab. 5.1:** Hydraulic and thermal constitutive laws

The first boundary condition (in the tab. 5.2) concerns the top of the column where there is a mixed condition representing gas and heat inflow-outflow. During the evaporation process the water leaves the column as vapour only at the top of the column due to the difference of the HR and temperature between the sample and the laboratory; therefore the boundary condition about the side of
The sample, the second one, is characterized only by the heat flux (energy was permitted to dissipate across the insulating layer of the sample). The boundary condition about the flux of water in gas phase is applied only at the top of the column and the values obtained are:

- $\beta_g = 0.0004$ m/s (it is the leakage coefficient for vapour non-advective flux);
- $\gamma_g = 5$ kg s$^{-1}$ MPa$^{-1}$ m$^{-2}$ (it is the leakage coefficient for gas advective flux);
- $\rho_g = 1.12$ kg/m$^3$ (gas density);
- $P_{g0} = 0.101325$ MPa (prescribed gas pressure of the laboratory);

The boundary condition of the heat flux is applied at the top and at the side of the column (because there are two boundary heat fluxes: one at the top of the column and another one along the side of the sample). The calibrated parameters are:

- $\gamma_e$ at the top is $0.1$ J s$^{-1}$ °C$^{-1}$
- $\gamma_e$ at the side is $10$ J s$^{-1}$ °C$^{-1}$.

<table>
<thead>
<tr>
<th>1</th>
<th>Boundary condition at the top of the column (eq. 5.27, 5.28)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prescribed mass fraction of water in gas phase</td>
<td>evolution of the laboratory</td>
</tr>
<tr>
<td>Prescribed gas pressure $P_{g0}$</td>
<td>0.101325 Mpa</td>
</tr>
<tr>
<td>Parameter of the boundary condition $\gamma_g$</td>
<td>$5$ kg s$^{-1}$ MPa$^{-1}$ m$^{-2}$</td>
</tr>
<tr>
<td>Parameter of the boundary condition $\beta$</td>
<td>0.0004 m/s</td>
</tr>
<tr>
<td>Prescribed gas density</td>
<td>1.12 kg/m$^3$</td>
</tr>
<tr>
<td>Prescribed temperature $T^*$</td>
<td>evolution of the laboratory</td>
</tr>
<tr>
<td>Parameter of the boundary condition $\gamma_e$</td>
<td>$0.1$ J s$^{-1}$ °C$^{-1}$</td>
</tr>
</tbody>
</table>

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<thead>
<tr>
<th>2</th>
<th>Boundary condition at the side of the column (eq. 5.28)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prescribed temperature $T^*$</td>
<td>evolution of the laboratory</td>
</tr>
<tr>
<td>Parameter of the boundary condition $\gamma_e$</td>
<td>$10$ J s$^{-1}$ °C$^{-1}$</td>
</tr>
</tbody>
</table>

**Tab. 5.2:** Boundary condition for liquid, vapour and heat
6 - RESULTS AND VERIFICATION OF THE NUMERIC MODEL

6.1 INTRODUCTION

Numerical simulation were carried out using the Code Bright v4, which uses the thermohydraulic model of Olivella et al. (1996b).

All the results of the model are used to calculate the ghaps in order to compare the values obtained by the sensors in the laboratory with those obtained with the model.

Moreover the graphs of the liquid, vapour and heat flow show their interaction in order to complete the representation of the behavior of this sample during an evaporation test.

6.2 EVOLUTION OF THE SUCTION

In the following figures (6.1,6.2,6.3,6.4,6.5) is shown the comparison between the evolution of the suction in the sensors and in the model during the evaporation process.

The suction ($s$) has been calculated considering that $s=P_g-P_l$.

![Graph showing the evolution of suction](image.png)

Fig. 6.1: Evolution of the suction in the model (s1model) and in the sensors (s1)
Fig. 6.2: Evolution of the suction in the model and in the sensors (s2)

Fig. 6.3: Evolution of the suction in the model and in the sensors (s3)

Fig. 6.4: Evolution of the suction in the model and in the sensors (s4)
The evolution is represented in the nodes where there were the sensors in the laboratory:

- s₁ corresponds in the model to the node 45 with a depth of 0.01 m;
- s₂ corresponds in the model to the node 35 with a depth of 0.03 m;
- s₃ corresponds in the model to the node 20 with a depth of 0.06 m;
- s₄ corresponds in the model to the node 11 with a depth of 0.09 m;
- s₅ corresponds in the model to the node 5 with a depth of 0.12 m.

The result that has been obtained in the model at the sensor 4 is really different with that of the sensors but this problem has been already shown in the chapter 3. In the laboratory they have measured abnormal values in the sensor 4 and it could be due to the greater energy of compaction that could have been applied at the surface of the first level, near to this sensor. For this reason we can notice a no good calibration between the sensor's values and the model.

The same problem there is in the graphs of the relative humidity.

During the calibration process of the graphs it has been analyzed the behavior of the model changing some parameters, considering that the processes are strongly coupled, i.e. all the parameters affect all the processes. It was noticed that:

- increasing $\beta$ (parameter of the boundary condition of the vapour flow) increases the suction of the model: it is due to the increase of $j_{gw}$ (the boundary mass flow of water in gas phase);
- increasing $\tau$ (tortuosity) increases the suction of the model: it is due to the increase of the diffusive flux;

![Graph showing the evolution of suction in the model and in the sensors (s5).](image-url)
increasing $\gamma_e$ (parameter of the boundary condition of the heat flow) increases the suction of the model: increasing $\gamma_e$ the model reaches quickly the temperature of the laboratory determining greater values of the temperature and so greater evaporations that causes increase of the suction in the sample;

- increasing $k_i$ (intrinsic permeability) increases the suction (but this parameter has a little influence on the suction because there is a low degree of saturation in the sample during all the evaporation test);

- decreasing $P$ (parameter of the WRC: measured pressure of air entry at 20 °C) there is an increase in suction;

- increasing $\lambda$ (shape function for the water retention curve and parameter of the relative permeability) there is an increase in the permeability that determines an increase in the liquid flux and suction.

### 6.3 EVOLUTION OF THE RELATIVE HUMIDITY (HR)

In this paragraph is shown the evolution of the relative humidity with the time at the same nodes that we have seen before.

It is shown the comparison between the evolution of this parameter in the sensors and in the model.

The evolution of the HR has been obtained with the psychrometric law (4.2) using the values of the liquid pressure, gas pressure and temperature calculated by the model.

![Fig. 6.6: Evolution of the relative humidity (HR) in the model and in the sensor (s1)](image)
Fig. 6.7: Evolution of the HR in the model and in the sensor (s2)

Fig. 6.8: Evolution of the HR in the model and in the sensor (s3)

Fig. 6.9: Evolution of the HR in the model and in the sensor (s4)
The best calibration of the relative humidity is displayed in the sensors 2 and 3 (Fig. 6.7, 6.8) and the same behavior has been noticed in the graphs of the suction in the same nodes (Fig. 6.2, 6.3) because the two parameters are related as is shown in the psychrometric law.

Moreover, the numerical model overestimates the relative humidity in the sensor 1 (so underestimates the suction in the same node).

The evolution of the relative humidity in the sensor 4 shows the same problem that we have seen before for the suction and it is due to the same reason.

Like it has been noticed in the laboratory, at the end of the test all the nodes (unless the node at the sensor 4) records values of the relative humidity which are like the values of the environment; it shows that all the water has evaporated.

### 6.4 EVOLUTION OF THE TEMPERATURE

The following graphs show the evolution of the temperature during the 309 days of simulated time at the same nodes that we have seen before.

In the first graph there is the comparison of the temperature of the sensor with the temperature of the model and the temperature that has been measured outside the sample in the laboratory.

It is shown that the temperature in the sample reaches the outside temperature after about 3500 hours. This result can be related with the graph 4.9 because after 3500 hours there is a small loss of water (small evaporation) due to the decrease of the temperature.

The temperature along the sample is almost constant (we will see it better in the next paragraph).
During the calibration of this graphs it has been noticed that the parameters that influenced mostly the evolution of the temperature are $\beta_g$ and $\gamma_c$ of the top and of the sides of the sample (parameters of the boundary conditions):

- Increasing $\gamma_c$ (at the top or/and at the sides) there is an increase in the temperature of the model that reaches quickly the temperature of the laboratory. In order to have the best calibration of the model the values of $\gamma_c$ are $0,1 \text{ J s}^{-1} \text{°C}^{-1}$ at the top and $10 \text{ J s}^{-1} \text{°C}^{-1}$ at the sides;
- The value of $\beta_g$ is low (0,0004 m/s) to avoid that during the first day the temperature of the model has a abnormal decrease of more than 1°C.

![Fig. 6.11: Evolution of the temperature in the model, in the sensor (s1) and outside in the laboratory](image1)

![Fig. 6.12: Evolution of the temperature in the model and in the sensor (s2)](image2)
Fig. 6.13: Evolution of the temperature in the model and in the sensor (s3)

Fig. 6.14: Evolution of the temperature in the model and in the sensor (s4)

Fig. 6.15: Evolution of the temperature in the model and in the sensor (s5)
In all the nodes the temperature at the end of the experiment reaches a value that is about 1°C less than the temperature at the beginning (about 21°C at the beginning and about 20°C at the end in all the nodes). The graphs (6.11, 6.12, 6.13, 6.14, 6.15) show that in the first 3500 hours the temperature of the model is a bit greater than that of the sensors, but after there is an almost perfect correspondence between the two evolution.

6.5 PROFILES OF THE TEMPERATURE WITH THE DEPTH

Figure 6.16 displays the profiles of the temperature computed for seven different times (at the days 30,60,90,120,190,250,309) with the experimental results.

The profiles of the temperatures show that this value has a small change along the sample. Temperature is almost constant along the column considering that the it is small (14 cm.) and that the initial temperatures of it are almost the same in all the sensors (s1: 21,12 °C; s2: 21,31; s3:21,15; s4: 21,24; s5:21,08). The values of the model have also the same trend of those of the sensors. There is initially an increase from 21,5 to 22,5 °C, after a decrease until 17,5°C and at the end the temperature is about 19,8°C which is almost the same temperature that has been measured outside the column in the laboratory (19,78 °C).
Comparing the values of the model with those of the sensors we can see also that there is a quite good calibration with a difference that is always less than 0,9 °C, considering that (as it is shown in the paragraph before) the model overestimates the sensor's values in the first part of the experiment.

6.6 PROFILES OF THE DEGREE OF SATURATION WITH THE DEPTH

Figure 6.17 displays the saturation profiles computed for seven different times (after 30,60,90,120,190,250,309 days) with the experimental results at the end of the experiment, after 309 days.

The initial average value of the degree of saturation that has been measured in the laboratory is 0,226. It shows that the column has a low water content already at the beginning.

Saturation profiles illustrate the progressive desaturation of the column from the top and at the end all the sample has a very low degree of saturation that is constant along the column.

The final value of the degree of saturation along all the column is about 0,07 and it is similar to that of the residual saturation (0,08). It shows that the modified equation of Van Genuchten represent in a good way the behavior of the sample considering also the saturation below the residual saturation and extending the WRC for high suctions (i.e. conditions of drying by evaporation) representing the oven dry branch that goes from the residual saturation to the ovendryness.

CIEMAT (Villar et al. 2012) measured the values of the saturation in the five sensors only at the end of the evaporation process. In the figure 6.17 it is illustrated also this profile with values that range from 0,065 to 0,076 (without considering the value of the sensor 4 for the same reason that we have seen before) and that are similar to those of the model.

The values of the degree of saturation measured by the model are a bit greater than the values of the laboratory at the top of the sample. This is in agreement with the lower suction that has been calculated by the model in the upper node (Fig. 6.1).
The advective flux of the liquid phase is calculated with the Darcy's law (5.14)

\[ \rho_l \cdot q_l (\text{kg}/(\text{s} \cdot \text{m}^2)). \]

Figure 6.18 displays the profiles of liquid water flux (kg/(s*\text{m}^2)) for the same days as the previous figures.

Liquid water flows upwards because of capillarity.

There is a liquid flux only upwards in the lower part of the sample and after about 120 days it is almost 0 kg/(s*\text{m}^2). This result is due to the very small amount of water that is in the column, because, as it has been shown before, there is a very low degree of saturation and so the small liquid flow is related to that.

An evaporation front is located where the liquid flux drops abruptly to zero. This front is located at about 0.07 m. of depth after 30 days and it advances deeper into the soil as the feeding liquid flux from the bottom diminishes over the time. During the evaporation test this front disappears after about 100 days when all the liquid flux (and the water content) is almost insignificant.

The evaporation front in an ideal front of the column where the water evaporates and above it the water can no longer flow as a liquid but there is only a vapour flux.
Fig. 6.18: Profiles liquid water flux - depth

### 6.8 VAPOUR WATER FLUX

The total mass flux of a species in a phase (e.g. flux of water in gas phase $j_g^w$) is in general the sum of two terms:

- the non-adveective flux: $i_g^w$, i.e. diffusive/dispersive flux;
- the adveective flux caused by fluid motion: $\theta_g^* q_g$, where $q_g$ is the Darcy flux and $\theta_g = \rho_g^* \omega_g^w$ is the vapour density;

In this case there isn't the adveective flux caused by solid motion, therefore the total vapour water flux is:

$$j_g^w = \rho_g^* \omega_g^* q_g + i_g^w$$ (6.1)

The relative contribution of each flux term to the total flux is not always the same. For instance, diffusion will become more important if advection is small.

### 6.8.1 ADVECTIVE VAPOUR FLUXES

The adveective flux of water in gas phase is calculated with the Darcy's law (m/s) (eq. 5.14).
The intrinsic permeability \((k_i)\) is the same that has been used for the advective liquid flux (because \(k_i\) depends only on the dimension and position of the pores).

![Advective vapour flux](image)

**Fig. 6.19:** Profiles advective vapour flux - depth

The figure 6.19 shows the advective vapour mass flux: \(\rho_g \cdot \omega_g \cdot w_g \cdot q_g\) (\(\text{kg}/(\text{s} \cdot \text{m}^2)\)).

The graph of the advective flux displays an upwards flow during all the evaporation test in all the column. Only at the end of the simulation there is a very small downwards flux in the lower part of the column.

The profile of the advective vapour flux after 30 days (the black line) shows that this flux increase upwards closed to the evaporation front (about 0.07 m. of depth) where the liquid flux decrease. The same behavior is displayed by the profile after 60 days (orange line) where the increase of the flow is at 0.11 m. of depth where the liquid flow decreases.

After this moment there is almost only an upwards vapour flux because the liquid flow and the degree of saturation are too low and the evaporation front disappeared because the advective vapour flux increase from the bottom of the sample without an abrupt increase.

### 6.8.2 DIFFUSIVE VAPOUR FLUXES

The diffusive vapour flux has been expressed by the Fick's law (5.12).
The trend of the profiles of the diffusive vapour flux (Fig. 6.20) are almost the same of the advective vapour flux but the values of the diffusive flow are bigger of about two orders of magnitude.

The graph of the diffusive vapour flux displays a upwards flow during all the evaporation test in all the column. Only at the end of the simulation there is a very small downwards flux in the lower part of the column.

As it is displayed in the graphs of the advective vapour flux, the profile of the diffusive vapour flux after 30 days shows the increase of the upwards flow. It is a further confirmation that after 30 days the evaporation front is at about 0,07 m. of depth. The same behavior is displayed by the profile after 60 days where the increase of the flow is at about 0,11 m. of depth where the liquid flow decreases. After this moment there is almost only an upwards vapour flux and it increases directly from the bottom of the sample.

As it is shown in the graphs, the values of the diffusive flux are much higher than the advective vapour flux and than the liquid flux; so the diffusive flux is the prevalent component of all the water (in liquid and gas phase) flux in the sample.

This upwards diffusive flux is due to the gradient of the water mass fraction in gas phase ($\omega_g^w$) of the sample. In the figure 6.21 are displayed the vapour density ($\rho_g\,\omega_g^w$) of the surface node (node 50) and that of outside the sample in
the laboratory. The last one is lower than that of the surface node and this explain also the upward diffusive flux.

![Graph](image-url)

**Fig. 6.21:** Comparison between the vapour density in the surface node (node 50) and the vapour density of the laboratory

### 6.9 LOSS OF WATER

In order to check the validity of the calibration of the model there is a comparison between the loss of water calculated by the model and that obtained in the laboratory by CIEMAT (Villar et al. 2012) (Fig. 6.22)

During the evaporation test Villar et al. have recorded the changes of mass of the column and it is greater in the first 3500 hours and then it changes more slowly coinciding with a period of oscillation of the temperature in the laboratory (Fig. 4.9).

At the end of the evaporation test in the laboratory there is a loss of water (change of the weight of the column) of 33.2 g.

During the evaporation process the water leaves the column as vapour only at the top of the column due to the difference of the gas pressure, temperature and water mass fraction in gas phase between the sample and the laboratory.

Integrating the evolution of the boundary water flow (expressed in kg/s and considering the negative values for the outflows) at the surface of the column during all the time of the evaporation process it has been obtained the total quantity of water (kg, in liquid and gas phase) that leaves the sample during the 309 days.
Moreover the output of the program considers that the column has an area of 1 m$^2$ and so this result has been modified, multiplying it by the area of the sample, considering that the sample's area is 0.0049 m$^2$.

The result of the model (red line) underestimates a bit the loss of water during the first 1000 hours. After it overestimates it a bit until 2500 hours and then, until the end of the evaporation test, there is a good correspondence between the two graphs considering that the loss of water calculated by the model at the end is 33.37 g.

![Fig. 6.22: Evolution of the loss of water (kg): values measured by CIEMAT (blu line), results of the calculation of the model (red line)](image)

During the calibration of the graph of the loss of water has been noticed that:

- increasing $\beta$ (parameter of the boundary condition of the vapour flow) there is an increase in the loss of water of the model: it is due to the increase of $j_{gw}$ (the boundary mass flow of water in gas phase);
- increasing $\tau$ (tortuosity) increases the loss of water: it is due to the increase of the diffusive flux;
- increasing $k_i$ (intrinsic permeability) increases the loss of water (but this parameter has a little influence on the suction because there is a low degree of saturation in the sample during all the evaporation test);
- increasing $\lambda$ (shape function for the water retention curve and parameter of the relative permeability) there is an increase in the permeability that determines an increase in the liquid flux and in the loss of water;
• increasing $\gamma_e$ (parameter of the boundary condition of the heat flow) the model reaches quickly the temperature of the laboratory determining greater values of the temperature and so greater evaporations that causes increase of the loss of water;
• increasing $\gamma_g$ (parameter of the boundary condition of the vapour flow) there is an increase in the loss of water of the model: it is due to the increase of $j_{gw}$ (the boundary mass flow of water in gas phase). However this parameter has a little influence in the change.

6.10 HEAT FLUX

Heat flux or thermal flux is the rate of heat energy transfer through a given surface. The SI derived unit of heat rate is joule per second, or watt. Heat flux is the heat rate per unit area. In SI units, heat flux is measured in [W/m$^2$].

The total heat flux is in general the sum of two terms:

• the conductive heat flux $i_c$;
• the advective heat flux $j_{adv}$.

The first one is the energy flux (J m$^{-2}$ s$^{-1}$) owing to conduction through the porous medium.

The second one is an advective flux of energy (J m$^{-2}$ s$^{-1}$) caused by mass motion. This flux can be divided in two parts:

• advective heat flux due to the liquid motion;
• advective heat flux due to gas motion (vapour motion).

\begin{equation}
  j_{adv} = j_{adv,l} + j_{adv,g} \tag{6.2}
\end{equation}

The total heat flux is (eq. 6.3):

\begin{equation}
  j_{heat} = i_c + j_{adv,l} + j_{adv,g} = \\
  = -\lambda \nabla T + C_w j_{liq} T + (q_g \rho_g \omega_g w + i_g w) E_w \quad [J/m^2/s]
\end{equation}

6.10.1 CONDUCTIVE HEAT FLUX

The constitutive law of the conductive heat flux $i_c$ is expressed by the Fourier's law (5.21)
The numerical model also enables us to study in detail heat fluxes. Figure 6.23 displays the conductive heat flux in the column after 30, 60, 90, 120, 190, 250, 309 days. Positive values of flux represent an upwards flux. The values of the conductive heat flow (upwards or downwards flow) are always very low during all the evaporation process. It is due to the constant value of the temperature along the column. In fact, as it was displayed before, the temperature along the column is always almost constant along the column and so the gradient of the temperature is very low.

The conductive heat flux is bigger along the column than at the top and it may be due to the fact that the $\gamma_e$ of the side of the sample is bigger than that of the top ($\gamma_{e,\text{side}} = 10; \gamma_{e,\text{top}} = 0.1$).

### 6.10.2 ADVECTIVE HEAT FLUX BY LIQUID WATER FLOW

The total heat flux is also caused by the advective heat flux that is due to the mass motion (liquid and vapour motion).
The liquid motion of the water along the column determines part of the advective heat flux which is an upwards flux.

As the figure 6.18 shows the liquid flux is negligible almost always during the evaporation test and considering that the advective heat flux due to liquid flux depends by the liquid flux it is expected a low intensity of this kind of heat flux.

The advective heat flux ($j_{\text{adv},l}$) caused by liquid water motion is expressed by the law (5.6).

The figure 6.24 displays the advective heat flux due to the liquid motion and as it was expected this heat is very low and the trend of the profiles is similar to that of the liquid water flux (Fig. 6.18).

### 6.10.3 ADVECTIVE HEAT FLUX BY VAPOUR FLOW

The advective heat flux is also due to the vapour flux (advective and diffusive vapour flux).

Also a non-advective mass flux causes an advective heat flux because a species inside a phase moves and transports energy.

The figure 6.25 displays the profiles of the advective heat flux due to the vapour motion for the same instants of the other previous graphs.
As it was expected the trend of the profiles is similar to that of the diffusive and advective vapour flux (Fig. 6.19, 6.20) and so there is almost always an upwards heat flux (only at the end in the lower part of the column there is a downwards flux).

The advective heat flux ($j_{adv,g}$) caused by advective and diffusive vapour motion is expressed by the law (5.7).

The figures 6.24 and 6.25 show that the advective heat flux is almost all caused by the vapour flux. In fact the vapour flux (more precisely the diffusive flux) is greater than the liquid flux and so the advective heat flux due to the vapour flux is about five orders of magnitude bigger than the one due to the liquid flux.

Moreover the figures 6.23, 6.24 and 6.25 show that the prevalent part of all the heat flux is due to the advective heat flux due to the vapour motion. This is in agreement with the other graphs of the model considering that the liquid flux is almost negligible (and so there is a little advective heat flux due to liquid water motion) and that the gradient of the temperature along the column is small (a constant temperature along the sample determines a small conductive heat flux).

The figure 6.25 shows that the advective heat flux by vapour flow (and so also the total heat flux) is upwards (unless at the end in the lower part of the sample). The upwards heat flux is in agreement with the reduction of the temperature along the sample. At the end of the evaporation test the temperature of the
column is about 20 °C which is almost 1°C less than its temperature at the beginning of the test. Therefore in order to obtain this reduction it was expected an upwards heat flow during the 309 days of test.

**6.11 SURFACE HEAT FLUX**

For energy the boundary condition has the general form expressed by the equation 5.28.

![Graph showing surface heat flux](image)

**Fig. 6.26**: Evolution of the loss of energy at the top of the column (J) (Code Bright)

Integrating the heat flow across the boundary (expressed in J/s and considering the negative values for the outflows) during all the time of the evaporation process it has been obtained the total quantity of energy (J) that leaves the sample during the 309 days of the evaporation test. Moreover the output of the program considers that the column has an area of 1m² and so this result has been modified, multiplying it by the area of the sample, considering that the sample's area is 0.0049 m².

The figure 6.26 displays that during the evaporation test there is a loss of energy due to the upwards flux of heat at the top of the sample. At the end of the test the total loss of energy is 7,946*10⁴ J. This upwards flux of heat is in agreement with the upwards total heat flux of the figure 5.34.
6.12 LATERAL HEAT FLUX

The second boundary heat flux is the lateral heat flux along the column. Even if the soil was placed in a cylinder of methacrylate there is a lateral heat flux and its evolution is expressed by Code Bright (in J/s) considering that the positive values are inflows. For energy the boundary condition has the general form expressed by the equation 5.28.

![Figure 6.27: Evolution of the lateral entry of energy (J) (Code Bright)](image)

Integrating the value of the heat flow across the sides of the sample (expressed in J/s and considering the negative values for the outflows) during all the time of the evaporation process it has been obtained a positive value. Therefore there is a quantity of energy (J) that goes inside the sample during the 309 days of the evaporation test.

The output of the program considers that the column has an area of 1m² and so this result has been modified, multiplying it by the area of the sample, considering that the sample's area is 0,0049 m².

The figure 6.27 displays that during the evaporation test there is an influx and so an entrance of energy along the sample.

At the end of the test the total quantity of energy that is entered is 7,09*10⁴ J.

The figures 6.26 and 6.27 show that the quantity of energy that leaves the column (at the top) is greater than the energy that goes inside (lateral entry). The difference between these quantities represents the total loss of energy of the column and it is in accordance with the decrease of temperature (about 1°C) that characterizes the soil at the end of the process.
7 - INFLUENCE OF β IN THE CALIBRATION

7.1 INTRODUCTION

Before reaching the calibration of the graphs and the final value of the parameters it was found a particular behavior of the sample due to an higher value of β.

Using a value of β higher than the one that has been used at the end of the calibration and changing the other parameters of only a small amount a good calibration was reached in some graphs.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Model</th>
<th>Model (2)</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>λ (shape function of the WRC)</td>
<td>0.016</td>
<td>0.01</td>
<td></td>
</tr>
<tr>
<td>P (pressure of the air entry at 20 °C)</td>
<td>0.24</td>
<td>0.25</td>
<td>Mpa</td>
</tr>
<tr>
<td>ki (intrinsic permeability)</td>
<td>1.45*10^{-15}</td>
<td>1.38*10^{-15}</td>
<td>m²</td>
</tr>
<tr>
<td>τ (tortuosity)</td>
<td>0.7</td>
<td>0.47</td>
<td></td>
</tr>
<tr>
<td>γg (parameter of the boundary condition)</td>
<td>5</td>
<td>14</td>
<td>kg s⁻¹ MPa⁻¹ m⁻²</td>
</tr>
<tr>
<td>γe.top (parameter of the boundary condition)</td>
<td>0.1</td>
<td>0.8</td>
<td>J s⁻¹ °C⁻¹</td>
</tr>
<tr>
<td>γe.lat (parameter of the boundary condition)</td>
<td>10</td>
<td>0.5</td>
<td>J s⁻¹ °C⁻¹</td>
</tr>
<tr>
<td>β (parameter of the boundary condition)</td>
<td>0.0004</td>
<td>0.01</td>
<td>m/s</td>
</tr>
</tbody>
</table>

Tab 7.1: Comparison of the parameters in the two modeling

Tab. 7.1 shows the difference between the parameters. The first column (model) displays the parameters of the final calibration of the model that we have already seen. The second column (model (2)) shows the changed parameters.

These different parameters enable a good calibration of the graphs of the suction, relative humidity and loss of water. Instead there isn’t a good result in the profiles of the degree of saturation and in the evolution of the temperature at the beginning because an abrupt and abnormal decrease of temperature was noticed during the first days of the test.

In this way it is noticed the influence of β in the calibration of the sample.

7.2 SUCTIONS AND RELATIVE HUMIDITY

Using these parameters a good calibration of the graphs of the suction and of the relative humidity was reached.

The figure 7.1 shows the evolution of the suction in the node 45 (close to the surface of the sample) and with these different parameters a better calibration of the suction in this node was obtained.
The greater value of $\beta$ (0.01) determines a higher suction and so permits a better calibration of this graph, mainly in the first half of the evolution where a perfect calibration was reached.

Fig. 7.1: Evolution of the suction in the model (s1model) and in the sensors (s1)

The figure 7.2 displays the evolution of the suction in the node 35 (sensor 2) and it shows a perfect calibration in the second half of the evolution.

Fig. 7.2: Evolution of the suction in the model (s2model) and in the sensors (s2)

Comparing the evolution of the suction in the nodes in the two models an increase of the suction at the top of the sample is noted when $\beta$ (parameter of the boundary condition of the vapour flow) increases.
This increase at the top of the sample is due to the increase in the boundary mass flow of water in gas phase \((j^w_g)\) at the top. Reducing \(\beta\) from 0.01 to 0.0004 there is a big decrease of the suction and in order to obtain a good calibration the final model has a smaller \(P\) and bigger values of the tortuosity \((\tau)\), intrinsic permeability \((k_i)\), \(\lambda\) (shape function for the water retention curve and parameter of the relative permeability) and \(\gamma_e\) at the side (parameter of the boundary condition of the heat flow).

**Fig. 7.3:** Evolution of the HR in the model and in the sensor (s1)

**Fig. 7.4:** Evolution of the HR in the model and in the sensor (s2)

The figures 7.3 and 7.4 display the evolution of the relative humidity (HR). Comparing the evolution of the HR in the two models it is displayed a better calibration at the top of the column using a greater value of \(\beta\). The graphs of the
HR in the sensors s1 and s2, displayed in the fig. 7.3 and 7.4, show that there is a better calibration than that obtained in the final model (fig 6.6, 6.7). However the improvement disappeared at the bottom (node 5) where the evolution of the suction and of the relative humidity is the same in both the models.

### 7.3 LOSS OF WATER

Using the parameters of the model (2) there is still a good correspondence between the loss of water of the model and that measured in the laboratory. Though the value of β is bigger (0.01), and so there should be an increase of the loss of water, the calibration was obtained reducing the values of τ (tortuosity), \(k_i\) (intrinsic permeability), \(\lambda\) (shape function for the water retention curve and parameter of the relative permeability) and \(\gamma_e\) at the side (parameter of the boundary condition of the heat flow).

![Fig. 7.5: Evolution of the loss of water (kg): values measured by CIEMAT (blu line), results of the calculation of the model (2) (red line)](image)

Considering the equation (5.27) of the boundary mass flux of water in gas phase \(j_{gw}^w\), in order to have this loss of water with a bigger value of β (parameter of the boundary condition of the vapour flow) the difference of the vapour density \(\left(\rho_g \omega_g^w\right)^0 - \left(\rho_g \omega_g^w\right)\) outside and at the surface of the sample is lower (as it is shown in the fig 7.6).
**7.4 TEMPERATURE**

One of the problem of the model (2) is the abrupt decrease of the temperature in the first days. It is an abnormal decrease that is due to the value of $\beta$, because the only way to avoid it is decreasing $\beta$ (parameter of the boundary condition of the vapour flow) (in fact the value of $\beta$ in the model is 0,004).

The figures 7.7 and 7.8 shows the evolution of the temperature in the sensors s1 and s2 (the sensors at the top of the column) and in the models. The main difference between the two graphs of the models is the already mentioned decrease of temperature that characterizes the model (2). This decrease was noted in all the five nodes analyzed (45,35,20,11,5) and it is of almost 2 °C.

It is due, maybe, to the fact that the initial values of the temperature have been measured in the laboratory (Villar et al. 2012) only in the five sensors and so there isn't a complete knowledge of the temperature along the column at the beginning of the evaporation test. However there isn't a real and sure explanation of this abrupt decrease.

After about 1000 hours there is a quite good correspondence between the two models.

The other parameters that influence the evolution of the temperature are $\gamma_e$ at the top and at the side of the column. Increasing these parameters there is an increase in the temperature of the model (because the outside temperature is higher than inside and in this way the model reaches soon that temperature) removing also the abrupt decrease of the temperature of the beginning.
Therefore in order to have a good calibration the choice of these two $\gamma_e$ is important because increasing them too much would avoid the initial decrease of temperature but there will be a bigger difference between the temperature of the model and that of the sensors during all the test (the temperature of the model would be like the temperature of the laboratory). Moreover it was noted that $\gamma_e$ at the top has a greater influence on the temperature.

**Fig. 7.7:** Evolution of the temperature in the model and in the model (2) in the node 45; and the evolution measured by the sensor (s1)

**Fig. 7.8:** Evolution of the temperature in the model and in the model (2) in the node 35; and the evolution measured by the sensor (s2)
### 7.5 WATER RETENTION CURVE AND PROFILES OF THE DEGREE OF SATURATION

The figure 7.9 displays the WRC expressed with the Modified Van Genuchten Model (considering the shape function of the equation \( \lambda=0.01 \) and \( P=0.25 \) MPa) and shows the values of degree of saturation and suction measured in the laboratory (the average final and initial value with the final values in the sensors s1, s2, s3, s5).

Though in the model (2) the graphs of the suction have a good calibration, in the water retention curve (WRC) there isn't a good calibration with the average initial value measured in the laboratory.

The problem with the calibration of the WRC in the model (2) explains the low values of degree of saturation that have been calculated by the program.

The initial degree of saturation that was measured in the laboratory is about 0.226, instead the model (2) has an initial saturation of about 0.18. Moreover the comparison at the end of the test between the values of the laboratory and that of the program show that the model underestimates the degree of saturation along all the sample.

**Fig. 7.9**: Water Retention Curve (WRC) - Modified Van Genuchten Model (model (2)) and initial and final values of the laboratory by CIEMAT
7.6 VAPOUR AND LIQUID FLUXES

The liquid flux obtained in the model (chapter 6.7) is very low and less than $5 \times 10^{-10} \text{ Kg/s/m}^2$.

The lower values of the degree of saturation of the model (2) determines a lower liquid water flux (which is no more than $4 \times 10^{-11} \text{ Kg/s/m}^2$) during all the evaporation.

However the trends of this profiles (fig. 7.11) are similar to that of the model and they show at the same depth the position and evolution of the evaporation front.
Fig. 7.11: Profiles liquid water flux - depth in the model (2)

The profiles of the advective and diffusive vapour flux of the model (2) are similar to that of the calibrated model.

The figure 7.12 shows the profiles of the diffusive vapour fluxes at the same instant of before and a small reduction in the diffusive flux compared to the flux
of the model can be noted. It is due to the reduction in the value of tortuosity ($\tau = 0.47$ in the model (2) and $\tau = 0.7$ in the model)

The figure 7.13 shows that also with these parameters (the ones of the model (2)) the liquid flux is negligible compared to the diffusive flux and the trends of the profiles are similar in the two models.
8 - SUMMARY AND CONCLUSIONS

The radioactive waste of low and intermediate level type generated in Spain are placed in the El Cabril centralized disposal facility. The waste, placed in cells of concrete, will be covered by a capillary barrier to guarantee the isolation of the waste, preventing the infiltration of the water. In order to study the behavior of the barrier there is a pilot test located in El Cabril.

In this thesis the superficial layer (vegetal soil) of this pilot test has been studied. Before using this material, the part with a dimension greater than 2 mm was removed by sieving.

This work consists of a one-dimensional modeling of the same evaporation test realized by CIEMAT (Villar et al. 2012) on a sample of 14 cm of topsoil. The experimental values used to calibrate the model are the porosity, the loss of water, the degree of saturation and the temperature, suction and relative humidity measured in the five sensors and outside the sample.

All the unknown parameters of the constitutive laws and of the boundary conditions of the soil are obtained by manual calibration adjusting the numerical model using the laboratory data and graphs. The other parameter are literatures values.

Numerical simulation were carried out using the Code Bright v4 considering the interaction between liquid, gas and heat flows in a soil under evaporation conditions.

The one-dimensional model reproduces quite accurately the experimental observation of the evolution of the suction, HR, temperature, loss of water and degree of saturation (this value is measured in the laboratory only at the end of the evaporation test).

The Water Retention Curve has been obtained with laboratory experiment (M.Villar 2011), with the laboratory values of suction and degree of saturation
measured at the end of the evaporation test (M. Villar 2012) and with the calibration of the model.

In order to consider the very low values of the degree of saturation, which are lower than the residual saturation at the end of the evaporation process, it was used the modified equation of Van Genuchten.

The parameters obtained for the WRC are:

- \( \lambda = 0.24 \)
- \( P = 0.016 \) MPa
- \( P_{\text{dry}} = 400 \) MPa
- \( \alpha = 0.16 \)
- \( S^0 = 0.08 \)

The other parameters that have been calibrated are the tortuosity \( (\tau = 0.7) \), the intrinsic permeability \( (k_i = 1.45 \times 10^{-15} \text{ m}^2) \) and the parameters of the boundary conditions \( (\gamma_g = 5 \text{ kg s}^{-1} \text{ MPa}^{-1} \text{ m}^{-2}) \), \( \gamma_e \) at the top \( (0.1 \text{ J s}^{-1} \text{ °C}^{-1}) \) and at the side of the column \( (10 \text{ J s}^{-1} \text{ °C}^{-1}) \).

From the calibrated model can be noticed that:

- At the end of the test the relative humidity in all the column is like that of the environment; it shows that all the available water has evaporated;
- evaporation is caused by the different temperature and relative humidity inside and outside the sample;
- the sample reaches the external temperature after 3500 hours; this result can be related to the small loss of water that there is after 3500 hours due to the decrease of the temperature;
- the temperature is almost always constant along the sample; so there isn't a vapour diffusive flux due to \( \nabla T \).
- the temperature at the end is about 1°C less than that at the beginning;
• the sample has always a low water content: the degree of saturation at the beginning is 0.226 and at the end it reaches a saturation of about 0.07 along all the column;
• it shows that there are oven dry condition (i.e. water content below the residual saturation) and so the modified equation of van Genuchten represents good the behavior of the soil;
• intrinsic permeability has little influence during the calibration caused by the low values of the degree of saturation;
• liquid flux is upwards but with low values due the low water content. The liquid flux is negligible compared to the vapour flux. The evaporation reduces the water content and the unsaturated hydraulic conductivity causing the evaporation front to move downwards until it disappears after 100 days when all the liquid flux is insignificant all along the column;
• the advective heat flux caused by the liquid flux is negligible due to the very low values of the liquid flux;
• vapour flux is always upwards (unless at the end in the lower part of the column)
• the diffusive vapour flux represent the prevalent part of all the liquid and vapour water flux and so the prevalent heat flux is the advective heat flux due to the vapour motion;
• the total heat flux is almost always upwards and it can be noted that the evaporation front moves down during the first days until it disappears;
• Evaporation tends to cool the column: the boundary heat flows show an inflow of energy through the lateral part of the column and an outflow at the top; the outflow is bigger than the inflow because the temperature in the model at the end of the test is 1°C less that the one at the beginning and so there is a dissipation of heat;
moreover it was noted the influence of β in the process: a larger value of this parameter causes an abrupt and abnormal decrease of the temperature of almost 2°C at the beginning of the evaporation test; This particular behavior hasn't a good and sure explanation.

In this way we have a characterization of the vegetal soil during the evaporation condition. In this situation the soil is almost dry, with low values of the degree of saturation and low value of the intrinsic permeability. The situation may be different in other conditions, for instance in case of rainfall events. In this other case there will be wetter conditions with an higher value of the intrinsic permeability that may influence more the interaction between the liquid, water and heat flow.
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