4. SIMULATION METHOD AND MODELLING

4.1 Introduction

The simulations were carried out using a two-dimensional geotechnical finite element software named PLAXIS. The software has been developed by PLAXIS BV, which is a company involved in research and development of numerical models for the characterization of the deformation behaviour of soils. PLAXIS is a finite element package specifically intended for the analysis of deformation and stability in geotechnical engineering projects. The characteristics of this software are robust calculation procedures and user-friendly input and output facilities. A brief summary of the important features of the program is given below.

- ***Graphical input of geometry models***: The input of soil layers, structures, construction stages, loads and boundary conditions is based on CAD drawing procedures, which allows for a detailed modelling of the geometry cross section. From this geometry model, a 2D finite element mesh is generated.
- ***Automatic mesh generation***: PLAXIS allows for fully automatic generation of unstructured finite element meshes with options for global and local mesh refinement. The mesh may contain thousands of elements.
- ***Interfaces***: Joint elements are available to model soil structure interaction. For example, these elements may be used to simulate the thin zone of intensely shearing material at the contact between a tunnel lining and the surrounding soil. Values of interface friction angle and adhesion are generally not the same as the friction angle and cohesion of the surrounding soil. Interfaces are used here to model prescribed fractures.
- ***Boundary conditions***: Fixities are prescribed displacements equal to zero. These conditions are applied to geometry lines as well as to geometry points in x and y directions. Prescribed displacements are special conditions that shall be imposed on geometry lines to control the displacements of these lines. Prescribed displacements shall be used in the models in order to cause a stress field.
- ***Material set database***: Material properties for soil, as well as for structural elements are entered in a project database. The most used materials in the present work are sandstones and shales which will be varied, concerning to their mechanical parameters, during the investigations, depending on the effects to be studied. The most important mechanical parameters here shall be the Young modulus, cohesion and the friction angle.
- ***Steady state pore pressure***: Complex pore pressure distributions may be generated on the basis of a combination of phreatic levels or direct input of water pressures. As an alternative, a steady state groundwater flow calculation can be performed to calculate the pore pressure distribution in problems that involve steady flow or seepage.

These features of the software make it suitable to study the problem of multi-layer fracturing. Especially its flexibility and calculation speed allow variation of a large number of conditions and parameters in order to evaluate their effect on the strain and stress distribution in multi-layer rocks. These models are described in the next section.

4.2 Models

4.2.1 Geometry

In order to simulate the investigations, a rectangular model has been built by means of the input program of Plaxis. A ***Plane Strain model*** shall be applied to a box of 50 m and 25 m horizontal and vertical extent, respectively (**Figure 6**). The models consist of three or five layers, depending on the effects to be studied.

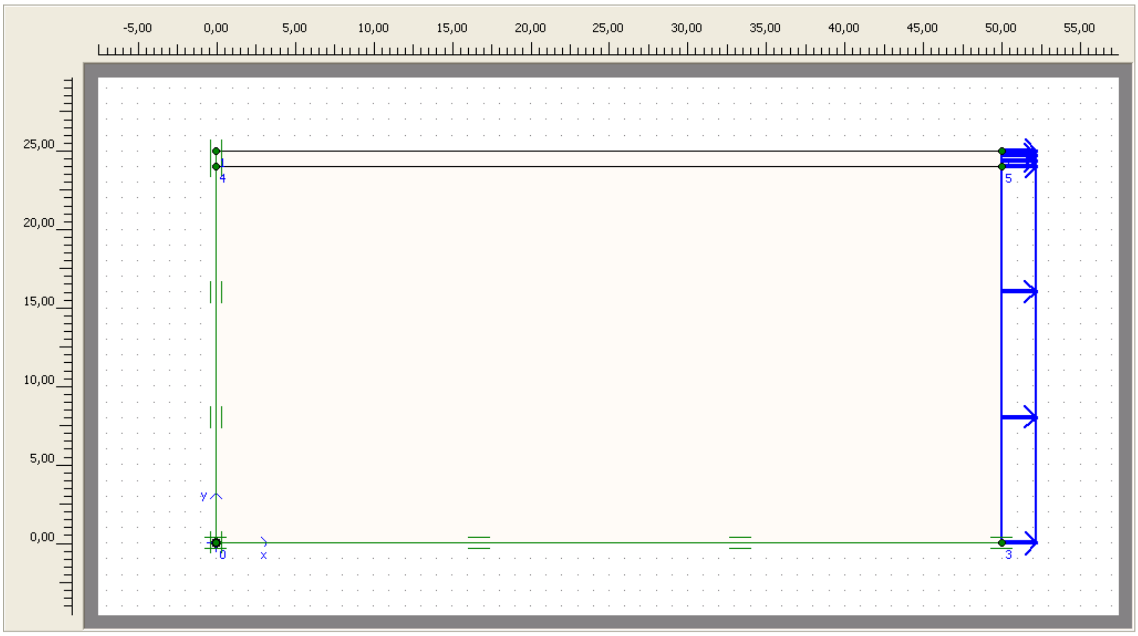

Figure 6. Example of the general model; three or five layers shall be applied here with different properties defining the competent and the incompetent layers. The box is 50 m and 25 m horizontal and vertical extent, respectively. There is an initial prescribed displacement of 10 cm, which shall be increased until 15 cm. Note that the prescribed displacement is not represented at the same scale as the box.

Notice that the prescribed displacement only has been applied at one of the sides (right side) whereas the other one (left side) is fixed. The model represents only the half part of the real model, which is symmetric to the present model's left margin.

4.2.2 Boundary conditions and material parameters

Some ***Boundary conditions*** have to be defined to simulate as real as possible the behaviour in nature.

Vertical fixities have been applied in the bottom of the models in order to not allow the vertical displacement in that part of the model. With it, it is intended to specify that the layer is in a certain depth, and therefore, it shall have some material below it. Also for this reason, a ***Heavy layer*** has been applied at the top of the model. This means, as a matter of fact, that the composed models shall have four and six layers, instead of three and five, respectively. However, the models shall be named as three- and five-layer models because it is assumed that the heavy layer acts as a boundary condition. This heavy layer has the same properties as the other materials, except the γ parameter (**Table 1**), which is 200 times bigger, representing the height of the overburden above the main part of the model. Actually, this heavy layer is introduced to simulate the overburden pressure acting on the model due to all the layers and different materials situated above it. Assigning the γ parameter 200 times bigger than normal specific weight values for shale to a 1 m thick shale layer, simulates an overburden of 200 m thickness, consisting of shales, above the three- or five-layer model.

Horizontal fixities at the left boundary have been applied to simulate that this boundary is a symmetry axis across which no displacement can occur. In the right margin of the model, a progressive horizontal displacement has been applied. In all simulations, an initial sequence of deformation steps was calculated up to a total displacement of 1 mm. This was followed by progressive, stepwise displacement up to a total of 15 mm. The prescribed displacements are applied in order to cause a constrained displacement so that a stress field is created. When it is required in the model, the prescribed displacements shall be increased by means of the multipliers' option in the Calculations Menu, as it shall be explained in the appropriate section.

MATERIAL'S SET TABLE						
PARAMETER		**Units**	Heavy Shale	Sandstone	Shale	Interfaces
Young Modulus	$\mathbf{E_{ref}}$	**kN/m²**	5E+05	5E+06	5E+05	5E+06
Poisson's Ratio	$\boldsymbol{\nu}$		0.14	0.19	0.14	0.19
Cohesion	$\mathbf{c_{ref}}$	**kN/m²**	5E+05	1E+06	5E+06	1E+06
Friction Angle	$\boldsymbol{\varphi}$	°	28	45	28	45
Dilatancy	$\boldsymbol{\psi}$	°	15	0.1	15	0.1
Specific Weight	$\boldsymbol{\gamma_{sat}}$	**kN/m³**	2000	18	18	18
	$\boldsymbol{\gamma_{unsat}}$	**kN/m³**	2000	20	20	20
Permeability	$\mathbf{k_x}$	**m/day**	1E-03	1E-03	1E-03	1E-03
	$\mathbf{k_y}$	**m/day**	1E-03	1E-03	1E-03	1E-03

Table 1. The figure shows the values of the different material parameters used in the models. The values of the material parameters are general values in the sense that they do not belong to any source. E_{ref}, c_{ref} and φ will be the varied parameters during modelling.

Material parameters have been applied depending on the material to simulate. Very common geological materials shall be dealt with here, and in nature mechanical parameters can vary in a wide range of values, but for this study, some approximated average values shall be taken. In the next table (**Table 1**) the different used materials and a very short description of these parameters are shown. These values have been used in the base case and in those simulation runs where the only one varied parameter was the height of the layer. In the other simulation runs always one single of these parameters was varied with respect to the base case. In order to carry out the investigations in the present work, the competent layer shall be represented by sandstones, and the incompetent layer shall be represented by shales.

One important fact to take into account is the presence of water or the groundwater flow. In the simulations it was assumed that the phreatic level has not reached the model and the materials simulated. Thus, the water pressure is zero in all the models and it has only been taken into account the overburden pressure or stresses of the materials.

4.3 Modelling procedure

As a first step, the required model is built using ***Plaxis Input***. There are some steps to follow in order to get the required construction of the model, as it is shown as follows.

4.3.1 File Menu

- Using the ***General Settings*** of the model (dimensions, geometry…) as it has been explained in the previous section.
- In the ***Geometry Menu*** it is possible to build the model with the geometry lines to draw the contour and the different layers. In the five-layer models, this step is followed by the definition of one or more fractures. Fractures are drawn also with the geometry lines, but it is important that interfaces are attributed by means of the same menu, in order to define in the model that these lines can suffer some displacements due to several loads (see **Table 1** for the interfaces parameters).
- The ***Loads Menu*** is used to apply the fixities to the model as it has been explained above. After that, prescribed displacements have to be attributed, and in the same menu there is an option to apply these prescribed displacements and vary them in the model depending on the needs.
- Next step is applying the different materials with their specific parameters to the model, by means of the ***Material Set Menu***. At the same time, this mentioned menu allows to create, change, edit or simply delete all the wished materials.
- Once the models have been completely built and all the features applied, an initial mesh is generated using the ***Mesh Menu***.

4.3.2 Initial Conditions Menu

Here it is possible to specify the water weight required, as well as the phreatic level or the flow.

- ***Geometry*** and ***Generate Menu*** are both used in this step to generate the initial water pressures (set to zero in the present work) and the initial stresses and geometry configuration.
- When the initial stresses are generated, it is possible, by means of the ***Stresses Menu***, to see the different distributions that have been reached by the model as

well as the plastic points and extreme overconsolidation ratios (OCR). The initial stresses in a soil body are influenced by the weight of the material and the history of its formation. This stress state is usually characterised by an initial vertical effective stress $\sigma'_{v,0}$. The initial horizontal effective stress $\sigma'_{h,0}$, is related to the initial vertical effective stress by the coefficient of lateral earth pressure, K_0 ($\sigma'_{h,0} = K_0 \cdot \sigma'_{v,0}$). In the generation of the stresses a value of K_0=0.5 is used for all the materials and layers.

A menu tree of the ***Input Menu*** and the ***Initial Conditions Menu*** is shown in the **Appendix** in order to succeed in a better understanding.

Once this step is finished, the next step is to proceed to carry on the calculation process, varying some features depending on the particular model which are investigated in that model run. All these possible changes are explained in the next section.

4.4 Calculations

In this section it shall be explained the calculation features applied to the software in order to obtain the expected results. Investigations have been divided into two different sets, depending on the number of the layers in the model. There are two general models, the three- and the five-layer model. Each model has been studied applying and varying some features or mechanical properties, which have been put on view below, where it is showed the different variations applied. The title of each section depends on what feature or mechanical parameter has been changed in order to carry on the study. In the next table (**Table 2**) it is possible to observe the changes of the features or the mechanical parameters in each model.

3 - layer	Base case		4.4.2.1	5.2.1.1
	H_h, H_{su} and H_{sb} (heights of the three layers -middle, upper and lower-)		4.4.2.2	5.2.1.2
	Mechanical parameters (competent layers)	E (Young modulus) c (cohesion) φ (friction angle)	4.4.2.3	5.2.1.3
	Mechanical parameters (incompetent layers)	E (Young modulus) c (cohesion) φ (friction angle)	4.4.2.4	5.2.1.4

5 - layer	Base case		4.4.3.1	5.2.2.1
	H_{sm} (height of the middle soft layer)		4.4.3.2	5.2.2.2
	Mechanical parameters (incompetent layers)	E (Young modulus) c (cohesion) φ (friction angle)	4.4.3.3	5.2.2.3
	Mechanical parameters (competent layers)	E (Young modulus) c (cohesion) φ (friction angle)	4.4.3.4	5.2.2.4
	Fracture spacing in the top competent layer		4.4.3.5	5.2.2.5

Table 2. The table shows the changes of the features and the mechanical parameters in each model. The number situated in the two last right columns shows respectively the section number where these changes have been applied to the models and the section number where the results have been showed and commented.

4.4.1 Procedures

Calculations in Plaxis must be defined by means of several steps before carrying out the investigations. The steps are defined as follows:

1. General features: definition of the phase number (1, 2 or 3) and the calculation type ('plastic' in the present work).
2. Parameters: definition of the control parameters and the loading input (staged construction or multipliers).
3. Multipliers: definition of the multipliers (total or incremental), only if this option has been chosen.
4. Preview of the input model ready for the calculations.

In the present work three phases have been used during the simulations (**Table 3**). In the phase no. 1 (Displacement) a prescribed displacement of 1 cm has been applied, except in two special runs for the Base Cases (three- and five-layer model), for each of which a second simulation with a prescribed displacement of 1 mm was run. Immediately afterwards, in the phase no. 2 (Multipliers 1), it has been increased the displacement until a value of 5 cm (and 5 mm respectively in the second models of the Base Cases). As a final step, in the phase no.3 (Multipliers 2), once more the value of the prescribed displacement has been increased until a value of 15 cm (or 15 mm respectively in the second models of the Base Cases). These steps have been used because it is possible, with Plaxis, to structure the calculations in all the steps required. The profit of this type of calculation is that the software can show the results and the output at the end of each phase, so it is easier to understand how it behaves. Thus, it is easier to determine visually the different changes in its behaviour. The observation of the behaviour at the end of each step can allow us to have a full view of the mechanical progression and behaviour of the model.

CALCULATION STEPS TABLE				
Identification	**Phase no.**	**Start from**	**Calculation**	**Loading Input**
Initial Phase	0	0	N/A	N/A
Displacement	1	0	Plastic	Staged Construction
Multipliers 1	2	1	Plastic	Total Multipliers
Multipliers 2	3	2	Plastic	Total Multipliers

Table 3. Calculation steps table used in the models.

4.4.2 Three-layer model

This model has been originally built of three layers with the same thickness for each one. This is not the main topic of the study, but it shall be a first approximation of the study in order to be able to see the several behaviours that can be expected in the next investigations. An example of the starting point model is shown in **Figure 7**. Different changed features or parameters are outlined immediately afterwards, with a brief explanation for each one.

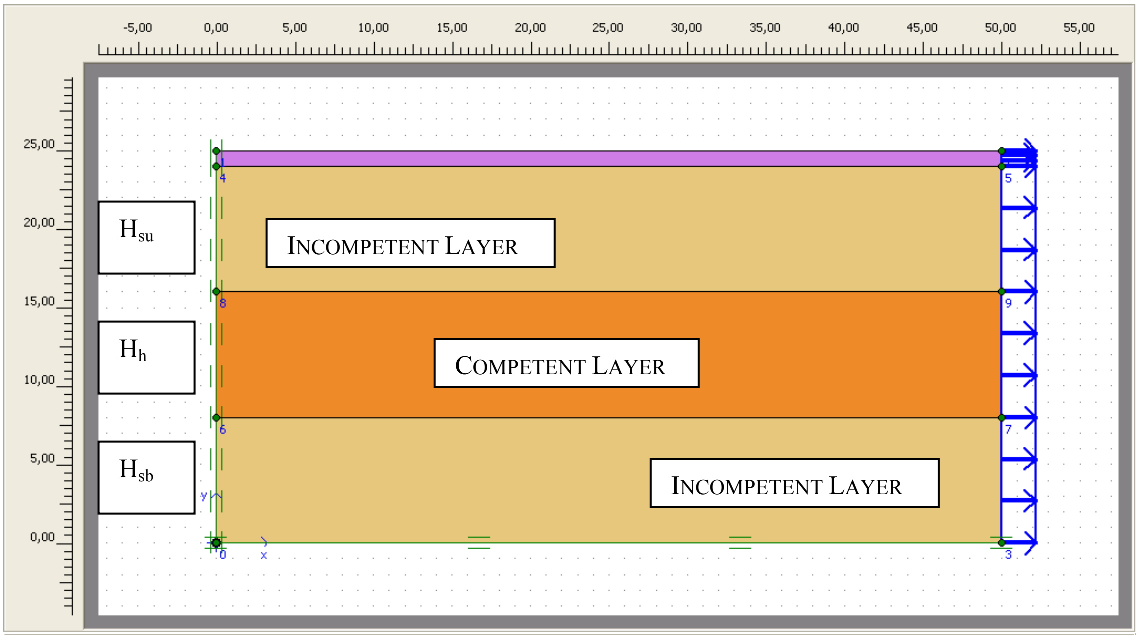

Figure 7. Example of the base case for the three-layer models. It illustrates the different boundary conditions applied (fixities and heavy top layer), the prescribed displacement as well as the materials used.

4.4.2.1 Base case

A base case of the three-layer model has been built here in order to show the initial model which shall be varied during the work. **Table 1** lists the initial parameters of this model. Also in the **Table 4**, at the end of this section, it is possible to observe the values, in thickness, used in this case.

4.4.2.2 Variations of H_h, H_{su} and H_{sb}

In this step the thickness of the middle competent layer and the two weak or incompetent layers shall be varied in order to observe the mechanical behaviour of this middle layer and the adjacent incompetent layers surrounding the middle one. The thickness of this middle layer has been named in short H_h, whereas the thickness of the weak upper layer has been called in short H_{su}, and finally the thickness of the weak layer in the bottom of the model has been called briefly H_{sb}. Thicknesses shall be varied by means of the geometry lines in the Input Menu, changing the height of the middle competent layer and, at the same time, changing also the heights of the two adjacent incompetent layers, thus maintaining the total height of the model and keeping the competent layer in the centre of the model. In the **Table 4**, at the end of this section, it is possible to observe the different values, in thickness, used in this case.

4.4.2.3 Variations of the mechanical properties in the competent layer

These models shall investigate the changes in the mechanical behaviour of the central competent layer if its mechanical properties are varied. The thickness of this competent layer shall be the same in all the calculations. It shall be observed the development of the model depending on these parameters. The main altered parameters shall be the Young modulus (E), cohesion (c) and the friction angle (φ). Always one of these parameters shall be varied whereas the others have the value given in Table 1. Mechanical properties of the two incompetent layers surrounding the central one shall be kept constant. In the **Table 4**, at the end of this section, it is possible to observe the different values of the main altered parameters used in this case.

4.4.2.4 Variations of the mechanical properties in the incompetent layers

In order to finish the investigations about the three-layer model, the behaviour of the incompetent layers shall be studied by means of changing the mechanical parameters of these two weak layers surrounding the competent one. The main altered parameters shall be the same ones as in the preceding model series, but here for the incompetent layer. Here the mechanical properties of the central competent layer shall be kept constant at the value of the base case (**Table 1**). Also in the **Table 4**, which it can be checked at the end of this section, it is possible to observe the different values, for the different main altered parameters which have been used in this case.

4.4.3 Five-layer model

This model consists of five layers. The variation in comparison with the first model (three-layer model) is that here not all the layers have the same thickness, not even in the base model. An example of the base model is shown in **Figure 8**.

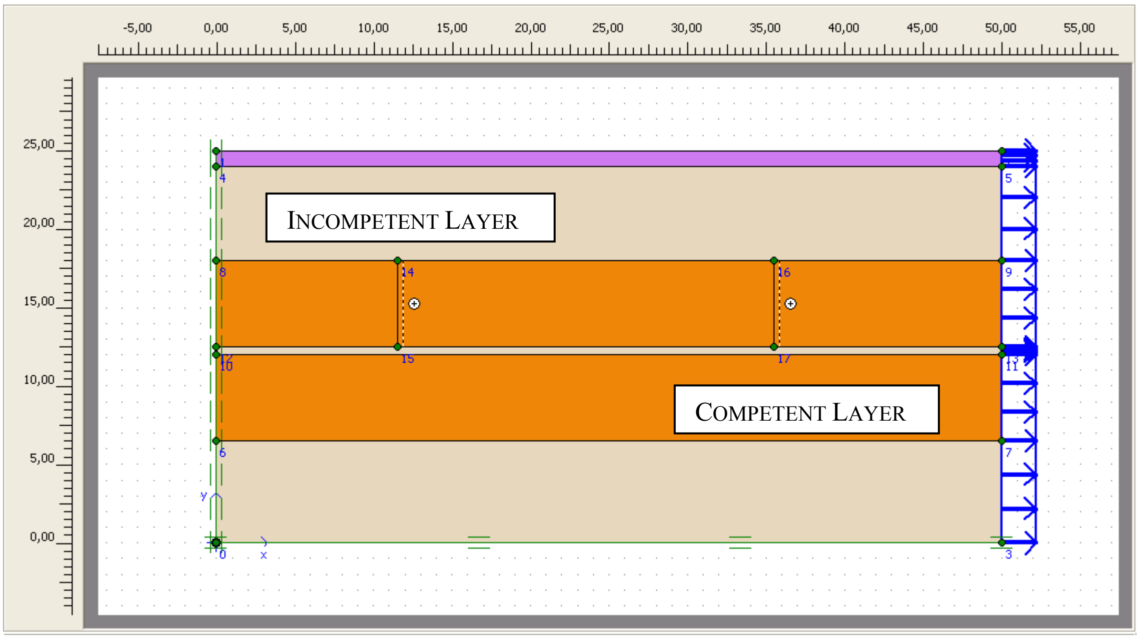

Figure 8. Example of the base case for the five-layer models. It can be observed the different boundary conditions applied (fixities and heavy top layer), the prescribed displacement as well as the materials used.

The central layer is a weak and very thin layer, surrounded by two competent layers of greater thickness. These three layers are surrounded by two weaker ones, which have the same mechanical properties as the central layer. One or several fractures will be placed in the top competent layer in the models. The main topic here is try to observe the effect of the fracture(s) in one or both of the two competent layers on the stress and strain distribution in these competent layers. Different changed features or parameters are shown immediately afterwards.

4.4.3.1 Base case

A base case of the five-layer model has been built here in order to show the initial model which shall be varied during the work. **Table 1** lists the initial parameters of this model. There shall be applied two vertical fractures in the top competent layer of the model, located at the points X=11.5 and X=35.5 from the origin.

4.4.3.2 Variations of H_{sm}

In this first step of this model the thickness of the middle incompetent layer shall be varied in order to observe the mechanical behaviour of this layer and of the adjacent competent ones. The thickness of this middle incompetent layer has been named in short H_{sm}, referring to the height of the middle soft layer. Thickness of the middle incompetent layer shall be varied by means of the geometry lines in the Input Menu, changing the height of this middle incompetent layer and, at the same time as before, changing also the heights of the upper and lower incompetent layers, but keeping the thicknesses of the competent ones in constant values, thus maintaining the total height of the model and keeping the incompetent layer in the centre of the model. It shall be interesting here, as well as in the following sections, to observe the behaviour and development of the fractures and different layers. **Table 4**, at the end of this section, is showed in order to observe the different values of H_{sm} used in this case.

4.4.3.3 Variations of the mechanical properties in the incompetent layers

The main objective in this part is to observe the influence of varying mechanical parameters of the incompetent layers. The thickness of all layers shall be the same in all the calculations. As in the previous model, the main altered parameters shall be the Young modulus (E), cohesion (c) and the friction angle (φ), but here for the three incompetent layers. Always one of these parameters shall be varied whereas the others have the value given in **Table 1**. Mechanical properties of the two competent layers surrounding the central incompetent one shall be kept constant. Also in the **Table 4**, which it can be checked at the end of this section, it is possible to observe the different values, for the different main altered parameters which have been used in this case.

4.4.3.4 Variations of the mechanical properties in the competent layers

Here we shall investigate the effect of a fracture or a small set of fractures if the mechanical properties of the competent layers are varied. The thicknesses of all layers shall be the same in all the calculations. Parameters shall be varied similar to the previous series, but here for the two competent layers. Parameters for the incompetent layers are as given in **Table 1**.

4.4.3.5 Variation of fracture spacing in the top competent layer

In order to finish this set of calculations, the behaviour of a small set of fractures situated only in the top competent layer shall be observed. As a first step one fracture shall be applied. There shall be applied successively more fractures in the same layer until arriving at a number of five fractures in the top competent layer. With this model it shall be observed the influence of the increasing fracture density in a competent layer. Height and mechanical parameters of all the layers shall not be varied in this model.

In order to have a recompilation of all the investigations and the varied parameters in the different models, **Table 4** shows all these features and where they can be observed.

MODEL	CASE	THICKNESS (m)	E (kPa)	c (kPa)	φ (°)	DISPLACEMENT	NUMBER OF FRACTURES	
Three-layer Model	Base Case	8 (each layer)	See **Table 1**			15 mm	0	3.a.1.
						15 cm	0	3.a.2.
	H_h, H_{su} and H_{sb} (variations of H_h)	4	See **Table 1**			15 cm	0	3.b.1.
		8						3.b.2.
		12						3.b.3.
	Mech. Prop. Comp. Layer	8	5.00E+05	1.00E+05	30	15 cm	0	3.c.1.
			5.00E+06	1.00E+06	45			3.c.2.
			1.00E+08	1.00E+07	60			3.c.3.
	Mech. Prop. Incomp. Layer	8	1.00E+04	5.00E+03	18	15 cm	0	3.d.1.
			5.00E+05	5.00E+05	28			3.d.2.
			5.00E+06	5.00E+06	38			3.d.3.

MODEL	CASE	THICKNESS (m)	E (kPa)	c (kPa)	φ (°)	DISPLACEMENT	NUMBER OF FRACTURES	
Five-layer Model	Base Case	See **Figure 8**	See **Table 1**			15 mm	2	5.a.1.
						15 cm	2	5.a.2.
	H_{sm}	0.5	See **Table 1**			15 cm	2	5.b.1.
		1.5						5.b.2.
		2.5						5.b.3.
	Mech. Prop. Incomp. Layers	See **Figure 8**	5.00E+04	1.00E+04	18	15 cm	2	5.c.1.
			5.00E+05	5.00E+05	28			5.c.2.
			1.00E+07	5.00E+06	38			5.c.3.
	Mech. Prop. Comp. Layers	See **Figure 8**	1.00E+05	1.00E+05	30	15 cm	2	5.d.1.
			5.00E+06	1.00E+06	45			5.d.2.
			1.00E+08	1.00E+07	60			5.d.3.
	Fracture Spacing	See **Figure 8**	See **Table 1**			15 cm	1	5.e.1.
							3	5.e.2.
							4	5.e.3.
							5	5.e.4.

Table 4. The table shows the values of all the parameters which have been used in the models. Last right column indicates a number of the investigation, and it will be used in the next section to be able to refer easily to an each one of the models.