POLLUTANT TRANSPORT MODELLING IN PARTIALLY SATURATED DEFORMABLE POROUS MEDIA

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Abstract. The main scope of this article is to carry out a mathematical framework and its corresponding finite element discretization for the solution of pollutant transport in partially saturated soils. A multiphase system with the interstitial voids in the grain matrix filled with water (liquid phase), water vapour and dry air (gas phase) and with pollutant substances, is assumed. The ensuing mathematical model involves equations of momentum balance, energy balance and mass balance of the whole multiphase system. Encouraging outcomes were achieved in several different examples.

1 INTRODUCTION

Environmental geomechanics span a wide number of engineering problems where the geomaterials mechanical equations are usually coupled with flux and mass transport equations. This area generally deals with pollutant transport problems through aquifers especially when partially saturated media is involved, because, under these circumstances, the solid phase usually undergoes large deformation and displacement due to the proper soil nature or due to the capillary pressure effect. Another relevant aspect of the environmental geomechanics science is to design safe containers for toxic wastes, nuclear wastes or pollutant leftovers, for this is a matter of prior importance in industrial societies.

Different authors have taken over this issue from several standpoints regarding different aspects or hypothesis. An early view of the problem may be found in Li and Zienkiewicz (1992). In this work, the fluid transport through porous media is simultaneously presented in one or two phases separated by an interface. No chemical reactions or components interchange between the phases are regarded and the capillary pressure is given in series form (Peaceman, 1977). Schrefler (2001), a mathematical framework assuming a multiphase porous system with voids filled with water, water vapour, dry air and pollutant along with a finite element discretization, is presented. Here, the pollutants may be mixed with the fluid phase or they may not, in which case, a new phase wherein this pollutants flow (*immiscible phase*) is considered. Similarly to the previous work, no chemical reaction between pollutant and the other phases is allowed.

Sheng and Smith (2002) present a two-dimensional finite element solution for various contaminants considering advection-dispersion transport based on previous works (Sheng and Smith, 2000). Juncosa et al. (2002), asserts the basic postulated for a mathematical framework for non isothermal multiphase flux with reactive transport and the solution for the former is undertaken. The media constituent mass balance (water, air and solute), the energy conservation principle and the equilibrium equations, describe a partial derivative system of equation that may be integrated using various approaches. In Klubertanz et al. (2003), the mathematical framework for the analysis of the miscible and immiscible flux trough porous media based on continuum mechanics was presented.

Finally, Schrefler (2001) and later on Schrefler and Pesavento (2004), relying on Hassanizadeh and Gray averaging theories (Hassanizadeh, 1986b; Hassanizadeh and Gray, 1979a,b, 1980, 1990), the analysis of isothermal flux transport is further extended to non isothermal flux bearing in mind the thermodynamics properties of the interface between the different porous media constituents (Lewis and Schrefler, 1998; Schrefler, 1995). In fact, it is the interface surface tension what holds the immiscibility between porous fluids. A null value of the surface tension conveys a null value of the capillary pressure as well, bringing on a constant fluid pressure.

In the present work, the analysis of immiscible pollutant transport through partially saturated soils coupled with the mechanical behaviour is undertaken. A mathematical framework assuming a multiphase porous media wherein the interstitial voids of the solid matrix are filled with water, dry air and pollutant is addressed as well as the solution of the arisen partial difference equation system using the finite element methods. The attained numerical model involves momentum, energy and mass balance equations.

2 REPRESENTATIVE ELEMENTAL VOLUME

In the classical mechanic, a continuum distribution of whatever particles exists (fluid or solids) for which the balance laws and constitutive relationships are valid, is taken for granted. The herein studied phenomena, occurs in domains occupied by different phases. There is an om-

nipresent phase, i.e., the solid one or solid skeleton, whose voids are taken to be filled with fluid (gas of liquid) separated by a membrane called interface. The difference between constituents and phases should be emphasised here: the phases are chemically homogeneous portions of the multiphase system which mechanical behaviour is assumed to be uniform. On the other hand, the constituents are the individual parts that yield the phases but acting each one independently, being the case in point the gaseous phase which may be constituted by a gas mix wherein each gas is a constituent.
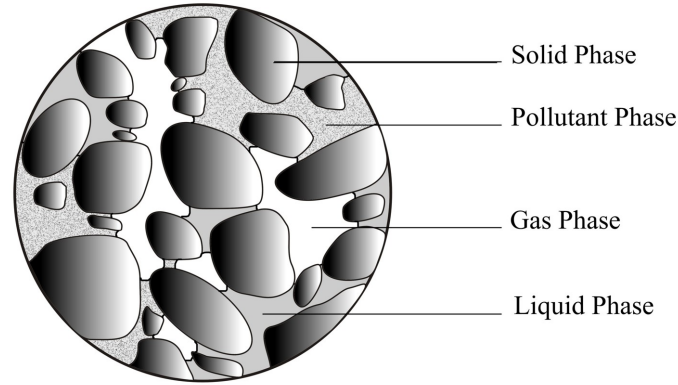

Figure 1: Representative elemental volume

There are two possible levels for describing the multiphase media intergranular configuration: The macroscopic and the microscopic level. At the microscopic level, the real porous media structure is regarded (see figure 1). The govern equations are established considering each constituent separately, giving rise to a complicated solution. Furthermore, the microscopic properties are usually awkward to assess. Considering the aforementioned reasons and adding that a microscopic description is far beyond the civil engineering goals (Di Rado, 2006), for the present work, a macroscopic description is adopted. One noteworthy feature of the macroscopic description is the fact that at each material point all the phases are assumed to be simultaneously present. In a volume fraction, the following elements may be found (Beneyto, 2003):

- Solid Phase: $\eta^s = 1 - n$, being $n = (dv^w + dv^g + dv^\pi)/dv$ the porosity and dv the differential volume of the i constituent.

- Liquid Phase: $\eta^w = nS_w$, being $S_w = dv^w/(dv^w + dv^g + dv^\pi)$ the water saturation degree.

- Gaseous Phase: $\eta^g = nS_g$, being $S_g = dv^g/(dv^w + dv^g + dv^\pi)$ the air saturation degree.

- Pollutant phase: $\eta^\pi = nS_\pi$, being $S_\pi = dv^\pi/(dv^w + dv^g + dv^\pi)$ the pollutant saturation degree.

From the aforesaid equations yields:

$$S_w + S_g + S_\pi = 1 \tag{1}$$

and the multiphase media density is

$$\rho = \rho_s + \rho_w + \rho_g + \rho_\pi = (1 - n)\rho^s + nS_w\rho^w + nS_g\rho^g + nS_\pi\rho^\pi \tag{2}$$

Within this condition and provided that the medium is constituted by different phases, any of them may be described relatively to any other previously defined, i.e., the solid one. Thereby, relative velocities of the liquid, gaseous and pollutant may be addressed:

$$v^{ws} = v^w - v^s \quad , \quad v^{gs} = v^g - v^s \quad , \quad v^{\pi s} = v^\pi - v^s \tag{3}$$

3 GOVERN EQUATION

3.1 Microscopic balance equations

The classical continuum mechanic balance equations will be taken into account in order to obtain the microscopic behaviour of an individual phase γ. For any thermodynamic attribute, ψ, the general conservation equation for a single phase may be written (Malvern, 1969; Oliver, 2000):

$$\frac{\partial \rho \psi}{\partial t} + \text{div}\,(\rho \psi \dot{\boldsymbol{r}}) - \text{div}\,\boldsymbol{i} - \rho\,\boldsymbol{b} = \rho\,\boldsymbol{G} \tag{4}$$

where $\dot{\boldsymbol{r}}$ is the phase local velocity in a fix spatial point, ρ is the density, $\boldsymbol{b}$ is the external supply, $\boldsymbol{i}$ is the associated flux vector and $\boldsymbol{G}$ is the internal net production of ψ.

To set up balance equations for a certain thermodynamic attribute, the state variables $\boldsymbol{i}$, $\boldsymbol{b}$ and $\boldsymbol{G}$ must been alternatively modified. Being a case in point, the mass balance equation is given by:

$$\psi = 1 \quad ; \quad \boldsymbol{i} = 0 \quad ; \quad \boldsymbol{b} = 0 \quad ; \quad \boldsymbol{G} = 0 \tag{5}$$

introducing these values in (4), the microscopic mass balance equation is given by:

$$\frac{\partial \rho}{\partial t} + \text{div}\,(\rho \dot{\boldsymbol{r}}) = 0 \tag{6}$$

3.2 Macroscopic balance equations

The macroscopic balance equations are obtained by the systematic application of the pioneer work of Hassanizadeh and Gray (1980) to the microscopic balance equations (4), in which for each constituent, the thermodynamic variable is substituted by the appropriate microscopic property (Lewis and Schrefler, 1998). The pollutant behaviour may be depicted in two different forms depending on its mixing capability with the fluid or with the gaseous phase. The most general situation, i.e. with immiscible pollutants, the behaviour may be described as another fluid phase, whereas with soluble pollutant, three possible transport processes must be considered: advection, diffusion and dispersion.

3.2.1 Solid Phase

From Eq. (6) and recalling the material time derivative of a spatial magnitude (Malvern, 1969) the mass balance expression for the solid phase is obtained:

$$\frac{\partial \rho_s}{\partial t} + \rho_s \text{div}\, v^s = 0 \tag{7}$$

where v^s is the solid skeleton velocity.

$$\text{div}\,(\rho_s v^s) = \rho_s \text{div}\, v^s + grad\,\rho_s \cdot v^s \tag{8}$$

Since (8) and taking into account (2), it is obtained:

$$\frac{(1-n)}{\rho^s}\frac{\partial \rho^s}{\partial t} - \frac{\partial n}{\partial t} + (1-n)\operatorname{div} v^s = 0 \tag{9}$$

3.2.2 Liquid Phase

The microscopic mass balance equation for the liquid phase is tantamount to the corresponding one for the solid phase (4) being the identity different form zero ($G \neq 0$) due to the water possibility of transforming into vapour and the other way around.

$$\frac{\partial \rho_w}{\partial t} + \rho_w \operatorname{div} v^w = -\dot{\boldsymbol{m}} \tag{10}$$

where v^w is the liquid phase mass velocity and $-\dot{\boldsymbol{m}}$ is the water amount per unit volume of transformed into vapour. Taking into account (2), it leads us to:

$$\frac{\partial (nS_w\rho^w)}{\partial t} + nS_w\rho^w \operatorname{div} v^w = -\dot{\boldsymbol{m}} \tag{11}$$

Working with the above formula and after some algebra as well as considering the Eq. (3) and (8) and adding the result to (9), the subsequent expression is yielded:

$$\frac{(1-n)}{\rho^s}\frac{\partial \rho^s}{\partial t} + \operatorname{div} v^s + \frac{n}{\rho^w}\frac{\partial \rho^w}{\partial t} + \frac{n}{S_w}\frac{\partial S_w}{\partial t} + \frac{1}{S_w\rho^w}\operatorname{div}(nS_w\rho^w \cdot v^{ws}) = -\frac{\dot{m}}{S_w\rho^w} \tag{12}$$

3.2.3 Gaseous Phase

The here considered gaseous phase is composed by two constituents: dry air (ga) and water vapour (gw). Since both elements are miscible and their physical behaviour is similar, they may be treated as a single phase occupying the same differential volume, nS_g. Regardless of the internal mass production due to self-chemical reactions, the microscopic balance equation for this phase is once more given by (6) (Hassanizadeh, 1986a).

$$\frac{\partial}{\partial t}(nS_g\rho^{ga}) + \operatorname{div}(nS_g\rho^{ga}v^{ga}) = 0 \tag{13}$$

Likewise, making use of the gw superscript, the vapour balance equation is obtained:

$$\frac{\partial}{\partial t}(nS_g\rho^{gw}) + \operatorname{div}(nS_g\rho^{gw}v^{gw}) = \dot{\boldsymbol{m}} \tag{14}$$

Clearly, given expressions (13) and (14), the mass balance equation for the dry air and water vapour mixture will be:

$$\frac{\partial}{\partial t}(nS_g\rho^g) + \operatorname{div}(nS_g\rho^g v^g) = \dot{\boldsymbol{m}} \tag{15}$$

with $\rho^g = \rho^{ga} + \rho^{gw}$ y $v^g = 1/\rho^g (\rho^{ga}v^{ga} + \rho^{gw}v^{gw})$

Working with eq. (15), an expression tantamount to eq. (11) is obtained:

$$\frac{\partial (nS_g\rho^g)}{\partial t} + nS_g\rho^g \operatorname{div} v^g = \dot{\boldsymbol{m}} \tag{16}$$

Once more, after some algebraic manipulation of the above with inclusion of expressions (3) and (8) and adding the remainder to equation (9), the subsequent relationship is yielded:

$$\frac{(1-n)}{\rho^s}\frac{\partial \rho^s}{\partial t} + \text{div } v^s + \frac{n}{S_g}\frac{\partial S_g}{\partial t} + \frac{n}{\rho^g}\frac{\partial \rho^g}{\partial t} + \frac{1}{S_g\rho^g}\text{div}\left(nS_g\rho^g \cdot v^{gs}\right) = \frac{\dot{\boldsymbol{m}}}{S_g\rho^g} \tag{17}$$

3.2.4 Immiscible Pollutant

When the pollutant existing in the porous media has no miscible property with any of the non solids phases, it is clearly taking part of a new phase, π. One way of coping with this phenomenon is to consider the pollutant behaviour similar to the liquid phase one (Schrefler, 2001), whereby it is possible to yield the conservation equations for the pollutant as well as it was done for the liquid phase. Therefore, the mass balance equation for immiscible pollutants will be likewise Eq. (12) but without the internal production term (source), $\dot{\boldsymbol{m}} = 0$.

$$\frac{(1-n)}{\rho^s}\frac{\partial \rho^s}{\partial t} + \text{div } v^s + \frac{n}{\rho^\pi}\frac{\partial \rho^\pi}{\partial t} + \frac{n}{S_\pi}\frac{\partial S_\pi}{\partial t} + \frac{1}{S_\pi\rho^\pi}\text{div}\left(nS_\pi\rho^\pi \cdot v^{\pi s}\right) = 0 \tag{18}$$

3.3 Constitutive and state relationships

To provide a complete description of the mechanical behaviour, the constitutive equations are required. The balance equations developed in the previous section take into account elaborate constitutive theories, especially when these equations are valid at the interfaces (Hassanizadeh and Gray, 1980).

3.3.1 Fluid phase stress tensor

By the application of the second law of thermodynamics to the porous media (Hassanizadeh and Gray, 1979b), the stress tensor for the fluid phase may be written as

$$\boldsymbol{t}^\gamma = -\eta^\gamma p^\gamma \boldsymbol{I} \tag{19}$$

being $\boldsymbol{I}$ the unit tensor, p^γ is the phase γ pressure and η^γ is the phase volume fraction. It may be clearly noticed that no deviatoric stresses are present in the fluid phase stress tensor.

3.3.2 Solid phase stress tensor

As well as in the previous section, by means of the use of the second law of thermodynamics for the porous media (Hassanizadeh and Gray, 1980), the stress tensor for the solid phase is conveyed:

$$\boldsymbol{t}^s = (1-n)\left(\boldsymbol{t}_e^s - \boldsymbol{I}p^s\right) \tag{20}$$

while the solid phase pressure is

$$p^s = S_w p^w + S_g p^g + S_\pi p^\pi \tag{21}$$

and the effective stress tensor is

$$\boldsymbol{\sigma}' = (1-n)\,\boldsymbol{t}_e^s \tag{22}$$

Introducing (21) in (20)

$$\boldsymbol{t}^s = (1-n)\left[\boldsymbol{t}^s_e - \boldsymbol{I}\left(S_w p^w + S_g p^g + S_\pi p^\pi\right)\right] \tag{23}$$

The volume fraction $(1-n)$ points out that $\boldsymbol{t}^s$ stands for is the stress per unit of area exerted over the solid phase. In order to obtain the total stress, $\boldsymbol{\sigma}$, the expressions derived for the liquid and the gaseous phases (23) must be added to (19), giving:

$$
\begin{aligned}
\boldsymbol{\sigma} = \boldsymbol{t}^s + \boldsymbol{t}^w + \boldsymbol{t}^g + \boldsymbol{t}^\pi = \\
(1-n)\left[\boldsymbol{t}^s_e - \boldsymbol{I}\left(S_w p^w + S_g p^g + S_\pi p^\pi\right)\right] - nS_w p^w \boldsymbol{I} - nS_g p^g \boldsymbol{I} - nS_\pi p^\pi \boldsymbol{I} = \\
(1-n)\boldsymbol{t}^s_e - \boldsymbol{I}\left(S_w p^w + S_g p^g + S_\pi p^\pi\right) \quad (24)
\end{aligned}
$$

The precedent equation may be arranged following the most well known form in soil mechanics (Fredlund and Rahardjo, 1993; Lambe and Whitman, 1979):

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}' + \boldsymbol{I}\left(p^w S_w + p^g S_g + p^\pi S_\pi\right) \tag{25}$$

3.3.3 Solid mass density

Considering a compressible solid mass, an expression for the time derivative of the solid mass density may be obtained from the mass conservation differential equation:

$$\frac{\partial\left(\rho^s V^s\right)}{\partial t} = 0 \tag{26}$$

Assuming that the solid mass density is function of p^s (21), of the temperature and of the first effective stress tensor invariant, it is obtained:

$$\frac{1}{\rho^s}\frac{\partial\rho^s}{\partial t} = -\frac{1}{V_s}\frac{\partial V_s}{\partial t} = \frac{1}{K_s}\frac{\partial p^s}{\partial t} - \beta_s\frac{\partial T}{\partial t} - \frac{1}{3\left(n-1\right)K_s}\frac{\partial\left(\mathrm{tr}\boldsymbol{\sigma}'\right)}{\partial t} \tag{27}$$

wherein the following expressions were regarded:

$$\frac{1}{\rho^s}\frac{\partial\rho^s}{\partial p^s} = \frac{1}{K_s} \tag{28}$$

$$\frac{1}{\rho^s}\frac{\partial\rho^s}{\partial T} = -\beta_s \tag{29}$$

$$\frac{1}{\rho^s}\frac{\partial\rho^s}{\partial\left(\mathrm{tr}\boldsymbol{\sigma}'\right)} = \frac{1}{3\left(n-1\right)K_s} \tag{30}$$

in the previous, K_s is the grain compressibility coefficient, β_s is the grain thermal expansion and $\mathrm{tr}\boldsymbol{\sigma}'$ is the first invariant of the stress tensor. Bearing in mind the constitutive relationship for the first invariant of the effective stress tensor (Malvern, 1969):

$$\frac{\partial\mathrm{tr}\boldsymbol{\sigma}'}{\partial t} = 3K_T\left(\mathrm{div}\boldsymbol{v}^s + \frac{1}{K_s}\frac{\partial p^s}{\partial t} - \beta_s\frac{\partial T}{\partial t}\right) \tag{31}$$

where, K_T, is the skeleton bulk modulus. Considering the Biot constant definition (Biot and Willis, 1957):

$$(1 - \alpha) = \frac{K_T}{K_s} \tag{32}$$

and expressions (31) and (27), it is obtained::

$$\frac{1}{\rho^s} \frac{\partial \rho^s}{\partial t} = \frac{1}{1 - n} \left[(\alpha - n) \frac{1}{K_s} \frac{\partial p^s}{\partial t} - \beta_s (\alpha - n) \frac{\partial T}{\partial t} - (1 - \alpha) \operatorname{div} v^s \right] \tag{33}$$

The incompressible grain condition, i.e. $1/K_s = 0$, $\alpha = 1$, whatsoever indicates a rigid or incompressible skeleton, since under load application, an interstitial voids re-arrangements is undertaken.

3.3.4 State equation for the liquid phase

The water solid state equation was developed by Fernandez (1972) and it is given by:

$$\rho^w = \rho^{wo} \exp\left[-\beta_w T + C_w (p^w - p^{wo})\right] \tag{34}$$

where the superscript o stands for the initial state, β_w is the thermal expansion coefficient and C_w is the compressibility coefficient. Taking the series expansion of (19) and disregarding the higher order terms, it is obtained

$$\rho^w = \rho^{wo} \left[1 - \beta_w T + C_w (p^w - p^{wo})\right] \tag{35}$$

being the time derivative:

$$\frac{1}{\rho^{wo}} \frac{\partial \rho^w}{\partial t} = \frac{1}{K_w} \frac{\partial p^w}{\partial t} - \beta_w \frac{\partial T}{\partial t} \tag{36}$$

where $K_w = 1/C_w$ is the water bulk modulus. The previous formula may be also obtained from the mass balance differential equation (Lewis and Schrefler, 1998).

3.3.5 State equation for the gaseous phase

The gaseous phase may be considered as a mixture of perfect ideal gases, dry air and water vapour. Therefore, it is possible to apply the ideal gas laws by relating the constituent partial pressure, the constituent mass concentration in the gaseous phase, $p^{g\gamma}$, of the γ component, and the absolute temperature θ. The perfect gas state equations applied to dry air (ga), to water vapour (qw) and to the air (g), are (Fredlund and Rahardjo, 1993):

$$p^{ga} = \rho^{ga} \theta R / M_a \tag{37}$$

$$p^{gw} = \rho^{gw} \theta R / M_w \tag{38}$$

$$\rho^g = \rho^{ga} + \rho^{gw} \tag{39}$$

$$p^g = p^{ga} + p^{gw} \tag{40}$$

$$M_g = \left(\frac{\rho^{gw}}{\rho^g} \frac{1}{M_w} + \frac{\rho^{ga}}{\rho^g} \frac{1}{M_a} \right)^{-1} \tag{41}$$

where M_γ is the constituent molar mass and R is the universal gas constant.

4 GENERAL FIELD EQUATIONS

Macroscopic balance laws are currently transformed by the introduction of the constitutive relationships previously defined in section 3.3.

4.1 Solid phase

The solid phase behaviour may be conveniently depicted using the lineal momentum balance equation, which is obtained from eq. (4) by appropriately setting the state variables i, b and G (Lewis and Schrefler, 1998).

$$\boldsymbol{L}^T \boldsymbol{\sigma} + \rho \boldsymbol{g} = 0 \tag{42}$$

being the differential operator:

$$\boldsymbol{L}^T = \begin{vmatrix} \partial/\partial x & 0 & 0 & \partial/\partial y & 0 & \partial/\partial z \\ 0 & \partial/\partial y & 0 & \partial/\partial x & \partial/\partial z & 0 \\ 0 & 0 & \partial/\partial z & 0 & \partial/\partial y & \partial/\partial x \end{vmatrix} \tag{43}$$

4.2 Liquid phase

Taking the Derivative of the degree saturation of the different phases (1) with respect to time and clearing $\partial S_g/\partial t$, it is obtained:

$$\frac{\partial S_g}{\partial t} = -\frac{\partial S_w}{\partial t} - \frac{\partial S_\pi}{\partial t} \tag{44}$$

Introducing the liquid phase state equation (36), the solid phase pressure definition (21) and the solid phase density (33) in the macroscopic balance of the liquid phase, (12), and constraining the problem to an isothermal condition,

$$\left[S_w^2 \frac{(\alpha - n)}{K_s} + \frac{nS_w}{K_w} \right] \frac{\partial p^w}{\partial t} + \left[\frac{(\alpha - n)}{K_s} S_w S_g \right] \frac{\partial p^g}{\partial t} + \left[\frac{(\alpha - n)}{K_s} S_w S_\pi \right] \frac{\partial p^\pi}{\partial t}$$
$$+ \alpha \, S_w m^T L \frac{\partial u}{\partial t} + \left[\frac{(\alpha - n)}{K_s} S_w p^w - \frac{(\alpha - n)}{K_s} S_w p^g + n \right] \frac{\partial S_w}{\partial t} + S_w \frac{(\alpha - n)}{K_s} \left[p^\pi - p^g \right] \frac{\partial S_\pi}{\partial t}$$
$$+ \frac{1}{\rho^w} \nabla^T \left[\frac{k k^{rw}}{\mu^w} \left(-\nabla p^w + \rho^w g \right) \right] = 0 \quad (45)$$

Terms like $\partial S_w/\partial t$ y $\partial S_\pi/\partial t$ may be written as

$$n \frac{\partial S_w}{\partial t} = n \frac{\partial S_w}{\partial p^{gw}} \frac{\partial p^{gw}}{\partial t} = C_w \frac{\partial p^{gw}}{\partial t} = C_w \left(\frac{\partial p^g}{\partial t} - \frac{\partial p^w}{\partial t} \right)$$
$$n \frac{\partial S_\pi}{\partial t} = n \frac{\partial S_\pi}{\partial p^{g\pi}} \frac{\partial p^{g\pi}}{\partial t} = C_\pi \frac{\partial p^{g\pi}}{\partial t} = C_\pi \left(\frac{\partial p^g}{\partial t} - \frac{\partial p^\pi}{\partial t} \right) \tag{46}$$

where $n\partial S_w/\partial p^{gw} = C_w$ is the derivative of the water saturation with respect to the suction which may be obtained with the aid of the soil characteristic curve $(S_w - p^{gw})$ (Fredlund and Xing, 1994; Beneyto et al., 2005). Since the π phase behaves like a fluid, an equivalent analysis may be achieved by the mere implementation of a new $S_\pi - p^{g\pi}$ curve which allows the assessment of the derivative $n\partial S_\pi/\partial p^{g\pi} = C_\pi$ as well as it was done for the water (Pao and

Lewis, 2002). One possibility is the adoption of a hyperbolic function (Bolzon et al., 1996) for the abovementioned $S_\pi - p^{g\pi}$ curve.

$$\alpha_{22}\frac{\partial p^w}{\partial t} + \alpha_{23}\frac{\partial p^g}{\partial t} + \alpha_{24}\frac{\partial p^\pi}{\partial t} + \alpha_{21}L\frac{\partial u}{\partial t} + \frac{1}{\rho^w}\nabla^T\left[\frac{kk^{rw}}{\mu^w}\left(-\nabla p^w + \rho^w g\right)\right] = 0 \qquad (47)$$

with

$$
\begin{aligned}
\alpha_{21} &= \alpha\ S_w m^T \\
\alpha_{22} &= \frac{(\alpha - n)}{K_s}S_w\left(S_w - p^w\frac{C_w}{n} + p^g\frac{C_w}{n}\right) + \frac{nS_w}{K_w} - C_w \\
\alpha_{23} &= \frac{(\alpha - n)}{K_s}S_w\left(S_g + p^w\frac{C_w}{n} - p^g\frac{C_w}{n} + (p^\pi - p^g)\frac{C_\pi}{n}\right) + C_w \\
\alpha_{24} &= \frac{(\alpha - n)}{K_s}S_w\left(S_\pi - (p^\pi - p^g)\frac{C_\pi}{n}\right)
\end{aligned}
\qquad (48)
$$

4.3 Gaseous phase

From the gaseous phase balance equation for isothermal processes (17) and regarding the state equation for the gaseous phase (41), the relative velocity definition (3), the solid phase density 33 and the expressions (44) and (46), the following mathematical statement is obtained:

$$
\begin{aligned}
&\left[\frac{(\alpha - n)}{K_s}S_g\left(S_w - \frac{C_w}{n}(p^w - p^g)\right) + C_w\right]\frac{\partial p^w}{\partial t} \\
&+ \left[\frac{(\alpha - n)}{K_s}S_g\left(S_g + \frac{C_w}{n}(p^w - p^g) + \frac{C_\pi}{n}(p^\pi - p^g)\right) - C_w - C_\pi + \frac{nS_g M_g}{\rho^g \theta R}\right]\frac{\partial p^g}{\partial t} \\
&\qquad + \left[\frac{(\alpha - n)}{K_s}S_g\left(S_\pi - \frac{C_\pi}{n}(p^\pi - p^g)\right) + C_\pi\right]\frac{\partial p^\pi}{\partial t} \\
&\qquad\qquad + \alpha S_g\ m^T L\frac{\partial u}{\partial t} + \frac{1}{\rho^g}\nabla^T\left[\frac{kk^{rg}}{\mu^g}\left(-\nabla p^g + \rho^g g\right)\right] = 0 \quad (49)
\end{aligned}
$$

which may be written similarly to the equation (47)

$$\alpha_{32}\frac{\partial p^w}{\partial t} + \alpha_{33}\frac{\partial p^g}{\partial t} + \alpha_{34}\frac{\partial p^\pi}{\partial t} + \alpha_{31}L\frac{\partial u}{\partial t} + \frac{1}{\rho^g}\nabla^T\left[\frac{kk^{rg}}{\mu^g}\left(-\nabla p^g + \rho^g g\right)\right] = 0 \qquad (50)$$

with

$$
\begin{aligned}
\alpha_{31} &= \alpha S_g\ m^T \\
\alpha_{32} &= \frac{(\alpha - n)}{K_s}S_g\left(S_w + \frac{C_w}{n}(p^g - p^w)\right) + C_w \\
\alpha_{33} &= \frac{(\alpha - n)}{K_s}S_g\left(S_g - \frac{C_w}{n}(p^g - p^w) - \frac{C_\pi}{n}(p^g - p^\pi)\right) - C_w - C_\pi + \frac{nS_g M_g}{\rho^g \theta R} \\
\alpha_{34} &= \frac{(\alpha - n)}{K_s}S_g\left(S_\pi + \frac{C_\pi}{n}(p^g - p^\pi)\right) + C_\pi
\end{aligned}
\qquad (51)
$$

4.4 Immiscible pollutant phase

Whenever the pollutant is unable to mix with the liquid phase and accordingly to what was settled herein, it is clearly forming a new phase, π. The mathematical framework may be stated likewise the liquid phase (Schrefler, 2001). From the immiscible pollutant mass balance equation for isothermal processes (18) and regarding expressions (33), (36), (44) and (46) it is obtained:

$$
\begin{aligned}
& \left[\frac{(\alpha - n)}{K_s} S_\pi \left[S_w - (p^w - p^g) \frac{C_w}{n} \right] \right] \frac{\partial p^w}{\partial t} \\
& \quad + \left[\frac{(\alpha - n)}{K_s} S_\pi \left[S_g + (p^w - p^g) \frac{C_w}{n} + (p^\pi - p^g) \frac{C_\pi}{n} \right] + C_\pi \right] \frac{\partial p^g}{\partial t} \\
& \qquad + \left[\frac{(\alpha - n)}{K_s} S_\pi \left[S_\pi - (p^\pi - p^g) \frac{C_\pi}{n} \right] + \frac{n S_\pi}{K_\pi} - C_\pi \right] \frac{\partial p^\pi}{\partial t} \\
& \qquad\qquad + \alpha \, S_\pi m^T L \frac{\partial u}{\partial t} + \frac{1}{\rho^\pi} \nabla^T \left[\frac{k k^{r\pi}}{\mu^\pi} \left(-\nabla p^\pi + \rho^\pi g \right) \right] = 0 \quad (52)
\end{aligned}
$$

which may be expressed likewise the equation (47)

$$
\alpha_{42} \frac{\partial p^w}{\partial t} + \alpha_{43} \frac{\partial p^g}{\partial t} + \alpha_{44} \frac{\partial p^\pi}{\partial t} + \alpha_{41} L \frac{\partial u}{\partial t} + \frac{1}{\rho^\pi} \nabla^T \left[\frac{k k^{r\pi}}{\mu^\pi} \left(-\nabla p^\pi + \rho^\pi g \right) \right] = 0 \qquad (53)
$$

with

$$
\begin{aligned}
\alpha_{41} &= \alpha \, S_\pi m^T \\
\alpha_{42} &= \frac{(\alpha - n)}{K_s} S_\pi \left[S_w - (p^w - p^g) \frac{C_w}{n} \right] \\
\alpha_{43} &= \frac{(\alpha - n)}{K_s} S_\pi \left[S_g + (p^w - p^g) \frac{C_w}{n} + (p^\pi - p^g) \frac{C_\pi}{n} \right] + C_\pi \\
\alpha_{44} &= \frac{(\alpha - n)}{K_s} S_\pi \left[S_\pi - (p^\pi - p^g) \frac{C_\pi}{n} \right] + \frac{n S_\pi}{K_\pi} - C_\pi
\end{aligned} \qquad (54)
$$

5 DISCREET MATHEMATICAL MODEL

By the application of Galerkin method to the differential system of equations described by equations (42), (47), (50) and (53), and dicretizing using the finite element method (Bathe, 1996), the following algebraic system is furnished:

$$
\boldsymbol{K}_E \frac{\partial \bar{\boldsymbol{u}}}{\partial t} + \boldsymbol{C}_{sw} \frac{\partial \bar{p}^w}{\partial t} + \boldsymbol{C}_{sg} \frac{\partial \bar{p}^g}{\partial t} + \boldsymbol{C}_{s\pi} \frac{\partial \bar{p}^\pi}{\partial t} = \frac{\partial \boldsymbol{f}^u}{\partial t} \tag{55}
$$

$$
\boldsymbol{P}_{ww} \frac{\partial \bar{p}^w}{\partial t} + \boldsymbol{C}_{wg} \frac{\partial \bar{p}^g}{\partial t} + \boldsymbol{C}_{w\pi} \frac{\partial \bar{p}^\pi}{\partial t} + \boldsymbol{C}_{ws} \frac{\partial \bar{\boldsymbol{u}}}{\partial t} + \boldsymbol{H}_{ww} \bar{p}^w = \boldsymbol{f}^w \tag{56}
$$

$$
\boldsymbol{C}_{gw} \frac{\partial \bar{p}^w}{\partial t} + \boldsymbol{P}_{gg} \frac{\partial \bar{p}^g}{\partial t} + \boldsymbol{C}_{g\pi} \frac{\partial \bar{p}^\pi}{\partial t} + \boldsymbol{C}_{gs} \frac{\partial \bar{\boldsymbol{u}}}{\partial t} + \boldsymbol{H}_{gg} \bar{p}^g = \boldsymbol{f}^g \tag{57}
$$

$$
\boldsymbol{C}_{\pi w} \frac{\partial \bar{p}^w}{\partial t} + \boldsymbol{C}_{\pi g} \frac{\partial \bar{p}^g}{\partial t} + \boldsymbol{P}_{\pi\pi} \frac{\partial \bar{p}^\pi}{\partial t} + \boldsymbol{C}_{\pi s} \frac{\partial \bar{\boldsymbol{u}}}{\partial t} + \boldsymbol{H}_{\pi\pi} \bar{p}^\pi = \boldsymbol{f}^\pi \tag{58}
$$

Re arranging the terms and using a matrix description, it is obtained

$$
\begin{bmatrix}
\boldsymbol{K}_E & \boldsymbol{C}_{sw} & \boldsymbol{C}_{sg} & \boldsymbol{C}_{s\pi} \\
\boldsymbol{C}_{ws} & \boldsymbol{P}_{ww} & \boldsymbol{C}_{wg} & \boldsymbol{C}_{w\pi} \\
\boldsymbol{C}_{gs} & \boldsymbol{C}_{gw} & \boldsymbol{P}_{gg} & \boldsymbol{C}_{g\pi} \\
\boldsymbol{C}_{\pi s} & \boldsymbol{C}_{\pi w} & \boldsymbol{C}_{\pi g} & \boldsymbol{P}_{\pi\pi}
\end{bmatrix}
+
\begin{bmatrix}
\dot{\bar{\boldsymbol{u}}} \\
\dot{\bar{p}}^w \\
\dot{\bar{p}}^g \\
\dot{\bar{p}}^\pi
\end{bmatrix}
+
\begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & \boldsymbol{H}_{ww} & 0 & 0 \\
0 & 0 & \boldsymbol{H}_{gg} & 0 \\
0 & 0 & 0 & \boldsymbol{H}_{\pi\pi}
\end{bmatrix}
\begin{bmatrix}
\bar{\boldsymbol{u}} \\
\bar{p}^w \\
\bar{p}^g \\
\bar{p}^\pi
\end{bmatrix}
=
\begin{bmatrix}
\dot{\boldsymbol{f}}^u \\
\boldsymbol{f}^w \\
\boldsymbol{f}^g \\
\boldsymbol{f}^\pi
\end{bmatrix}
$$

(59)

All the matrices and vectors are presented in the appendix 1.

6 NUMERICAL EXAMPLES

6.1 Unidimentional soil column problem

The following example consists in a non saturated soil column with liquid and gaseous substances as well as another immiscible substance gathered in the solid skeleton voids. The sample may be treated as a unidimensional model.

The physical and geometric data of the problem are given as follows: Wide $B = 0.10m$; height $H = 1.00m$; load $q = 10.0Kpa$; Young's modulus $E = 1000.0Kpa$; Poisson's ratio $\mu = 0.3$; internal friction $\phi = 30° = 0,5236rad$; cohesion $c = 50.0Kpa$; initial void ratio $e_0 = 2.0$; vertical permeability coefficient $k_y = 0.00864m/dia$; water and pollutant compressibility coefficient $K_f = K_\pi = 1000000.0Kpa$; initial water saturation degree $S_w = 0.50$; initial pollutant saturation degree $S_\pi = 0.40$. The pore pressures on the top surface are set to zero (atmospheric pressure), whereas the boundary conditions for displacements are indicated in figure 2.
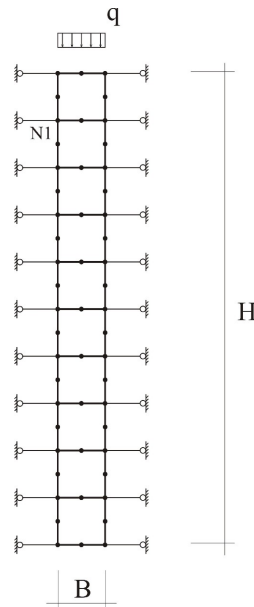

Figure 2: FEM Mesh and boundary condition

In figure 3a, 3b, 3c and 3d, plots standing for displacements vs. time (settlement evolution), the pollutant saturation vs. time as well as the pore water and pore pollutant values vs. time, were respectively presented.

A further discussion on the results shown in figure 3 allows pointing out that the pore pressure evolution is indeed in agreement with the solid phase deformation as well as with the saturation

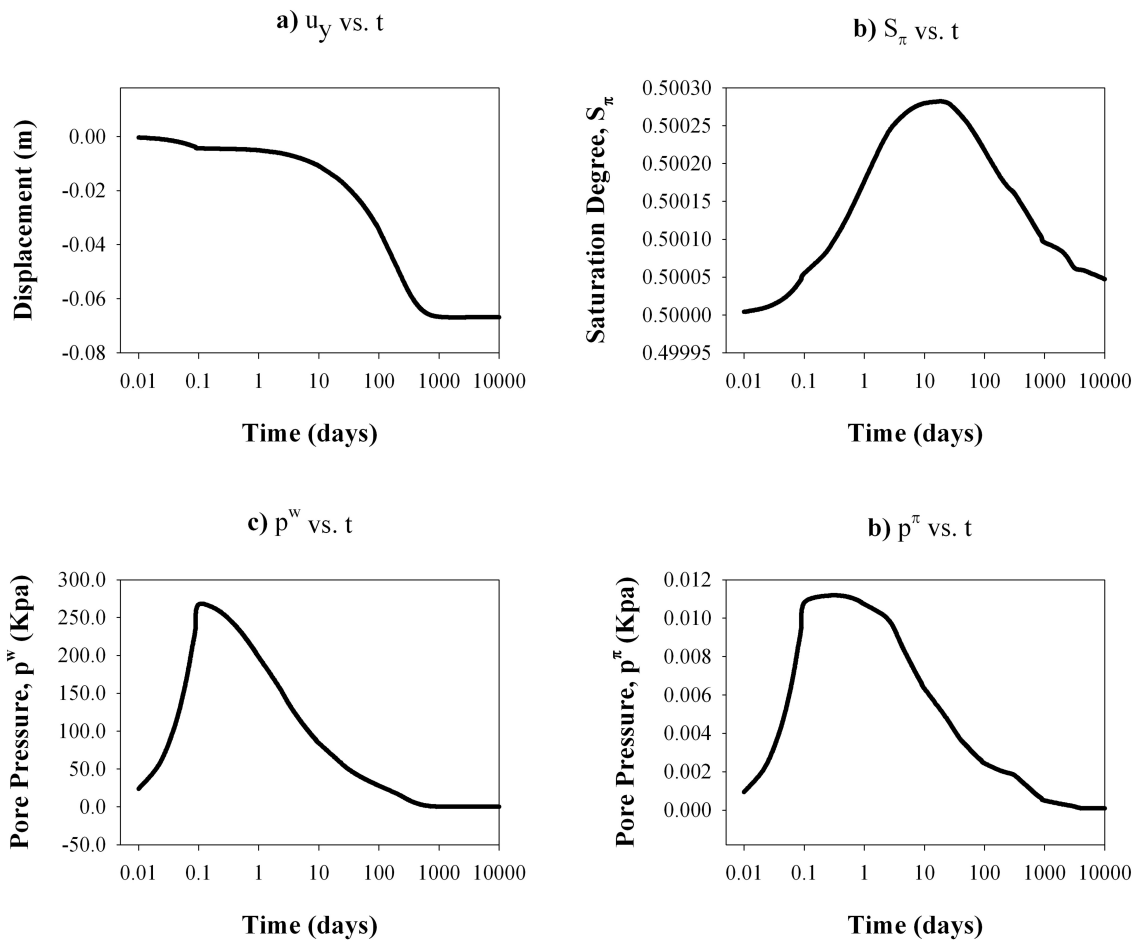degree decrease due to the reduction of the interstitial voids with the load process evolution.

a) u_y vs. t

b) S_π vs. t

c) p^w vs. t

b) p^π vs. t

Figure 3: Unidimentional soil column. Numerical result: a) Displacement vs. Time ; b) Pollutant saturation degree vs. Time ; c) Water pore pressure vs. Time ; d) Pollutant pore pressure vs. Time

6.2 Aquifer exploitation

The next example consists in an aquifer exploitation trough a typical soil profile found in the Northeast region of the Argentine Republic (NEA in spanish). The superficial layer is constituted by a low saturation sand (*soil 1*), the following layer is constituted by a saturated clay-type soil with a considerably low permeability coefficient (*soil 2*) and the last and deepest layer, is constituted by an almost saturated sand with the presence of an immiscible pollutant (*soil 3*) in its voids.

The problem data is given as follows: Height $H = 2.00m$; wide $B = 2.00m$; diameter of the well $d = 0.20m$. The physical characteristics of the different soil layers are given in table 1.

The finite element mesh used for this example, is constituted by 286 serendipity rectangular eight nodes elements. In figure 4, the displacement boundary conditions as well as the mentioned finite element mesh, is presented.

Likewise the previous example, the pore pressure for the nodes in contact with the atmosphere was set to zero. Finally, figures 6 and 5 shows respectively the pollutant and water pore pressure evolution.

Soils properties	Soil 1	Soil 2	Soil 3
Young´s modulus, $E[Kpa]$	3000.0	1500.0	2500.0
Poisson´s ratio, μ	0.3	0.3	0.3
Specific gravity, $\gamma[tn/m^3]$	2.0	2.0	2.5
Internal friction, $\phi[rad]$	0,5236	0,5236	0,5236
Cohesion, $c[Kpa]$	0.0	50.0	50.0
initial void ratio, e_0	1.0	2.0	1.0
Grains compressibility, $K_s[Kpa]$	1000000.0	1000000.0	1000000.0
Horizontal permeability coefficient, $k_x[m/dia]$	1.728	0.001728	0.01728
Vertical permeability coefficient, $k_y[m/dia]$	0.864	0.000864	0.00864
Water initial water saturation degree, S_w	0.40	0.50	0.40
Pollutant initial water saturation degree, S_π	0.00	0.50	0.50

Table 1: Physical properties of a NEA characteristic ground profile
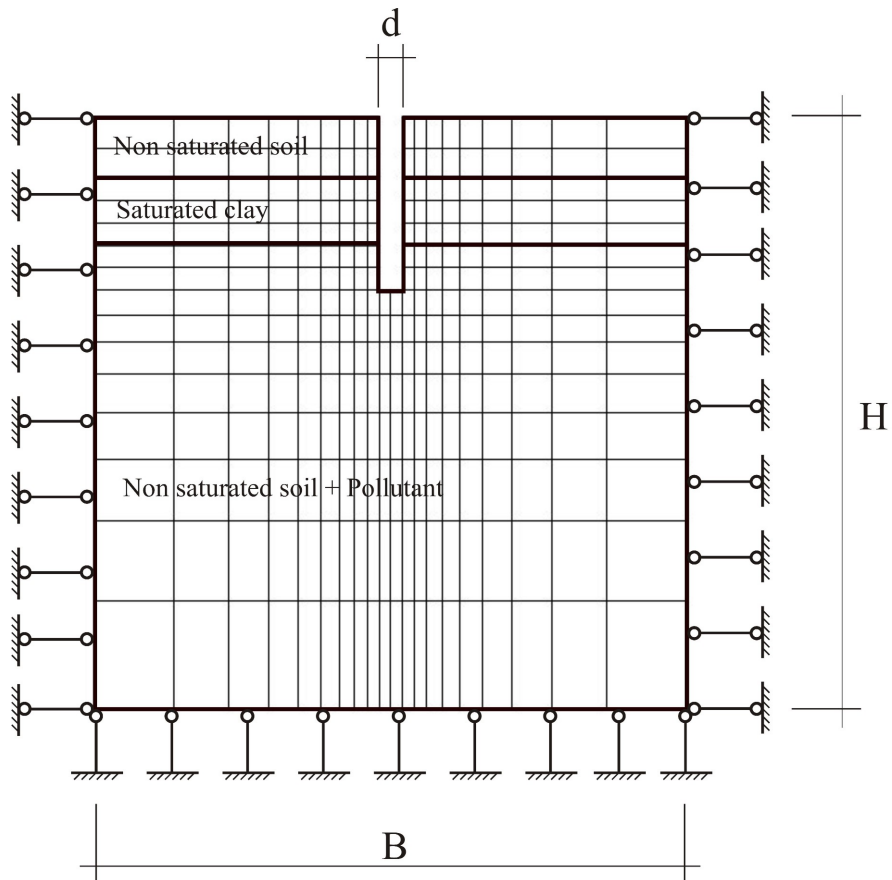

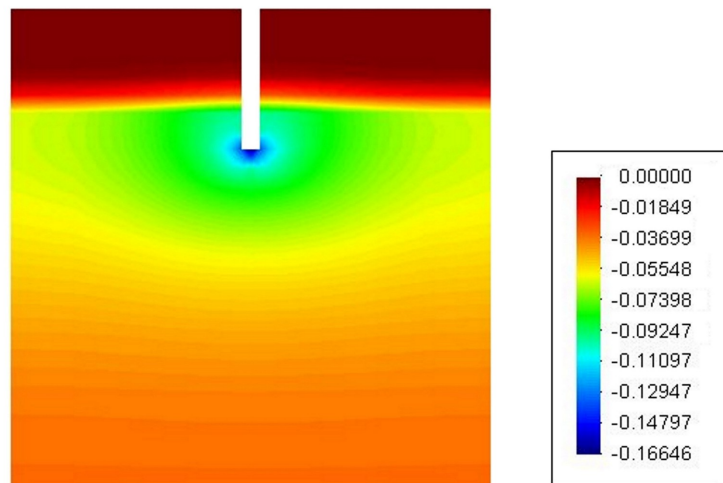Figure 4: FEM Mesh and boundary conditions (286 elements)
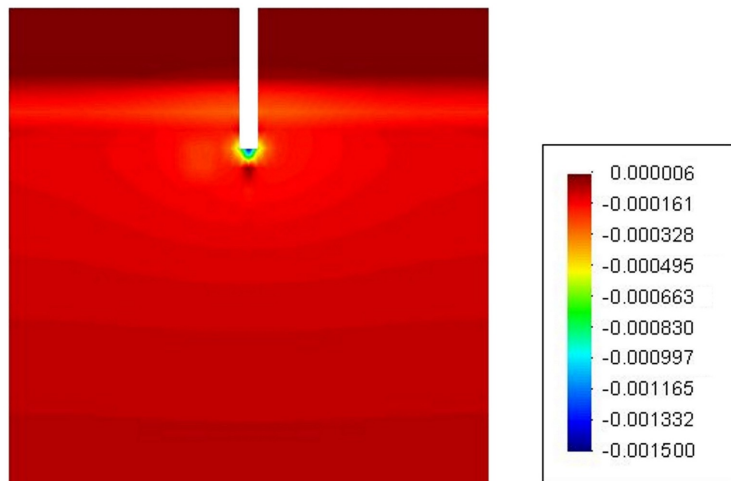
Figure 5: Pore water pressure at 30 hs

Figure 6: Pollutant pressure at 30 hs

7   CONCLUSIONS

A coupled mathematical framework for the solution of pore pressures and displacements of a non saturated porous media with three fluid phases in isothermal conditions was presented. Furthermore, the solution of the aforementioned problem using the finite element method was carried out. Encouraging outcomes were obtained based on the general compatibility between the different variables values.

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APPENDIX 1

$$\boldsymbol{K}_E = \int_\Omega \boldsymbol{B}^T \boldsymbol{D}_E \boldsymbol{B} \; d\Omega \qquad\qquad \boldsymbol{B} = \boldsymbol{L}\boldsymbol{N}_u$$

$$\boldsymbol{C}_{sw} = \int_\Omega \boldsymbol{B}^T \alpha_{12} \boldsymbol{N}_p \; d\Omega \qquad \boldsymbol{C}_{ws} = \int_\Omega \boldsymbol{N}_u^T \alpha_{21} \boldsymbol{B} \; d\Omega$$

$$\boldsymbol{C}_{sg} = \int_\Omega \boldsymbol{B}^T \alpha_{13} \boldsymbol{N}_p \; d\Omega \qquad \boldsymbol{C}_{gs} = \int_\Omega \boldsymbol{N}_u^T \alpha_{31} \boldsymbol{B} \; d\Omega$$

$$\boldsymbol{C}_{s\pi} = \int_\Omega \boldsymbol{B}^T \alpha_{14} \boldsymbol{N}_p \; d\Omega \qquad \boldsymbol{C}_{\pi s} = \int_\Omega \boldsymbol{N}_u^T \alpha_{41} \boldsymbol{B} \; d\Omega$$

$$\boldsymbol{C}_{wg} = \int_\Omega \boldsymbol{N}_p^T \alpha_{23} \boldsymbol{N}_p \; d\Omega \quad \boldsymbol{C}_{gw} = \int_\Omega \boldsymbol{N}_p^T \alpha_{32} \boldsymbol{N}_p \; d\Omega$$

$$\boldsymbol{C}_{w\pi} = \int_\Omega \boldsymbol{N}_p^T \alpha_{24} \boldsymbol{N}_p \; d\Omega \quad \boldsymbol{C}_{\pi w} = \int_\Omega \boldsymbol{N}_p^T \alpha_{42} \boldsymbol{N}_p \; d\Omega$$

$$\boldsymbol{C}_{g\pi} = \int_\Omega \boldsymbol{N}_p^T \alpha_{34} \boldsymbol{N}_p \; d\Omega \quad \boldsymbol{C}_{\pi g} = \int_\Omega \boldsymbol{N}_p^T \alpha_{43} \boldsymbol{N}_p \; d\Omega$$

$$\boldsymbol{P}_{ww} = \int_\Omega \boldsymbol{N}_p^T \alpha_{22} \boldsymbol{N}_p \; d\Omega \quad \boldsymbol{P}_{gg} = \int_\Omega \boldsymbol{N}_p^T \alpha_{33} \boldsymbol{N}_p \; d\Omega$$

$$\boldsymbol{P}_{\pi\pi} = \int_\Omega \boldsymbol{N}_p^T \alpha_{44} \boldsymbol{N}_p \; d\Omega$$

$$\boldsymbol{H}_{ww} = \frac{1}{S_w \rho^w} \int_\Omega (\nabla \boldsymbol{N}_p)^T \frac{\boldsymbol{k} k^{rw}}{\mu^w} \nabla \boldsymbol{N}_p \; d\Omega$$

$$\boldsymbol{H}_{gg} = \frac{1}{S_g \rho^g} \int_\Omega (\nabla \boldsymbol{N}_p)^T \frac{\boldsymbol{k} k^{rg}}{\mu^g} \nabla \boldsymbol{N}_p \; d\Omega$$

$$\boldsymbol{H}_{\pi\pi} = \frac{1}{S_\pi \rho^\pi} \int_\Omega (\nabla \boldsymbol{N}_p)^T \frac{\boldsymbol{k} k^{r\pi}}{\mu^\pi} \nabla \boldsymbol{N}_p \; d\Omega$$

$$\boldsymbol{f}^u = \int_\Omega \boldsymbol{N}_u^T \left((1-n)\,\rho^s + nS_w\rho^w + nS_g\rho^g + nS_\pi\rho^\pi \right) \boldsymbol{g}\; d\Omega + \int_{\Gamma_u^q} \boldsymbol{N}_u^T \bar{\boldsymbol{t}}\; d\Gamma_u^q$$

$$\boldsymbol{f}^w = \frac{1}{S_w\rho^w} \int_\Omega \left(\nabla \boldsymbol{N}_p \right)^T \frac{\boldsymbol{k}k^{rw}}{\mu^w} \rho^w \boldsymbol{g}\; d\Omega - \int_{\Gamma_w^q} \boldsymbol{N}_p^T \frac{\boldsymbol{q}^w}{\rho^w}\; d\Gamma$$

$$\boldsymbol{f}^g = \frac{1}{S_g\rho^g} \int_\Omega \left(\nabla \boldsymbol{N}_p \right)^T \frac{\boldsymbol{k}k^{rg}}{\mu^g} \rho^g \boldsymbol{g}\; d\Omega - \int_{\Gamma_g^q} \boldsymbol{N}_p^T \frac{\boldsymbol{q}^g}{\rho^g}\; d\Gamma$$

$$\boldsymbol{f}^\pi = \frac{1}{S_\pi\rho^\pi} \int_\Omega \left(\nabla \boldsymbol{N}_p \right)^T \frac{\boldsymbol{k}k^{r\pi}}{\mu^\pi} \rho^\pi \boldsymbol{g}\; d\Omega - \int_{\Gamma_\pi^q} \boldsymbol{N}_p^T \frac{\boldsymbol{q}^\pi}{\rho^\pi}\; d\Gamma$$