QUATERNIONS TO MODEL NON-ISOTHERMAL POROELASTIC PHENOMENA

Mario-César Suárez Arriaga and Fernando Samaniego V.

Faculty of Physics and Mathematical Sciences, Michoacán University
Edificio B Cd. Universitaria
Morelia, Mich., 58060, Mexico
e-mail: mcsa50@gmail.com

ABSTRACT

Quaternions are hypercomplex quantities in four dimensions (q_0, q_1, q_2, q_3); they are a generalization of the classical two-dimensional complex numbers $(x, y) = x + i\,y$, where $i^2 = -1$. Quaternions satisfy all the algebraic properties of the traditional complex numbers except that their multiplication law is not commutative. They have important applications in aeronautics, space flight dynamics, robotics, control theory, signal processing, and in computer graphics because of their stability and ability to represent three-dimensional rotations. In this paper we present for the first time, an original application of quaternions to model non-isothermal poroelasticity.

It is well known that the presence of a moving fluid in elastic porous rocks modifies their mechanical response. Poroelasticity explains how the fluid inside the pores bears a portion of the total load supported by the rock. The other part of the load is supported by the skeleton. The total deformation of geothermal rocks originates from lithostatic compression, pore pressure and thermal stresses. The introduction of the volumetric Gibbs free enthalpy as a fundamental thermodynamic potential, allows to include the thermal stresses directly. We introduce the thermoporoelastic theory by defining poroelastic coefficients coupling four quaternions: two for the bulk rock, one for the fluid and one for the total thermal expansion/contraction. The need of the fourth dimension appears naturally and permits to extend the theory of linear elasticity to geothermal rocks, taking into account the effect of both the fluid pressure and the temperature changes. Isothermal poroelasticity contains 16 different coefficients, but only four of them are independent. Introducing four volumetric thermal dilation coefficients, one for the fluid and three for the skeleton, a complete set of parameters for non-isothermal rocks are obtained. We show how the set of quaternions we are introducing is equivalent to a 4D-tensorial poroelastic model. In other words, the thermoporoelastic functions mimic the algebraic structure of a non-commutative "field".

To illustrate the practical use of this formulation some applications are outlined: full deduction of the classical Biot's theory coupled to thermal stresses. Construction of a general, well posed mathematical model to represent the physical behavior of geothermal rocks. Deformations of a non-isothermal reservoir, solved with finite elements, are included. These results can be applied to geothermal and hydrocarbon reservoirs, and to deep aquifers.

INTRODUCTION

All crustal rocks forming natural reservoirs are poroelastic. The fluid inside the pores and any temperature change affect their geomechanical properties. This elasticity is evidenced by the compression resulting from the pore pressure decline, which can shorten the pore volume. This reduction of the pore volume can be the principal source of fluid released from storage. On the other hand, any variation of temperature induces a thermo-poroelastic behavior that influences the elastic response of rocks. The expansivity of rocks is relatively small, but its effects can produce an increase in permeability and severe structural damages in rocks subjected to strong temperature gradients (Bundschuh and Suárez, 2010), as happens during the injection of cold fluids. This mechanism is of great importance in enhanced oil reservoirs and geothermal systems, when the injected cold fluid circulates in the underground. This transport can change both the permeability and the rock thermal conductivity. To develop our proposed four-dimensional model, we need to introduce first the main properties of quaternions, which will be a new mathematical tool to represent thermoporoelastic phenomena.

PROPERTIES OF QUATERNIONS

Algebraic definitions

We can define the quaternions as hypercomplex numbers in a four-dimensional space $q \in \mathbb{H} \cong \mathbb{R}^4$ (this symbol $\cong$ means that there is an isomorphism between both spaces, the first one is denoted by $\mathbb{H}$ in honor of Sir William Rowan Hamilton); they satisfy

two basic operations, addition and multiplication, defined as follows. Let q and p be two quaternions such that: $q = (q_0, q_1, q_2, q_3)$ and $p = (p_0, p_1, p_2, p_3)$, where all their individual components are real numbers ($p_n, q_n \in \mathbb{R}^1$, $n = 0, 1, 2, 3$).

Addition:
$$p + q = (p_0 + q_0, p_1 + q_1, p_2 + q_2, p_3 + q_3) \tag{0}$$

Product:
$$
\begin{aligned}
p * q = (&p_0 q_0 - p_1 q_1 - p_2 q_2 - p_3 q_3, \\
&p_0 q_1 + p_1 q_0 + p_2 q_3 - p_3 q_2, \\
&p_0 q_2 + p_2 q_0 + p_3 q_1 - p_1 q_3, \\
&p_0 q_3 + p_3 q_0 + p_1 q_2 - p_2 q_1)
\end{aligned} \tag{1}
$$

Two quaternions p and q are equal if and only if each one of their four components are equal:

$$p = q \iff p_n = q_n, \forall n = 0, 1, 2, 3$$

To obtain a vectorial representation of q, we define the following unit vectors of $\mathbb{R}^4 \cong \mathbb{H}$: $h = (1, 0, 0, 0)$, $i = (0, 1, 0, 0)$, $j = (0, 0, 1, 0)$ and $k = (0, 0, 0, 1)$. In this way, every quaternion can be written as a linear combination of four-dimensional basis vectors:

$$q = q_0 h + q_1 i + q_2 j + q_3 k \tag{2}$$

In this context, q is a thermoporoelastic function, which will be defined later in this paper. The unit vectors satisfy the following multiplication table which is built on from definition (1):

Table 1: *Quaternions products of the unit vectors (Hamilton, 1843; after Graves, 1882).*

*	h	i	j	k
h	1	i	j	k
i	i	-1	k	- j
j	j	- k	-1	i
k	k	j	- i	-1

Using this table, we deduce another hypercomplex form of any quaternion in terms of simple complex numbers:
$$
\begin{aligned}
q = q_0 h + q_1 i + q_2 j + q_3 k = \\
= (q_0 + q_1 i) + (q_2 + q_3 i) j = z_1 + z_2 j
\end{aligned} \tag{3}
$$

Where $z_1 = q_0 + q_1 i$ and $z_2 = q_2 + q_3 i$ are traditional complex quantities, z_1 and $z_2 \in \mathbb{C} \cong \mathbb{R}^2$; and $i * j = k$. Therefore, the hypercomplex polar form of q is:

$$q = z_1 + z_2 j = r_1 e^{i\theta_1} + r_2 e^{i\theta_2} j \tag{4}$$
where: $e^{i\theta_n} = Cos\,\theta_n + i\,Sin\,\theta_n\ (n = 1, 2)$

Each individual complex part of the quaternion q has a very simple geometric representation illustrated by the following two-dimensional graph.
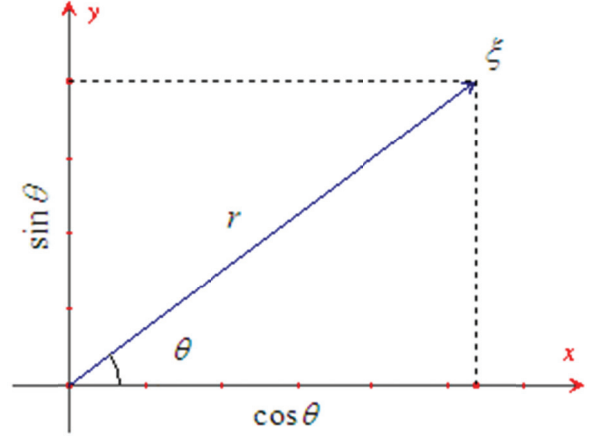

Figure 1: *Geometric representation of each complex part of q, where $\xi = r\,(Cos\,\theta + i\,Sin\,\theta)$.*

Matrix representations in $\mathbb{H}$

We can build quaternions into complex matrices and also into real matrices. The first one uses the hypercomplex form of equation (3):

$$
q = q_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + q_1 \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} + q_2 \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} + q_3 \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}
$$

$$
= \begin{pmatrix} q_0 + q_1 i & q_2 + q_3 i \\ -q_2 + q_3 i & q_0 - q_1 i \end{pmatrix} = \begin{pmatrix} z_1 & z_2 \\ -\bar{z}_2 & \bar{z}_1 \end{pmatrix}
$$

where: $\bar{z}_1 = q_0 - q_1 i$, $\bar{z}_2 = q_2 - q_3 i$
$$\tag{5}$$

The symbols in the last line are called the complex conjugates of z_1 and z_2 respectively. The second matrix form of quaternions uses the following four-dimensional objects:

$$
\mathbf{1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \mathbb{I} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix},
$$

$$
\mathbb{J} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \quad \mathbb{K} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}
$$

$$\tag{6}$$

In terms of these unit and anti-symmetrical matrices, any quaternion can be expressed as a linear combination of arrays, which have the following property:

$$\mathbf{1}^2 = +\mathbf{1}, \ \mathbb{I}^2 = \mathbb{J}^2 = \mathbb{K}^2 = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = -\mathbf{1}$$

$$q = q_0 \mathbf{1} + q_1 \mathbb{I} + q_2 \mathbb{J} + q_3 \mathbb{K} = \begin{pmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{pmatrix} \tag{7}$$

Note that the square matrix property $(.)^2 = -\mathbf{1}$, is also satisfied by the complex (2×2) matrices of equation (5). The matrix representation (7) allows to define, in an alternative way, the quaternion multiplication (1) as a four-dimensional, skew-symmetric matrix-vector product:

$$q * p = \begin{pmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{pmatrix} \cdot \begin{pmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{pmatrix} =$$

$$= \begin{pmatrix} q_0 p_0 - q_1 p_1 - q_2 p_2 - q_3 p_3 \\ q_1 p_0 + q_0 p_1 - q_3 p_2 + q_2 p_3 \\ q_2 p_0 + q_3 p_1 + q_0 p_2 - q_1 p_3 \\ q_3 p_0 - q_2 p_1 + q_1 p_2 + q_0 p_3 \end{pmatrix} \neq p * q \tag{8}$$

This result compared to equation (1) demonstrates the non-commutative nature of quaternion multiplication. From equation (2) a third matrix representation is deduced in the form of a diagonal (4×4) array for every $q \in \mathbb{H}$:

$$q = \begin{pmatrix} q_0 & 0 & 0 & 0 \\ 0 & q_1 & 0 & 0 \\ 0 & 0 & q_2 & 0 \\ 0 & 0 & 0 & q_3 \end{pmatrix} \tag{9}$$

If we separate the matrix $q_0 \mathbf{1}$ from the global array (7), we observe that each quaternion can be represented by the sum of a real diagonal matrix plus an anti-symmetrical matrix called the imaginary matrix part of the quaternion:

$$q = q_0 \mathbf{1} + \mathbb{A} \quad \Leftrightarrow$$

$$q = q_0 \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & -q_1 & -q_2 & -q_3 \\ q_1 & 0 & -q_3 & q_2 \\ q_2 & q_3 & 0 & -q_1 \\ q_3 & -q_2 & q_1 & 0 \end{pmatrix} \tag{10}$$

It is well known that any anti-symmetrical matrix represents a pure rotation where (q_1, q_2, q_3) are the corresponding components of the rotation vector.

Hybrid scalar-vector representation in $\mathbb{H}$

The result (10) suggests the following hybrid scalar-vectorial definition of a quaternion which clearly separates its two parts:

$$q = q_0 \, h + Q = q_0 + Q \tag{11a}$$
$$Q = q_1 \, i + q_2 \, j + q_3 \, k$$

The term q_0 is the real scalar part of q, and Q is its imaginary vector part. Replacing definition (11a) into equation (8) and after doing some algebra we arrive to the following practical result which is useful to compute quaternion products in terms of classic vector operations:

$$q = q_0 \, h + Q , \ p = p_0 \, h + P \quad \Rightarrow$$
$$p * q = (p_0 q_0 - P \cdot Q) h + q_0 P + p_0 Q + P \times Q \tag{11b}$$

where $P \cdot Q$ represents the scalar product and $P \times Q$ is the vectorial product of P and Q respectively. Because of the fact that $P \times Q \neq Q \times P$ we confirm again that the quaternion multiplication is a non-commutative operation.

Arithmetic properties

Quaternions satisfy all the algebraic and arithmetic properties of the classical two-dimensional complex numbers, except the multiplication commutative law (Hamilton, 1853; Kuipers, 1999). The main properties of $q \in \mathbb{H}$ are summarized as follows:

1. **Additive inverse**: $-q = -q_0 h - Q$, $q + (-q) = 0$
2. **Hypercomplex Conjugate**: $\bar{q} = q_0 \, h - Q$
3. **Norm of q:** $|q| = \sqrt{q * \bar{q}} = \sqrt{q_0^2 + q_1^2 + q_2^2 + q_3^2}$
4. **Multiplicative Inverse**: $q^{-1} = \dfrac{\bar{q}}{q * \bar{q}}$, $q * q^{-1} = 1$
5. **Division of quaternions**: $\dfrac{p}{q} = p * q^{-1} = \dfrac{p * \bar{q}}{q * \bar{q}}$
6. **Normalized quaternion:** if $q * \bar{q} = 1 \Rightarrow q^{-1} = \bar{q}$

The addition is commutative and associative; the multiplication is associative but non-commutative; both operations obey the distribution law. The set $\mathbb{H}$

of quaternions, along with the addition, product and properties already defined, has an algebraic structure called a non-commutative division ring, or simply an anti-commutative algebra. The future usefulness of quaternions was clearly envisioned by its creator:

"Time is said to have only one dimension, and space to have three dimensions. ... The mathematical quaternion partakes of both these elements; in technical language it may be said to be time plus space, or space plus time: and in this sense it has, or at least involves a reference to, four dimensions. And how the One of Time, of Space the Three, Might in the Chain of Symbols girdled be. ... quaternions would be found to have a powerful influence as an instrument of research."
 (William Rowan Hamilton; quoted in Graves, 1882).

The triple product of quaternions conjugate

Let $q = q_0 + Q$ be a non-zero quaternion and $v \in \mathbb{R}^3$ be a vector or pure imaginary quaternion ($v_0 = 0$). The application of equation (11b) to the triple product of q, its conjugate $q_0 - Q$ and v gives the following result:

$$q * v * \overline{q} = \left(q_0^2 - Q \cdot Q \right) v + 2 (Q \cdot v) Q + 2\, q_0\, Q \times v \quad (12)$$

If q is a normalized quaternion of unit norm:

$$q * v * \overline{q} = \left(2\, q_0^2 - 1 \right) v + 2 (Q \cdot v) Q + 2\, q_0\, Q \times v \quad (13)$$

Rotations in three dimensions using $q \in \mathbb{H}$

We can perform easily three-dimensional rotations using quaternions and unit vectors to define an axis. A rotation in $\mathbb{R}^3$ about a unit vector u by an angle θ can be computed using the following unit q and the triple product of quaternions:

$$q = q_0 + Q = Cos\frac{\theta}{2} + u\, Sin\frac{\theta}{2} \ \Rightarrow$$

$$w = q * v * \overline{q} = \left(2\, Cos^2 \frac{\theta}{2} - 1 \right) v + \quad (14)$$

$$+ 2 (u \cdot v) u\, Sin^2 \frac{\theta}{2} + 2\, Cos\frac{\theta}{2} Sin\frac{\theta}{2}\, u \times v$$

and therefore $w \in \mathbb{R}^3$. A series of two connected successive rotations, first q and then p, is computed using the following formula:

$$q = Cos\frac{\theta_1}{2} + u_1\, Sin\frac{\theta_1}{2}, \ p = Cos\frac{\theta_2}{2} + u_2\, Sin\frac{\theta_2}{2}$$

$$\Rightarrow w = p * (q * v * \overline{q}) * \overline{p} = (p * q) * v * (\overline{q} * \overline{p}) \quad (15)$$

LINEAR POROELASTICITY IN TERMS OF QUATERNIONS $q \in \mathbb{H}$

A key question that arises when developing the very basic poroelastic equations is: why do we need a four-dimensional space in poroelasticity? If we perform an experiment in a simple, non-porous solid under an uniaxial stress state, the resulting relationship between the stress σ_x and the strain ε_x is a one-dimensional equation:

$$\sigma_x = E\, \varepsilon_x \quad (16a)$$

Where E is the Young's modulus. But if we carry out the same one-dimensional experiment in a porous rock, because of the fluid contained in the pores, we obtain two simultaneous linear relationships that are equivalent to a (2×2) matrix equation (Bundschuh and Suárez, 2010), which corresponds to a two-dimensional formula:

$$\sigma_x = K_U \varepsilon_x - C\zeta \text{, and } p_f = -C\varepsilon_x + M\zeta$$

$$\Leftrightarrow \ \begin{pmatrix} \sigma_x \\ p_f \end{pmatrix} = \begin{pmatrix} K_U & -C \\ -C & M \end{pmatrix} \cdot \begin{pmatrix} \varepsilon_x \\ \zeta \end{pmatrix} \quad (16b)$$

Where K_U is the undrained bulk modulus (Appendix), C is a coefficient representing deformations coupling between the solid grains and the fluid, M is a parameter characterizing the fluid elastic properties, p_f is the fluid-pore pressure, and ζ is a special strain representing the variation of the fluid mass content in the pores. Using only the parameter K_U we obtain similar 2D relationships:

$$\begin{pmatrix} \sigma_x \\ p_f \end{pmatrix} = \begin{pmatrix} K_U & -K_U B \\ -K_U B & \dfrac{K_U B}{b} \end{pmatrix} \cdot \begin{pmatrix} \varepsilon_x \\ \zeta \end{pmatrix} \quad (16c)$$

Where $b = C/M$ is a quotient called the Biot-Willis coefficient (Biot & Willis, 1957); B is the Skempton coefficient ($B = C/K_U$). The inverse matrix equation of (16b,c) is:

$$\begin{pmatrix} \varepsilon_x \\ \zeta \end{pmatrix} = \begin{pmatrix} K_B^{-1} & H^{-1} \\ H^{-1} & R^{-1} \end{pmatrix} \cdot \begin{pmatrix} \sigma_x \\ p_f \end{pmatrix} \quad (16d)$$

Where $K_B^{-1} = C_B$ is the bulk compressibility, K_B is called the drained bulk modulus; H^{-1} represents an expansion coefficient and R^{-1} is an unconstrained specific storage modulus (Wang, 2000). In terms of these moduli, the Biot and Skempton coefficients are defined as: $b = K_B/H$ and $B = R/H$, respectively. These coefficients represent properties that are not encountered in standard elasticity of simple solids. The experimental definitions of these poroelastic moduli are in the Appendix.

Equation (16d) reveals that changes in σ_x and p_f produce changes in ε_x, which require fluid to be added or removed from storage because ζ also changes as a function of σ_x and p_f. After this observational result, we conclude that the fluid contained in the pores of the rock acts inside a second hidden spatial dimension, although the experiment was done in only one dimension. This result is immediately generalized to two- and three-dimensional experiments: an extra third or fourth spatial dimension will always appear because of the fluid contained in the pores. At this point, a natural question arises: what are the quaternions properties that are useful in poroelasticity?

The fundamental poroelastic relationship in $\mathbb{H}$
In order to introduce our model, we define first the following poroelastic quaternions for homogeneous, isotropic, porous rocks.

$$q_\sigma = p_f\, h + \sigma_x\, i + \sigma_y\, j + \sigma_z\, k$$
$$q_\varepsilon = 0\, h + \varepsilon_x\, i + \varepsilon_y\, j + \varepsilon_z\, k$$
$$q_B = -\frac{C}{\lambda}\varepsilon_B\, h + \varepsilon_B\, i + \varepsilon_B\, j + \varepsilon_B\, k \qquad (17)$$
$$q_p = \frac{M}{b}\zeta\, h - p_f\, i - p_f\, j - p_f\, k$$

Because of the physical symbols involved, we name the quaternions: q_σ the stress, q_ε the pure strain, q_B the volumetric strain, and q_p the fluid pressure. These expressions do not contain shear strains (ε_{ij}), because changes in the fluid pressure or in compressions are supposed not to induce shears (Wang, 2000). The fundamental linear relationship among the quaternions in equation (17) is very simple:

$$\boxed{q_\sigma = 2G\, q_\varepsilon + \lambda\, q_B + b\, q_p} \quad \Leftrightarrow$$
$$p_f = -C\,\varepsilon_B + M\,\zeta \qquad (18)$$
$$\sigma_n = 2G\,\varepsilon_n + \lambda\,\varepsilon_B - b\, p_f,\ (n = x, y, z)$$

The symbols in equations (17) and (18) are of common use: σ_n ($n = x$, y, z) holds for the three normal stresses acting in the rock; ε_n are the normal strains describing the elastic response of the porous rock; $\varepsilon_B = \varepsilon_x + \varepsilon_y + \varepsilon_z$ is the volumetric strain, G and λ are poroelastic coefficients. The rigidity modulus G represents the rock response to shear; the Lamé module $\lambda = K_B - 2G/3$ measures the rock response to compression under drained conditions. In terms of quaternions it is straightforward to invert the stress-strain relationship (18). For example:

$$q_\varepsilon = \frac{1}{2G}\left(q_\sigma - \lambda\, q_B - b\, q_p\right) \qquad (19)$$

From this equation we deduce the inverted components relationships:

$$\zeta = b\,\varepsilon_B + \frac{p_f}{M}$$
$$\varepsilon_n = \frac{\sigma_n}{2G} - \frac{\lambda}{2G}\varepsilon_B + \frac{b}{2G}p_f;\ \ n = x, y, z \qquad (20)$$

After doing some algebra we deduce other common inverse expressions (Biot, 1941; Wang, 2000):

$$\zeta = \frac{\sigma_M}{H} + \frac{p_f}{R}$$
$$\varepsilon_n = \frac{\sigma_n}{2G} - 3\frac{v}{E}\sigma_M + \frac{p_f}{3H};\ \ n = x, y, z \qquad (21)$$
$$\sigma_M = K_B\,\varepsilon_B - C\,\zeta = \frac{\sigma_x + \sigma_y + \sigma_z}{3}$$

Where σ_M is the average of the normal stresses, and v is the Poisson's module. If the rock is anisotropic and inhomogeneous, the corresponding quaternions are defined as follows:

$$q_\sigma = p_f h + \sigma_x\, i + \sigma_y\, j + \sigma_z\, k$$
$$q_\varepsilon = 0\, h + \varepsilon_x\, i + \varepsilon_y\, j + \varepsilon_z\, k$$
$$q_B = \varepsilon_B\, h + \varepsilon_B\, i + \varepsilon_B\, j + \varepsilon_B\, k \qquad (22)$$
$$q_p = \zeta\, h - p_f\, i - p_f\, j - p_f\, k$$

The fundamental linear relationship among the non-isotropic quaternions can be written similarly as in equation (18) using the following diagonal matrices (quaternions) of poroelastic coefficients:

$$\mathbf{G} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & G_x & 0 & 0 \\ 0 & 0 & G_y & 0 \\ 0 & 0 & 0 & G_z \end{pmatrix},\ \mathbf{\Lambda} = \begin{pmatrix} -C & 0 & 0 & 0 \\ 0 & \lambda_x & 0 & 0 \\ 0 & 0 & \lambda_y & 0 \\ 0 & 0 & 0 & \lambda_z \end{pmatrix}$$
$$\mathbf{b} = \begin{pmatrix} M & 0 & 0 & 0 \\ 0 & -b_x & 0 & 0 \\ 0 & 0 & -b_y & 0 \\ 0 & 0 & 0 & -b_z \end{pmatrix} \quad \Rightarrow \qquad (23)$$

The fundamental anisotropic stress-strain relationship in terms of quaternions is a linear combination of matrix - quaternion products:

$$\boxed{q_\sigma = 2\mathbf{G}\cdot q_\varepsilon + \mathbf{\Lambda}\cdot q_B + \mathbf{b}\cdot q_p} \qquad (24)$$

Note that we use here the common matrix-vector product, and not the quaternion multiplication (1), its direct use still needs more research. Equation (24) is valid for both isotropic and non-isotropic rocks.

Inclusion of the shear stresses σ_{ij} and Biot's theory

Note that there are no shear stresses nor shear strains involved in quaternions (17) and (22). They are going to be introduced in a different way. We define two symmetric matrices $\boldsymbol{\sigma}_G$ and $\boldsymbol{\varepsilon}_G$. The first one contains the shear stresses and the second one the shear strains. Equations (23) and (24) are diagonal matrices of type (9) containing only principal stresses and strains. Both influence the bulk rock deformation through tension or compression in the principal axes. Since there are no shear tensions in the fluid, the pore fluid pressure affects only the three normal strains ε_n ($n = x, y, z$), as shown in equation (20). Therefore the shear stresses can only work on the shear strains:

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \sigma_{xy} & \sigma_{xz} \\ 0 & \sigma_{xy} & 0 & \sigma_{yz} \\ 0 & \sigma_{xz} & \sigma_{yz} & 0 \end{pmatrix} = 2\,\mathbf{G}_0 \cdot \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_{xy} & \varepsilon_{xz} \\ 0 & \varepsilon_{xy} & 0 & \varepsilon_{yz} \\ 0 & \varepsilon_{xz} & \varepsilon_{yz} & 0 \end{pmatrix}$$

$$\mathbf{G}_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & G_{xx} & G_{xy} & G_{xz} \\ 0 & G_{xy} & G_{yy} & G_{yz} \\ 0 & G_{xz} & G_{yz} & G_{zz} \end{pmatrix} \quad \text{is the shear matrix}$$

$$\boldsymbol{\sigma}_G = 2\,\mathbf{G}_0 \cdot \boldsymbol{\varepsilon}_G \;\Leftrightarrow\; \sigma_{nm} = 2\,G_{nm}\,\varepsilon_{nm} \quad (n, m = x, y, z) \tag{25}$$

Where the full shear matrix $\mathbf{G}_0$ holds for anisotropic rocks. Note that the shear strains and corresponding stresses cannot be represented by quaternions. Formula (25) completes the set of linear poroelastic equations when added to Eq. (24) in matrix form:

$$\boxed{q_\sigma + \boldsymbol{\sigma}_G = 2\,\mathbf{G}\cdot q_\varepsilon + 2\,\mathbf{G}_0 \cdot \boldsymbol{\varepsilon}_G + \boldsymbol{\Lambda}\cdot q_B + \mathbf{b}\cdot q_p} \tag{26}$$

If the rock is isotropic and homogeneous the full set of four-dimensional arrays is simply:

$$\begin{pmatrix} p_f & 0 & 0 & 0 \\ 0 & \sigma_x & \sigma_{xy} & \sigma_{xz} \\ 0 & \sigma_{xy} & \sigma_y & \sigma_{yz} \\ 0 & \sigma_{xz} & \sigma_{yz} & \sigma_z \end{pmatrix} = 2\,G \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \varepsilon_x & \varepsilon_{xy} & \varepsilon_{xz} \\ 0 & \varepsilon_{xy} & \varepsilon_y & \varepsilon_{yz} \\ 0 & \varepsilon_{xz} & \varepsilon_{yz} & \varepsilon_z \end{pmatrix} +$$

$$\varepsilon_B \begin{pmatrix} -C & 0 & 0 & 0 \\ 0 & \lambda & 0 & 0 \\ 0 & 0 & \lambda & 0 \\ 0 & 0 & 0 & \lambda \end{pmatrix} - b \begin{pmatrix} -\dfrac{M}{b}\zeta & 0 & 0 & 0 \\ 0 & p_f & 0 & 0 \\ 0 & 0 & p_f & 0 \\ 0 & 0 & 0 & p_f \end{pmatrix} \tag{27}$$

Equation (26) corresponds to the formulation of the theory for anisotropic rocks in terms of quaternions and shear matrices. The connections among the individual components of equation (27) are known as Biot's linear poroelastic theory for isotropic rocks (Biot, 1941, 1955). The components of equation (27) can be written in compact form (δ_{nm} is the unit tensor):

$$\text{for } n, m = x, y, z \;\rightarrow$$
$$\sigma_{nm} = \left(\lambda\,\varepsilon_B\,\delta_{nm} + 2\,G\,\varepsilon_{nm}\right) - b\,p_f\,\delta_{nm} \tag{28}$$

The term τ_{nm} is called the Terzaghi effective stress, which acts only in the solid matrix:

$$\tau_{nm} = \lambda\,e_B\,\delta_{nm} + 2\,G\,\varepsilon_{nm} \tag{29}$$

Another important fact concerning the inclusion of the shear stress-strains is that the shear matrices connected with linear poroelasticity are symmetric arrays. A special case of the spectral theorem in linear algebra (Lang, 1969) establishes that any real symmetric (4×4) matrix $\mathbf{M}$ can be transformed into a diagonal matrix $\mathbf{D}$ in the following way:

$$\mathbb{M} \rightarrow \quad \mathbb{U}^T \cdot \mathbb{M} \cdot \mathbb{U} = \mathbb{D}, \text{ where: } \mathbb{U}^T = \mathbb{U}^{-1} \tag{30}$$

The matrix $\mathbf{U}$ is called an orthogonal matrix and is built on the eigenvectors of $\mathbf{M}$. The corresponding basis of eigenvectors for the four-dimensional space $\mathbb{R}^4$ is orthogonal. The matrices representing the quaternions in the fundamental equations (18), (24) and (26) are all symmetric. Therefore, any poroelastic matrix equation, which includes shear stresses and shear strains, can be transformed into a diagonal matrix and, consequently it can be represented by a quaternion of type (9) which is valid for every $q \in \mathbb{H}$.

THERMOPOROELASTICITY IN TERMS OF QUATERNIONS $q \in \mathbb{H}$

The basic thermodynamic potentials in porous rocks are the internal energy and the specific enthalpy for the fluid phase. The free energy describes the solid matrix while for the skeleton the appropriate potential is the free enthalpy (Bundschuh and Suárez, 2010). In this section we focus only on isotropic, homogeneous geothermal rocks.

The Gibbs free enthalpy for the porous rock

The volumetric Gibbs free internal enthalpy g_S is defined as the algebraic difference of the enthalpy h_S minus the product of the absolute temperature T and the skeleton entropy S_S per unit volume of rock:

$$g_S\left(\varepsilon_i, p_f, T\right) = h_S - T\,S_S \quad \left[\text{J/m}^3 = \text{Pa}\right] \tag{31}$$

If the process is reversible and there is no energy dissipation in the rock, the total differential of this thermodynamic potential is useful to describe the skeleton thermal behavior with shear strains and porosity φ included (Coussy, 1991; Bundschuh and Suárez, 2010):

$$d\,g_S = \sigma_{ij}\,d\varepsilon_{ij} - \varphi\,dp_f - S_S\,dT \qquad (32)$$

These differential equations are integrated between an initial state g_S^0 ($\varepsilon_i = 0$, $p_f = p_0$, $T = T_0$) ($i, j = x, y, z$) at zero strain, and a final state g_S (ε_{ij}, p_f, T). Note that an initial temperature T_0 and an initial pore pressure p_0 are needed because both thermodynamic variables T and p_f are changing in non-isothermal processes:

$$\int_{g_S^0}^{g_S} d\,g_S = \int_0^{\varepsilon_i} \sigma_{ij}\,\partial\varepsilon_{ij} - \int_{p_0}^{p_f} \varphi\,\partial p_f - \int_{T_0}^T S_S\,\partial T \qquad (33)$$

After integrating equations (33), an exact, analytic expression for the Gibbs potential of the skeleton is obtained:

Initial State: $g_S^0 = g_S\left(\varepsilon_{ij} = 0, p_f = p_0, T = T_0\right)$;

Final State: for $(i, j = x, y, z)$ and for $t > 0$:

$$g_S\left(\varepsilon_{ij}, p_f\ T\right) =$$

$$\sigma_M^0\,\varepsilon_B + \left(\sigma_{ij}^0 - \sigma_M^0\delta_{ij}\right)\left(\varepsilon_{ij} - \frac{\varepsilon_B}{3}\delta_{ij}\right) - \varphi_0 p_f - S_S^0\,T$$

$$+ \frac{K_B}{2}\left(\varepsilon_B\right)^2 - \varphi\gamma_\varphi\left(p_f - p_0\right)\left(T - T_0\right)$$

$$- \left(p_f - p_0\right)b\varepsilon_B - K_B\gamma_B\left(T - T_0\right)\varepsilon_B$$

$$- \frac{\left(p_f - p_0\right)^2}{2}\frac{K_f - M\varphi}{K_f M} - \frac{C_V\left(T - T_0\right)^2}{2T_0}$$

$$+ G\left(\varepsilon_{ij} - \frac{\varepsilon_B}{3}\delta_{ij}\right)^2$$

$$(34)$$

Where K_f is the bulk modulus of the fluid. The parameters γ_B and γ_φ [1/K] are volumetric thermal dilatation coefficients. The first one γ_B measures the bulk dilatation of the skeleton, while γ_φ is related to the variation of the porosity when the temperature changes:

$$\gamma_B = \frac{1}{V_B}\left(\frac{\partial V_B}{\partial T}\right)_\sigma, \quad \gamma_\varphi = \frac{1}{\varphi}\left(\frac{\partial\varphi}{\partial T}\right)_{p_f} \qquad (35)$$

C_V is the skeleton volumetric heat capacity under constant deformations. The thermodynamic behavior

of the porous rock is obtained by computing the following partial derivatives:

$$\sigma_{ij} = \frac{\partial g_S}{\partial\varepsilon_{ij}}, \quad \varphi = -\frac{\partial g_S}{\partial p}, \quad S_S = -\frac{\partial g_S}{\partial T} \qquad (36)$$

Thermodynamics of the fluid mass content

The symbol ζ represents the variation of the fluid content in the pores defined as follows (Biot, 1941):

$$m_f = \rho_f\varphi \rightarrow \zeta = \frac{\Delta m_f}{\rho_0} = \frac{\rho_f\Delta\varphi + \varphi\Delta\rho_f}{\rho_0} \qquad (37a)$$

Where m_f is the fluid mass content per unit rock volume, ρ_f is the fluid density, ρ_0 is a reference density, φ is the effective porosity and Δ represents a change in the corresponding variable. An explicit thermodynamic expression for ζ can be obtained by differentiating m_f in equation (37):

$$d\zeta = \frac{d\,m_f}{\rho_f} = \varphi\frac{d\rho_f}{\rho_f} + d\varphi \qquad (37b)$$

The fluid density is a function of both, the fluid pressure and the temperature $\rho_f(p_f, T)$, thus:

$$\frac{d\rho_f}{\rho_f} = \frac{1}{\rho_f}\frac{\partial\rho_f}{\partial p_f}d\,p_f + \frac{1}{\rho_f}\frac{\partial\rho_f}{\partial T}dT \qquad (38)$$

The fluid compressibility C_f and the fluid thermal expansivity γ_f are defined as:

$$C_f = \frac{1}{K_f} = \frac{1}{\rho_f}\left(\frac{\partial\rho_f}{\partial p_f}\right)_T$$

$$\gamma_f = \frac{1}{V_f}\left(\frac{\partial V_f}{\partial T}\right)_{p_f} = -\frac{1}{\rho_f}\left(\frac{\partial\rho_f}{\partial T}\right)_{p_f} \qquad (39)$$

We define another thermal expansion coefficient γ_m, which measures the changes in the fluid mass content when the average stress σ_M and p_f are held constant:

$$\gamma_m = \frac{1}{m_f}\left(\frac{\partial m_f}{\partial T}\right)_{\sigma_M, p_f} =$$

$$\frac{1}{\varphi}\left(\frac{\partial\varphi}{\partial T}\right)_{p_f} + \frac{1}{\rho_f}\left(\frac{\partial\rho_f}{\partial T}\right)_{p_f} = \gamma_\varphi - \gamma_f \qquad (40)$$

Substituting the coefficients (39) into equation (37b):

$$d\zeta = d\varphi + \frac{\varphi}{K_f}dp_f - \varphi\gamma_f dT \qquad (41)$$

Integrating this expression, between the initial and final states, and replacing the result into equation (36) for the porosity we obtain:

$$\zeta = b\,\varepsilon_B + \frac{p - p_0}{M} + \varphi\gamma_m\left(T - T_0\right) \qquad (42)$$

Equation (42) is a useful expression for the variation of the fluid content in a linear non-isothermal process.

The thermoporoelastic relationship in ℍ

With the previous results, we can define the thermal stress quaternion q_T for thermoporoelastic rocks:

$$q_T = \Delta T\left(\varphi h + i + j + k\right) \qquad (43)$$

Where $\Delta T = T - T_0$. The corresponding matrix of thermal expansivity coefficients is the following diagonal array:

$$\mathbf{\Gamma} = \begin{pmatrix} M\gamma_m & 0 & 0 & 0 \\ 0 & K_B\gamma_B & 0 & 0 \\ 0 & 0 & K_B\gamma_B & 0 \\ 0 & 0 & 0 & K_B\gamma_B \end{pmatrix} \qquad (44a)$$

The linear relationship among the quaternions in non-isothermal processes is:

$$\boxed{q_\sigma = 2\mathbf{G}\cdot q_\varepsilon + \mathbf{\Lambda}\cdot q_B + \mathbf{b}\cdot q_p - \mathbf{\Gamma}\cdot q_T} \qquad (44b)$$

In terms of four-dimensional matrices, the equation relating stresses and strains in isotropic rocks is deduced directly:

$$q_\sigma = \varepsilon_B \begin{pmatrix} -C & 0 & 0 & 0 \\ 0 & \lambda & 0 & 0 \\ 0 & 0 & \lambda & 0 \\ 0 & 0 & 0 & \lambda \end{pmatrix} + 2G \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \varepsilon_x & 0 & 0 \\ 0 & 0 & \varepsilon_y & 0 \\ 0 & 0 & 0 & \varepsilon_z \end{pmatrix}$$

$$-\Delta p \begin{pmatrix} A_p & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & b \end{pmatrix} - K_B\,\Delta T \begin{pmatrix} A_T & 0 & 0 & 0 \\ 0 & \gamma_B & 0 & 0 \\ 0 & 0 & \gamma_B & 0 \\ 0 & 0 & 0 & \gamma_B \end{pmatrix}$$

$$(44c)$$

Where:

$$\Delta p = p - p_0,\quad A_p = -\frac{M\,\zeta}{p - p_0},\quad A_T = \frac{M\varphi}{K_B}\gamma_m$$

Note that every quaternion is equivalent to a diagonal matrix. The fact that linear thermoporoelasticity theory can be represented by quaternions is very important because all quaternions properties, that are useful in this context, can be applied to geothermal rocks deformations. This allows to the development and discovery of other unknown poroelastic processes.

Some numerical values of the poroelastic moduli and the thermal expansivity coefficients

To construct the following table of poroelastic coefficients the basic experimental data set used was $\{E, G, \varphi, K_S \text{ and } K_f\}$ (see Appendix).

Table 2: Poroelastic coefficients of different rocks.

Rock Type	φ (%)	E (GPa)	ν	ν_U	G (GPa)	λ (GPa)	λ_U (GPa)
[0]	65.0	0.18	0.01	0.49	0.09	.001	6.1
[1]	26.0	9.7	0.15	0.31	4.2	1.8	7.3
[2]	19.0	13.1	0.17	0.30	5.6	2.9	10.9
[3]	13.0	30.5	0.26	0.32	12.1	13.1	23.2
[4]	8.5	35.8	0.31	0.32	13.7	21.7	24.8
[5]	2.0	60.0	0.25	0.27	24.0	24.2	28.3
[6]	0.5	42.2	0.42	0.42	14.9	73.9	74.0

Rock Type	K_B (GPa)	K_U (GPa)	K_S (GPa)	B	b	M (GPa)	R (GPa)
[0]	0.062	6.2	10^5	0.99	1.0	6.1	0.06
[1]	4.6	10.1	42.0	0.61	0.89	6.9	3.2
[2]	6.6	14.6	28.9	0.71	0.77	13.4	6.1
[3]	21.2	31.2	72.6	0.46	0.71	20.0	13.6
[4]	30.8	33.9	49.7	0.24	0.38	21.6	19.6
[5]	40.0	44.3	50.0	0.49	0.19	107.3	97.0
[6]	83.8	83.9	85.0	0.06	0.01	384.3	384.0

The rock types are:

[0].- Clay, (K_f = 3.9 GPa).
[1].- Boise sandstone, (K_f = 2.0 GPa).
[2].- Berea sandstone (K_f = 3.5 GPa);
[3].- Indiana limestone, (K_f = 3.1 GPa).
[4].- Andesite, (K_f = 2.1 GPa, p_k = 250 bar, T = 25°C).
[5].- Tennessee marble, (K_f = 3.5 GPa).
[6].- Rock with celestite, (K_f = 2.0 GPa)

References used: Rocks [0], [1], [2] and [3], Wang (2000); [4], [5] and [6], Bundschuh and Suárez (2010). The figures in italics were estimated using poroelastic formulas. Rocks of type [0] and [6] are representative of the two limit cases of linear poroelastic theory, for $b \approx 1$ and $b \approx 0$, respectively. In this section, we also give some experimental values of the volumetric thermal dilatation coefficients γ_B, γ_f, γ_φ, γ_m and γ_U [1/K]. As a general trend, thermal expansion increases when temperature

rises. The volumetric thermal expansivity γ_B is about 10^{-5} K^{-1} for solids, 10^{-4} K^{-1} for liquids and 10^{-3} K^{-1} for gases. For the expansivity of the pores in granite we estimated $\gamma_\varphi \approx 1.7 \times 10^{-4}$ K^{-1}. For water, at 80°C and 100 bar, $\gamma_f = 6.3 \times 10^{-4}$ K^{-1}. For low porosity hard volcanic rocks, having a porosity $\varphi = 0.0018$, $b = 0.3$, and $B = 0.9$, Guéguen & Boutéca (2004) published the values $\gamma_B = 5.0 \times 10^{-5}$ K^{-1}, $\gamma_m = -46.0 \times 10^{-5}$ K^{-1} and $\gamma_U = 5.075 \times 10^{-5}$ K^{-1} and the corresponding bulk moduli $K_B = 27$ GPa and $K_U = 38$ GPa. Using these data, the corresponding variations of the fluid mass content and of the fluid pressure p for drained and undrained conditions are:

$$\left(\frac{\partial \zeta}{\partial T}\right)_{\varepsilon_B, p} = \varphi \gamma_m - b \gamma_B = -1.58 \times 10^{-5} \left[\frac{1}{K}\right]$$

$$\left(\frac{\partial p}{\partial T}\right)_{\varepsilon_B, \zeta} = -\frac{B K_U}{b}\left(\varphi \gamma_m - b \gamma_B\right) = 18.04 \times 10^5$$

$$\left(\frac{\partial p_U}{\partial T}\right)_{p_k, \zeta} = -\frac{B K_B}{b}\varphi \gamma_m = 0.67 \times 10^5$$

units in the last two equations: $\left[\dfrac{Pa}{K}\right]$

These numerical values confirm that in low porosity and low permeability rocks, the thermal variation of the fluid content is very small because of the short hydraulic parameters. For the same reason, a significant fluid pressure increase occurs in the presence of thermal stresses, specifically in undrained conditions. This is a common case when injection of cold water takes place in hot dry rock reservoirs. The values presented in Table 2 were obtained under isothermal conditions. But there are evidences suggesting a great sensitivity of the poroelastic parameters with regard to temperature changes in non-isothermal processes (Suárez, 2010). For example, the bulk modulus of cold water at 25°C is equal to 2.1 GPa (Table 2); whereas the bulk modulus of hot water is lower under deep geothermal conditions ($K_f = 0.45$ GPa at 250°C), producing larger variations of the fluid content and inducing higher thermoporoelastic deformations. Therefore, the poroelastic deformations can be much higher in geothermal reservoirs than in cold isothermal aquifers. This effect is more important in high porosity sedimentary rocks. Figure 2 shows the relationship between b, the Biot-Willis modulus and the bulk modulus of water K_f (equation 45), which depends on both, the temperature and the fluid pressure (Bundschuh and Suárez, 2010):

$$2K_S b = \left(K_U - K_B\right) + $$
$$+\sqrt{\left(K_U - K_B\right)^2 - 4\left(1 - K_S / K_f\right)\left(K_U - K_B\right)K_S \varphi} \quad (45)$$
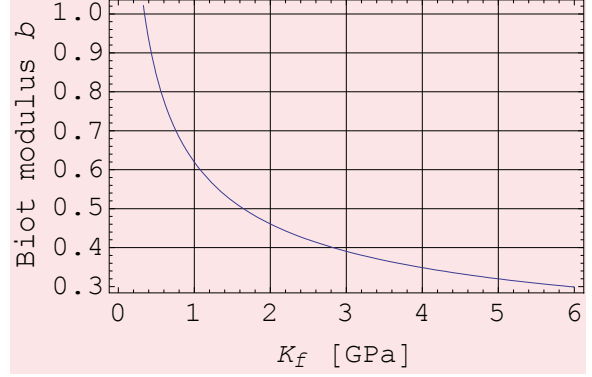

Figure 2: The Biot-Willis coefficient as a function of the bulk modulus of water.

A GENERAL POROELASTIC MODEL IN 3D

The fundamental law of dynamic poroelasticity in two-dimensions is (Bundschuh and Suárez, 2010):

$$\rho\begin{pmatrix}\dfrac{\partial^2 u_x}{\partial t^2} \\[2mm] \dfrac{\partial^2 u_y}{\partial t^2}\end{pmatrix} = \begin{pmatrix} C_0 \dfrac{\partial^2 u_x}{\partial x^2} + 2G \dfrac{\partial^2 u_x}{\partial y^2} + C_0 \dfrac{\partial^2 u_y}{\partial x \partial y} + F_x \\[3mm] C_0 \dfrac{\partial^2 u_y}{\partial y^2} + 2G \dfrac{\partial^2 u_y}{\partial x^2} + C_0 \dfrac{\partial^2 u_x}{\partial x \partial y} + F_y \end{pmatrix}$$

$$\vec{u}(t) = \left(u_x, u_y\right), \quad \frac{\sqrt{u_x^2 + u_y^2}}{L_0} \ll 1, \qquad (46)$$

$$C_0 = \lambda + b C + 2G + 2C\varphi + M\varphi^2$$

Where (u_x, u_y) are the components of the displacement vector; (F_x, F_y) are the components of the external body force acting on the porous rock; the left term in equation (46) is the vectorial acceleration and ρ is the average density, when ρ_f and ρ_s are the fluid and solid phase densities respectively; L_0 is a representative dimension of the porous skeleton. This general model is valid only for small, reversible deformations of Hookean poroelastic rocks. We consider only the important case of static poroelastic equations when the external body force is the vertical gravitational force per unit bulk volume and the acceleration in equation (46) is zero. The governing poroelastostatic equations in condensed tensorial notation is equivalent to the following formula:

$$G \nabla^2 u_i + \left(\lambda + G\right)\frac{\partial^2 u_i}{\partial i \, \partial j} - b\frac{\partial p_f}{\partial i} + F_i = 0 \qquad (47)$$
$$\text{for } \{i, j = x, y, z\}$$

Equation (47) is coupling the poroelastic mechanism between the pore pressure and the displacement of the porous rock particles. Two drained coefficients λ and G emerge because the coupling term is the fluid pressure.

The mathematical model of a poroelastic rock, fully saturated with a moving fluid, is a coupled group of partial differential equations governing the fluid flow inside the pores of the deformable skeleton. All the coefficients, concepts and relationships described in previous sections are sufficient to develop this model. We only need to define the unknowns and methodically arrange the appropriate equations. There are twelve fundamental unknown variables in three dimensional thermoporoelasticity: the six stresses (σ_{ij}) of equation (27); the three coordinates (u_x, u_y, u_z) of the relative fluid-solid displacement; the variation of the fluid content ζ (Eq. 20), the pore pressure p_f (Eq. 18), and the temperature T (Eq. 43). The six strain components (ε_{ij}) can be computed using either the quaternion equation (19) or their definition in terms of the vector displacement. The corresponding equations of the previously mentioned unknowns are the seven components relating stresses, strains and the pore pressure (Eq. 26) or (Eq. 27), the three partial differential equations obtained from the equilibrium conditions in the skeleton (Eq. 47), the eleventh equation comes from the conservation of the fluid mass relating ζ with the Darcy's law through the fluid pressure (Eq. 20); while the final twelfth comes from the general heat flow equation in geothermal reservoirs, which includes conduction and convection through an advective term related to the transport of energy by the moving fluid in the pores:

$$c_p \rho \frac{\partial T}{\partial t} - \vec{\nabla} \cdot \left(\mathbf{k}_T \cdot \vec{\nabla} T \right) + \vec{\nabla} \cdot \left(c_p \rho T \, \vec{v} \right) = Q_H \quad (48)$$

Where vector v represents the Darcy's fluid velocity, c_p is the specific heat coefficient at constant pressure, $\mathbf{k}_T$ is the thermal conductivity tensor, and Q_H [W/m³] is the volumetric thermal energy production. This group of equations provides an equilibrated system that can be numerically solved using different numerical techniques.

SOLUTION OF THE POROELASTIC MODEL USING FINITE ELEMENTS: A 2D EXAMPLE

Equation (47) includes Biot's poroelastic theory. It can be formulated and numerically solved using the Finite Element Method (FEM). Let Ω be the bulk volume of the porous rock, and let $\partial\Omega$ be its boundary, u is the set of admissible displacements in equation (46); there is a volumetric force and a force acting on the surface $\partial\Omega$. After doing some algebra (Liu and Quek, 2003) we arrive to a FEM fundamental equation for every element V^e in the discretization of Ω composed of N_e finite elements:

$$\mathbf{K}^e \cdot \vec{d}^{\,e} + \mathbf{M}^e \cdot \frac{\partial^2 \vec{d}^{\,e}}{\partial t^2} = \vec{F}^{\,e}; \quad e = 1, N_e \quad (49)$$

d^e is a vector containing the displacements of the nodes in each V^e. Equation (49) approximates the displacement u of the poroelastic rock. F^e is the vector of total nodal forces. $\mathbf{K}^e$ and $\mathbf{M}^e$ are the stiffness and equivalent mass matrices for each finite element V^e. The mathematical definitions of both matrices are:

$$\mathbf{K}^e = \int_{V^e} \mathbf{B}^T \cdot \mathbf{C}_B \cdot \mathbf{B} \, dV \; ; \; \mathbf{B} = \mathbf{L} \cdot \mathbf{N} \, ;$$

$$\mathbf{M}^e = \int_{V^e} \rho \, \mathbf{N}^T \cdot \mathbf{N} \, dV \; ; \; e = 1, N_e \quad (50)$$

Where $\mathbf{C}_B$ is an array of poroelastic coefficients, N is the matrix of shape functions that interpolate the displacements, L is a matrix differential operator and array B is called the strain poroelastic matrix. To illustrate the model (49), two-dimensional strains of an elastic aquifer are presented, including the form in which a temperature change can affect its poroelastic deformation. In the first example, we assume that the aquifer contains cold water at 20°C (1000 kg/m³). In a second example, we consider an uniform aquifer temperature of 250°C. In both cases water obeys Darcy's law for head h. Three sedimentary layers overlay an impermeable bedrock in a 5000 m long basin where faulting creates a bedrock step (BS) near the mountain front (Figure 3). The sediment stack totals 420 m at the deepest point of the basin ($x = 0$ m) but thins to 120 m above the step ($x > 4000$ m). The top two layers of the sequence are each 20 m thick. The first and third layers are aquifers; the middle layer is relatively impermeable to flow.
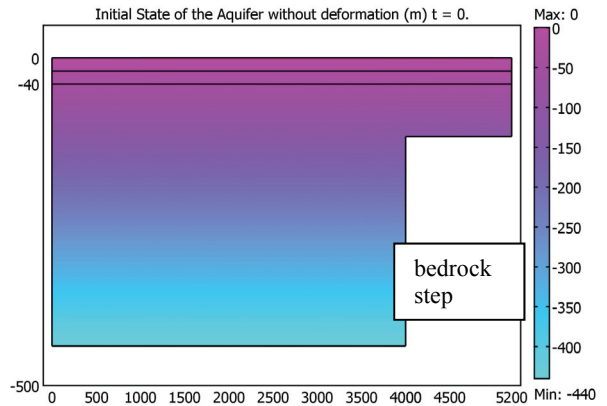

Figure 3: Initial state and aquifer's geometry with the impermeable bedrock in the basin.

The two examples presented herein were programmed and solved using the finite element software COMSOL–Multiphysics (2009) for this well-known problem of linked fluid flow and solid

deformation near a bedrock step in a sedimentary basin described in a previous publication (Leake & Hsieh, 1997).

The problem concerns the impact of pumping for a basin filled with sediments draping an impervious fault block. The flow field is initially at steady state, but pumping from the lower aquifer reduces hydraulic head by 6 m per year at the basin center (under isothermal conditions). The head drop moves fluid away from the step. The fluid supply in the upper reservoir is limitless. The period of interest is 10 years. Streamlines represent the fluid to porous rock coupling. The second simulation was performed for a poroelastic coupled deformation when the water in the aquifer corresponds to geothermal conditions (fluid density of 800.4 kg/m^3, temperature of 250 °C, and pressure of 50 bar). The rock is poroelastic, homogeneous and obeys quaternion equation (18). Water obeys Darcy's law for head h (K_X, K_Y are the hydraulic conductivities and S_S is the specific storage):

$$\frac{\partial}{\partial x}\left(K_X\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_Y\frac{\partial h}{\partial y}\right)+q_V = S_S\frac{\partial h}{\partial t} \qquad (51)$$

For the computations, data of Table 3 were used. In the first example for the Biot-Willis coefficient we assume that $b = 0.3$; in the second example $b = 0.9$ because it was affected by the higher temperature through the water bulk modulus (Fig. 2).

Table 3:   Parameters used in the simulations.

Hydraulic conductivity, upper & lower aquifers	K_X 25 m/day	Poroelastic storage coeff. upper aquifer	S_S 10^{-6}
Hydraulic conductivity confining layer	K_Y 0.01 m/day	Poroelastic storage coeff., lower aquifer	S_S 10^{-5}
Biot-Willis coefficient (cold water at 20°C)	b 0.3	Biot-Willis coefficient (hot water, at 250°C)	b 0.9
Young's modulus	E 8×10^8 Pa	Poisson's ratio	ν 0.25

The corresponding FE mesh has 2967 elements excluding the bedrock step (Fig. 3). Figures (4) and (5) show the horizontal strains in the aquifer for cold and hot water respectively. Figures (6) and (7) show the aquifer vertical deformation after 10 years of pumping with cold and hot water respectively.
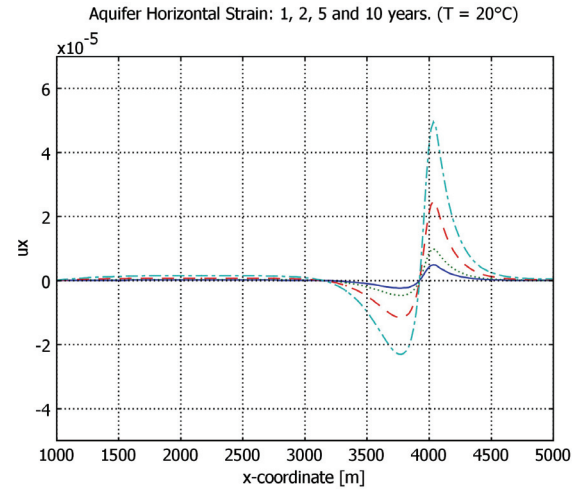

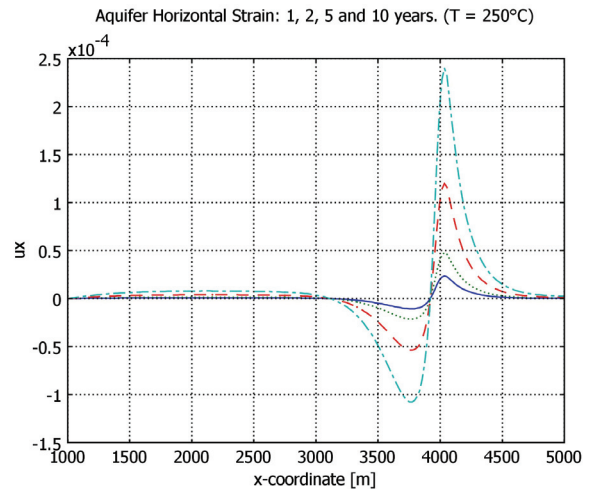Figure 4: Horizontal strain at the basin containing cold water at 20°C.

Figure 5: Horizontal strain at the basin containing hot water at 250°C.

CONCLUSIONS

■ A general thermoporoelastic linear model based on quaternions was introduced. This new formulation is equivalent to a 4D-tensorial model, which contains the classic Biot's theory. The model takes into account, in a simple way, both the fluid pressure and the temperature effects in porous rock deformations.

■ The examples presented suggest the influence of temperature changes on the poroelastic strains and on the coefficients. The poroelastic deformations are much higher in geothermal reservoirs than in isothermal aquifers. For cold water, the estimated value of ε_z is about $-1.5 \cdot 10^{-4}$, while for hot water ε_z is about $-7.5 \cdot 10^{-4}$.
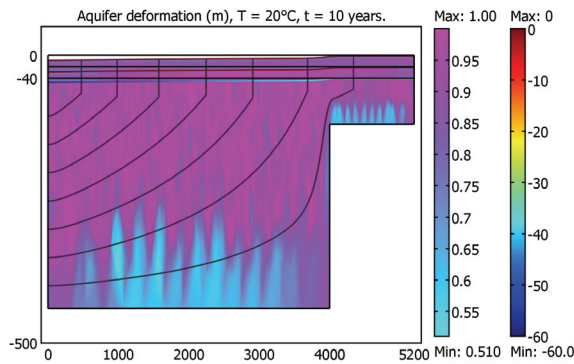
Figure 6: Poroelastic deformation of the basin for the BS problem with cold water (20°C).
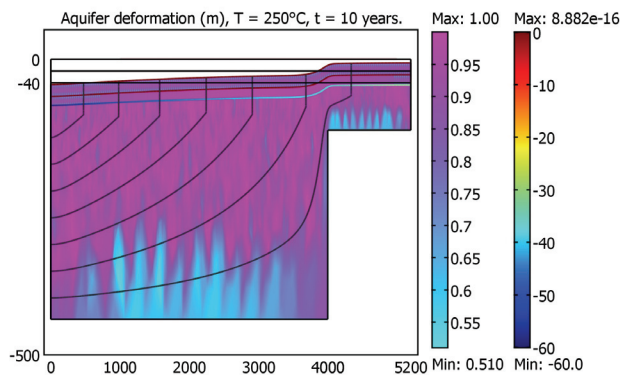

Figure 7: Poroelastic deformation of the basin for the BS problem with hot water (250°C).

REFERENCES

Biot, M. A. (1941), "General theory of three-dimensional consolidation", *Journal of Appl. Physics*, **12**, 155–164.

Biot, M. A. (1955), "Theory of elasticity and consolidation for a porous anisotropic solid", *Journal of Appl. Physics*, **26**, 182–185.

Biot, M. A. and Willis, D. G. (1957), " The elastic coefficients of the theory of consolidation", *Journal of Appl. Mechanics*, **24**, 594–601.

Biot, M. A. (1962), " Mechanics of deformation and acoustic propagation in porous media" *Journal of Applied Physics*, **33/4**, 1482–1498.

Bundschuh,J. and Suárez, M.C. (2010), "Introduction to the Numerical Modeling of Groundwater and Geothermal Systems: Fundamentals of Mass, Energy and Solute Transport in Poroelastic Rocks", 525 pp., ISBN: 978-0415-401678.

COMSOL (2009), "Coupled flow laws solved with COMSOL Multiphysics® 3.5a", COMSOL AB, User's Manual, Stockholm, Sweden.

Coussy, O. (1991). "Mécanique des Milieux Poreux", Editions Technip, Paris.

Gueguen, Y. and Bouteca, M. (editors; 2004), "Mechanics of fluid - saturated rocks". *International Geophysics Series* 89, Elsevier-Academic Press, New York, NY.

Graves, R. P. (1882), "Life of Sir William Rowan Hamilton", published in three volumes: Vol. 1, 1882, Vol. 2, 1885, Vol. 3, 1889. Dublin University Press.

Hamilton, W. R. (1853), "Lectures on Quaternions", a set of lectures delivered by Hamilton between 1848 and 1853 in the Trinity College of Dublin. Hodges and Smith, Grafton-Street. The original text can be read at this web site:

http://dlxs2.library.cornell.edu/cgi/t/text/pageviewer-idx?c=math&cc=math&idno=05230001&q1=Lectures+on+Quaternions&frm=frameset&view=image&seq=9

Hamilton, Edwin (son of Sir William Hamilton) published the book "Elements of Quaternions" in 1866, Dublin University Press. C. Jasper prepared a 2nd edition in two volumes; the 1st one in 1899 and the 2nd in 1901, published by Longmans, Green & Co.

Kuipers, J. B. (1999), "Quaternions and Rotation Sequences: a Primer with Applications to Orbits, Aerospace, and Virtual Reality", Princeton University Press, 371 pp, ISBN: 0-691-10298-8.

Lang, S. (1969), "Linear Algebra", 294 pp., Addison-Wesley Pub. Co., New York.

Leake, S. A. and Hsieh, P. A. (1997), "Simulation of Deformation of Sediments from Decline of Ground-Water Levels in an Aquifer Underlain by a Bedrock Step". US Geological Survey Open File Report 97 – 47.

Liu, G. R. and Quek, S. (2003), "The finite element method—A practical course", Butterworth-Heinemann, Bristol, UK.

Suárez, A. M. C. (2010), "A Four-Dimensional Formulation of Geothermal Poroelasticity", Proceedings of the World Geothermal Congress, pp. 1-10. Bali, Indonesia, 25-29 April 2010.

Wang, H. F. (2000), " Theory of linear poroelasticity - with applications to geomechanics and hydrogeology", Princenton University Press, NJ.

APPENDIX - NOMENCLATURE

Poroelastic coefficients: experimental definitions

In experimental poroelasticity, there are four different types of bulk moduli and two types of deformations, drained and undrained. Both modes represent limiting responses of the rock (Biot, 1941; Wang, 2000):

Drained conditions: The rock is confined and subjected to support an external hydrostatic pressure σ_H. The fluid in the pores is allowed to escape and the total stress is entirely supported by the rock skeleton. The deformations are achieved at constant pore fluid pressure p_f. Biot (1962) called this state, "an open system".

Undrained conditions: Deformations are measured at constant fluid mass content m_f ($\Delta \zeta = 0$). The rock is entirely submerged in a fluid in such a way that the external hydrostatic pressure is balanced by the pore pressure ($\sigma_H = - p_f$). The fluid in the pores remains constant; no fluid is allowed to move into or out of the control volume. The fluid remains trapped in the skeleton. For Biot (1962) this state was characteristic of a "closed system".

Bulk elastic modulus: The drained bulk coefficient K_B is one of the central concepts in poroelasticity; it is experimentally defined as the ratio of the change in confining lithostatic pressure p_k relative to the volumetric strains when the fluid pressure remains constant, under isothermal conditions:

$$\frac{1}{C_B} = K_B = -\left(\frac{\partial p_k}{\partial \varepsilon_B} \right)_{p_f} \qquad (A1)$$

Undrained bulk compressibility: The undrained bulk modulus K_U measures the resistance of the bulk rock against deformations produced by the confining lithostatic pressure when the fluid content ζ remains constant:

$$\frac{1}{C_U} = K_U = -\left(\frac{\partial p_k}{\partial \varepsilon_B} \right)_{\zeta} \qquad (A2)$$

Compressibility of the solid phase: The elastic modulus K_S measures the resistance of the solid rock against deformations produced by changes on hydrostatic compression ($\sigma_H = - p_f$) when the differential pressure $p_d = p_k - p_f$ remains constant:

$$\frac{1}{C_S} = K_S = -\left(\frac{\partial p_f}{\partial \varepsilon_S} \right)_{p_d} \qquad (A3)$$

Compressibility of the fluid phase: The isothermal compressibility of the fluid C_f is defined as the change of fluid volume with respect to the effective pressure change per unit volume:

$$\frac{1}{K_f} = C_f = -\frac{1}{V_f}\left(\frac{\partial V_f}{\partial p_f} \right)_T = \frac{1}{\rho_f}\left(\frac{\partial \rho_f}{\partial p_f} \right)_T \qquad (A4)$$

Compressibility of the pore volume: The unjacketed compressibility of the pore volume C_φ, is defined as the change of pore volume with respect to the pore pressure change per unit volume when p_d remains constant:

$$\frac{1}{K_\varphi} = C_\varphi = \frac{-1}{V_\Phi}\left(\frac{\partial V_\Phi}{\partial p_f} \right)_{p_d} = \frac{-1}{\varphi}\left(\frac{\partial \varphi}{\partial p_k} \right)_{p_d} \qquad (A5)$$

The Biot-Willis Coefficient: This fundamental parameter is equal to the change of pressure p_k with respect to the fluid pressure change when the total volumetric strain remains constant:

$$b = \left(\frac{\partial p_k}{\partial p_f} \right)_\varepsilon = 1 - \frac{K_B}{K_S} = \varphi\frac{K_B}{K_\Phi} = \left(\frac{\partial V_\Phi}{\partial V_B} \right)_{p_f} \qquad (A6)$$

The last expression in (A6) gives another definition of b as the ratio of pore volume change to total bulk volume change under drained conditions. This equation also provides two ways of computing the drained bulk modulus of the pore space K_Φ. These formulae are obtained from experiments in which the pore fluid can flow in or out of the pores to maintain the pore pressure constant.

The poroelastic expansion coefficient: $H^{-1} = 1/H$ describes how much ΔV_B changes when p_f changes while keeping the applied stress σ constant; $1/H$ also measures the changes of ζ when σ changes and p_f remains constant:

$$\frac{1}{H} = \left(\frac{\partial \varepsilon_B}{\partial p_f} \right)_\sigma = \left(\frac{\partial \zeta}{\partial \sigma} \right)_{p_f} \qquad (A7)$$

The unconstrained specific storage coefficient: 1/R measures the changes of ζ when p_f changes when the applied stress σ remains constant. Its numerical value is determined by the compressibility of the frame, the pores, the fluid and the solid phase:

$$\frac{1}{R} = \left(\frac{\partial \zeta}{\partial p_f} \right)_\sigma \qquad (A8)$$

The constrained specific storage coefficient: $1/M$ is equal to the change of ζ when p_f changes, and it is measured at constant strain. This parameter can be expressed in terms of the three fundamental ones previously defined:

$$\frac{1}{M} = \left(\frac{\partial \zeta}{\partial p_f}\right)_{\varepsilon_B} = \frac{1}{R} - \frac{K_B}{H^2} \qquad (A9)$$

Deformations coupling coefficient: The parameter C represents the coupling of deformations between the solid grains and the fluid:

$$C = \frac{K_B}{H} M \;\Rightarrow\; b = \frac{K_B}{H} = \frac{C}{M} \qquad (A10)$$

The Skempton coefficient: B represents the change in pore pressure when the applied stress changes for undrained conditions:

$$B = \left(\frac{\Delta p_f}{\Delta p_k}\right)_{m_f} = -\left(\frac{\Delta p_f}{\Delta \sigma}\right)_{\zeta} = \frac{R}{H} \qquad (A11)$$