

## Moisture and temperature effects on rocks materials and natural erosion energy

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### Abstract

Materials interact with pollutant in a very complex manner, the possibility of erosion, adsorption, desorption, transportation, deposition, and phase change will appear because of the interaction between the pollutant and the material surface. The effect of many other environmental effects also appear, like the effect of rain water in breaking away tiny rock particles (grit productivity). All the actions mentioned or any one of them may causes high damage or weaken the structure. This research highlights the importance of specific physical properties and material weakness, the effect of specific environmental factors (humidity, rain, and temperature) on materials, such as building materials and the potential occurrence places of cracks in the material, by knowing the quality of the material.

**Keywords:** Theoretical Study; hygrothermal model; Energy; Erosion; Matlab.

### Introduction:

Materials and pollutants interact in a variety of ways, Dry deposition, direct deposition of gaseous pollutants on the surface, varies with factors such as wind speed, direction and relative humidity [14]. The response of the gas reaction with limestone is enhance, if the relative humidity is above 80 per cent. Wet deposition, and delivery of gaseous pollutants on the surface, by integrating them into the water, varies with factors such as surface geometry. Where the surface is exposed to precipitation and runoff, wet chemical reactions such as a solution may be formed, then deposition occurs. The matrix of calcium carbonate or calcium carbonate rock are susceptible to reaction with acidic solutions. Porous materials, whatever their chemical composition, are likely to be susceptible to degradation from acidic solutions, it also provides a large pore size of a large area of chemical reactions [14]. Similarly, porous material will also be broken or vulnerable to the actions of salt, and salt can penetrate into tight spaces where expansion can exercise a lot of pressure on the material. Finally, the presence and movement of moisture in materials, facilitated by high porosity, can enhance and change the focus of agents of weathering and help the harmful activity.

Glass also undergoes a chemical change in contaminated environment [19], although this may not be obvious at first visually modern glass. Sodium which can be out of the surface layers of the modern glass is able to infiltrate to sulfur and carbon atmosphere of carbon dioxide. The degree of change is largely dependent on the presence of moisture (how long they stay wet), and the concentration of contaminants present and the supply of oxygen to the surface of the reaction. If the oxygen supply is cut off by the formation of a layer of weathering products, feedback can slow down dramatically. Oxidized layers may, in fact, constitute a protective barrier for another change on the surface of the metal. If these oxide layers become wet, however, there may be a fast response for an electro-chemical reaction, and promote change.

Many sets of interrelated factors determine how the interaction of materials with atmospheric pollutants and the form of decay. Unfortunately, it is often difficult to establish a clear relationship and distinctive one-to-one between pollutants and forms of decay. It is likely that the same pollutants can produce different forms of decay depending on the specific circumstances of the interactions, or it may be that the same shape produced by a variety of pollutants. It is also important to note that some reactions will only happen if the pollutants or environmental parameter

level crosses a critical threshold. Salt weathering, for example, may not happen unless the pore spaces are filled with stress and can be exercised on the walls of the pores [17].

The term decay is the process that causes a loss of a part of the material or a decrease in the material contents at a rate proportional to its current value [17].

The term phase change is any change in the chemical (change in concentrations) or structural component of the material under microscopic vision [13]

It is more than 60 years since Huntington and Dickey [9] used molecular- level models for studying dislocations disadvantage in solids, then followed by Cotterill and Doyama [5] to study the dislocations positions in face centered cubic metals through a molecular level model. Rattan, Winfree, and Ahrens [15] compared distribution of energy densities in the medium, in the presence of phase change with the compressing distribution in a material incapable of phase change. Knowles, Winfree, and Ahrens [10] found that the ratio of energy density decreases as the loading rate increases is due to the fact that the dissipation rate associated with the phase change increases with loading rate.

The environmental circumstances may cause changes in building materials, such as phase change or decay, and sometimes the two effects together where Phase change gets facilitating decay. Song, Ma, & Li [18] tried to change the environment disadvantage towards benefits, using SMA (Shape memory Alloys) to preserve the buildings from cracking as a result of environmental factors. Tariku, Kumaran, and Fazio [20] develop a transient model that solves the coupled heat, air and moisture transfer through multilayered porous media , they found that the thermal and moisture dynamic responses of building enclosures, essential inputs for whole building hygrothermal models, have strong impact on the overall performance. This is due to the fact that the moisture stored in the structure affects the indoor humidity and energy flow across the structure. Abahri , Belarbi, and Trabelsi [1], studied the effect of heat and moisture coupling on environmental material building subjected to summer and winter weather conditions. Their simulation results show that the thermal diffusion affects strongly the moisture migration in the building envelope (wall) . But the contribution of the moisture terms in energy balance equation has few incidences on temperatures values.

Graue, Siegesmund, and Oyhantcabal [7] investigated crust formation on limestone, sandstone, and volcanic rock from Cologne cathedral to identify the impact of pollution. Buseti, Mish, and Rech [4] developed a numerical tool for modeling finite deformation of reservoir rocks presenting an attempt to eliminate the main limitations of idealized methods that cannot account for the complexity of rock deformation.

This research highlights the importance of specific physical properties in studying materials weakness, the interaction between pollutants, and the effect of pollutant on materials, such as building materials and the potential occurrence places of cracks in the material by knowing the material component of elements.

• **Theoretical description**

**Transport phenomena and retardation**

Transport phenomena almost caused by the environmental circumstances, mass transport is the most common phenomena in materials interaction with the state of natural affairs, the diffusion or disperse on is concerned with the concentration difference of the material contents[2,3,12].

The fundamental formula for the conservation principle must take heat transport into account, so the conservation of energy can be expressed by the general continuity equation:

$$\frac{\partial}{\partial t} E = \frac{\partial}{\partial x} j_{Ex} + \frac{\partial}{\partial y} j_{Ey} + \frac{\partial}{\partial z} j_{Ez} + Q \text{ ----- (1)}$$

Where  $j_{Ex}, j_{Ey}, j_{Ez}$  represents energy fluxes in the three space directions, t is the time, E is the energy as a function of (x,y,z,t). Q stand for heat transportation for the whole process, in terms of Q all sources and sinks are generated. If Q(x,y,z,t) is positive, there is a source in time t at position r(x,y,z); if Q(x,y,z,t) is negative, there is a sink in time t at position r(x,y,z). Equation (1) states

that the amount of change of E in time is equal to the local flux budget. The continuity equation is derived from the budget of a control volume, i.e. a volume of finite small extensions  $\Delta x, \Delta y$ , and  $\Delta z$  in (3D). The process which causes a natural tendency to level out concentration difference is the diffusion. In the molecular scale, diffusion is a random motion of molecules in all directions. If there is a net flux in one direction from high to low concentration, then the diffusive flux equals to:

$$j = -D\nabla c \quad \text{----- (2)}$$

The term D in the last equation stands for the (factor of proportionality), it is the diffusion constant or the diffusivity. c is the concentration for any physical term. For example, in the heat diffusion, c stands for temperature and D for thermal conductivity, in the case of mass diffusion, c stands for the atomic concentration & D for diffusivity. The minus sign in equation (2) guarantees that the direction of the net flux is from high to low concentrations. When both diffusion and dispersion are considered, the flux vector in x- direction results as the sum of both contributions [8]:

$$j = -D\nabla c + vc \quad \text{----- (3)}$$

Where D is the diffusivity (a measure of the capability of a substance or energy to be diffused or to allow something to pass by diffusion). One of the most common side effects on the building materials is the humidity effects, or the rain water retarding in the pours material. Equation (3) shows that if advection is present and in fluid flowing through a homogeneous porous medium, the diffusivity is not constant, but shows a strong dependency on the flow velocity. Regarding the mass conservation equation [6,16]:

$$\theta \frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left( D \frac{\partial c}{\partial x} - vc \right) + q \quad \text{----- (4)}$$

Where q represents the heat flux,  $\theta$  represents the volumetric water content. In the case of constant velocity v and constant D and in three dimensions, the above equation becomes:

$$\theta \frac{\partial c}{\partial t} = \nabla \cdot (\theta D \nabla c - vc) + q \quad \text{----- (5)}$$

The last equation is the mass transport equation.

In pollutant interaction with materials, some portions of the solid material change its phase due to chemical reactions in the presence of environmental factors.

Let c = the fluid phase concentration and  $c_s$  the solid phase concentration, also the concentration of any phase is adjusted if the concentration of the other phase is changing according to the following equation [3]:

$$c_s = K_d c \quad \text{----- (6)}$$

Where  $K_d$  is the ratio between solid phase and liquid phase concentrations.

The expression for mass balance neglecting sorption exchange will be as follows [8, 21]:

$$\frac{\partial}{\partial t} (\theta c) = -\nabla \cdot (\theta j) \quad \text{----- (7)}$$

$$\frac{\partial}{\partial t} (\rho_b c_s) = -\nabla \cdot (\rho_b j_s) \quad \text{----- (8)}$$

Where  $j_s$  represents the flux in the solid material, and  $\rho_b$  is the bulk density of the porous medium plus the liquid. The relation between the bulk density and the density of the solid material  $\rho_s$  is:

$$\rho_b = (1 - \theta) \rho_s \quad \text{----- (9)}$$

Retardation is the fraction of an analyte in the mobile phase of a chromatographic system. In the case of fast sorption and by adding the two equations noted as (7& 8) to each other:

$$\frac{\partial}{\partial t} (\theta c + \rho_b c_s) = -\nabla \cdot (\theta j) - \nabla \cdot (\rho_b j_s) \quad \text{----- (10)}$$

This yield to

$$\frac{\partial}{\partial t}(R\theta c) = -\nabla \cdot (\theta j) - \nabla \cdot (\rho_b j_s) \text{ ----- (11)}$$

Where R is called the retardation factor, given by the following equation [21]:

$$R = 1 + \frac{\rho_b c_s}{\theta c} \text{ ----- (12)}$$

In the case of linear isotherm  $\frac{c_s}{c} = K_d$  (linear isotherm describes the equilibrium of the sorption or desorption of a material at a surface (more general at a surface boundary) at constant temperature

$$R = 1 + \frac{\rho_b}{\theta} K_d \text{ ----- (13)}$$

• **Entropy change**

One of the most common side damage is the effect of humidity and rain water on the porous medium. As a result of the existence of water within the materials slots, the growth of the entropy in any part of material must equal at least the sum of the entropy flux across the boundary and the entropy production in the interior of that part.

$$\partial_t (\rho_b \eta) \geq -\nabla \cdot \left(\frac{q}{T}\right) + \rho_b \left(\frac{r}{T}\right) \text{ ----- (14)}$$

$\eta$  = the entropy density, T= temperature, r= the external heat supply in (W/Kg.m), and q= the referential heat flux (W/ m<sup>2</sup>)

The environmental factors, like heat and humidity on the materials, have a thermodynamical explanation of fragility [2]. To calculate the energy required to do these changes, and according to the first and second low of thermodynamic,

$$\int F \cdot dx = dU - Tds \text{ ----- (15)}$$

Where F represents force, U internal energy, T temperature, and S represents the entropy.

$$\int \frac{\sum m_i}{R} a \cdot dx = dU - Tds \text{ ----- (16)}$$

The entropy change  $\frac{ds}{dt} \geq -\nabla \cdot \left(\frac{q}{T}\right) + \rho_b \left(\frac{r}{T}\right) \text{ ----- (17)}$

Regarding the mass transport and from the retardation definition, (it's the act or intruder result of delaying mass) [11].

The retardation factor could be written as (The rate of the new phase mass ( $\sum m_i$ ) to the total mass of the substance (M)).

$$R = \frac{\sum m_i}{M} \text{ ----- (18)}$$

Substituting equation (17) in equation (16).

$$\int \frac{\sum m_i}{R} a \cdot dx = dU - T \left( \nabla \cdot \frac{q}{T} + \rho_b \frac{r}{T} \right) \text{ ----- (19)}$$

Substituting the retardation factor from equation (13) in the previous equation

$$\int \frac{\sum_i m_i \cdot a}{1 + \frac{\rho_b \cdot c_s}{\theta \cdot c}} dx = dU - \nabla \cdot q + \rho_b q \text{ ----- (20)}$$

Where  $\theta$  is the porosity  $\theta = 1 - \frac{\rho_b}{\rho_s}$

Let  $\sum_i m_i = m$

$$\int \frac{m \cdot a}{1 + \frac{\rho_b \cdot c_s}{\theta \cdot c}} dx = dU - \nabla \cdot q + \rho_b q \text{ ----- (21)}$$

$\rho_b$  is the bulk density ( the density of solid containing water from rain & humidity), and  $\rho_s$  = density of the solid phase material.

$$m \cdot a \cdot x = (dU - \nabla \cdot q + \rho_b q) \cdot (1 + \frac{\rho_b}{\theta} K_d) \text{ ----- (22)}$$

$$m \cdot a \cdot x = (dU - \nabla \cdot q + \rho_b q) \cdot (1 + \frac{\rho_b}{(1 - \frac{\rho_b}{\rho_s})} K_d) \text{ ----- (23)}$$

$$m \cdot a \cdot x = (dU - \nabla \cdot q + \rho_b q) (1 + \frac{\rho_b}{(\rho_s - \rho_b)} K_d \rho_s) \text{ ----- (24)}$$

But  $m \cdot a \cdot x = E$

$$E = (dU - \nabla \cdot q + \rho_b q) + (dU - \nabla \cdot q + \rho_b q) (\frac{\rho_b}{\rho_s - \rho_b} K_d \rho_s) \text{ ----- (25)}$$

$$E = (dU - \nabla \cdot q + \rho_b q) + (dU - \nabla \cdot q + \rho_b q) (\frac{\rho_b \rho_s}{\rho_s - \rho_b} K_d) \text{ ----- (26)}$$

The last equation states that the total energy E supplied by the material to resist any kind of material deformation due to the environmental circumstances, is the sum of the change in the internal energy of the material dU, the internal heat stocked inside the material  $\nabla \cdot q$ , the external heat subjected on the material  $\rho_b q$ , and the effect of mass loss denoted by factors between the

second brackets in the right side of the last equation  $(\frac{\rho_b \rho_s}{\rho_s - \rho_b} K_d)$ .

Explaining and understanding this molecular choreography will let us reduce material damage through controlling the effect of pollutant molecular reaction dynamics. Every molecule will regarded as simple harmonic oscillator and according to Hooks law the energy for every molecule  $E_1$  describes by the following equation:

$$E_1 = \frac{1}{2} kx^2 \text{ ----- (27)}$$

Where k represents the oscillator constant which differs with the material, x is the oscillator displacement from its original position. For n oscillators in three dimensions, the oscillation energy as a function of position mesh shown in fig (1) shows line of adjacent peaks. The presence of these regions at the energy surfaces shows the possibility of the presence of many molecules under the action of higher energy due to high oscillating frequency. Adding deformation energy E (as

expressed in equation (26)) to  $E_1$  may cause cracks in the materials body. So, knowing the material contents and environmental conditions that affects the material, make it easy to find out where the occurrence of cracking, or erosion in material.

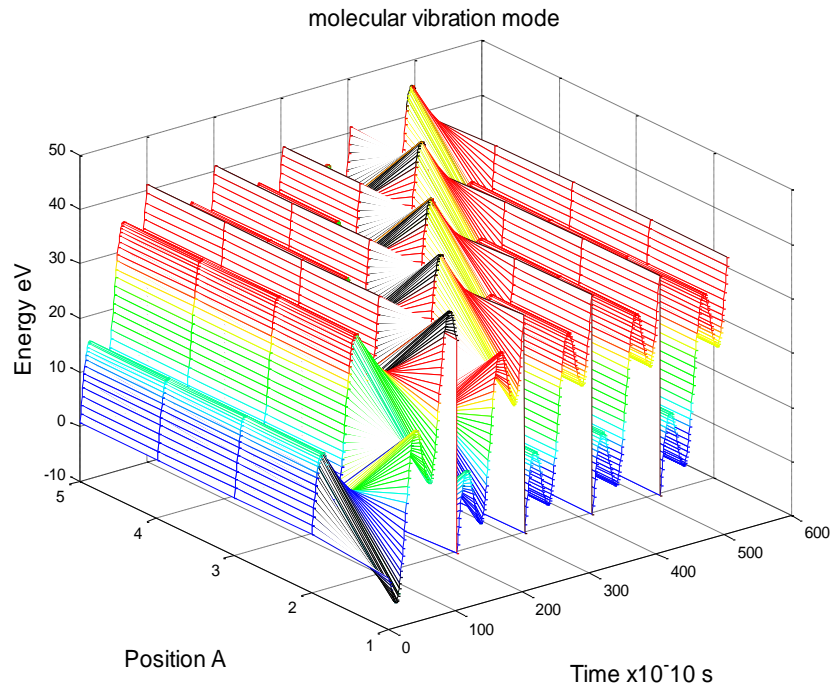


Fig (1) represents molecular vibration energy

Our results agree with the results of Tariku, Kumaran, and Fazio 2010[10], where they found that the essential factors affecting the whole building have strong impact on the overall performance because the moisture stored in the structure affects the indoor humidity and energy flow across the structure.

**Conclusions**

This article discussed the amount of energy required to deform the material in the presence of phase change under the influence of the natural environments. Energy crystalline bonding is the key factor in corrosion resistance which is based on the nature of the material used; this energy described by equation 22, shows the sum of change in the internal energy of the material  $dU$ , the internal heat stocked inside the material  $\nabla.q$ , the external heat subjected on the material  $\rho_o q$ , and

the effect of mass loss denoted by  $(\frac{\rho_b \rho_s}{\rho_s - \rho_b} K_d)$ . For n oscillators in three dimensions, the

oscillation energy as a function of position mesh shown in fig (1) shows line of adjacent peaks. The presence of these regions at the energy surfaces shows the possibility of the presence of many molecules under the action of higher energy due to high oscillating frequency. Adding deformation energy E to the oscillating energy for 3n molecules may cause cracks in a specified regions of materials body. So, knowing the material contents and environmental conditions that affects the material, make it easy to find out where the occurrence of cracking or erosion in material.

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## تأثير الرطوبة ودرجة الحرارة على المواد الصلبة والصخور وطاقة تأكلها الطبيعية

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### المخلص

تتفاعل المواد الصلبة مع الملوثات بطريقة معقدة جداً، إمكانية التآكل، الامتصاص، انتقال الجزيئات من و الى المادة، الترسيب، وتغير طور المادة الصلبة تظهر بسبب التفاعل بين الملوثات و سطح المادة. ويظهر ايضاً تأثير العديد من الآثار البيئية الأخرى مثل الضغط المسلط على المادة من قطرات المطر عند هطولها و ضغط جريان السيول التي تفصل جزيئات الصخور الصغيرة و تنقلها بعيداً (إنتاج حصى). جميع التأثيرات المذكورة أو أي واحد منها قد يسبب اضرار عالية أو إضعاف بنية و متانة المواد. يبرز هذا البحث أهمية خصائص فيزيائية محددة في اضعاف المواد، وتأثير الملوثات على بعض المواد مثل مواد البناء والأماكن المحتملة لحدوث تشققات في المواد من خلال معرفة نوعية المادة. يناقش هذا البحث كمية الطاقة اللازمة لتشوه المادة الصلبة نتيجة الظروف الطبيعية. إن هذا البحث يسلط الضوء على الطاقة اللازمة لتشوه المادة حيث أنها تساوي التغير في الطاقة الداخلية الكلية اللازمة للتشوه زائد الحرارة الداخلية المخزونة داخل المادة زائد الحرارة الخارجية المسلطة على المادة، بالإضافة الى تأثيرات فقد الكتلة. و يحدد البحث مناطق الضعف في كل مادة، و التي تكون عرضة أكثر للتشوه اعتماداً على نوع المادة المستخدمة.

**الكلمات المفتاحية:** دراسة نظرية، تحول الطور، الطاقة، تآكل المادة، ماثلاب.