Moisture and temperature effects on rocks materials and natural erosion energy

Zina Al-Shadidi

Department of physics, Faculty of Education/ Sabr, Aden University, Aden, Yemen
zabaqer@yahoo.com

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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

Moisture and temperature effects on rocks materials and natural ............... Zina Al - Shadidi

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, and 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
moister 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. Abahi, 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. Busetti, Mish, and
Reches [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 cased 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:

$$\frac{\partial}{\partial t} E = \frac{\partial}{\partial x} J_{Ex} + \frac{\partial}{\partial y} J_{Ey} + \frac{\partial}{\partial z} J_{Ez} + Q \hspace{1cm} \hspace{1cm} (1)$$

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

Moisture and temperature effects on rocks materials and natural …………Zina Al -Shadidi

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 \( \Delta t, \Delta y, \) 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:

\[
j = -D \nabla c \]

(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]:

\[
j = -D \nabla c + vc \]

(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 porous 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]:

\[
\theta \frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \theta(D \frac{\partial c}{\partial x} - vc) + q \]

(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:

\[
\theta \frac{\partial c}{\partial t} = \nabla \theta(D \nabla c - vc) + q \]

(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]:

\[
c_s = K_sc \]

(6)

Where \( K_s \) is the ratio between solid phase and liquid phase concentrations.

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

\[
\frac{\partial}{\partial t} (\theta c) = -\nabla (\theta j) \]

(7)

\[
\frac{\partial}{\partial t} (\rho_s c_s) = -\nabla (\rho_b j_s) \]

(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:

\[
\rho_b = (1-\theta)\rho_s \]

(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:

\[
\frac{\partial}{\partial t} (\theta c + \rho_b c_s) = -\nabla (\theta j) - \nabla (\rho_b j_s) \]

(10)
Moisture and temperature effects on rocks materials and natural properties ………………Zina Al-Shadidi

This yield to

\[ \frac{\partial}{\partial t}(R \dot{\theta}) = -\nabla.(\theta \dot{f}) - \nabla.\left(\rho_b \dot{f} \right) \]  

(11)

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

\[ R = 1 + \frac{\rho_b c_s}{\theta c} \]  

(12)

In the case of linear isotherm \( \frac{c_f}{c} = K_d \) (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

\[ R = 1 + \frac{\rho_b}{\theta} K_d \]  

(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.

\[ \dot{c}_i(\rho, \eta) \geq -\nabla.\left(\frac{q}{T}\right) + \rho_b \left(\frac{r}{T}\right) \]  

(14)

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

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,

\[ \int F \cdot dx = dU - Tds \]  

(15)

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

\[ \int \frac{i}{R} m_i a \cdot dx = dU - Tds \]  

(16)

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

(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 \( M \)).

\[ R = \frac{\sum m_i}{M} \]  

(18)

Substituting equation (17) in equation (16).

\[ \int \frac{i}{R} m_i a \cdot dx = dU - T(\nabla.\frac{q}{T} + \rho_b \frac{r}{T}) \]  

(19)

Substituting the retardation factor from equation (13) in the previous equation.
Moisture and temperature effects on rock materials and natural  

\[ \int \frac{\sum m_i a}{1 + \frac{\rho_b c_s}{\theta c}} \, dx = dU - \nabla q + \rho_b q \]  \hspace{1cm} (20)

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

Let \( \sum m_i = m \)

\[ \int \frac{ma}{1 + \frac{\rho_b c_s}{\theta c}} \, dx = dU - \nabla q + \rho_b q \]  \hspace{1cm} (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.

\[ m a x = (dU - \nabla q + \rho_b q)(1 + \frac{\rho_b}{\theta} K_d) \]  \hspace{1cm} (22)

\[ m a x = (dU - \nabla q + \rho_b q)(1 + \frac{\rho_b}{\rho_s} - K_d) \]  \hspace{1cm} (23)

\[ m a x = (dU - \nabla q + \rho_b q)(1 + \frac{\rho_b}{\rho_s - \rho_b} K_d \rho_s) \]  \hspace{1cm} (24)

But \( m a x = E \)

\[ E = (dU - \nabla q + \rho_b q) + (dU - \nabla q + \rho_o q)(\frac{\rho_b}{\rho_s - \rho_b} K_d \rho_s) \]  \hspace{1cm} (25)

\[ E = (dU - \nabla q + \rho_b q) + (dU - \nabla q + \rho_o q)(\frac{\rho_b \rho_s}{\rho_s - \rho_b} K_d) \]  \hspace{1cm} (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 \( \nabla q \), 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 \( E_i \) describes by the following equation:

\[ E_i = \frac{1}{2} kx^2 \]  \hspace{1cm} (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

Moisture and temperature effects on rocks materials and natural

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.

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 \( \nabla \cdot q \), the external heat subjected on the material \( \rho_0 q \), and the effect of mass loss denoted by \( \left( \frac{\rho_b \rho_s - K_d}{\rho_s - \rho_b} \right) \). 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 \( 3\pi \) 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.
Moisture and temperature effects on rocks materials and natural………………Zina Al -Shadidi

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Moisture and temperature effects on rocks materials and natural.............Zina Al-Shadidi

تأثير الرطوبة ودرجة الحرارة على المواد الصلبة والصخور وطاقة تآكلها الطبيعية
زيينة الشديدي
قسم الفيزياء، كلية التربية صبر، جامعة عدن- عدن/ اليمن
zabaqer@yahoo.com
DOI: https://doi.org/10.47372/uajnas.2017.n2.a20

الملخص
تتفاعل المواد الصلبة مع الملوثات بطريقة معقدة جداً. إمكانية التآكل، الامتصاص، انتقال الجزيئات من و إلى المادة، الترسيب، وتغير طور المادة الصلبة تظهر بسبب التفاعل بين الملوثات وسطح المادة.
ويظهر أيضاً تأثير العديد من الأثار البيئية الأخرى مثل الضغط المسلط على المادة من قطرات المطر عند هطولها وضغط جريان السبوائل، التي تفصل جزيئات الصخور الصغيرة وتقللها قليلاً (إنتاج حصى). جميع التآثرات المذكورة أو أي واحد منها قد يسبب اضرار عالية أو إضعاف بنية ومتانة المواد. يتوقع هذا البحث أهمية خصائص فيزيائية محددة في اضعاف المواد، وتأثير الملوثات على بعض المواد مثل مواد البناء والأحماض المحتملة لدبيوت تشكقات في المواد من خلال معرفة نوعية المادة.
وتطرق 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 لتشوه زائد الحرارة الداخلية المخزونة داخل المادة زائد الحرارة الخارجية المسلطة على المادة، بالإضافة إلى تأثيرات فقد الكتلة. يحدد البحث مناطق الضعف في كل مادة، والتي تكون عرضة لتشوه اعتماداً على نوع المادة المستخدمة.

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