A new theoretical mineral dissolution rate equation for physicochemical factors

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The dissolution rate of minerals is affected by not only physical factors but also chemical factors, such as temperature, solid applied stress, pore water pressure and pH. In general, previous studies on mineral dissolution have dissociated these physical and chemical factors. In this paper, we propose a new dissolution rate equation for quartz dissolution that considers the physical and chemical effects of dissolution. Therefore, the reaction rate constant \( k \), which is the most important factor in the calculation of the reaction rate, was separated into three individual terms: temperature, solid applied stress and pore water pressure. Finally, the theoretical dissolution rate equation is proposed in this study; the equation contains all of the parameters that are related to the dissolution mechanism, such as temperature, solid applied stress at contact zone, pore pressure and pH conditions. To verify the proposed equation, it is compared with the experimental results, which were collected under various physical and chemical conditions; the equation is found to fit the experimental data well.

Keywords: physico-chemical effects, quartz dissolution, dissolution rate equation, adsorption, Arrhenius equation

INTRODUCTION

The mineral crystals of a porous media can be dissolved under high stress conditions, even at low temperatures. These dissolved species can then be transported by diffusion or by advective flux mechanisms to nearby or distant locations (Stumm and Morgan, 1996). Rock deformation by physico-chemical processes has been reported by many researchers (Ganor et al., 2003; Stumm, 1992), especially for quartz dissolution (Berger et al., 1994; Brady and Walther, 1989; Dove, 1994; Ganor et al., 1995; Ganor and Lasaga, 1998; Gratz and Bird, 1993; Lahann and Roberson, 1980; Yasuhara et al., 2003, 2007). Brady and Walther (1989) studied the effect of pH on quartz dissolution at 25°C and reported the silicate dissolution rates for various pH conditions. These authors stated that the correlation between the metal-oxygen site potentials and the pH-dependent surface detachment reactions permits the estimation of the dissolution rates of a large number of silicates for a pH range of 5 to 12.

Yasuhara et al. (2003) investigated the relationship between dissolution mass, diffusive mass and precipitation mass fluxes under applied stress and temperature conditions using a mechanical model of the compaction of granular aggregates. These authors reported that the pressure solution proceeds rapidly from the initial state, in which the amount of grain-to-grain contact is so small that there is a strong enhancement of the local stress, and the initial porosity rapidly decreases with time. The dissolution and associated compaction cease as the intergranular stresses approach the critical stress level, which leads to an equilibrium state (Yasuhara et al., 2007).

For an elementary solution between A and B, the classical reaction can be represented using the activated complex theory (ACT) (Stumm and Morgan, 1996):

\[
A + B \rightleftharpoons \text{Product}
\]

where \( k^* \) is the forward rate coefficient, and \( K^* \) is the equilibrium reaction constant (Fig. 1). According to this theory, the reaction rate constant \( k \) is represented by \( k = K^*k^* \). \( K^* \) can be represented using the standard Gibbs energy \( \Delta G^0 \) value in the reaction, the standard enthalpy \( \Delta H^0 \) value and the standard entropy \( \Delta S^0 \) value of the reaction as

\[
K^* = e^{-\frac{\Delta G^0}{RT}} = e^{-\frac{\Delta H^0}{RT} + \frac{\Delta S^0}{R}}.
\]

In addition, \( k^* \) is represented as

\[
k^* = \frac{k_BT}{h}.
\]
where $h$ is Planck’s constant, and $k_B$ is Boltzmann’s constant (Benjamin, 2002). Using Eqs. (2) and (3), the reaction rate constant ($k$) is then rewritten as

$$k = \frac{k_B T}{h} e^{-\Delta G^*/RT} = \left(\frac{k_B T}{h} e^{-\Delta G^*/R}\right) e^{-\Delta A^*/RT}. \quad (4)$$

However, it is difficult to explain the effects of the physico-chemical factors on the reaction rate using Eq. (4) because this equation can only be used to describe the temperature effect of the reaction rate. Therefore, we proposed new terms of the reaction rate constants ($k_p$, $k_w$) that depend not only on temperature but also on the solid applied stress and pore water pressure. We separated these three terms into $k_p$, $k_w$, and $k_r$. The term $k_r$ depends on temperature, and this term has been studied by many other researchers, including Arrhenius, who suggested an empirical equation for the temperature dependence using experimental results. However, $k_p$ and $k_w$, which include the solid applied stress and the pore water pressure effects, were not well understood until the present work. In this study, the new reaction rate constant was first proposed that involves the applied solid stress and water pore pressure effects, and this reaction rate constant was derived using the relationship between the Gibbs free energy and the applied stress values. To provide one equation that includes the proposed reaction rate constants and pH effect, the developed adsorption theory, which combine the Freundlich and Langmuir adsorption theories, was used. Finally, the new dissolution rate equation for quartz dissolution was proposed, which was developed by considering the physical and chemical effects of the reaction rate process. Although the new equation is complex, it may be useful because this proposed equation involves both the physical and chemical factors that affect quartz dissolution in one equation. To verify the applicability of this new equation, it was compared with the results of a previous study, and the results were in good agreement.

**THE EFFECT OF TEMPERATURE ON QUARTZ DISSOLUTION**

The dissolution reaction between quartz and water can be represented as

$$SiO_2 + 2H_2O \rightarrow (SiO_2 \cdot 2H_2O) \rightarrow H_4SiO_4, \quad (5)$$

where $K$ is the thermodynamic equilibrium constant and $k^*$ is the rate coefficient for the formation ‘forward’. This process is schematically represented in Fig. 2 (Atkins and Paula, 2002).

For a first-order reaction, the dissolution rate ($v$) of Eq. (5) is represented by

$$\frac{Rate(v)}{\rho_r} = k \cdot X_{abs}. \quad (6)$$

FIG. 1. The potential energy along a one-dimensional reaction coordinate for an elementary reaction. $E_0$ is the difference in the zero-point energies between the reactants and the activated complex, $AB^*$; $\Delta E$ is the energy difference between the reactants and the products. $E_a = E_b$ is the activation energy of the elementary process (Stumm and Morgan, 1996).
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\[ k(s^{-1}) \] is a rate constant that is determined by
\[ k = K^*k^*, \]
where \( k^* \) is a rate constant, \( K^* \) is the surface concentration of the ions on the site, and \( \rho_r \) (mol/cm²) is the density of the reactive sites on the mineral’s surface (Ganor and Lasaga, 1998). In this equation, \( k \) depends on environmental conditions, such as the temperature, solid applied stress and pore water pressure, and \( X_{ads} \) depends on the pH.

**Temperature dependence**

To understand the effect of temperature on the rate constant, the Arrhenius equation was used, which postulates that the reaction rate constant \( (k) \) is known to be temperature \((T)\) dependent; this constant is determined experimentally using

\[ k = A e^{-E_a/RT}, \]

where \( A \) is the frequency factor, \( E_a (J/mol) \) is the activation energy, and \( R (J/mol/K) \) is the gas constant. The logarithmic form of Eq. (7) is given as

\[ \ln k = \ln A - \frac{E_a}{RT}. \]

However, the relationship between the activity energy \( (E_a) \) and the standard enthalpy \((\Delta H^0)\) was introduced as (Stumm and Morgan, 1996)

\[ E_a = \Delta H^0 + RT. \]

Thus, the Arrhenius equation is confirmed using the ACT treatment, and the expression of \( k \) in terms of \( \Delta S^0 \) and \(-E_a \) is given as

\[ k = e^{\frac{k_B T}{h} e^{\Delta S^0/RT} e^{-E_a/RT}}. \]

**A SUGGESTION FOR A NEW DISSOLUTION RATE EQUATION**

To date, many researchers have studied the effect of temperature and other factors on pressure solutions. However, almost all of these researchers have studied the physical and chemical effects on dissolution separately, making it difficult to understand the exact dissolution behavior under complex environmental conditions. For this reason, we propose a new dissolution rate equation that accounts for the effects of the physical and chemical
factors that affect dissolution. In this newly proposed equation, the physical effects are determined using the thermodynamic and small strain theories, and the chemical effects are determined using the adsorption theories on the mineral’s surface.

Based on this equation, it is possible to examine the exact behavior of the mineral dissolution under complex physico-chemical environmental conditions, such as a deep underground environment.

**The effect of solid applied stress**

Physically, the energy that is stored in the dissolved part of a solid is released during the process of stress dissolution. Using an analogy to the Arrhenius approach from Eq. (7), which accounts for the temperature effect, this process suggests that the effect of the stress that is generated in the solid part may be introduced using the following form:

$$ k = A^* e^{E_s/RT}, $$

(12)

where $E_s$ (J/mol) is the mechanical energy that is related to the solid applied stress, and $A^*$ is the coefficient. The authors refer to Eq. (12) as the stress-Arrhenius equation.

Let us assume that the material is hyper-elastic, with an internal energy per unit mass $u(\varepsilon, s, c_\alpha)$, where $\varepsilon$ is the strain, $s$ is the entropy, and $c_\alpha$ is the concentration of the $\alpha$-th chemical species. Because quartz exhibits a high degree of stiffness, the small strain theory (Bonet and Wood, 1997) was used. Next, the Cauchy stress, $s$ (N/m$^2$), can be represented (Bonet and Wood, 1997; Chadwick, 1999) as

$$ s = \frac{du}{d\varepsilon}. $$

(13)

By differentiating Eq. (13) with respect to strain ($\varepsilon$), the elastic tensor $D_{ijkl}$ was determined as follows:

$$ D_{ijkl} = \frac{\partial s_{ij}}{\partial \varepsilon_{kl}} = -\frac{\partial}{\partial \varepsilon_{kl}} \left( \frac{du}{d\varepsilon} \right) = -\frac{\partial}{\partial \varepsilon_{kl}} \left( \frac{\partial u}{\partial \varepsilon_{ij}} \right) = \frac{\partial^2 u}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} = D_{ijkl}. $$

(14)

Next, the enthalpy, $h(\sigma, s, c_\alpha)$, was introduced, which is defined by the internal energy and the stress tensor as follows:

$$ h(\sigma, s, c_\alpha) = u(\varepsilon, s, c_\alpha) - s \cdot \varepsilon, $$

(15)

where $\sigma$ is the stress tensor that acts on the solid and ($\varepsilon$) represents the tensor inner product. The variation enthalpy ($dh$) was defined as follows:

$$ dh = du - \varepsilon \cdot (d\sigma) = Tds - \varepsilon \cdot d\sigma. $$

(16)

Because the variation of internal energy ($du$) is defined as $dh = du = Tds + \sigma \cdot d\varepsilon$, the strain and temperature can be determined using $\varepsilon = -(\partial h)/(\partial \sigma)$ and $T = -(\partial h)/(\partial s)$ according to the Paff form.

Using Eq. (16), the compliance tensor $C_{ijkl}$ is defined as

$$ C_{ijkl} = \frac{\partial e_{ij}}{\partial \sigma_{kl}} = -\frac{\partial}{\partial \sigma_{kl}} \left( \frac{\partial h}{\partial \sigma_{ij}} \right) = -\frac{\partial}{\partial \sigma_{kl}} \left( \frac{\partial h}{\partial \sigma_{ij}} \right) = \frac{\partial e_{ij}}{\partial \sigma_{kl}} = C_{ijkl}. $$

(17)

Finally, the increase in the mechanical energy that is related to the solid applied stress and strain can be calculated as follows:

$$ \sigma_{ij} e_{ij} = \frac{d}{dt} \left( \frac{1}{2} D_{ijkl} e_{ij} e_{kl} \right) = \frac{d}{dt} \left( \frac{1}{2} C_{ijkl} \sigma_{ij} \sigma_{kl} \right). $$

(18)

We define the mechanical energy ($E_m$) that is related to the solid applied stress and the strain in the dissolution using the following equation:

$$ E_m = \frac{1}{2} D_{ijkl} e_{ij} e_{kl} = \frac{1}{2} C_{ijkl} \sigma_{ij} \sigma_{kl}. $$

(19)

**The effect of the pore water pressure**

To determine the effect of the pore pressure on the pressure solution, Eq. (4) can be used as follows:

$$ \frac{\partial k}{\partial p} = \frac{k}{RT} \left( \frac{\partial G_0}{\partial \rho} \right)_T = \frac{k}{RT} e_p. $$

(20)

$$ e_p = -\frac{\partial G_0}{\partial \rho} \bigg|_T $$

(21)

where $e_p$ is the volumetric strain that is generated on a solid part (e.g., quartz) due to the pore water pressure. Thus, in a form that is similar to the Arrhenius equation (Eq. (7)), the effect of the pore pressure can be given by

$$ k = A^* e^{E_p/RT}, \quad E_p = \int e_p dp \quad (22) $$

where $A^*$ is the coefficient for the pore water stress.
The effect of ion adsorption

The thermodynamic equilibrium constant \( (K^*) \) is related to the adsorption mechanism of the ions on the mineral’s surface. During the adsorption process, the fractional coverage of the adsorbate, \( \theta \), is defined according to Whittaker et al. (2000) as

\[
\theta = \frac{\text{number of adsorbate molecules per unit area on the solid surface}}{\text{total number of adsorbate molecules per unit area}}.
\]

(23)

The rate of adsorption \( (d\theta/dt) \) can then be determined by observing the change in the fractional coverage over time. The rate of change of the surface coverage due to adsorption is proportional to the pressure and the number of vacant sites, \( N(1 - \theta) \), whereas \( N \) is the total number of adsorbed layers (\( N = 1 \) in the Langmuir isotherm theory):

\[
\frac{d\theta}{dt} = k_aP_a(1 - \theta),
\]

(24)

where \( k_a \) is the adsorption rate constant and \( P_a \) is the partial pressure of an \( \alpha \) ion. The rate of change of \( \theta \) that is due to desorption is proportional to the number of adsorbed species, \( N \theta \):

\[
\frac{d\theta}{dt} = -k_d\theta,
\]

(25)

where \( k_d \) is the desorption rate constant. At equilibrium, the adsorption and desorption rates are equal; in other words, the sum of the two rates is zero, and solving for \( \theta \) yields the Langmuir isotherm (Erbil, 2006; Stumm and Morgan, 1996):

\[
\theta = \frac{k_aP_a}{k_d + k_aP_a} = \frac{b_\alpha a_\alpha}{1 + b_\alpha a_\alpha}.
\]

(26)

where

\[
b_\alpha = \frac{k}{k_d}
\]

(27)

is termed the adsorption coefficient for the chemical species \( \alpha \) and is the same as the equilibrium constant \( (K^*) \). For adsorption from liquid solutions, the solution concentration, \( c_\alpha \), can be used instead of \( P_a \) (Erbil, 2006).

Therefore, when a dilute solution flows into porous media, Eq. (26) can be expressed as

\[
\theta = \frac{b_\alpha c_\alpha}{1 + b_\alpha c_\alpha}.
\]

(28)

In a practical solution, the concentration can be represented using the following relationship (Stumm and Morgan, 1996):

\[
\gamma_\alpha = \frac{a_\alpha}{c_\alpha}.
\]

(29)

Next, the Langmuir isotherm equation (Eq. (26)) can be rewritten as

\[
\theta = \frac{b_\alpha a_\alpha}{1 + b_\alpha a_\alpha}.
\]

(30)

where \( \gamma_\alpha \) is assumed to be one (Stumm and Morgan, 1996).

On the surface of a crystal, defects that are related to the dissolution of the crystal structure are commonly observed. On these nonuniform surfaces, the following formulation devised by Freundlich may be fitted to the experimental data:

\[
\theta = \left( \frac{b_\alpha a_\alpha}{1 + b_\alpha a_\alpha} \right)^{1/m}.
\]

(31)

This formula yields a nonlinear equilibrium adsorption isotherm. In this equation, \( b_\alpha \) is the distribution coefficient; and \( m \) is a coefficient that is larger than unity, which is dependent on the mineral surface conditions. Equation (31) is known as the ‘generalized Freundlich isotherm’.

In this research, we combined these two isotherm equations under the assumption that the adsorption mechanism was controlled by the mineral surface conditions and that the adsorption layer was only one layer. We call the following equation the Freundlich Langmuir Isotherm Equation:

\[
\theta = \frac{b_\alpha a_\alpha^{1/m}}{1 + b_\alpha a_\alpha^{1/m}}.
\]

(32)

APPLICATION OF THE PROPOSED MODEL

The concentration of an ion that is chemisorbed onto the surface of a mineral (\( X_{\text{ads}} \)) can be described using many types of adsorption isotherms. In the present study, the concentration of the sorbed protons was represented using the newly proposed Freundlich Langmuir Isotherm equation (Eq. (32)):

\[
X_{\text{ads}} = F \cdot \frac{b_\alpha a_\alpha^{1/m}}{1 + b_\alpha a_\alpha^{1/m}}.
\]

(33)

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be rewritten in terms of the activity of a proton ($a_{H}^+$) using Eq. (29). Next, by substituting Eq. (33) into Eq. (9), the dissolution rate equation can be obtained, which includes the pH condition, as follows:

$$Rate(v) = \rho \cdot F \cdot \frac{b_0 a_{H}^+ \exp\left(\frac{\Delta S}{R} + \frac{\Delta H}{RT}\right)}{1 + b_0 a_{H}^+ \exp\left(\frac{\Delta S}{R} + \frac{\Delta H}{RT}\right)}.$$  (34)

To devise a dissolution rate equation that includes physico-chemical conditions, such as temperature, the solid applied stress, the pore water pressure and pH conditions, we substituted Eqs. (11), (15) and (22) into Eq. (34). Thus, the dissolution rate equation, called the Freundlich Langmuir Dissolution Model (FLD-Model equation), which includes the physical and chemical effects, can be obtained as

$$Rate(v) = \rho \cdot F \cdot A^T e^{-E_s/RT} e^{E_s/RT} \frac{b_0 a_{H}^+ \exp\left(\frac{\Delta S}{R} + \frac{\Delta H}{RT}\right)}{1 + b_0 a_{H}^+ \exp\left(\frac{\Delta S}{R} + \frac{\Delta H}{RT}\right)}.$$  (35)

where $b_0 = e^{-\Delta G_0/R}$.

In this equation, $A^T$ is the total frequency factor ($s^{-1}$) concerning the temperature, solid applied stress and pore water pressure on dissolution, and $m$ is defined by the surface conditions.

To examine the applicability of the newly proposed FLD-model to quartz dissolution, the proposed model was compared with other experimental results. In this research, the thermodynamic properties of silica were obtained from the results of Gunnarsson and Arnórsson (2000), who determined the thermodynamic properties and the Arrhenius parameter $(A)$ using the relationship between $\ln k$ and $1/T$ of the silicate mineral, as presented in Table 1 and Fig. 4.

The results of the FLD model (Eq. (35)) were compared with the experimental data that were presented by Brady and Walther (1989), Wollast and Chou (1986), Knauss and Wolery (1988) and Knauss and Copenhaver (1995), who performed experiments under various pH and temperature conditions. Figure 5 presents the results of the suggested FLD model and the experimental data. The results of the FLD model fit well with the experimental results, using the constant terms of $1/m$ and $\rho / FA^T$ in Eq. (35) calculated using the fitting curve (listed in Table 2).

The slope ($1/m$) of the dissolution rate increases as the temperature increases, and the constant term ($\rho / FA^T$) of the dissolution rate also increases as the temperature increases, as observed in Figs. 6 and 7, respectively.

The relationship equations of $1/m$ and $\rho / FA^T$ across the temperature range 298–343 K are

$$1/m = 0.03T - 0.66 \quad (36)$$

$$\rho / FA^T = 1.24 \times 10^{-24} e^{0.11T}. \quad (37)$$

To determine the effect of the applied stress on dissolution, the results from the newly proposed equation were compared with experimental data under various temperature and applied stress conditions by Choi et al. (2011). They assumed that the pore pressure between contact parts of specimen is zero. The results demonstrated that the effect of applied stress at a high temperature is greater than that at a low temperature. In other words, the effect of applied stress on quartz dissolution at a low temperature was less pronounced compared with that at a high temperature, and the activation energy that was related to temperature and mechanical energy was more significantly affected by high temperature than by low temperature (Fig. 8).
A new dissolution equation for physicochemical factors result, it is clear that the activation energy for the applied stress increases as the temperature increases. The slope of the dissolution rate ($1/m$) at a high temperature is steeper than that at a low temperature. The equations of Fig. 4. Experimental results of the quartz dissolution in pure water at Psat (Gunnarsson and Arnórsson, 2000).

Fig. 5. The relationship between the results of the FLD-Model under various temperatures (line with open triangles, circles, and squares) and the experimental results from previous researchers across several pH conditions.

merical results in this case. From these results, the values of the compliance tensor are approximately 100 MPa at an applied stress of 7 MPa and approximately 800 MPa at an applied stress of 21 MPa. As demonstrated by this result, it is clear that the activation energy for the applied stress increases as the temperature increases. The slope of the dissolution rate ($1/m$) at a high temperature is steeper than that at a low temperature. The equations of A new dissolution equation for physicochemical factors
Fig. 8. The relationship between the dissolution rate and the solid applied stress under different temperature conditions (lines represent the results of the FLD-Model in this study, and the open triangles and squares are the results from Choi et al. (2011)).

Fig. 6. The relationship between $1/m$ and the temperature.

Fig. 7. The relationship between the $r_{FAT}$ value and the temperature.

the activation energy for the dissolution rate equation that considers the effects of physical and chemical factors on the mechanisms of this process, we separated the activation energy ($E_a$) into three factors: temperature ($E_{aT}$), solid applied stress ($E_{as}$), and pore water pressure ($E_{ap}$). We then proposed a rate constant ($k$) for each physico-chemical factor using these activation energies. We proposed a new adsorption equation because ion adsorption significantly affects the dissolution process on the mineral surfaces. Hence, we combined the Freundlich and Langmuir isotherms to create a new isotherm equation, called the Freundlich-Langmuir isotherm.

Finally, a new dissolution rate equation was proposed, which included the effects of temperature, applied stress, pore water pressure and pH on the quartz dissolution mechanism. The applicability of the newly proposed model was compared with the existing experimental results. From these comparisons, the following results were observed:

1. The FLD-model fits well with the experimental results for various pH and temperature conditions. In particular, the suggested equation fits the experimental results well for the relevant applied stress and temperature conditions.
2. The increasing ratio ($1/m$) of dissolution in the new FLD-Model increases as the temperature increases.
3. The activation energy for applied stress ($E_{as}$) at high temperature is greater than that at low temperature.
4. The newly suggested FLD-model explains the physico-chemical effect on the quartz dissolution mechanism under complex conditions.

The effect of applied stress on dissolution under low temperature was not significant when compared with that under high temperature. The reason for this result is that the interaction between the activation energies for temperature and applied stress is very strongly affected by increasing temperature. Due to the unavailability of the experimental data that resulted from the consideration of the effects of pore pressure on quartz dissolution, the proposed model was tested by selecting zero for these parameters. Therefore, the presented equation must be further tested with the data provided by pore pressure experiments on quartz dissolution.

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**REFERENCES**


**Nomenclature**

K*: Equilibrium reaction constant

k*: Forward rate coefficient

k: Reaction rate constant (s$^{-1}$)

$\Delta h^0$: Standard Gibbs energy (J/mol)

$\Delta H^0$: Standard enthalpy (J/mol)

$\Delta S^0$: Standard entropy (J/mol/K)

b: Plank’s constant (6.626 $\times$ 10$^{-34}$ Js)

$k_b$: Boltzmann constant (1.3805 $\times$ 10$^{-23}$ J/K)

R: Gas constant (8.314 J/mol/K)

$X_s$: Surface concentration of the ions on the sites

$\rho_s$: The density of the reactive sites on the mineral’s surface (mol/cm$^2$)

A: Frequency factor (s$^{-1}$)

A*: Coefficient for stress (s$^{-1}$)

A**: Coefficient for pure water stress (s$^{-1}$)

E$_f$: Activation energy (J/mol)

$\gamma_a$: Cauchy stress (N/m$^2$)

$\phi$: Internal energy per unit mass (N/m$^2$)

$e$: Strain

$\sigma$: Entropy (J/mol/K)

$c_a$: Concentration of the a-th chemical species (mol)

$D_{ij}$: Elastic tensor

$C_{ijkl}$: Compliance tensor

$\theta$: Fraction coverage of the adsorbate

$k_a$: Adsorption rate constant (s$^{-1}$)

$P_a$: Partial pressure of $\alpha$-ion (N/m$^2$)

$a_{\alpha}$: Activation of $\alpha$-ion

$\gamma_{\alpha}$: Activity coefficient relating activities and concentrations

F: Maximum surface coverage

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