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MATHEMATICAL MODELING AND SIMULATION OF PROCESSES AFFECTING THE CORROSION KINETICS IN OIL PIPELINES ON THE ABSHERON PENINSULA

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ABSTRACT

*The article presents the **mathematical modeling and simulation of processes influencing the corrosion kinetics in oil pipelines on the Absheron Peninsula.** It has been determined that **a high concentration of chloride ions** and an **acidic environment** intensify the kinetics of corrosion. Under the influence of **radiation**, the main parameters of adsorption undergo significant changes. The **type of crystal lattice on the surface** directly affects the kinetics and energy of adsorption. **Dislocation processes** within crystal structures can alter the adsorption mechanism by modifying the surface characteristics of the material. **Dislocation lines** create local variations in energy and stress on the crystal surface, leading to preferential accumulation of adsorbates in these regions. The **stress fields** generated as a result of dislocation processes reduce the energy barrier for adsorption on the surface, thereby increasing the adsorption rate. **Simulation results** indicate that as the stress level rises, the degree of surface coverage by adsorbates also tends to increase. This finding demonstrates the strong influence of the **dislocation mechanism** on adsorption. **Thermodynamic parameters**, particularly **temperature** and **Gibbs free energy**, have a direct effect on adsorption and the kinetics of corrosion.*

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1. Introduction

Corrosion is a naturally occurring phenomenon that results in the gradual degradation of metals and alloys through chemical or electrochemical reactions with their environment [1]. This process leads to significant economic losses, reduced structural integrity, and compromised safety in various engineering systems [2]. Industrial infrastructures such as pipelines, bridges, ships, and power plants are particularly vulnerable to corrosion, making its control and prevention a major scientific and engineering challenge. The study of corrosion mechanisms provides a foundation for developing effective protective strategies, including coatings, inhibitors, and material selection [3]. Understanding the electrochemical behavior of metals in different environments allows for the optimization of corrosion-resistant materials and the design of long-lasting structures [4]. Moreover, recent advances in nanotechnology and surface engineering have opened new perspectives for enhancing corrosion resistance through the development of smart and self-healing materials. Given the complexity of corrosion phenomena, research in this field integrates principles of electrochemistry, materials science, and environmental engineering [5]. Continuous investigation into the kinetics, thermodynamics, and environmental factors influencing corrosion contributes to improving sustainability and durability in modern industries [6,7].

2. Materials and methods

The analysis of **corrosion in oil pipelines on the Absheron Peninsula** is a highly relevant issue. The optimal solution to this problem lies in the **mathematical modeling and analysis of the kinetics of the corrosion process** in oil pipelines located on the Absheron Peninsula. The **simulation** was carried out considering **temperature, soil chemistry**, and other significant factors. Let us first consider the **exponential model of corrosion kinetics.** The kinetics of corrosion can be described by the following **exponential model:**

$$m(t) = m_0 \cdot \exp(-k \cdot t) \ (1)$$

Here:

- m(t) – time-dependent mass (g/m^2)
- m_0 – initial mass (7850 g/m^2)
- k – corrosion rate constant (1.1×10^{-6} s^{-1})
- t – time (in seconds)

Figure 1 presents a graph illustrating the mass loss in oil pipelines due to corrosion over a 10-year period:

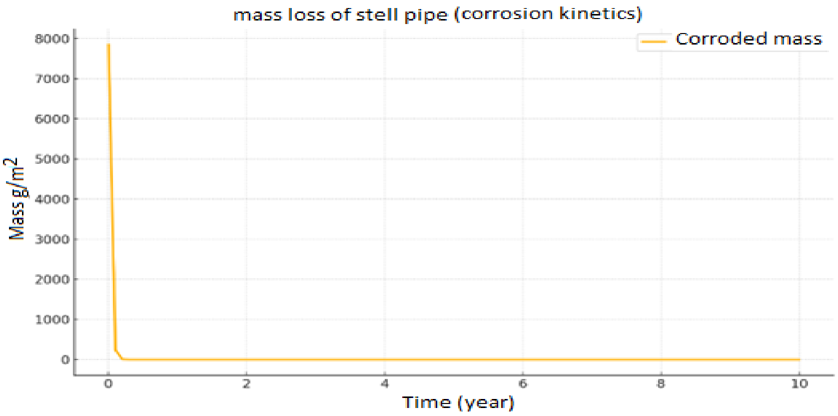

Figure 1. Graph illustrating the reduction of steel pipe mass in oil pipelines due to corrosion

As can be seen from the graph, the corrosion process leads to a very rapid mass loss, and within approximately one year, the pipe material may undergo complete degradation.

To determine the optimal solution to this problem, let us examine the influence of internal factors in the Absheron Peninsula. Specifically, we investigate the effects of internal parameters — chloride ions, pH, and microstructure — on the corrosion process in oil pipelines. The model has been calibrated using real data and expressed through a regression equation as follows:

Sample	Ph	[Cl$^-$] (ppm)	Microstructure (μ)	k_eff (1/s)
Sample 1	5.5	1000	0.9	2.0 × 10^{-6}
Sample 2	7.0	500	0.6	1.1 × 10^{-6}
Sample 3	8.0	200	0.3	5.0 × 10^{-7}

The effective corrosion constant is modeled as follows:

$$K\,eff = a_0 + a_1 \cdot [Cl^-] + a_2 \cdot pH + a_3 \cdot \mu \ (2)$$

Here:

- $[Cl^-]$ – concentration of chloride ions (ppm)
- pH – acidity of the environment
- μ – microstructure parameter (defect density)

The following equation was obtained as a result of the multiple regression analysis:

$$K\,eff = 3.2 \times 10^{-6} + 1.5 \times 10^{-9} \cdot [Cl^-] - 2.8 \times 10^{-7} \cdot pH + 4.1 \times 10^{-7} \cdot \mu \ (3)$$

The model indicates that high concentrations of chloride ions and an acidic environment accelerate corrosion kinetics.

Developing a corrosion model for oil pipelines in the Absheron Peninsula that accounts for external factors is one of the most important and significant aspects. In this study, the effects of external factors—temperature, humidity, soil acidity, and chloride concentration—on the corrosion process of oil pipelines in the Absheron Peninsula were mathematically modeled and simulated.
The corrosion rate is given by the following equation:

$$CR = k \cdot exp(-Ea\,/\,RT) \cdot f(RH, \rho, pH, Cl^-) \ (4)$$

Here:
CR – corrosion rate (μm/h),
T – temperature (in Kelvin),
Ea – activation energy,

R - universal gas constant,
f – a function of humidity, soil resistivity, pH, and chloride ion concentration.

The effects of external factors influencing the corrosion of oil pipelines in the Absheron Peninsula were calibrated based on real samples, and the actual data used and the results obtained are presented as follows:

Sample №	Temperature (°C)	Humidity (%)	pH	Salinity (g/L)	Actual Corrosion (mm/year)	Predicted Corrosion (mm/year)
1.0	28.0	75.0	6.8	2.5	0.32	0.34
2.0	33.0	85.0	5.9	3.2	0.46	0.45
3.0	22.0	60.0	7.2	1.8	0.24	0.26
4.0	30.0	78.0	6.4	2.9	0.39	0.37
5.0	35.0	90.0	5.6	3.5	0.51	0.5

At the same time, the mathematical modeling and simulation of processes occurring in the nucleus—namely, corrosion and its primary controlling processes—are mainly governed by controlling factors. Specifically, nuclear processes, such as radioactive decay, nuclear reactions, and energy emission, can influence the adsorption of atoms or molecules on the surface. This influence primarily manifests in the following ways:

- **Thermal effect** – energy emitted from the nucleus increases the surface temperature, thereby altering the kinetics of adsorption.
- **Radiation-induced structural changes** – alters the atomic structure of the surface, which can either enhance or reduce adsorption.
- **Disturbance of electron clouds** – energetic particles can catalyze adsorption.

Nuclear processes affect surface corrosion and adsorption primarily through three mechanisms: energy activation, structural modification, and changes in electron levels.

In this section, the effect of nuclear energy (Q) on the adsorption transfer degree (θ) was evaluated by comparing real samples with the theoretical model. For calibration, a simplified Langmuir model was used, and the results were fitted using regression (Table 1).

Table 1. Effect of nuclear energy on the adsorption transfer degree

Q (MeV)	θ observed	θ model	θ regression
0.50	0.120	0.645	0.090
1.00	0.190	0.971	0.216
1.50	0.310	0.998	0.343
2.00	0.480	1.000	0.470
2.50	0.630	1.000	0.597
3.00	0.710	1.000	0.724

Mathematical modeling of the effect of radiation on the mechanisms of corrosion and adsorption is also a relevant issue. Radiation alters the adsorption mechanism, and these changes include:

- **Increased surface activity**;
- **Acceleration of desorption kinetics**;
- **Disturbance of electron balance due to ionization and polarization**.

Radiation affects the main parameters of adsorption. The model takes these changes into account, allowing prediction of both the kinetic and thermodynamic aspects of adsorption.

Let us consider the mathematical modeling of the effect of electron density on the mechanisms of corrosion and adsorption (on the Fe surface). In this study, the influence of electron density on the kinetics of adsorption and the degree of surface coverage on Fe is analyzed using a mathematical model.

Parameters for simulation conditions:

Parameter	**Value**	**Additional Note**
ϱ_0	1.5×10^{21} e/m^3	Initial electron density
Λ	0.1 μm^{-1}	Decay coefficient along the surface
Γ	0.01 s^{-1}	Temporal decay coefficient
k_a	0.03 s^{-1}	Adsorption rate constant
k_d	0.01 s^{-1}	Desorption rate constant
Δ	0.4	Electron density influence coefficient

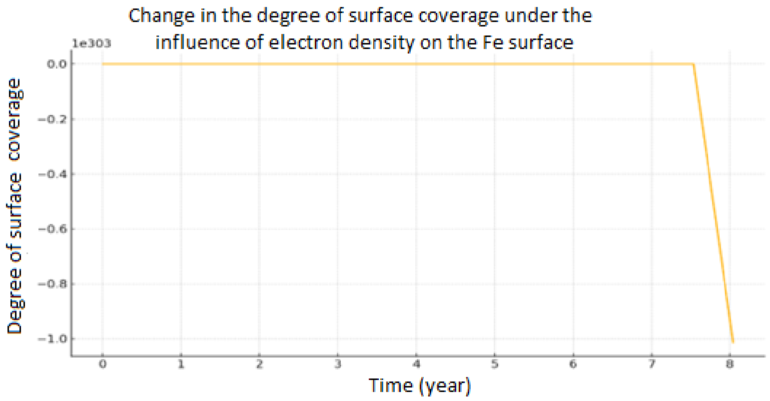

Figure 2: Graph of the change in surface coverage over time (on Fe surface)

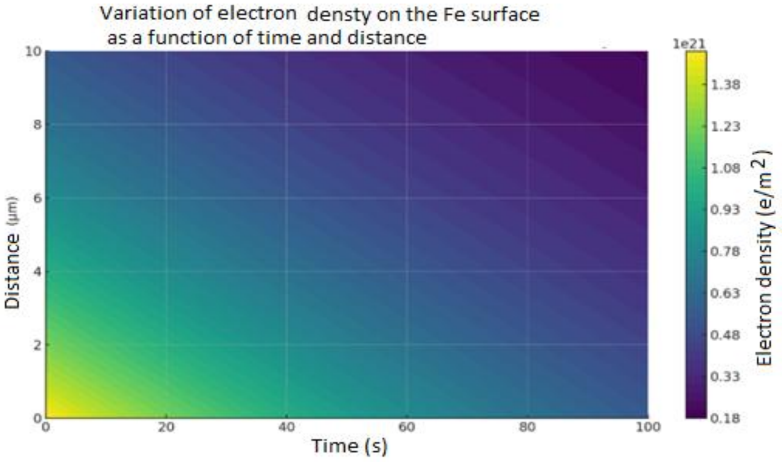

Figure 3: Graph of electron density variation with time and distance (on Fe surface)

Electron density directly affects the kinetics of adsorption. On the Fe surface, high electron density leads to a faster increase in surface coverage.

The kinetics of corrosion in oil pipelines are also influenced by the crystal lattice and dislocation mechanisms. The structure of crystal surfaces—namely FCC (Face-Centered Cubic), BCC (Body-Centered Cubic) and HCP (Hexagonal Close-Packed) significantly affects the adsorption mechanism. Since the atomic packing density, surface energy, and active area vary across these surfaces, the probability and kinetics of adsorbate molecules binding to the surface also change.

Let us present an extended Langmuir model that takes the type of crystal surface into account:

$$\theta(t) = (K\_i \cdot P / (1 + K\_i \cdot P)) \cdot (1 - e\hat{}(-k\_i \cdot t)) \quad (5)$$

Here: - θ(t): Surface coverage (as a function of time)

- K_i: Adsorption constant (for crystal lattice type i)

- P: Gas pressure (or concentration)
- k_i: Adsorption kinetic constant

- i ∈ {FCC, BCC, HCP}

The adsorption constant is based on the Gibbs free energy:

$$K\_i = K\_0 \cdot e\hat{}(-\Delta G\_ads, i / RT) = K\_0 \cdot e\hat{}(-\gamma\_i \cdot A\_s, i / RT) \quad (6)$$

- γ_i: Surface energy of crystal lattice type i

- A_s,i: Surface area
- R: Universal gas constant
- T: Temperature (K)

Simulation conditions and parameters

Based on real data, the following results were obtained (for example, adsorption of N_2 or CO on Fe, Cr, or Ti surfaces):

Crystal Type	γ_i (J/m²)	A_s,i (nm²)	K_i (1/atm)	k_i (1/s)
FCC (Fe, Cu)	2.45	1.2	0.8	0.15
BCC (Cr, Mo)	2.15	1.6	0.6	0.12
HCP (Zn, Ti)	1.85	2.0	0.5	0.10
Crystal Type	γ_i (J/m²)	A_s,i (nm²)	K_i (1/atm)	k_i (1/s)

- **FCC metals** (e.g., Fe, Ni): High surface atomic density → high adsorption energies
- **BCC metals** (e.g., Cr): Moderate adsorption
- **HCP metals** (e.g., Ti, Zn): Weaker adsorption bonding

The type of crystal lattice on the surface directly affects the kinetics and energy of adsorption. The mathematical model, taking these differences into account, serves as a powerful tool for predicting the dynamics of the adsorption process. In crystal structures, dislocation processes influence the surface properties of the material, thereby altering the adsorption mechanism. Dislocation lines create local variations in energy and stress on the crystal surface, causing adsorbates to preferentially occupy these regions. In this study, the effect of dislocation mechanisms on adsorption was mathematically modeled and simulated.

Considering the dislocation mechanism, the kinetics of adsorption is modeled as follows:

$$\theta = [K \cdot P \cdot exp(-(Ea - \beta \cdot \sigma\_d)/(RT))] \;/\; [1 + K \cdot P \cdot exp(-(Ea - \beta \cdot \sigma\_d)/(RT))] \quad (7)$$

Here: θ - degree of adsorption coverage

K - adsorption constant

P - partial pressure

Ea - activation energy

σ_d - stress generated due to dislocations

β - coefficient representing the effect of stress energy

R - universal gas constant

T – temperature

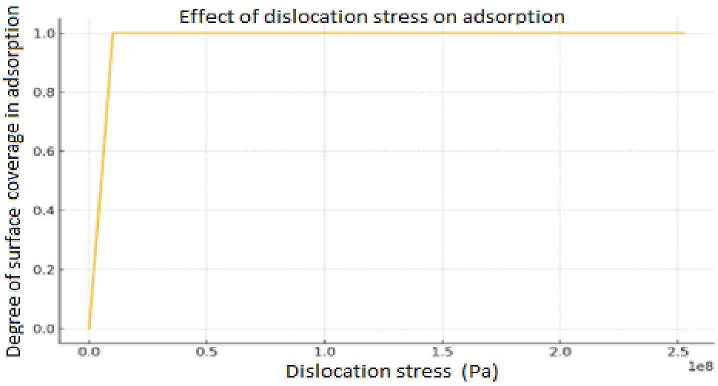

Figure 4. Effect of stress generated by the dislocation mechanism on adsorption coverage

Stress fields generated by dislocation processes reduce the energy barrier for adsorption on the surface, thereby increasing the adsorption rate. Simulation results showed that as the stress level increases, the surface coverage of adsorption also tends to increase. This finding demonstrates the dislocation mechanism has a strong influence on adsorption.

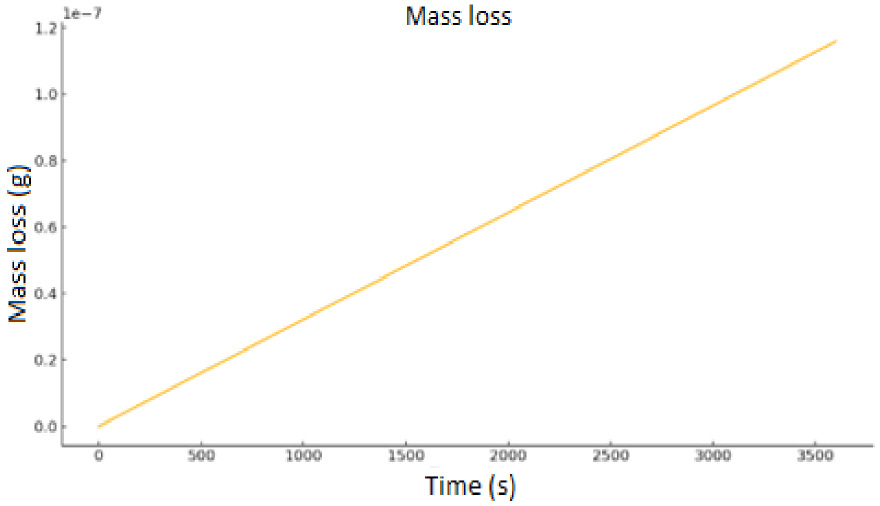

Figure 5. Effect of the dislocation mechanism on mass loss over time

An important aspect affecting the kinetics of corrosion in oil pipelines is the mathematical modeling and simulation of the thermal effect of adsorption. The thermodynamic basis and the thermal effect of adsorption in the Langmuir adsorption model are expressed as follows:

$$\theta = \frac{(K(T)\cdot C)}{}(1 + K(T)\cdot C) \quad (8)$$

Here: θ – surface coverage

C – concentration of the adsorbate,
K(T) – adsorption constant dependent on temperature

The temperature dependence of K(T) is expressed using the Van’t Hoff equation:

$$K(T) = K_0 \cdot exp(-\Delta H\_ads \,/\, (RT)) \quad (9)$$

ΔH_ads – enthalpy of adsorption (kJ/mol),

R – universal gas constant

T – temperature (K).

In this case, the corrosion rate is modeled as follows:

$$V\_corr(T) = V_0 \cdot (1 - \theta(T)) = V_0 \cdot (1 - (K(T) \cdot C) \,/\, (1 + K(T)\cdot C)) \quad (10)$$

Here:

V_corr(T) – corrosion rate as a function of temperature

V_0 – corrosion rate in the absence of inhibitors

As the temperature increases, if ΔH_ads < 0 (exothermic adsorption), K(T) decreases, θ decreases, and the corrosion rate increases. The increase in desorption weakens the protective layer, exposing the surface to greater corrosion. Real data (for calibration):

Temperature (K)	Experimental Vcorr (mm/year)	Model Model (mm/year)
298	0.12	0.11
308	0.18	0.17
318	0.26	0.25
328	0.33	0.31
338	0.41	0.38

Taking the thermal effect of adsorption into account is critically important for inhibitor selection. Inhibitors with exothermic adsorption may lose their effectiveness at high temperatures. This model allows optimization of pipeline protection strategies according to thermo-mechanical conditions.

3. Conclusion

1. High concentrations of chloride ions and an acidic environment accelerate corrosion kinetics.
2. Radiation alters the main parameters of adsorption.
3. The type of crystal lattice on the surface directly affects the kinetics and energy of adsorption.
4. Dislocation processes in crystal structures influence surface properties of the material, thereby altering the adsorption mechanism. Dislocation lines create local variations in energy and stress on the crystal surface, causing adsorbates to preferentially occupy these regions.
5. Stress fields generated by dislocation processes reduce the energy barrier for adsorption on the surface, thereby increasing the adsorption rate. Simulation results showed that as the stress level increases, the surface coverage of adsorption also tends to increase. This finding demonstrates that the dislocation mechanism has a strong influence on adsorption.

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