

2D Materials as Protective Coating against Low and Middle Temperature (100°C - 300°C) Corrosion-Erosion in Waste to Energy Plant: Case of Graphene

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Abstract

The combustion of MSW contains several species which if liberated into the flue gas will participate in erosion-corrosion reactions with the alloy surface and with the oxide layers. Actually with the evolution of material science and the discovery of 2D materials, we can handle that situation as well as possible. The graphene as 2D material presents a lot of advantage due to its physical properties such: melting point, boiling point and thermal conductivity, which can help to manage the problem of low and middle temperature (100°C - 300°C) erosion-corrosion into the boiler wall of waste to energy. The aim of the study was focused on analyzing the resistance at low and middle temperature (100°C - 300°C) in the enclosed environment and the corrosion-erosion resistance abilities of the graphene sheet as the 2D protective coating material. This paper analyzed the possibility of using the graphene in the aggressive environment which is waste to energy boiler. The results obtained from this study after simulation using ANSYS software which is one of the best software for simulations showed that Graphene protects the furnace walls against corrosion-erosion for temperatures lower than 400°C and that in the presence of certain impurities such as: sodium (Na), sulfur (S), chloride (Cl) and Phosphorous (P), Sodium Chloride (NaCl), Hydrogen Chloride (HCl), Dioxide of Carbon (CO₂) and Dioxide of Sulfur (SO₂).

Keywords

Waste to Energy (WTE), Municipal Solid Waste (MSW), Erosion-Corrosion, Temperature Corrosion, 2D Materials, Graphene

1. Introduction

Municipal Solid Waste (MSW) becomes a point of focus globally due to its harmful effects on the environment and human health if it is not managed properly. MSW was proved globally to be used as a resource, and it has a major opportunity in the realm of conversion technologies [1]. The combustion of Municipal Solids Wastes (MSW) contains several species which if liberated into the flue gas can participate in corrosion reactions and erosion with the alloy surface and with the oxide layers. Other than the significant concentration of chlorine, there is a large concentration of ash, which can contain alkali metals such as sodium and potassium or heavy metals, such as zinc and lead (Table 1). There is also an appreciable amount of sulfur in waste streams like textiles. There is roughly 5 - 10 times more chlorine in MSW than sulfur [2].

When we observe the combustion of MSW we can see quickly there is a different than that of any other fuels because of its heterogeneous nature. The corrosion mechanism can be indicated by: metal oxides (oxidation) [3], metal sulfides (sulfidation), mixtures sulfides (sulfidation) and oxides (oxidation), metal carbides (carburization) and metal chlorides (chlorination) [2].

By the way, Graphene consists of a single layer of carbon atoms arranged in a hexagonal lattice is a 2D materials which present a lot of advantages due to its physical properties [5] [6] (Table 2) which make it a good candidate as a protective solution against low and middle temperature corrosion-erosion into boiler walls.

2. Effect of Temperature on Graphene

Understanding the effect of thermally driven metal degradation is essential because of the temperatures present in industrial processes such as in: heat exchangers, boiler, and gas turbines.

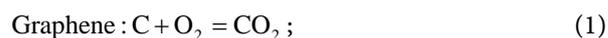
The graphene has been employed as anti-oxidation coatings because of their ambient thermal stability [7] [8] [9]. Thermal oxidation stimulates exothermic chemical reaction for graphene as follows [10]:

Table 1. Impurities which influence corrosion-erosion damage of boiler combustion gas environment in WTE plant [4].

	Kind of MSW	MSW
Contaminants of fuel (wet base)	Ash (wet base)	Large
	Cl (dry base)	A little
	S (dry base)	Large
Ash constituents	Alkaline metals (K,Na)	Large
	Alkaline earth metal (Ca, Mg)	Large but fluctuated
	Heavy metal (Zn, Pb)	Large
	Others (Fe, P)	Large but fluctuated
Corrosion of formed environment		Severe

Table 2. Physical properties of graphene.

Denomination	Properties
Appearance	Black solid
Molecular weight	12.01
Weight	0.77 mg/m ²
tensile strength	over 1 Tpa
Melting point	3652°C - 3697°C (sublimes)
Boiling point	4200°C
Density	2.267 g/cm ³
Electronegativity	2.55 Paulings
Heat fusion	117 kJ/mol
Heat vaporization	128 K-Cal/gm atom at 4612°C
Thermal conductivity	3000 - 4000 W·m ⁻¹ ·K ⁻¹
Flexibility	20% of its initial size without breaking it
Optical	2.3% of white light

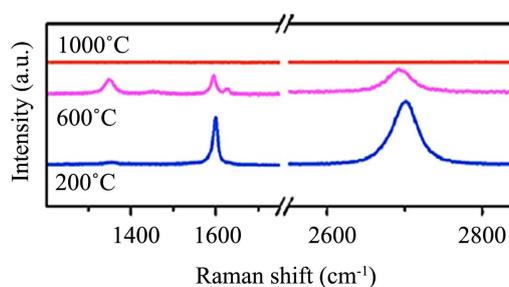


With $\Delta H_f = -393$ kJ/mole.

The activation energy required to form an initial vacancy in graphene is ~ 7.5 eV and the formation energy of subsequent vacancies decreases when adjacent atoms are sequentially detached [11]. Thus, subsequent removal of the carbon from the initial vacancy requires minimal energy.

Analyzing the Raman spectroscopy performed at different locations under a range of temperatures (up to 1000°C) elucidated the stability of corresponding 2D materials. By analyzing **Figure 1**, we can see that after 600°C, the absence of characteristics Raman peak means that for such temperatures the graphene starts to deteriorate. Meaning, under 600°C graphene coatings is acceptable.

Therefore, we will focus our study on medium and low temperatures in a closed and aggressive environment. Then, we will analyze the erosion corrosion resistance of Graphene as a 2D material in order to highlight its ability to protect the materials behind it. To achieve this objective we will run simulations using ANSYS software.

**Figure 1.** Raman spectra temperature evolution of Graphene [10].

3. Simulation Methodology

To solve our problem we use ANSYS software which is a good one for analysis of possibility of using the graphene single layer to protect the boiler walls into waste to energy plant against erosion-corrosion. For that, we have used ANSYS software.

3.1. Flow Simulation

A transient computational fluent dynamic (CFD) simulation applying a pressure-based solver was employed to solve the density weighted Reynolds-averaged Navier-Stokes (RANS) equations, as follows [12]:

$$\begin{cases} \frac{\partial \tilde{\rho} u_i}{\partial x_i} = 0 \\ \frac{\partial \tilde{\rho} u_i u_j}{\partial x_i} = \frac{\partial \tilde{\rho} u_i'' u_j''}{\partial x_i} - \frac{\partial p}{\partial x} + \frac{\partial \tau_{ij}}{\partial x_i} + \tilde{\rho} g_i \end{cases} \quad (2)$$

ρ : Density (kg/m³)

u_i : Favre-averaged velocity in tensor notation

x, y, z : Direction of coordinate axes

i, j, k : Tensorial indices

$\tilde{\cdot}$: Fluctuations with respect to a Reynolds averaging

$\overline{\cdot}$: Fluctuations with respect to a Favre averaging

g : Gravity (m/s²)

u_b, u_i : Reynolds stress (kg/m·s²)

u_i : Favre-averaged velocity in tensor notation

u_i : Resolved fluctuating velocity components

p : Pressure (Pa)

$$\frac{\partial \tilde{\rho} h u_j}{\partial x_i} = \frac{\partial \tilde{\rho} h'' u_j''}{\partial x_i} - \frac{\partial \tilde{p}}{\partial x} - \frac{\partial \tilde{J}_i^Z}{\partial x_i} + \tau_{ij} \frac{\partial u_i}{\partial x_i} + q_i + q_r, \quad (3)$$

With:

h : Enthalpy (j/kg)

J_i^Z : Diffusive flux of chemical species

q_b, q_r : The generic source term and reaction heat term

$$\frac{\partial \tilde{\rho} Y_z u_i}{\partial x_i} = \frac{\partial \tilde{\rho} Y_z''}{\partial x_i} - \frac{\partial \tilde{J}_i^Z}{\partial x_i} + \dot{R}_z, \quad (4)$$

Y : Mass fraction of species

R_z : Production rate of z th component

Where, the stress tensor, τ_{ij} , is given by [12]:

$$\tau_{ij} = \left[u \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \frac{2}{3} u \frac{\partial u_i}{\partial x_j} \delta_{ij}, \quad (5)$$

The species product by diffusive flux of combustion is defined by the Fick's law:

$$\widetilde{J}_i^z = \frac{u_t}{S_{ck}} \frac{\partial Y_z}{\partial x_i}, \quad (6)$$

u_t : Turbulent eddy viscosity (kg·m/s).

S_c : Schmidt number.

3.2. Radiation Modeling

To solve the problem in the present work, we use the discrete ordinates (DO) model of the radiative transfer Equation (RTE), considering the absorption and emission effects [12]:

$$\frac{dI(\mathbf{r}, \mathbf{s})}{ds} + (a + \sigma_s)I(\mathbf{r}, \mathbf{s}) = an^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} (\mathbf{r}, \mathbf{s})(\mathbf{r}, \mathbf{s})\Phi(\mathbf{r}, \mathbf{s})d\Omega, \quad (7)$$

I : Radiation intensity and

$(a + \sigma_s)$: The optical thickness of the medium

a : Absorption coefficient

\mathbf{r} : Position vector

Φ : Porosity

\mathbf{s} : Direction vector

n : Refractive index

The S2S model assumes any absorption, emission, or scattering of radiation by the medium can be ignored; as a result, reducing the computational cost by only considering the surface-to-surface radiation. In this model, the radiation heat transfer to a surface from another surface is a direct function of the surface-to-surface view factor. Therefore, the radiation energy balance for each surface follows the equation below [12]

$$q_{out,k} = \varepsilon_k \sigma T_k^4 + \rho_k \sum_{j=1}^N F_{kj} q_{out,j}, \quad (8)$$

F_{kj} : The view factor between surface k and surface j .

3.3. Combustion Modeling

Combustion inside the burner and furnace domains was modeled using the eddy-dissipation model (EDM). It should be noted that, because in the gas-fired furnace the burners create high velocity combustion products, the Arrhenius chemical kinetic calculations were not considered thereby the computational cost is significantly reduced. In EDM, the species transport formulation for the local mass fraction species (Y_z), for the z th species, was solved assuming that the reaction rates were dominated by turbulence. Therefore, the species transport equation becomes as follows [13]:

$$\frac{\partial}{\partial t}(\rho Y_z) + \nabla \cdot (\rho \bar{v} Y_z) = -\nabla \cdot \bar{J}_z + \dot{R}_z + \dot{S}_z, \quad (9)$$

\dot{S}_z : Source term of z th component.

3.4. Turbulence Model

The standard k - ε model uses model transport equations to obtain dissipation

rate k and turbulence kinetic energy k . Hence, the model transport equation for k can be obtained by applying the precise equation, whereas the model transport equation for k can be determined through the application of physical reasoning. Thus, to derive the k - ε model, assuming a complete turbulent flow with an insignificant molecular viscosity, making this k - ε model only applicable in flows which are fully turbulent. Hence, alterations are needed to improve both the model's applicability and its performance. Two model variants that use ANSYS Fluent are the k - ε model and realizable k - ε model, as formulated below [14]

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(u + \frac{u_i}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + G_k + G_b - \rho \varepsilon - T_M + S_k \quad (10)$$

$$\begin{aligned} & \frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) \\ & = \frac{\partial}{\partial x_j} \left[\left(u + \frac{u_i}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} + S_\varepsilon \end{aligned} \quad (11)$$

where:

G_k = production of turbulence kinetic energy due to velocity gradients.

G_b = generation of turbulence kinetic energy due to buoyancy.

T_M = contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate.

$C_{1\varepsilon}, C_{2\varepsilon}, C_{3\varepsilon}$: constants.

$\sigma_k, \sigma_\varepsilon$: turbulent Prandtl numbers for k and, respectively.

S_k, S_ε : the sources terms defined by the users.

3.5. Erosion Model

Here, we will present the erosion model using the experimental formula below [15]:

$$R_{erosion} = \sum_{p=1}^{N_{particle}} \frac{\dot{m}_p C(d_p) f(\alpha) \omega^{b(\omega)}}{A_{face}}, \quad (12)$$

$C(d_p)$ = function of particle

α = impact angle of the particle path with the wall face

$f(\alpha)$ = function of impact angle

ω = relative velocity of particle

$b(\omega)$ = function of relative particle velocity

A_{face} = area of the cell face at the wall

Default values are: $C = 1.8 \times 10^{-9}$, $f = 1$ and $b = 0$

Using the Tulsa Angle Dependent Model, Equation (30), can be rewrite as describe below:

$$ER = 1559 e^{-6} B^{-0.59} F_s \omega^{1.75} f(\alpha) \quad (13)$$

The Equation (13) will rewrite by making substitutions as follows:

$$\begin{aligned} \omega^{1.75} &= \omega^{b(\omega)} \\ 1559 e^{-6} B^{-0.59} F &= C(d_p) \end{aligned}$$

3.6. Assumptions and Boundary Conditions

To make these simulations, some assumptions and boundary conditions are required, such as:

The boiler is considered as a cube box;

We consider the a single layer graphene sheet with the size: 500 mm (long) and 250 mm (large);

The temperature into the boiler is considered variable;

We considered the pressure into boiler at 4 Mpa;

The graphene sheet is applied inside of wall of rectangular cube, meaning it already coated;

For our research we consider mechanical exfoliation as the production method of graphene and Chemical Vapor Deposition as method for coating and

The substrate is the steel.

3.7. Exposure Elements

Following elements will be used for the simulation:

Chemical elements: sodium (Na), sulfur (S), chloride (Cl) and Phosphorous (P)

Gases and composite elements: Sodium Chloride (NaCl), Hydrogen Chloride (HCl), Dioxide of Carbone (CO₂) and Dioxide of Sulfur (SO₂).

We choice to simulate the behavior of graphene in front of these elements because they are the dominants elements met into WTE.

3.8. ANSYS Input

See [Table 3](#) and [Table 4](#).

Table 3. Chemical elements characteristics to input.

Elements	density (kg/m ³)	Cp (J/kg·K)	Thermal conductivity (W/m·K)	Viscosity (kg/m·s)
sodium (Na)	970	1230	140	0.072
Chloride (Cl)	3.21	21.8	0.0089	0.0156
Sulfur (S)	2070	710	0.205	0.00409
Potassium (K)	860	750	100	0.072
Phosphorous (P)	1.82	0.77	0.236	0.00106

Table 4. Characteristics of composite chemical elements to input.

Gases	density (kg/m ³)	Cp (J/kg·K)	Thermal conductivity (W/m·K)	Viscosity (kg/m·s)
NaCl	0.00188	880	3.22	0.0328
HCl	450.14	799	0.01906	0.0000156
SO ₂	1296	148	0.0177	0.00002285
KCl	1980	690	6.53	0.000228
CO ₂	1.98	1040	20.769	0.00002485

4. Results and Analysis

This chapter is devoted to simulation of erosion resistance of graphene sheet at certain temperature and the corrosion analysis because we cannot make the last one on ANSYS software. The simulation will be made such as:

Step 1. Simulation of Temperature resistance of graphene sheet alone coated the boiler walls.

Step 2. Temperature resistance Simulation of the graphene sheet coated the boiler walls in presence of some chemical elements.

Step 3. Erosion Simulation of the ability of graphene sheet coated the boiler wall in presence of some chemical element and gases.

Step 4. Analysis of Corrosion barrier of graphene sheet.

4.1. Temperature Resistance of Graphene Sheet Coated the Boiler Walls

4.1.1. Geometry

In order to have convincing results as mentioned in the hypotheses, we will coat Graphene sheets (one layer) on the walls of a closed box which represents the walls of an oven. Below **Figure 2**, the geometry used for our simulation.

4.1.2. Mesh

After defining our geometry, we need to define the appropriate mesh which is important for the calculations.

Below **Figure 3** is the mesh.

4.1.3. Data Analysis

To exploit the data collect after running our simulation will be drop the data the table for further analysis.

We categorize the data obtained in three Classes such as:

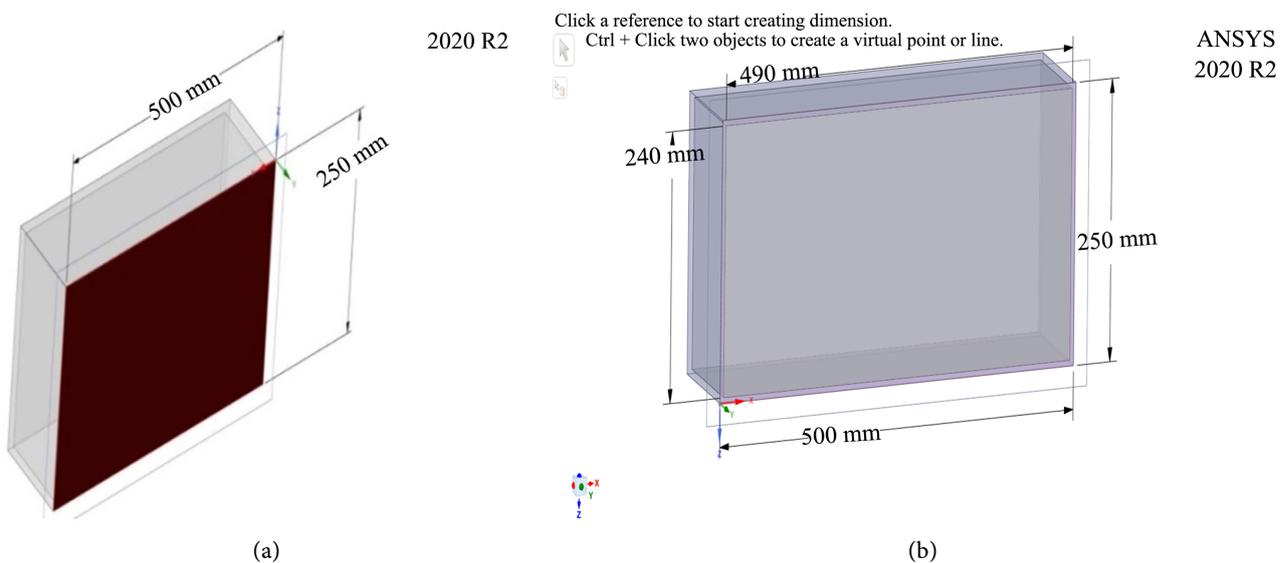


Figure 2. (a) The geometry of boiler with graphene coated on the wall (Graphene is the brown); (b) The geometry size.

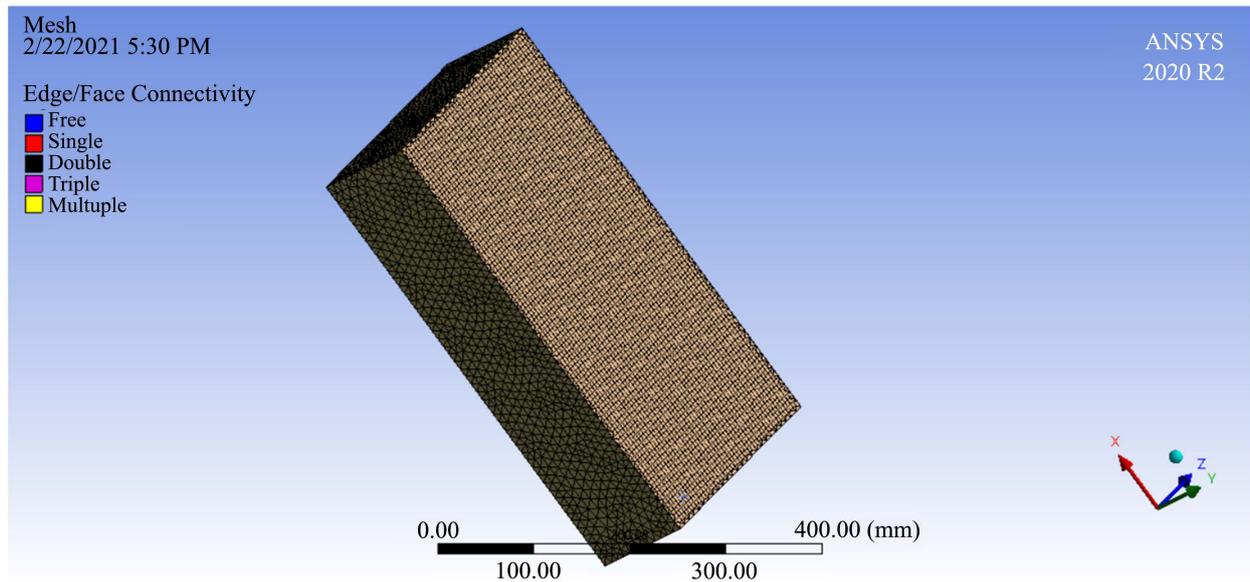


Figure 3. Study structure mesh.

Class 1: [148°C - 1067.85°C], represented by blue and blue bright on the **Figure 4**, what means a graphene sheet work well;

Class 2: [1067°C - 2905.85°C], represented by green and yellow on the **Figure 4**, meaning graphene sheet still supporting and work with increases of temperature;

Class 3: [3212.85°C - 4743.85°C], represented yellow red and red on the **Figure 4**, meaning the graphene sheet cannot support and work.

Thereby, the graphene sheet resists well and can protect the wall of boiler against any attack due to the temperature between (148°C - 761.85°C).

4.2. Temperature Resistance Simulation in Presence of Some Chemical Elements

4.2.1. Simulation of Graphene Sheet Coated the Boiler Walls in Presence of: Sodium (Na), Chloride (Cl), Sulfur (S) and Phosphorous (P)

See **Figures 5-8**.

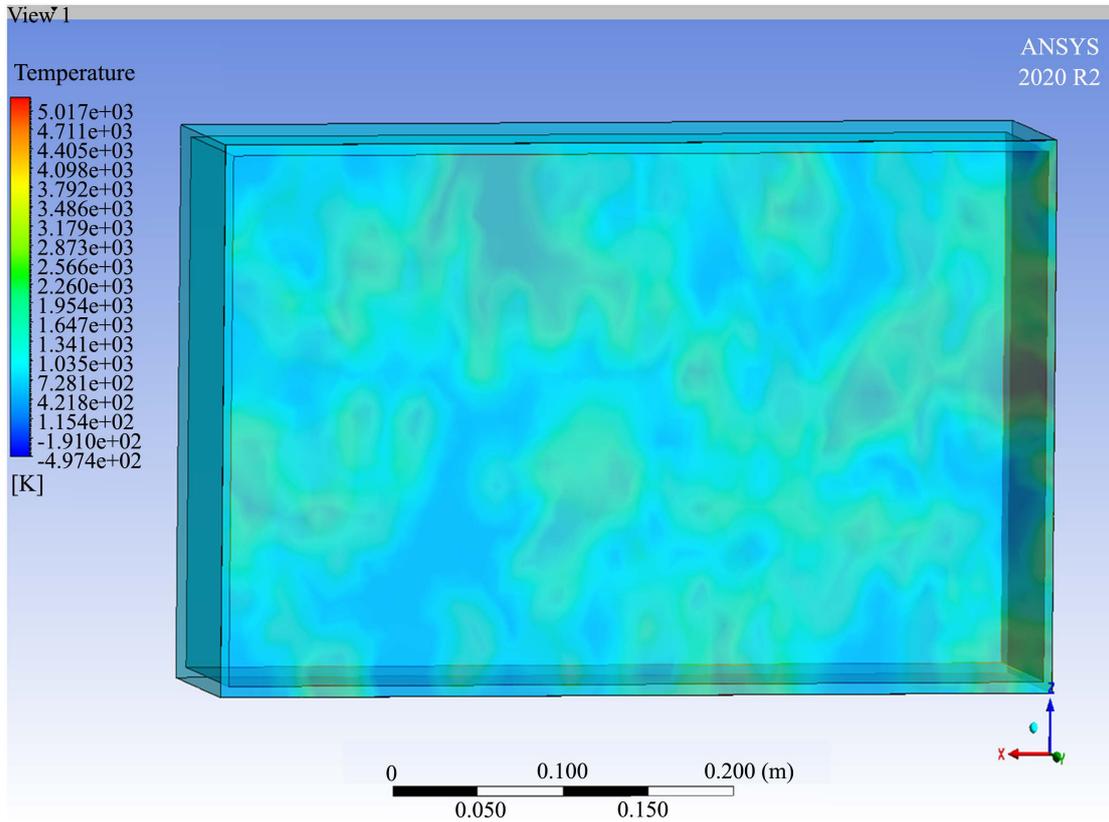
4.2.2. Data Analysis

We have simulated the behavior of graphene coated at some range of temperature and in presence some chemical selected elements, such as: Sodium, Chloride, Sulfur and Phosphor.

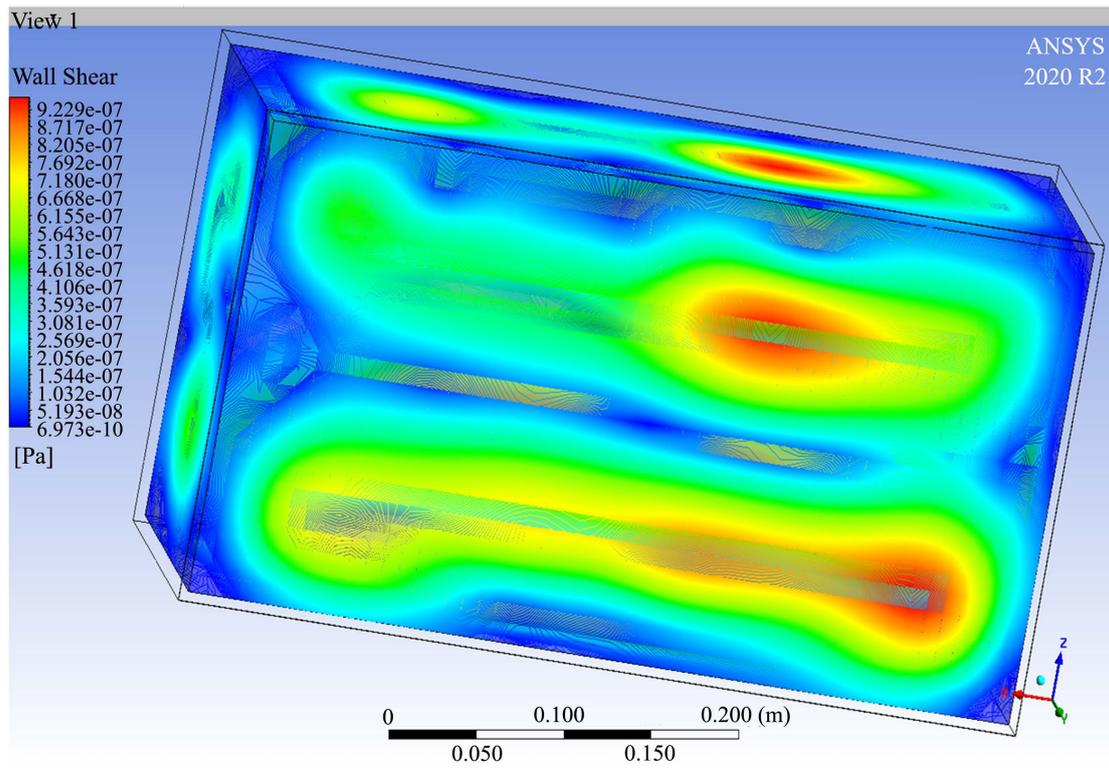
To analyze the data obtained from this simulation we will follow the approach used in point 3.1, the results of these simulations are synthesized on the following tables.

4.2.3. Results of Simulation of Graphene Coated the Boiler Wall Containing Sodium (Na)

After this simulation, we have categorized the behavior of the graphene sheet in three Classes, such as:



(a)



(b)

Figure 4. (a) Temperature the resistance of Graphene coated; (b) The wall shear.

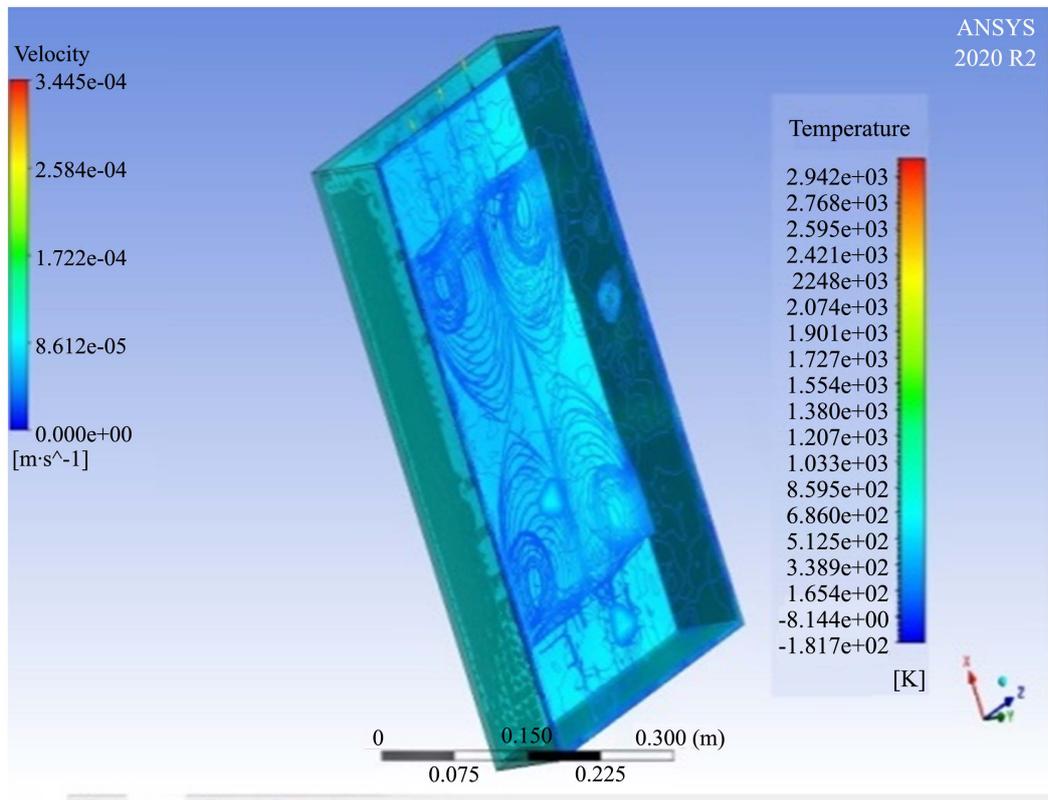


Figure 5. Graphene-sodium (Na).

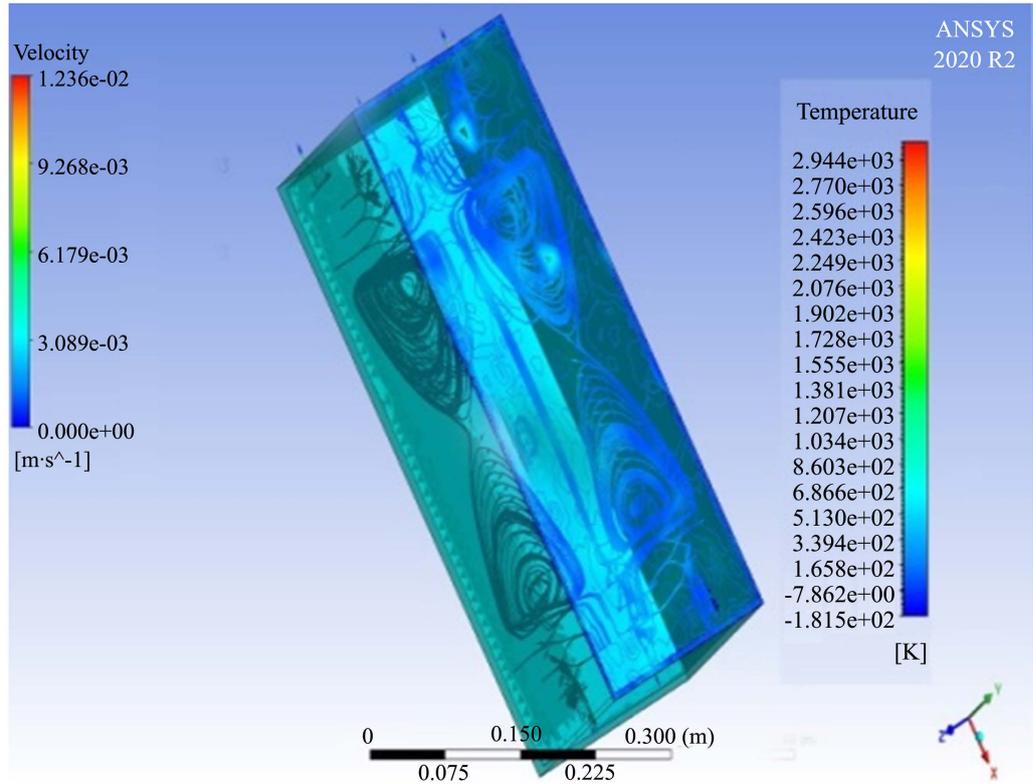


Figure 6. Graphene-Chloride.

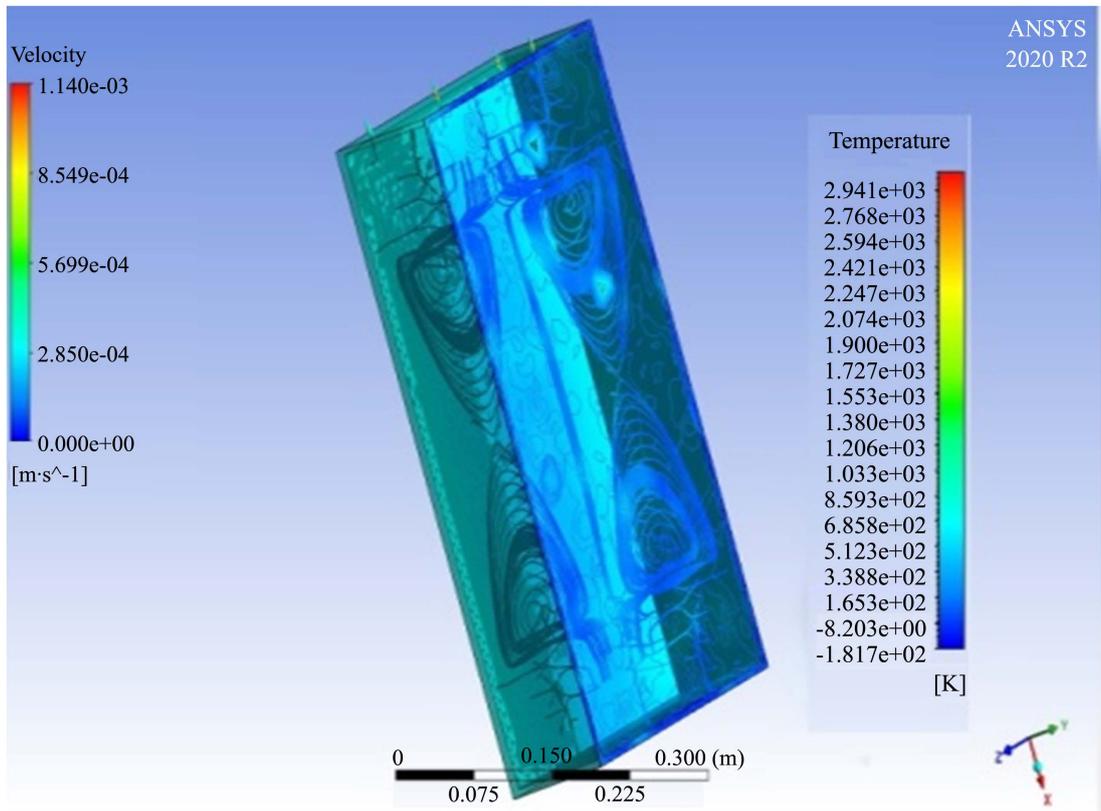


Figure 7. Graphene-Sulfur.

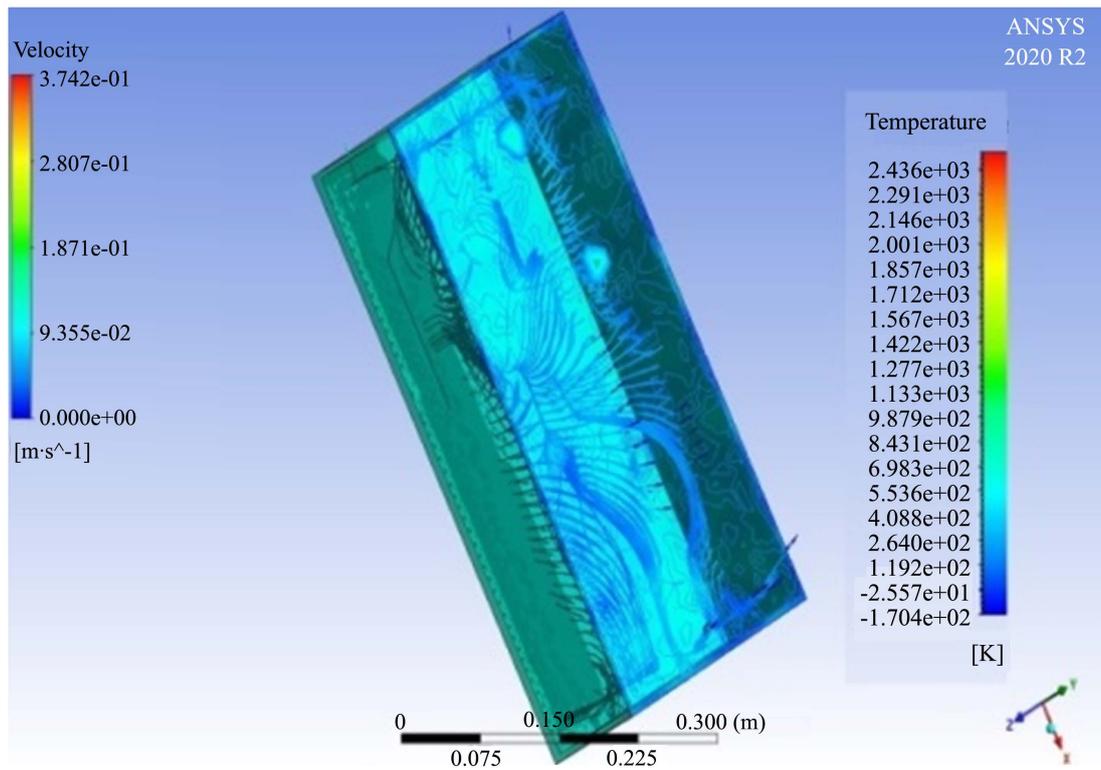


Figure 8. The Graphene-Phosphorous.

Class 1: [64.85°C - 412.85°C], represented by bleu and bleu bright on the **Figure 5**, which mean the graphene sheet work normally;

Class 2: [585.85°C - 1627.85°C], represented by green and yellow on the **Figure 5**, meaning graphene sheet still supporting and work but structural transformation due to the temperature happen;

Class 3: [2321.85°C - 2668.85°C], represented yellow red and red on the **Figure 5**, meaning the graphene sheet cannot work because we are near to the melting point and boiling.

4.2.4. Results of Temperature Resistance Simulation of Graphene Coated the Boiler Walls Containing Chloride (Cl)

For this case we have:

Class 1: [65.85°C - 412.85°C], represented by bleu and bleu bright on the **Figure 6**, what means a graphene sheet work well;

Class 2: [586.85°C - 1628.85°C], graphene sheet still supporting and work but structural transformation due to the temperature happen;

Class 3: [1802.85°C - 2670.85°C], represented yellow red and red on the **Figure 6**, meaning the graphene sheet cannot work because we are near to the melting point and boiling.

4.2.5. Results of Simulation of Graphene Coated the Boiler Wall Containing of Sulfur (S)

After this simulation, we have categorized the behavior of the graphene sheet in three classes, such as:

Class 1: [238.85°C - 411.85°C], represented by bleu and bleu bright on the **Figure 7**, what means a graphene sheet work well;

Class 2: [585.85°C - 1279.85°C], represented by green and yellow on the **Figure 7**, meaning graphene sheet still supporting and work with increases of temperature;

Class 3: [1800.85°C - 2667.85°C], represented yellow red and red on the **Figure 7**, meaning the graphene sheet cannot support and work.

4.2.6. Results of Temperature Resistance Simulation of Graphene Coated the Boiler Walls Containing of Phosphorous (P)

After this simulation, we have categorized the behavior of the graphene sheet in three Classes, such as:

Class 1: [180.75°C - 793.85°C], represented by bleu and bleu bright on the **Figure 8**, what means a graphene sheet work well;

Class 2: [800°C - 2634.85°C], represented by green and yellow on the **Figure 8**, meaning graphene sheet still supporting and work with increases of temperature;

Class 3: [2650°C - 5088.85°C], represented yellow red and red on the **Figure 8**, meaning the graphene sheet cannot support and work.

4.2.7. Average Comment

In the **Table 5** and **Figure 9**, we compare the limit of all these simulation results. We observe a significant difference between data of simulation graphene working alone when it coat at the boiler walls and data of simulation of graphene in presence of some chemical elements which are considered as pollutants and dangerous for the boiler walls. Thus, these elements reduce the protective capacity of Graphene approximately by half but the graphene still good.

Considering the temperature values into the table above graphene can perfectly work without convenient with all selected chemical elements until a max of 400°C.

4.3. Erosion Simulation of Graphene Sheet Coated the Boiler Walls

For this simulation we still using, the geometry and mesh at the point 4.1.1. We will simulate the erosion behavior of graphene coated the boiler walls in presence of gases and one simple chemical element such as: HCl, SO₂, KCl, P and CO₂.

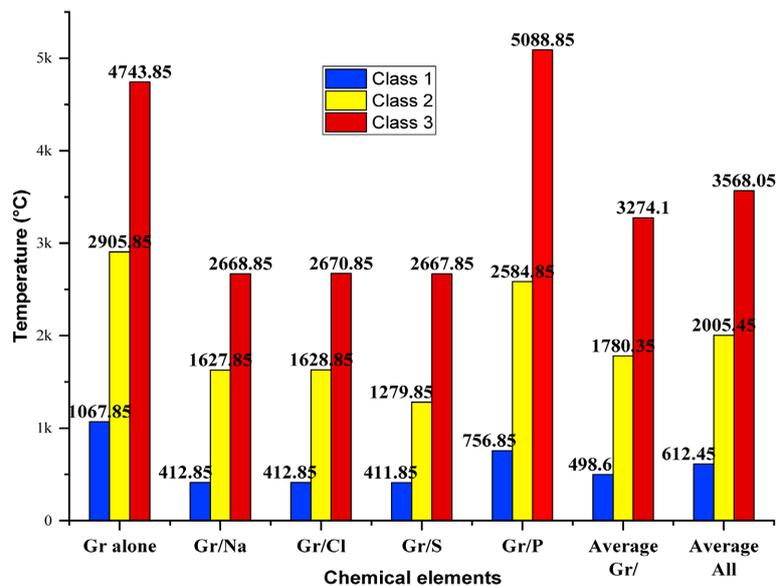


Figure 9. Limit values.

Table 5. The average of each category.

Designation	Class 1 (temperature °C)	Class 2 (temperature °C)	Class 3 (temperature °C)
Gr alone	1067.85	2905.85	4743.85
Gr/Na	412.85	1627.85	2668.85
Gr/Cl	412.85	1628.85	2670.85
Gr/S	411.85	1279.85	2667.85
Gr/P	756.85	2584.85	5088.85
Average Gr	498.6	1780.35	3274.1
Average All	612.45	2005.45	3568.05

4.3.1. Erosion Simulation of Graphene in Presence of HCL

Analysis

Comment

By analyzing the results presents above on the table and figure, we have:

Class 1: $\leq 610.45^\circ\text{C}$, represented by bleu and bleu bright on the **Figure 10(b)**, what means a graphene sheet work well without any problem; in the **Figure 11**, we can observe the erosion rate is approximately zero;

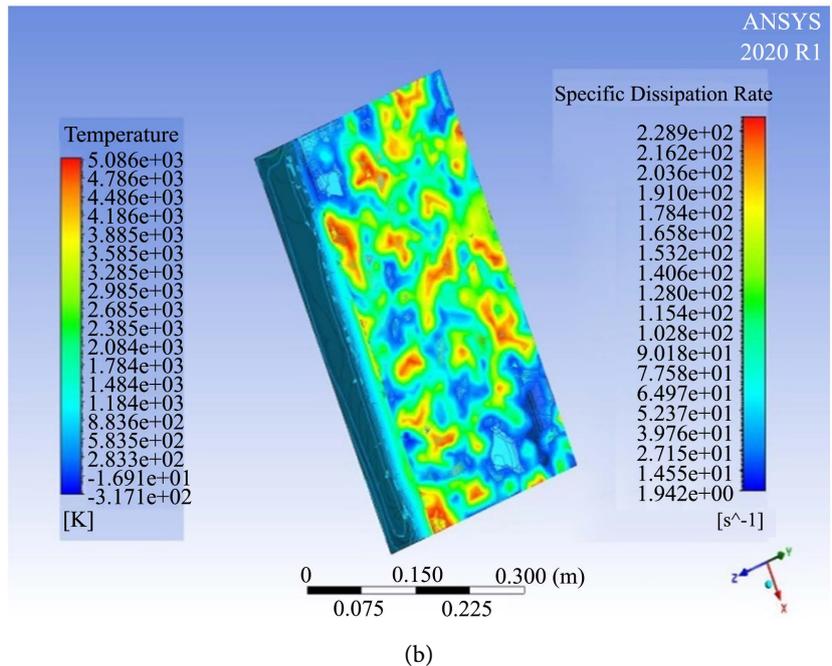
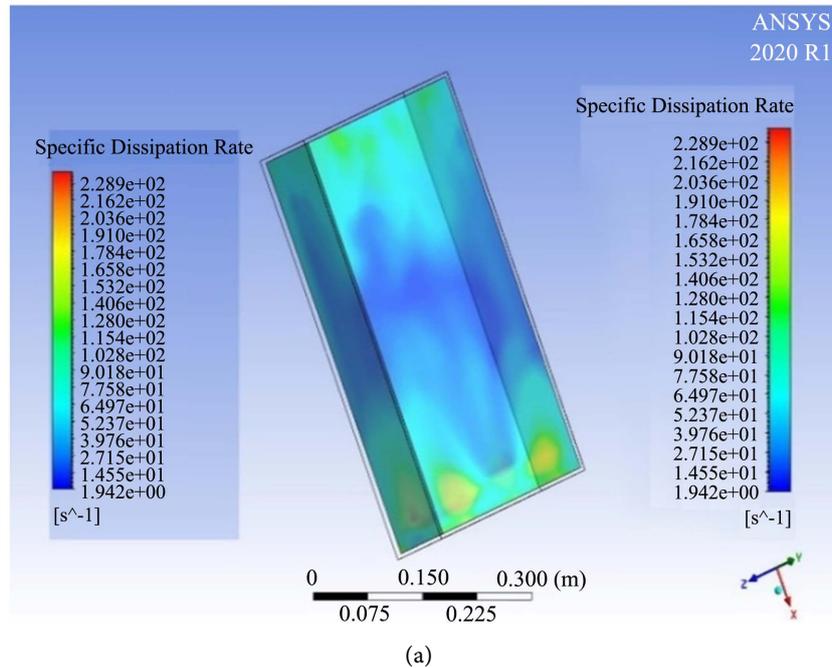


Figure 10. (a) Specific dissipation rate of graphene in presence of HCL; (b) Specific dissipation rate at some range of temperature.

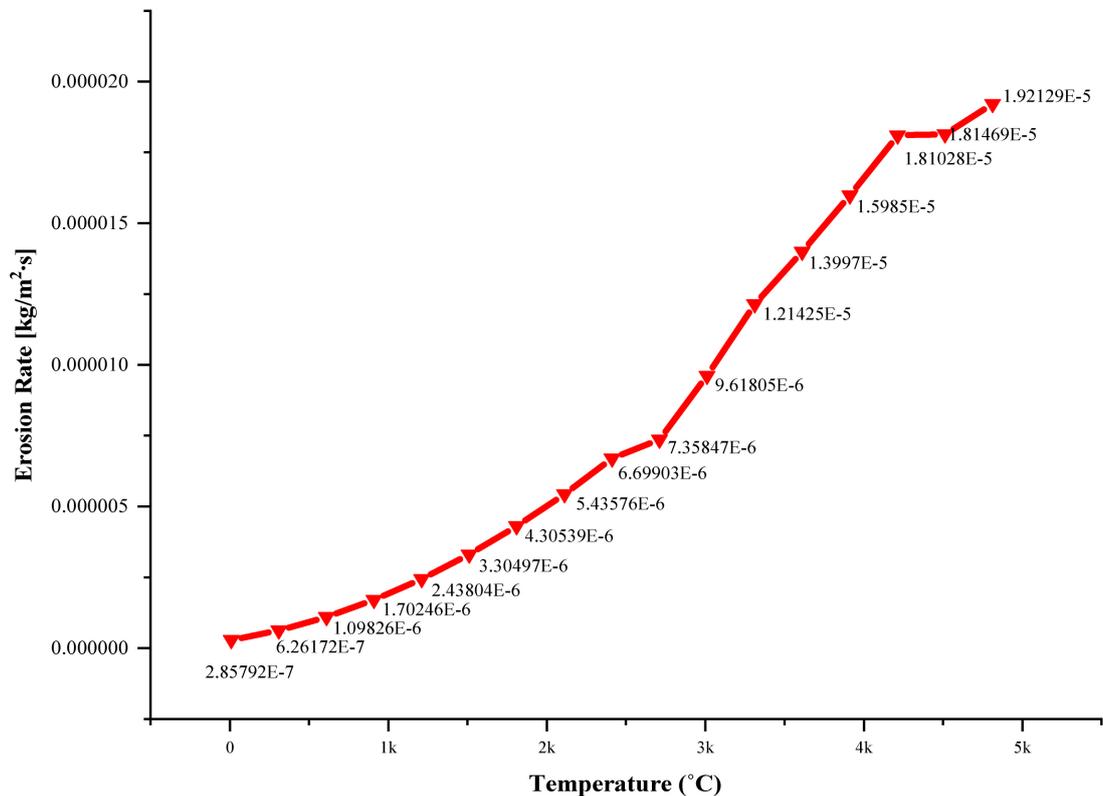


Figure 11. Erosion due by temperature change in the boiler full of HCl.

Class 2: [910.85°C - 2711.85°C], represented by green and yellow on the **Figure 10(b)**, meaning graphene sheet still supporting and work with increases of temperature;

Class 3: [3011.85°C - 4812.85°C], represented yellow red and red on the **Figure 10(b)**, meaning the graphene sheet cannot support and work.

4.3.2. Erosion Simulation of Graphene in Presence of SO₂

Analysis

Comment

By analyzing the results presents above on the table and figure, we have:

Class 1: ≤754.85°C, represented by bleu and bleu bright on the **Figure 12(b)**, what means a graphene sheet work well without any problem; and we observe the erosion rate is approximately zero (**Figure 13**);

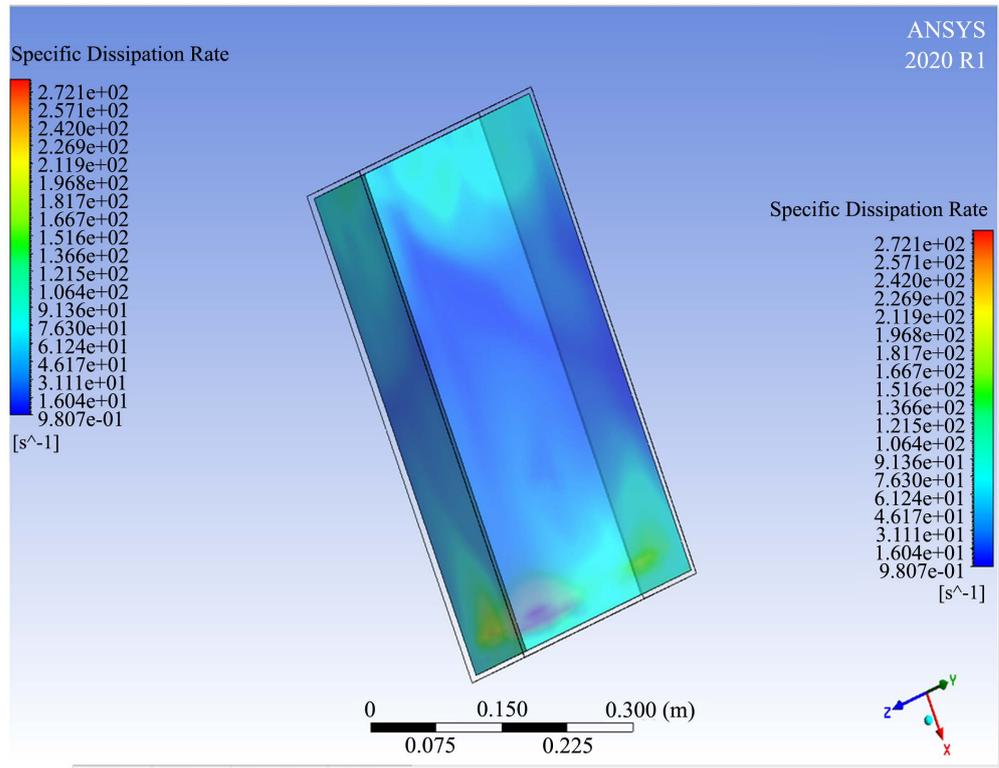
Class 2: [800°C - 2527.85°C], represented by green and yellow on the **Figure 12(b)**, meaning graphene sheet still supporting and work with increases of temperature;

Class 3: [2600°C - 4890.85°C], represented yellow red and red on the **Figure 12(b)**, meaning the graphene sheet cannot support and work.

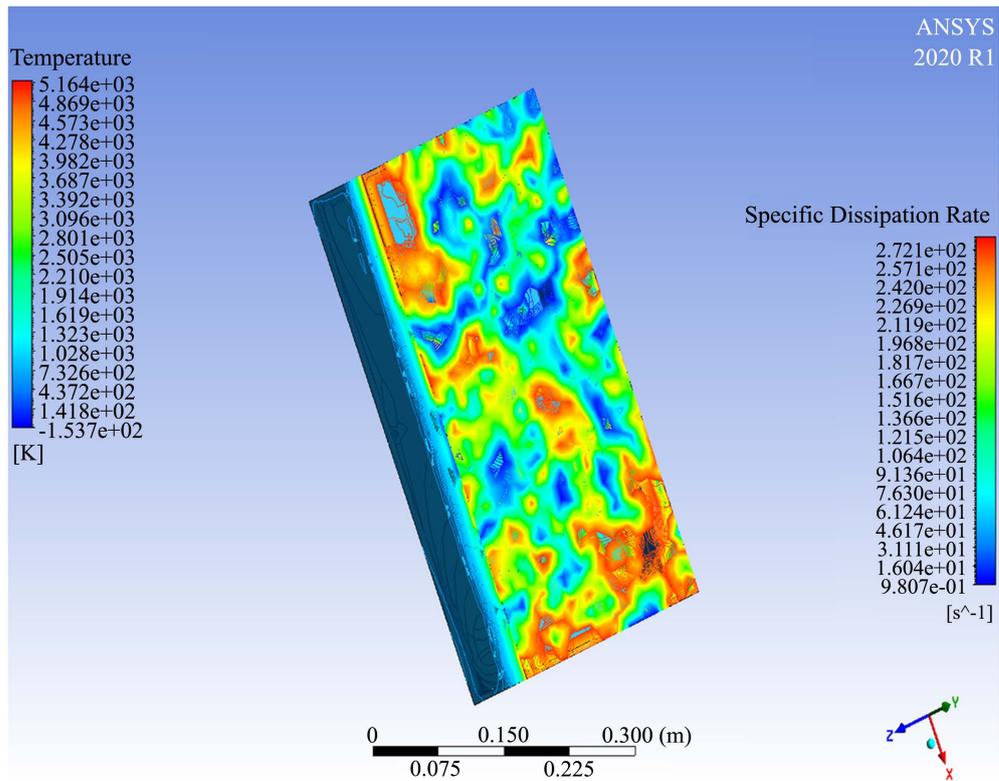
4.3.3. Erosion Simulation of Graphene in Presence of KCl

Analysis

Comment



(a)



(b)

Figure 12. (a) Specific dissipation rate of graphene in presence of SO₂; (b) Specific dissipation rate at some range of temperature.

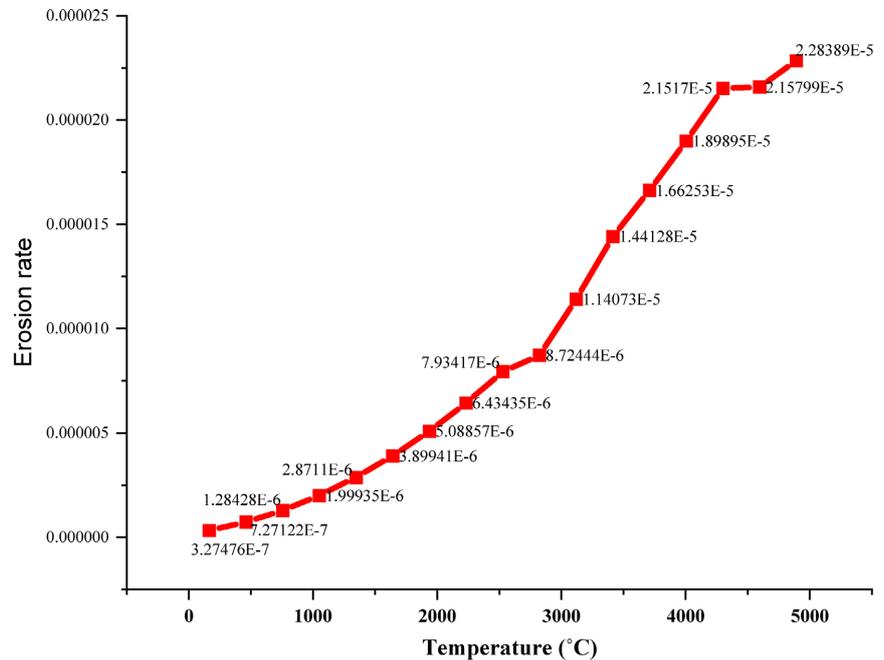


Figure 13. Erosion due by temperature change in the boiler filled of SO_2 .

By analyzing the results presents above on the table and figure, we have:

Class 1: $\leq 794.85^\circ\text{C}$, represented by bleu and bleu bright on the **Figure 14(b)**, what means a graphene sheet work well without any problem; in the **Figure 15**, we can observe the erosion rate is approximately zero;

Class 2: $[800^\circ\text{C} - 2634.85^\circ\text{C}]$: represented by green and yellow on the **Figure 14(b)**, meaning graphene sheet still supporting and work with increases of temperature;

Class 3: $[2700^\circ\text{C} - 5088.85^\circ\text{C}]$, represented yellow red and red on the **Figure 14(b)**, meaning the graphene sheet cannot support and work.

4.3.4. Erosion Simulation of Graphene in Presence of Phosphorous Analysis

Comment

By analyzing the results presents above on the table and figure, we have:

Class 1: $\leq 756.85^\circ\text{C}$, represented by bleu and bleu bright on the **Figure 16(b)**, what means a graphene sheet work well without any problem; in the **Figure 17**, we can observe the erosion rate is approximately zero;

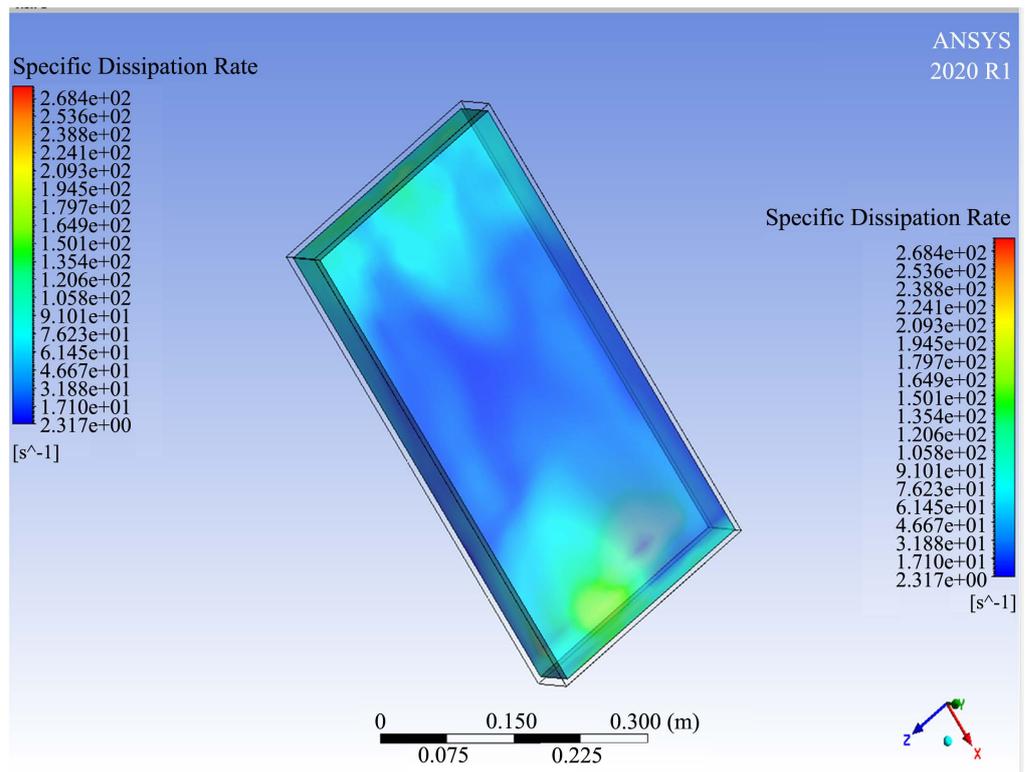
Class 2: $[800^\circ\text{C} - 2584.85^\circ\text{C}]$, represented by green and yellow on the **Figure 16(b)**, meaning graphene sheet still supporting and work with increases of temperature;

Class 3: $[2600^\circ\text{C} - 5088.85^\circ\text{C}]$, represented yellow red and red on the **Figure 16(b)**, meaning the graphene sheet cannot support and work.

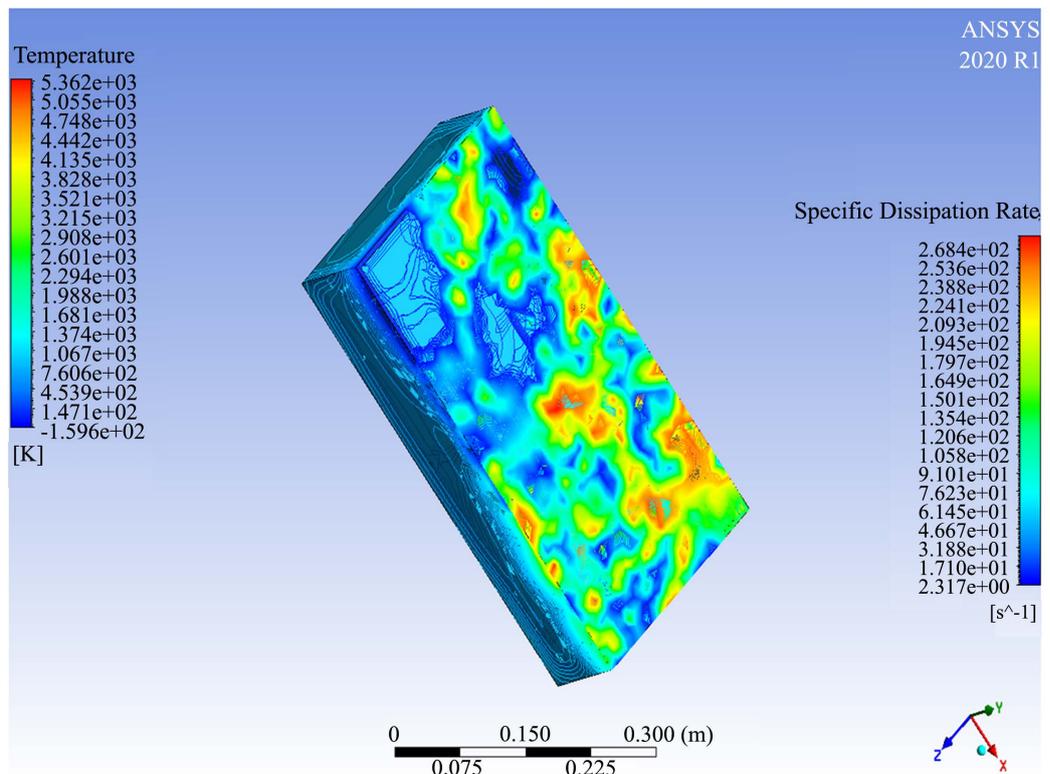
4.3.5. Erosion Simulation of Graphene in Presence of CO_2

Analysis

Comment



(a)



(b)

Figure 14. (a) Specific dissipation rate of graphene in presence of KCl; (b) Specific dissipation rate at some range of temperature.

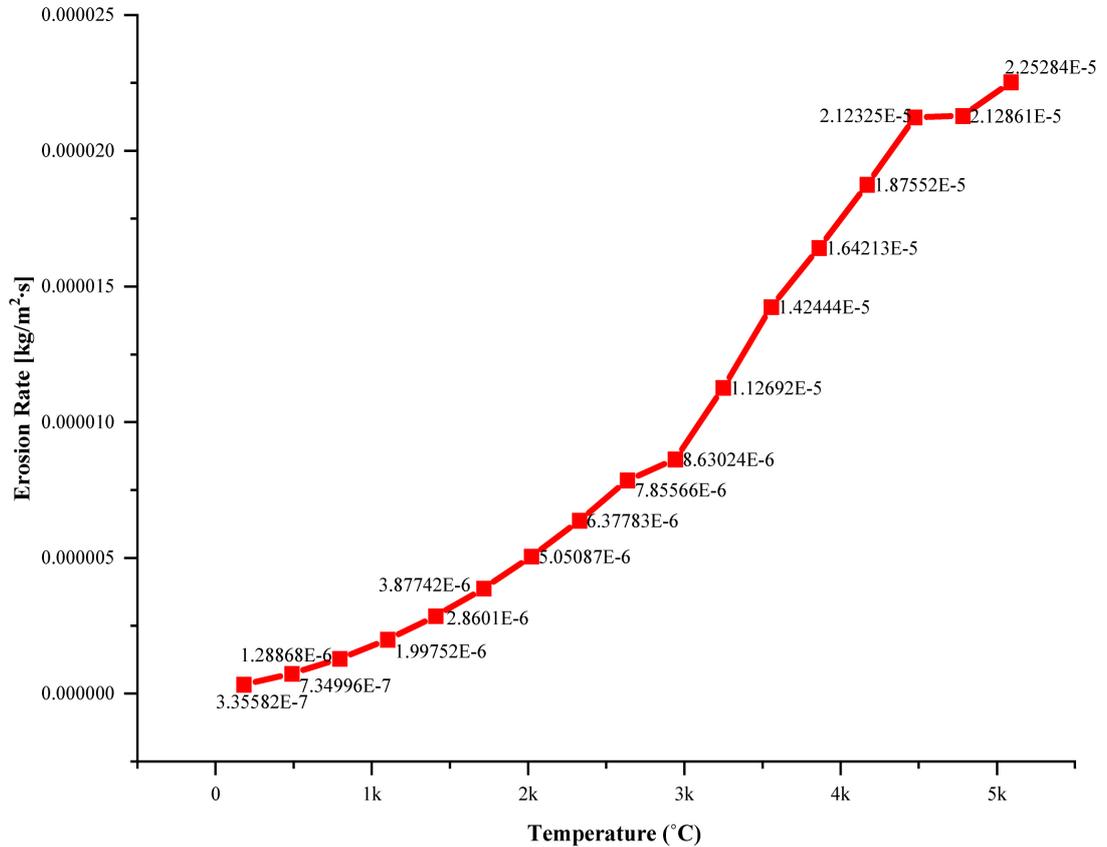


Figure 15. Erosion due by temperature change in the boiler full of KCl.

By analyzing the results presents above on the table and figure, we have:

Class 1: $\leq 743.85^{\circ}\text{C}$, represented by bleu and bleu bright on the **Figure 18(b)**, what means a graphene sheet work well without any problem; in the **Figure 19**, we can observe the erosion rate is approximately zero;

Class 2: $[800^{\circ}\text{C} - 2527.85^{\circ}\text{C}]$, represented by green and yellow on the **Figure 18(b)**, meaning graphene sheet still supporting and work with increases of temperature;

Class 3: $[2600^{\circ}\text{C} - 4890.85^{\circ}\text{C}]$, represented yellow red and red on the **Figure 18(b)**, meaning the graphene sheet cannot support and work.

4.3.6. Average

For all of those cases presented above, we will look the average what is presented in the **Table 6** below.

Regarding to data of this table, graphene combined with chemical and some gases will ensure a good protection of boiler walls against erosion until at 460°C .

4.4. Corrosion Analysis

Corrosion is a chemical phenomenon which ANSYS cannot do. Therefore, we will proceed by analytic method to solve this issue. That method is a microscopic analysis aspect of graphene:

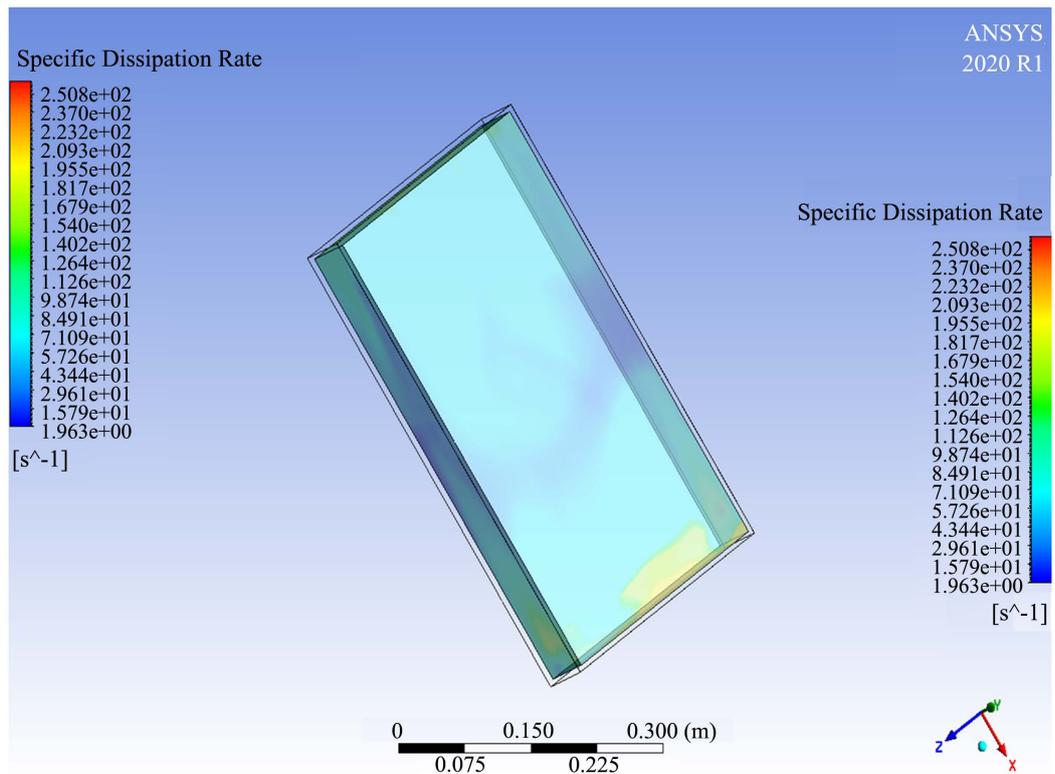
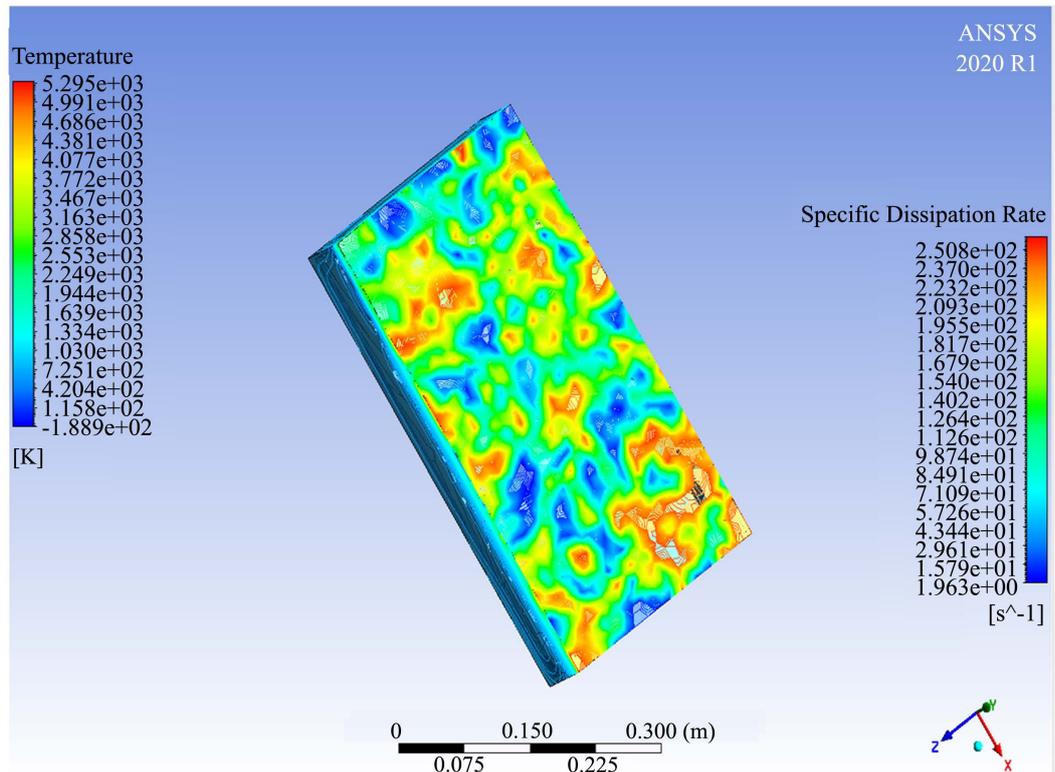


Figure 16. (a) Specific dissipation rate of graphene in presence of P; (b) Specific dissipation rate at some range of temperature.

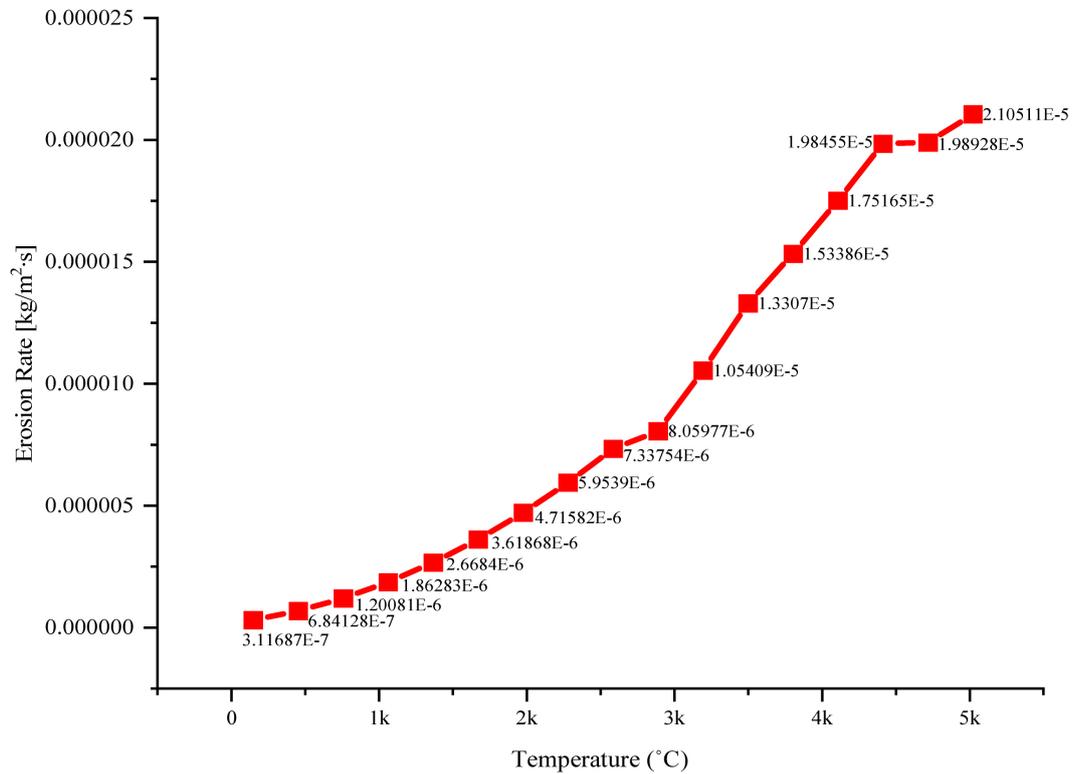
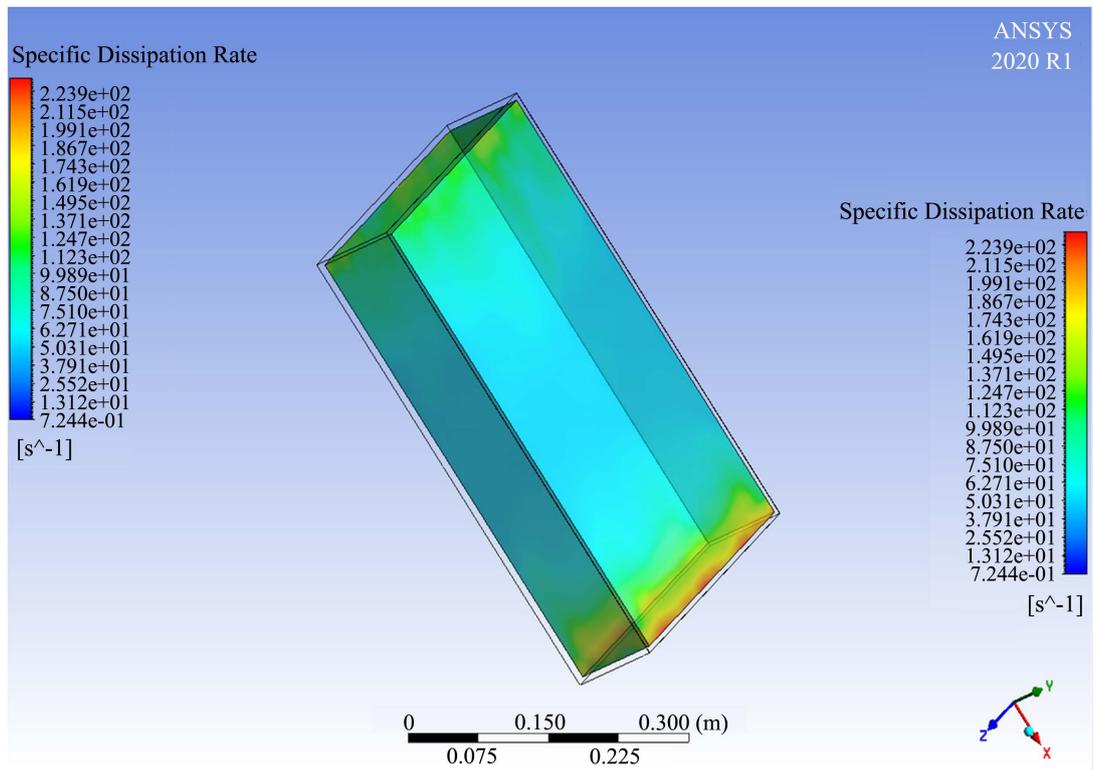


Figure 17. Erosion due by temperature change in the boiler full of P.

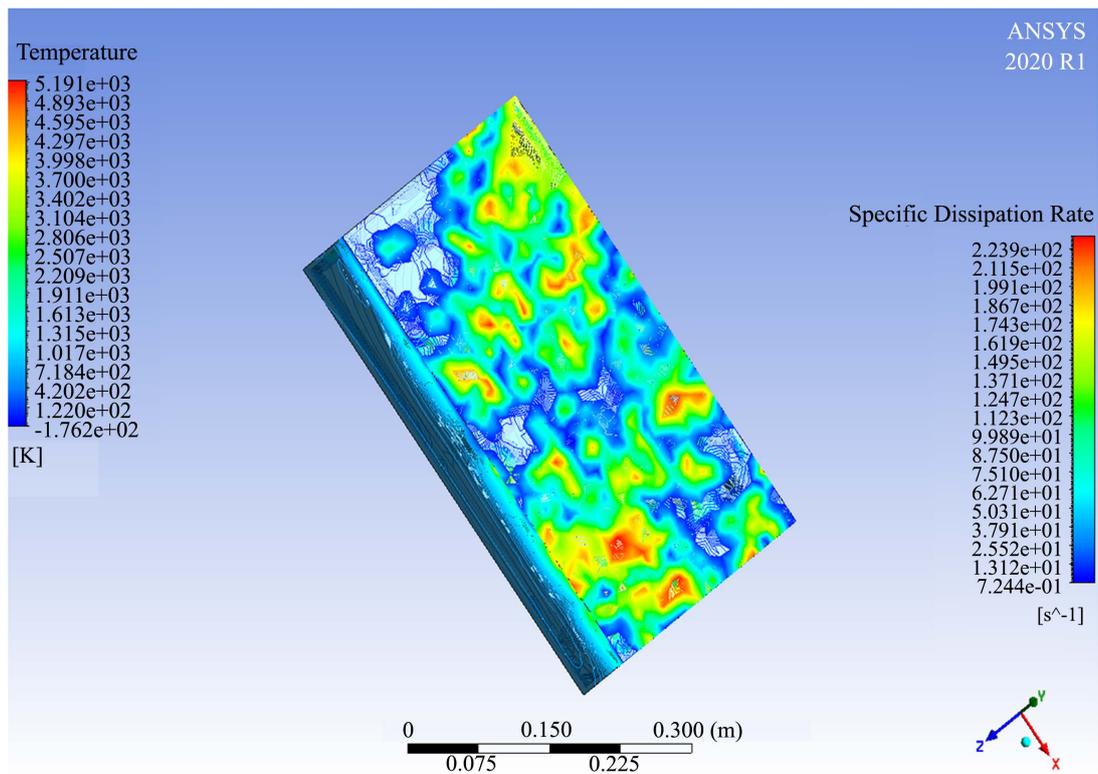
Table 6. The average of graphene resistance.

	Class1		Class2		Class3	
	Average T [°C]	Erosion rate average	Average T [°C]	Erosion rate average	Average T [°C]	Erosion rate average
Gr-HCl	460.45	9.28172E-07	1961.35	4.92361E-06	3912.42	1.5315E-05
Gr-SO ₂	459.45	7.79625E-07	1788.85	4.70449E-06	3856.98	1.70119E-05
Gr-KCl	487.35	7.86419E-07	1867.85	4.6699E-06	4015.1	1.67959E-05
Gr-P	452.02	7.32208E-07	1823.02	4.35953E-06	3955.85	1.5694E-05
Gr-CO ₂	445.38	6.40244E-07	1787.02	3.86828E-06	3874.35	1.39958E-05
Average	460.93	7.73334E-07	1845.62	0.000004505161	3922.94	0.000015762541

- Firstly, we analyze the pore diameter (Table 7) of the carbon ring in terms of the electron density is smaller than the kinetic diameter of various gases and chemicals elements, such as: He, H₂, CO₂, O₂, N₂, and CH₄. For that we can take an example of the pore diameter of an octagon ring (considering electron density) is only 1.5 Å. Only large vacancies with a size above 5Å, that is, two lattice parameters, can be penetrated by the gas molecule.
- Secondly, we refer to the relation (1), the initial energy to form vacancy in the graphene structure is approximately to 7.5 eV [16] and according to the Raman Spectra of temperature evolution (Figure 5), and graphene conserve that energy for the temperature under 700°C.



(a)



(b)

Figure 18. (a) Specific dissipation rate of graphene in presence of CO₂; (b) Specific dissipation rate at some range of temperature.

Table 7. The kinetic diameters of some common molecules present in WTE.

Molecule		Molecular weight	Kinetic diameter (pm)	Kinetic diameter (Å)
Name	Formula			
Hydrogen	H ₂	2	289	2.89
Helium	He	4	260	2.6
Methane	CH ₄	16	380	3.8
Water	H ₂ O	18	265	2.65
Nitrogen	N ₂	28	364	3.64
Carbon monoxide	CO	28	376	3.76
Nitric oxide	NO	30	317	3.17
Oxygen	O ₂	32	346	3.46
Hydrogen sulfide	H ₂ S	34	360	3.6
Hydrogen chloride	HCl	36	320	3.2
Carbon dioxide	CO ₂	44	330	3.3
Nitrous oxide	N ₂ O	44	330	3.3
Sulfur dioxide	SO ₂	64	360	3.6
Chlorine	Cl ₂	70	320	3.2

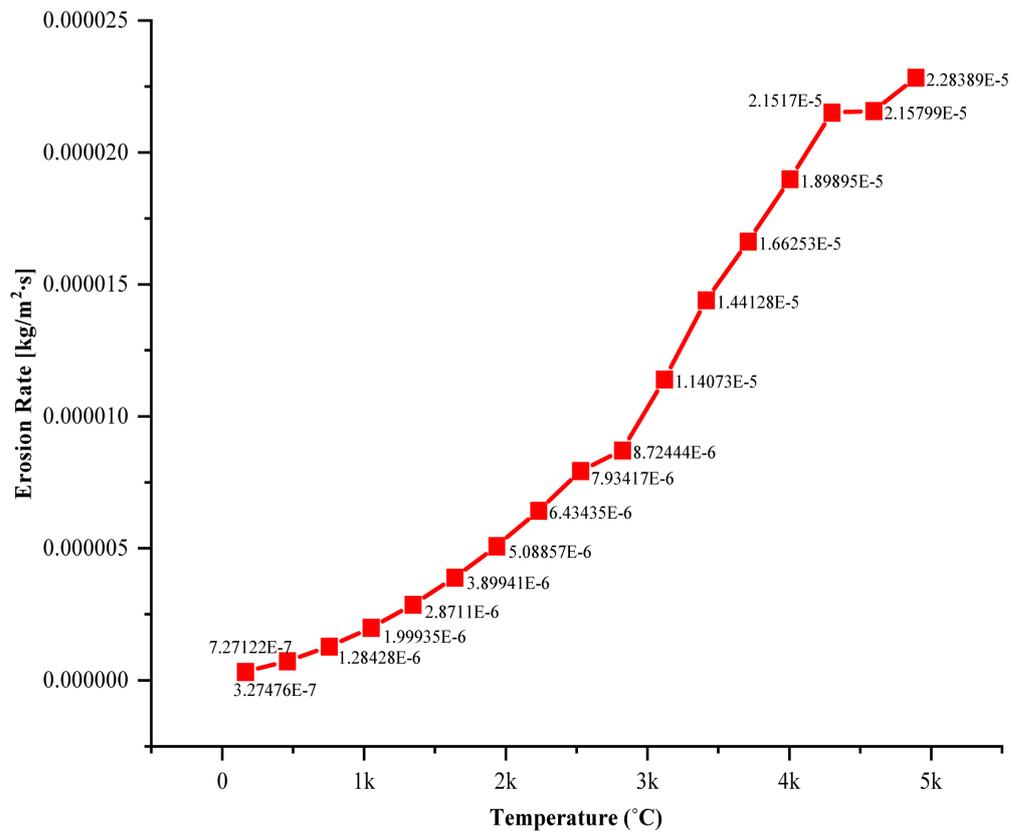


Figure 19. Erosion due by temperature change in the boiler full of CO₂.

The hexagonal pore lattice diameter of graphene is 0.246 nm and with a measured C-C bond length of 0.14 nm, the Graphene is considering the nuclei of the carbon atoms. When the Van der Waals radii (0.11 nm) pore diameter is reduced to 0.064 nm the carbon atoms are considered. The graphene ensures minimal permeability when the pore lattice present a small geometric and that even for smaller atoms such as helium. Moreover, the dense and delocalized electron cloud of π -conjugated carbon network in Graphene blocks the Class within its close packed aromatic rings and poses a repelling field to the reactive atom or molecule, consequently providing a physical separation between the refined metal surface and environmental reactants.

This energy barrier for a single layer coating of graphene is high enough to block the diffusion of oxygen to the underlying metal interface. The energy barrier magnitude of varies with molecular permission through the graphene lattice and the path of the atomic, suggesting that graphene can be the thinnest ever known corrosion barrier.

5. Conclusions and Suggestions

The arrival of new materials such as 2D materials (Graphene), a new door opens to mitigate or combat corrosion-erosion due to temperature by using the thermal properties of these materials (graphene).

Analyzing the graphene sheet at some range of temperature, also at the pressure of 4 MPa and in presence of some chemical elements, such as: Na, Cl, S and P. Thus, the results of simulation revealed a perfect protection of boiler walls by the graphene sheet, such as:

- With Na: the graphene sheet will ensure a good protection for the temperature $\leq 412.85^\circ\text{C}$;
- With Cl: the graphene sheet will ensure a good protection for the temperature $\leq 412.85^\circ\text{C}$;
- With S: the graphene sheet will ensure a good protection for the temperature $\leq 411.85^\circ\text{C}$ and
- With P: the graphene sheet will ensure a good protection for the temperature $\leq 700^\circ\text{C}$;

With all these elements combined in the boiler, Graphene sheet provides good wall protection for temperatures $\leq 415.6^\circ\text{C}$.

After that, we analyzed the erosion caused by the contaminating elements contained in the boiler, such as: hydrogen chloride, sulfur dioxide, phosphorus, potassium chloride and carbon dioxide. It turns out that the graphene sheet coating the walls of the boiler protects these perfectly for temperatures $\leq 700^\circ\text{C}$.

Comparing the results of the simulation of the empty boiler and the one filled with impurities represented by some chemical elements, we note a reduction of approximately half of the resistive capacity of Graphene, that is to say 1067°C to 415.85°C . In spite of this, it continues to protect the coated wall.

The graphene can handle well the problem of corrosion-erosion in general

and the problem of corrosion-erosion due to temperature. It is excellent candidate as anticorrosion-erosion coatings because of the great impermeability to all gases and salts (what is one of the responsible of corrosion into boiler in WTE) [17]. The Graphene-coated steel exhibits outstanding anti-corrosion-erosion properties.

Finally, graphene as a 2D material used in this study offers a great protection against corrosion-erosion for temperatures below 400°C, which will increase the life of the wall of the WTE boiler operating under temperatures lower than the above mentioned, this directly implies the life of the WTE.

Furthermore, our objective was to test and prove the use of Graphene in an aggressive and closed environment. Being able to work in an aggressive environment, Graphene can certainly be applied to other scales and environments as protection against corrosion-erosion.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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