Mathematical models predict corrosion inhibition

Subjects: Others

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The use of corrosion inhibitors is an important method to retard the process of metallic attack by corrosion. The construction of mathematical models from theoretical-computational and experimental data obtained for different molecules is one of the most attractive alternatives in the analysis of corrosion prevention, whose objective is to define those molecular characteristics that are common in high-performance corrosion inhibitors.

corrosion inhibition organic inhibitors theoretical studies molecular descriptors mathematical models

1. Introduction

Corrosion is defined as the destructive attack of a material by reaction with its environment. This process is a worldwide, significant problem because of the economic damage and safety loss it may lead to. The losses originating from corrosion can be categorized as direct and indirect, and the latter includes economic losses caused by plant shutdowns, efficiency reduction, costly maintenance, and contamination of products whose overall impact will ultimately require over-design. The direct losses include the cost of replacing corroded structures, fixing damaged machinery, and substituting some of its components [1].

Corrosion control can be achieved by recognizing and understanding the mechanisms associated with this process. It is possible to prevent corrosion by using corrosion-resistant materials and protective systems.

The selection of materials; which can be metallic, non-metallic or alloys, is a key factor in the prevention of corrosion processes, as well as the consideration of the temperature, the type of environment and the general conditions to which the material is subjected. In such selection, both the mechanical and physical analyses of the materials' properties play a very important role. However, such selection is limited by the availability and cost of materials. This limitation forces the industry to resort to the corrosion protection offered by metallic or non-metallic coatings and anodic or cathodic processes for metal protection, as well as to carefully select the appropriate geometrical configurations to prevent corrosive conditions and to avoid the use of bimetallic couples, which can be responsible for favoring the corrosion process. Corrosion protection can also be achieved by promoting the formation of Ni and Cr protective barriers or by protecting a substrate (steel) with sacrificing materials such as Zn, Al or Cd [2].

The environments to which metals are exposed make them prone to corrosion. A less aggressive environment can be obtained by removing constituents that facilitate corrosion, modifying the temperature, dehumidifying the air, removing dissolved O_2 or solid particles, controlling the pH or adding corrosion inhibitors . The usage of inhibitors is one of the most practical methods for protection against corrosion in acidic, alkaline, saline, and other aggressive environments [3][4].

The following sections include:

- The definition of a corrosion inhibitor and the structural characteristics associated with an inhibitor molecule; a brief mention is made of the techniques that allow evaluating the performance of corrosion inhibitors in the protection of metal surfaces exposed to aggressive environments.
- The factors that increase the corrosion process and those that can be modified to prevent this phenomenon are briefly mentioned.
- The most important data such as molecules and inhibition efficiencies obtained by different techniques and experimental conditions have been summarized, taking into account the functional group of greatest interest to the study authors. Information related to the descriptors used in the theoretical analysis of corrosion inhibitors has been collected.
- Finally, a table has been generated with examples of some mathematical models obtained to evaluate corrosion inhibitor molecules, in which it is possible to observe the most common descriptors to predict the corrosion phenomenon.

2. Corrosion Inhibitors

Corrosion inhibitors are chemical substances that are added to aggressive environments in small concentrations to decrease the corrosion rate. These substances can react with either a metal surface or its surroundings providing protection to the surface, although it has been observed that corrosion inhibitors generally work by forming an adsorbed film. Corrosion inhibitors are an appropriate option for metal protection when these are exposed to aggressive media, such as, acidic solutions (widely employed for industrial cleaning), oil well acidification, and petrochemical processes [5].

Corrosion inhibitors can be introduced into the aggressive environment in a single application or continuously by gradual and controlled additions. The single addition is possible in static systems at low temperature and where friction is negligible. Gradual addition is necessary for systems where variation in flow and temperature degrade the integrity of the protective film formed on the metal surface, either by physisorption or chemisorption. The stability of the corrosion inhibitor films can be compromised by the concentration levels of the inhibitor in the medium [6]. Comparative studies performed to determine inhibition effects are generally performed without shaking. Therefore, the existence of a significant effect of immersion time on the quality of the formed film of an inhibitor is reasonable.

An important number of compounds have been used for the corrosion protection of metals exposed to aggressive media. Their effectiveness is associated to their chemical composition, molecular structure, alkyl chain length (or molecular volume), planarity, presence of lone pairs of electrons in heteroatoms (e.g., S, N, O, P), affinity for the metallic surface, dipole moment, presence of π-electrons (unsaturation or aromatic ring) and energy of frontier molecular orbitals. The efficiency ($E\%$) of corrosion inhibitors is measured by applying the Equation (1) to experimental data obtained by techniques such as weight loss (WL), potentiodynamic polarization (PP), and electrochemical impedance spectroscopy (EIS):

$$E\% = \frac{(CR_u - CR_i)}{CR_u} \times 100. \qquad \text{Equation (1)}$$

where CR_u is the corrosion rate of the uninhibited system and CR_i is the rate of the inhibited system.

The mechanisms through which corrosion inhibitors can be bounded to the metal or the metal oxide surface may be physisorption, chemisorption, complexation or precipitation. The film formed by corrosion inhibitors prevents the access of oxygen to the cathode and the diffusion of hydrogen away from it, or simply inhibits metal dissolution (anodic inhibitors). Inhibition efficiency can be altered by modifying the system parameters such as pH, temperature, metal composition, type of inhibitor and molecular structure of the corrosion inhibitor [7]. An important factor associated with the corrosion process is surface roughness. The increase in the surface roughness of alloys (magnesium, titanium-based), stainless steels, copper, and aluminum increases the pitting susceptibility and the corrosion rate [8].

According to observations performed in presence of compounds with heteroatoms in their structure, the corrosion inhibition efficiency follows this tendency: O < N < S < P. This behaviour is also associated with the electronegative character of the involved atoms [9][10]. There is a growing interest in defining the best molecular characteristics of a corrosion inhibitor in addition to the effects associated with the presence of heteroatoms, while also taking factors such as cost, toxicity, availability and environmental friendliness into account [2].

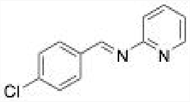
The following sections contain a review of some of the molecules studied as corrosion inhibitors in different environments. In the cases where the number of compounds evaluated by the authors was larger than four, only the best two and the worst two corrosion inhibitors are included, there is also mentioned the total number of corrosion inhibitors (N_{CI}) employed in every analysis. For almost all of the studies reviewed in this paper, the corrosion inhibition efficiencies tabulated correspond to the values obtained at the highest inhibitor concentration. It is worth noting that the most efficient corrosion inhibitors tended to be complex molecules with more than one heteroatom in their structure; however, for the purpose of this review, corrosion inhibitors have been classified according to the heteroatom considered of higher interest by the referenced researchers.

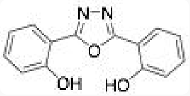
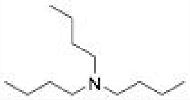
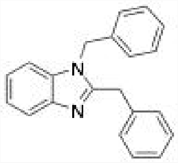
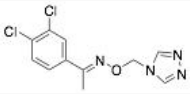
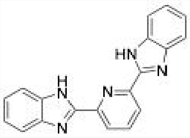
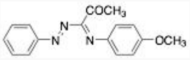
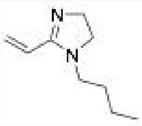
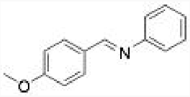
The following sections summarize the analysis conditions employed by different researchers and the corrosion inhibition efficiencies obtained by the different techniques; weight loss (Ef_{WL}), potentiodynamic polarization (Ef_{PP}), and electrochemical impedance spectroscopy (Ef_{EIS}), at those conditions. Cases where the theoretical analysis (TA) was applied (A) or not (NA) are mentioned. There is an important number of experimental conditions (Exp.C.) that affect the corrosion inhibition efficiency, among these factors we find: the metallic surface (Met) and the exposure time (t) of this in inhibited and uninhibited solutions, temperature (T), aggressive media and its concentration (Media), as well as the corrosion inhibitor concentration (Co), nature of the anion in the corrosive medium, type of metal, and pH [11] [12]. The immersion time (a) can affect the natural oxide film of some metallic surfaces, (b) can be responsible for increasing the thickness of the layer formed by corrosion products, which can reduce the corrosion rate, (c) may favour or not the increase of corrosion inhibitor adsorption leading to the formation of uniform and stable films of corrosion inhibitors.

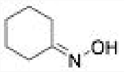
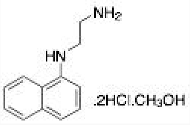
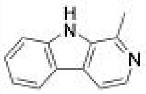
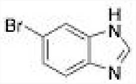
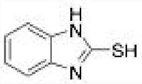
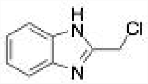
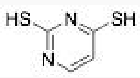
3. N-Containing Corrosion Inhibitors

An important number of molecules evaluated as corrosion inhibitors in acidic media contain N-atoms and the structural properties that are characteristic of high-performance corrosion inhibitors. Table 1 shows some examples of the N-containing corrosion inhibitors evaluated by different researchers.

Table 1. N-containing corrosion inhibitors

Example	Corrosion Inhibitor	$Ef_{WL}/Ef_{PP}/Ef_{EIS}$	Ref
	**(4-Chloro-benzylidene-pyridine-2-yl-amine)**	**99.5/99.6/99.6**	[13]
Exp. C. N_{CI}: 3, Met: mild steel, Media: HCl 1.0 M, Co: 2×10^{-4}–1×10^{-2} M, t: 24 h (WL), T: 25 °C, TA: A			

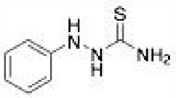
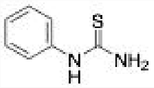
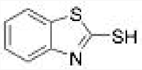
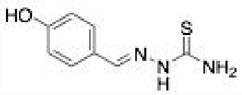
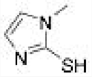
	2,5-bis(2-hydroxyphenyl)-1,3,4-oxadiazole	98.2/94.7/99.1	[14]
Exp. C. N_{Cl}: 2, Met: mild steel, Media: HCl 1.0 M, 0.5 M H_2SO_4, Co: 20–80 mg•L^{-1}, t: 24 h (WL), 20 h (EIS), T: 30 °C, TA: NA			
	Tributylamine	97.8/-/-	[15]
Exp. C. N_{Cl}: 23, Met: 13% Cr steel, Media: HCl (15%*w*/*v*), Co: 2%*w*/*v* inhibitor and 0.6% *w*/*v* formaldehyde (used to minimize hydrogen penetration), t: 3 h, T.: 60 °C, TA: A			
	1,2-bisbenzylbenzimidazole	96	[16]
Exp. C. N_{Cl}: 11, Met: iron, Media: HCl 1.0 M. The analysis technique and the rest of the experimental conditions are not specified. TA: A			
	3,4-Dichloro-acetophenone-O-1′-(1′.3′.4′-triazolyl)-metheneoxime (DATM)	92.8/98.7/98.7	[10]
Exp. C. N_{Cl}: 3, Met: mild steel, Media: HCl 1.0 M, Co:1×10^{-5}–1×10^{-3} M, t: 3 h (WL), 30 min (PP), T: 25 °C, TA: A			
	* 2,6-bis-(2-benzimidazolyl) pyridine	-/94–96/97.0	[17]
Exp. C. N_{Cl}: 4, Met: mild steel, Media: HCl 1.0 M, Co: 0.1–1.0 mM, t: 1–96 h (WL), 45 min (PP), T.: 30 °C, TA: NA			
	1-(4-Methyloxyphenylimino)-1-(phenylhydrazono)-propan-2-one	-/95.9/96.2	[18]
Exp. C. N_{Cl}: 5, Met: mild steel, Media: HCl 1.0 M, Co: 5×10^{-6}–7.5×10^{-5} M, t: 30 min, T: 25 °C, TA: NA			
	1-Butyl-2-propylene-2-imidazoline	95.1/-/-	[19]
Exp. C. N_{Cl}: 34, Met: stainless steel, Media: HCl 5%, Co: ≈0.1 M, t: 48 h, T: T_R (room temperature), TA: A			
	Aniline, N-(p-methoxybenzylidene)	-/94.0/-	[20]

Exp. C. N_{Cl}: 4, Met: aluminium, Media: HCl 2.0 N, Co: 10^{-5}–10^{-2} M, t:-, T: 30 °C, TA: NA			
	Cyclohexanone oxime	93.9/98.4/95.2	[21]
Exp. C. N_{Cl}: 3, Met: aluminium, Media: HCl 1.0 M, Co: 0.2–2.0 mM, t: 2 h, T: 20–50 °C, TA: NA			
	N-1-napththylethylenediamine dihydrochloride monomethanolate	90.2/88.1/87.9	[12]
Exp. C. N_{Cl}: 1, Met: carbon steel, Media: H_2SO_4 0.5 M, Co: 10^{-5}–10^{-2} M, t: 2 h (WL), 30 min (PP), T: 25 °C, TA: NA			
	1-Methyl-9H-pyrido[3 ,4-b]indole	-/89.0/93.0	[22]
Exp. C. N_{Cl}: 2, Met: C38 steel, Media: H_3PO_4 2.0 M, Co:10^{-5}–10^{-2} M, t: 2 h, 30 min, T: 30 °C, TA: A			
	6-Bromo-1H-benzimidazole	-/-/89.4	[23]
Exp. C. N_{Cl}: 15, Met: carbon steel, Media: HCl 1.0 M, Co:0.1–10 mM, t: 30 min, T: T_R, TA: A			
	2-Mercaptobenzimidazole	-/88.7/90.4	[5]
Exp. C. N_{Cl}: 3, Met: mild steel, Media: HCl 1.0 M, Co: 50–250 ppm, t: 30 min, T: 25 °C, TA: NA			
	2-Chloromethylbenzimidazole	-/-/69.7	[24]
Exp. C. N_{Cl}: 6, Met: carbon steel, Media: HCl 1.0 M, Co: 1×10^{-3} M, t: -, T: T_R, TA: A			
	2,4-Dimercaptopyrimidine	43.0/-/-	[7] [25]
Exp. C. N_{Cl}: 14, Met: Aramco iron, Media: HCl 2.0 M, Co: 1×10^{-3} M, t: 1 h, T: 40 °C, TA: A			
Simbology: TA: theoretical analysis, A: applied, NA: not applied, Exp. C.: experimental conditions; N_{Cl}: number of corrosion inhibitors, Co: inhibitor concentration, t: exposure time, T: temperature, $Ef_{WL}/Ef_{PP}/Ef_{EIS}$: corrosion inhibition efficiencies obtained by weight loss (WL), potentiodynamic polarization (PP), and electrochemical impedance spectroscopy (EIS), respectively.			

4. S-Containing Corrosion Inhibitors

Many authors have reported the beneficial effect of the sulphur atom in the molecular structure of corrosion inhibitors. Table 2 includes some examples of the S-containing corrosion inhibitors evaluated by different groups of researchers. The molecules were ordered from highest to lowest efficiency, considering the best inhibitor in each group.

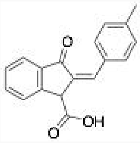
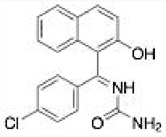
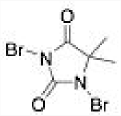
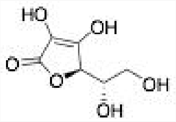
Table 2. S-containing corrosion inhibitors

Example	**Corrosion Inhibitor**	**$Ef_{WL}/Ef_{PP}/Ef_{EIS}$**	**Ref**
	**1-Phenyl thiosemicarbazide**	**-/100.0/-**	[26] [27]
Exp. C. N_{CI}: 10, Met: mild steel, Media: H_2SO_4, Co: 1 mM·dm^{-3}, t: -, T: 30 °C. TA: A			
	**Phenylthiourea (PTU)**	**-/-/97.2**	[28]
Exp. C. N_{CI}: 3, Met: mild steel, Media: H_2SO_4 0.1 M, Co: 1–10 mM, t:1 h, T: T_R, TA: NA			
	**2-Mercaptobenzothiazole**	**-/97/-**	[29]
Exp. C. N_{CI}: 1, Met: Steel (API 5L X52), Media: H_2SO_4 1.0 M, Co: 10^{-4-}–10^{-3} M, t: 30 min, T: 25 °C, TA: A			
	**4-Hydroxybenzaldehyde thiosemicarbazone**	**-/97.0/90.0**	[30]
Exp. C. N_{CI}: 6, Met: carbon steel, Media: HCl 1.0 M, Co: 10^{-4}–10^{-2} M, t: 30 min, T: 25 °C, TA: NA			
	**2-Mercapto-1-methylimidazole**	**90.4 /95.5/-**	[31]
Exp. C. N_{CI}: 1, Met: carbon steel, Media: $HClO_4$ 1.0 M, Co: 7.5 × 10^{-5}–2.5 × 10^{-3} M, t:1 h, T: 30 °C, TA: NA			
Simbology: TA: theoretical analysis, A: applied, NA: not applied, Exp. C.: experimental conditions; N_{CI}: number of corrosion inhibitors, Co: inhibitor concentration, t: exposure time, T: temperature, $Ef_{WL}/Ef_{PP}/Ef_{EIS}$: corrosion inhibition efficiencies obtained by weight loss (WL), potentiodynamic polarization (PP), and electrochemical impedance spectroscopy (EIS), respectively.			

5. O-Containing Corrosion Inhibitors

Many authors have studied the effect of the oxygen atom in the molecular structure of corrosion inhibitors. Table 3 includes examples of molecules that have been analyzed to observe the effect of oxygen on corrosion inhibition efficiency. The experimental conditions and efficiencies obtained using different techniques are also included.

Table 3. O-containing corrosion inhibitors

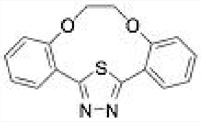
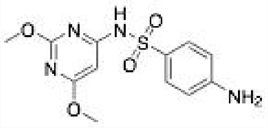
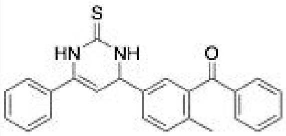
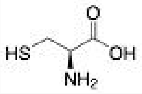
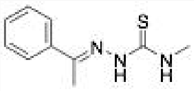
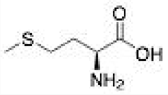
Example	Corrosion Inhibitor	$Ef_{WL}/Ef_{PP}/Ef_{EIS}$	Ref
	2-(4-Methylbenzylidene)-3-oxo-2,3-dihydro-1H-indene-1-carboxylic acid	92.0/93.9/92.6	[32]
Exp. C. NCI: 3, Met: mild steel, Media: HCl 1.0 M, Co: 10^{-6}–10^{-3} M, t: 6 h, T: 30 °C, TA: NA			
	1-((4-Chlorophenyl)(2-hydroxynaphtalen-1-yl)(phenyl) methyl)urea (CPHU)	90/92.0/-	[33]
Exp. C. NCI: 3, Met: mild steel, Media: H_2SO_4 0.5 M, Co: 2–10 ppm, t: 24 h (WL) and 30 min (PP), T: 20 °C, TA:A			
	1,3-Dibromo-5,5-dimethylhydantoin	-/89.8/91.4	[34]
Exp. C. NCI: 6, Met: mild steel, Media: HCl 0.5 M, Co: 10–50 ppm, t: 30 min, T: 30 °C, TA:A			
	L-ascorbic acid	69.0/-/-	[35]
Exp. C. NCI: 1, Met: mild steel, Media: H_2SO_4 0.01 M, Co: 10^{-7}–10^{-3} M, t: -, T: T_R, TA: NA			
Simbology: TA: theoretical analysis, A: applied, NA: not applied, Exp. C.: experimental conditions; N_{CI}: number of corrosion inhibitors, Co: inhibitor concentration, t: exposure time, T: temperature, $Ef_{WL}/Ef_{PP}/Ef_{EIS}$: corrosion inhibition efficiencies obtained by weight loss (WL), potentiodynamic polarization (PP), and electrochemical impedance spectroscopy (EIS), respectively.			

6. Multi-Heteroatom-Containing Corrosion Inhibitors

For the selection of high-performance corrosion inhibitors, some researchers tend to choose molecules with a high number of heteroatoms (Table 4), or molecules featuring the characteristics of better corrosion inhibitors. However, it has been found that some heteroatoms work more efficiently as adsorption centres than others, or that the presence of certain substituents increases the electron density of the functional groups leading to stronger interaction between the corrosion inhibitor and the metallic surface.

Table 4. Multi-heteroatom containing corrosion inhibitors

Example	Corrosion Inhibitor	$Ef_{WL}/Ef_{PP}/Ef_{EIS}$	Ref

	**(2,3,8,9-Dibenzo-4,7-dioxa-13-thia-11,12-diazabicyclo[8.2.1]trideca-10,12-diene (1-MCTH)**	**97.7/-/-**	[36]
Exp. C. NCI: 5, Met: mild steel, Media: 1.0 M HCl, Co: 1 × 10^{-6}–1 × 10^{-4} M, t: 24 h (WL), T: 30 °C, TA: A			
	**Sulphadimethoxine**	**93.8/84.0/92.1**	[4]
Exp. C. NCI: 5, Met: mild steel, Media:1.0 M HCl, Co: 1–5 × 10^{-5} M, t: 30 min, T: 30–50 °C, TA: A			
	**5-Benzoyl-4-tolyl-6-phenyl-1,2,3,4-tetrahydro-2-thioxopyrimidine**	**-/93.0/93.0**	[37] [38]
Exp. C. NCI: 2, Met: stainless steel, Media:1.0 M HCl, Co:1 × 10^{-4}–5 × 10^{-3} mol·dm^{-3}, t: 30 min, T: 25 °C. The experimental data were obtained by Caliskan, et al. . TA: A			
	**L-Cysteine**	**82.2/-/-**	[39]
Exp. C. NCI: 4, Met: mild steel, Media:0.1 M HCl, Co: 0.1–0.5 g·L^{-1}, t: 24, 168 h, T: 30, 60 °C, TA: A			
	**(E)-N-methyl-2-(1-phenylethylidene)hydrazinecarbothioamide PHCARB**	**80.7/-/-**	[40]
Exp. C. NCI: 4, Met: mild steel, Media:0.1 M HCl, Co: 1–5 × 10^{-4} M, t: 168 h, T: 30 °C, TA: A			
	**Methionine**	**72.7/84.6/85.8**	[41]
Exp. C. NCI: 16, Met: Armco iron, Media: HCl 1.0 M, Co: 10^{-3} M, et: 6 h (WL), 10 y 30 min (PP), T: 35 °C, TA: A			
Simbology: TA: theoretical analysis, A: applied, NA: not applied, Exp. C.: experimental conditions; NCI: number of corrosion inhibitors. Co: inhibitor concentration, t: exposure time, T: temperature, Ef_{WL}/Ef_{PP}/Ef_{EIS}: corrosion inhibition efficiencies obtained by weight loss (WL), potentiodynamic polarization (PP), and electrochemical impedance spectroscopy (EIS), respectively.			

7. Molecular Descriptors Associated to Corrosion Inhibitors

There is a growing interest in the development of quantum-chemical studies because the inhibition activity of molecules can be associated with certain theoretical parameters, such as the highest occupied molecular orbital energy (E_{HOMO}), the lowest unoccupied molecular orbital (E_{LUMO}), dipole moment and Mulliken atomic charges. The quantum parameters of organic inhibitors can be used to study their interaction with a metallic surface. Molecular dynamics simulation is helpful to study the adsorption of inhibitors on a metallic surface because it provides molecular-level information on the way the inhibitor is adsorbed on the metal. Theoretical and computational chemistry is a useful, powerful tool to choose the most appropriate inhibitor by understanding the inhibition mechanism before performing any experiment [42]. QSAR applied to corrosion analysis is a theoretical method convenient to correlate certain molecular structural parameters and the corrosion inhibition efficiency of a group of compounds with similar characteristics; it is a model of pattern recognition that can be implemented to define a trend in the corrosion efficiency scanning the variations in the inhibitor structural parameters. The QSAR approach was initially used in pharmacology in 1964 because Hansch and Leo observed that the variation of pharmacological efficiency of drugs might be explained in terms of different variables related to the molecular substituents. One of the main objectives of QSAR studies is to reduce the cost of research [26]. QSAR can be advantageous in the identification of compounds with high yields and characteristics that might be desirable from an environmental point of view. It is recommended to include a large number of compounds with similar backbones to enhance the QSAR accuracy; however, as stated by Mousavi and co-workers, that is in itself a disadvantage of this model since it might be difficult to find a large number of compounds with similar backbones and their corrosion inhibition experimental data obtained under the same conditions [42]. Some authors have mentioned that the cluster model based on density-functional theory (DFT) calculations is a suitable tool for modelling the inhibitor–surface interaction mechanism and for describing the effect of the inhibitor structural nature and the metal of interest. This method considers factors such as, inhibitor molecule, metal, and solvent which are ignored by the QSAR analysis. The cluster model evaluates the inhibitor–surface interaction energy vs. the experimental corrosion inhibition. The main advantage of the DFT calculation is to help researchers theoretically identify corrosion inhibitors that exhibit low interaction energies and discard them from the investigation, whereas the objective of QSAR is fundamentally based on two questions: 1) what structural and electronic properties of a molecule determine its activity, and 2) what structural and electronic properties can be altered to improve such activity [25].

As mentioned, the development of mathematical models (linear and non-linear) is possible through the analysis of quantum-chemical parameters and experimental data obtained from compounds with similar characteristics. Table 5 includes some examples of typical descriptors studied to understand the characteristic molecular factors of a good corrosion inhibitor.

Table 5. Examples of descriptors used in the theoretical analysis of corrosion inhibitors.

Quantum Descriptor	Symbol	Description	Reference
Energy of the highest occupied molecular orbital	E_{HOMO}	**Associated with the electron-donating ability of a molecule.**	[3]
Energy of the lowest unoccupied molecular orbital	E_{LUMO}	**Indicates the ability of the molecule to accept electrons.**	[31]
Ionization potential	**IP**	**It is a descriptor of the chemical reactivity of atoms and molecules. *IP* is the minimum energy required to remove an electron from an atom.**	[43]

Electron affinity	A	It is a property that determines how susceptible a molecule is towards the attack of a nucleophile.	[44]
Dipole moment	µD	The dipole moment is considered a measure of the stability of the formed complex on a metal surface. It is an indicator of the asymmetry in the molecular charge distribution. It is related to the hydrophobic character of the molecules.	[27] [33] [45] [46]
Energy gap	ΔE	$\Delta E = E_{HOMO} – E_{LUMO}$ It has been mentioned that the successful adsorption and proper efficiency of an inhibitor have been characterized by a high E_{HOMO}, a low E_{LUMO}, and a small energy gap. The lower the ΔE is, the higher the stability of the metal-inhibitor interaction.	[17][45][47]
Fraction of electron transferred	ΔN	If $\Delta N > 3.6$, the inhibition efficiency increases	[17]
Global hardness	η	It is a parameter associated with the resistance of an atom to transfer its charge.	[17]
Softness	σ	The σ shows the reactivity of the inhibitor molecules in terms of charge transfer.	[17]
Electronegativity	χ	The electronegativity measures the power of a group of atoms to attract electrons towards itself.	[17]
Electrophilicity index	ω	It is a reactivity descriptor that allows the quantitative classification of the global electrophilic nature of a molecule. This descriptor has been proposed as a measure of energy lowering due to maximal electron flow between donor and acceptor.	[10] [48]
Electrodonating power	ω^-	A descriptor associated with the ability of a species to donate electrons.	[49]
Electroaccepting power	ω^+	A descriptor associated with the ability of a species to accept electrons.	[49]
Dipole polarizability	α	α is a measure of the mean polarizability. Higher values of α enable a strong adsorption process.	[10]
Fukui functions	f_k^+, f_k^-	These functions indicate the part of the molecule where nucleophilic, electrophilic, and radical attack is most likely to occur.	[44]
Partition coefficient	Log P	Log P is a hydrophobic parameter of a molecule.	[50]

8. Mathematical Models Applied to Predict the Corrosion Inhibition Efficiency

Computational analysis and experimental techniques such as electrochemical impedance spectroscopy, potentiodynamic polarization, and weight loss, have been used by researchers for the generation of mathematical models that allow to define those molecular features associated with good protectors against corrosion. Computational techniques are also useful to analyse the mechanisms of action of corrosion inhibitors. Researchers usually take advantage of experimental databases of compounds previously tested as corrosion inhibitors in different media and for several metals with the aim of generating predictive models and reducing costs and time invested in analysis.

Among the objectives of the construction of mathematical models are (a) the understanding of the action mechanisms of the evaluated compounds and, (b) the design of new corrosion inhibitors with desirable properties for metal protection.

Table 6 includes some examples of mathematical models generated to analyse the corrosion inhibition efficiency of different organic molecules and their corresponding determination coefficients (R^2).

Table 6. Examples of mathematical models generated for corrosion analysis.

Molecules Evaluated	Theoretical Calculation	Mathematical Model	R^2	Ref.
Schiff base	**AM1 semi-empirical method**	$IE_{exp}\,(\%) = 2.084E_{HOMO} - 3.041E_{LUMO} + 115.772$	**1.00**	[3]
		$IE_{Theor} = \frac{(-604.90E_{HOMO}+5864.86E_{LUMO}+1190.06\mu_D-642.67)C}{[1+(-604.90E_{HOMO}+5864.86E_{LUMO}+1190.06\mu_D-642.67)C]}$	**0.98**	
Amines, thioureas, acetylenic alcohols	**AM1 methodology was used for most descriptors, PC model provided the volume calculations**	Unknown environment 'matrix'	**0.98**	[15]
		$lnK_{ads} = 1.52M - 0.79P + 0.53C_{12} + 0.80NT - 0.66NOH$	**0.86**	
		$\mathrm{lnK_{ads}}= -2.688 \times 10^{-2}A_1 + 0.115A_2 + 4.530 \times 10^{-2}A_3 + 8.762 \times 10^{-2}NB - 1.305 \times 10^{-2}NC$ $+0.102NCS - 4.518 \times 10^{-2}NT - 5.172 \times 10^{-2}NOH - 1.099 \times 10^{-3}NCR + 4.996 \times 10^{-2}NR$ $-6.338 \times 10^{-2}N - 0.114ED + 0.184M + 0.180P - 6.838 \times 10^{-2}C + 8.092 \times 10^{-2}C_{12}$ $-4.783 \times 10^{-2}C_{13} - 1.130 \times 10^{-2}C_{14} - 0.167C_1 - 0.152C_2 - 0.122E_{HOMO}$ $-7.838 \times 10^{-2}\mathrm{E_{LUMO}} - 7.004 \times 10^{-3}\Delta\mathrm{E} + 0.109\mu + 0.141\mathrm{V}$	**0.85**	
Triazole derivatives	**Density Functional Theory (DFT), B3LYP/6-31G**	$IE_{Theor} = \frac{(18.38E_{HOMO}-7.28E_{LUMO}-0.012V+123.36)C}{[1+(18.38E_{HOMO}-7.28E_{LUMO}-0.012V+123.36)C]}$ **Derived QSAR equation in gas phase**	**0.94**	[10]

		$IE_{Theor} = \frac{(-2.19E_{HOMO} - 1.24E_{LUMO} - 0.014V - 10.94)C}{[1 + (-2.19E_{HOMO} - 1.24E_{LUMO} - 0.014V - 10.94)C]}$ **Derived QSAR equation in aqueous phase**	**0.95**	
Imidazole derivatives	**Restricted Hartree–Fock level (RHF) using MINDO/3, MNDO, PM3 and AM1 semi-empirical SCF-MO methods.**	$IE_{exp}\left(\%\right) = 1174.95 + 214.612E_{HOMO} - 16.793E_{LUMO}$ **Gas phase (series 1)**	**0.90**	[16]
		$IE_{exp}\left(\%\right) = 517.7 + 53.8E_{HOMO} - 1.97E_{LUMO}$ **Aqueous phase (series 1)**	**0.82**	
		$IE_{exp}\left(\%\right) = 2420.86 + 295.67E_{HOMO} - 30.08E_{LUMO}$ **Gas phase (series 2)**	**0.97**	
		$IE_{exp}\left(\%\right) = 601.53 + 63.07E_{HOMO} - 1.405E_{LUMO}$ **Aqueous phase (series 2)**	**0.99**	
Imidazole and benzimidazole derivatives	---	$IE_{exp}\left(\%\right) = 38.47 + 20.21n\left(N\right) - 7.98N\left(O + NH_2\right) + 14.94\eta^{+} - 17.93\eta^{-}$	**0.97**	[19]
Indole derivatives	**DFT, B3LYP functional and 6-31G(2d,2p) basis**	$R_{ct} = 150 + (-359539E_{HOMO} + 1585825E_{LUMO})C$	**0.97**	[36]
		$R_{ct} = 150 + (-402535E_{HOMO} + 960146E_{LUMO})C$	**0.97**	
Imidazole and benzimidazole derivatives	**DFT: PBE/6-311++G ****	$E_{exp}\left(\%\right) = 5130.95 - 32.03\chi + 533.4bq^{ISO} + 0.37V + 1433.78q_{N1}$	**0.92**	[24]
Imidazole, benzimidazole and pyridine derivatives	**DFT: PBE/B3LYP/M06, using the orbital basis 6-31G* and 6-311++G****	$IE_{exp}\left(\%\right) = 92.965 + 0.152V + 35.337\omega^{-} + 3.592bq_{ANS}$	**0.75**	[23]
Pyrimidine derivatives	**DFT BLYP/DNP**	$IE_{exp}\left(\%\right) = -4.324\mu - 46.527\Delta E + 376.48q_{N1}$	**0.98**	[25]
Thiosemicarbazides	**PM3 and MNDO method.**	$IE_{Theor} = \frac{(-6.7E_{HOMO} - 5.9E_{LUMO} - 3.5\mu - 43.7)C}{[1 + (-6.7E_{HOMO} - 5.9E_{LUMO} - 3.5\mu - 43.7)C]} \times 100$	**0.84**	[27]
		$IE_{Theor} = \frac{(227.2 + 23.5E_{HOMO} - 3.8\mu)C}{[1 + (227.2 + 23.5E_{HOMO} - 3.8\mu)C]} \times 100$	**0.92**	
Thiosemicarbazides/ Thiosemicarbazones	**Data obtained from literature**	$IE_{exp} = \frac{e^{-2.5219E_{HOMO} - 0.5119\mu_D - 18.1761}C}{(1 + e^{-2.5219E_{HOMO} - 0.5119\mu_D - 18.1761}C)}$	**0.89**	[26]

		$\mathrm{IE_{exp}}=\frac{\mathrm{e}^{263.12\Delta\mathrm{E}-17.26\Delta\mathrm{E2}-999.22}\mathrm{C}}{1+\mathrm{e}^{263.12\Delta\mathrm{E}-17.26\Delta\mathrm{E2}-999.22}}$	**0.88**	
2-Mercaptobenzothiazole	**DFT: B3LYP/6-31+G***	$IE_{Theor}=\frac{(2.23E_{HOMO}-8.37E_{LUMO}+5.47\Delta E+1.76\Delta N+6.47\mu+119.8V+2.07)C}{[1+(2.23E_{HOMO}-8.37E_{LUMO}+5.47\Delta E+1.76\Delta N+6.47\mu+119.8V+2.07)C]}\times 100$	**0.96**	[29]
Urea derivatives	**DFT: B3LYP/6-31G**	$\Delta E=-0.0024IEexp-4.3145$	**0.95**	[33]
		$E_{HOMO}=-0.0107IE_{\mathrm{exp}}-4.88596$	**0.93**	
Hydantoin derivatives	**DFT: B3LYP/6-31G+(d,p)**	$IE_{Theor}=129.054-0.181Mwt-6.550\,\Delta\,E-174.884\,\Delta\,N+0.484BE$	**1.00**	[34]
		$IE_{Theor}=\frac{(9.1\times10^{13}Mwt+4.9\times10^{14}\Delta N+9.7\times10^{13}\Delta E+2.4\times10^{13}BE-5.9\times10^{13})}{(1+1.8\times10^{13}Mwt+1.8\times10^{16}\Delta N+8.1\times10^{14}\Delta E-1.2\times10^{13}BE-7.2\times10^{15})}$	**0.99**	
Polyether compounds	**DFT B3LYP/6-31G(d,p)**	$R_t=5+\left(2.710^7E_{HOMO}-7.610^7E_{LUMO}+3.910^6\mu\right)C$	**0.81**	[36]
Sulphonamide derivatives	**DFT: B3LYP/6-311+G(d,p)**	$IE_{\mathrm{exp}}\,(\%)=\frac{(2.47\omega+8.56\times10^{-2}E_{LUMO}-5.27\times10^{-2}\mu+6.20\eta-4.11\times10^{-2}LogP-21.81)*5000}{(1+(2.47\omega+8.56\times10^{-2}E_{LUMO}-5.27\times10^{-2}\mu+6.20\eta-4.11\times10^{-2}LogP-21.81)*50)}$	**1.00**	[4]
		$IE_{\mathrm{exp}}\,(\%)=\frac{(-1.44\Delta E+3.48E_{LUMO}-3.50E_{HOMO}+1.07\eta+1.75\omega^{+}-17.85)*5000}{(1+(-1.44\Delta E+3.48E_{LUMO}-3.50E_{HOMO}+1.07\eta+1.75\omega^{+}-17.85)*50)}$	**0.99**	
Pyrimidine compounds	**B3LYP/6-311++G(d,p)**	$IE_{Theor}\,(\%)=9.255\times10^{1}-3.213\times10^{-3}\frac{\chi}{C_1}+3.432\times10^{-7}\frac{\mu}{C_2^2}-1.768\times10^{-10}\frac{\Delta E}{C_3^3}-5.859\frac{E_{HOMO}}{C_4^4}$ *** equation for BTPTT, phase gas**	**0.98**	[37]
		$IE_{Theor}\,(\%)=9.326\times10^{1}+6.249\times10^{-4}\frac{E_{HOMO}}{C_1}-1.093\times10^{-7}\frac{E_{LUMO}}{C_2^2}$	**0.99**	
Amino acids	**PM6, PM3, MNDO and RM1 for semi-empirical studies. DFT. Local selectivity**	$IE_{exp}=125.80E_{HOMO}-121.83E_{LUMO}+1402.96$ **PM6 Hamiltonian**	**0.93**	[51]
		$IE_{Theor}=\frac{(1.085E_{HOMO}+1.114E_{LUMO}+\Delta E+4.128\mu)C}{[1+(1.085E_{HOMO}+1.114E_{LUMO}+\Delta E+4.128\mu)C]}\times 100$ **AM1 Hamiltonian, gas phase**	**0.86**	
		$IE_{Theor}=\frac{(0.896E_{HOMO}+1.38E_{LUMO}+\Delta E+\mu+1.694E_{diel}+18.38)C}{[1+(0.896E_{HOMO}+1.38E_{LUMO}+\Delta E+\mu+1.694E_{diel}+18.38)C]}\times 100$ **RM1 Hamiltonian, aqueous phase**	**0.96**	
Carbozones	**AM1, PM6, PM3, MNDO and RM1 Hamiltonians.**	$IE_{exp}\,(\%)=-14.686E_{HOMO}-48.966$	**0.94**	[40]

	Correlation MP2, basis STO-3G	$IE_{Theor} = \frac{(1.0176E_{HOMO}+0.9743E_{LUMO}+1.0351\Delta E+\cos A+\cos V+428.6731)C}{[1+(1.0176E_{HOMO}+0.9743E_{LUMO}+1.0351\Delta E+\cos A+\cos V+428.6731)C]}$	**0.83**	
Simbology				
Austin Model 1: AM1, Modified Intermediate Neglect of Differential Overlap: MNDO, Modified Neglect of Diatomic Overlap: MNDO, Parametric Method 3: PM3, Self consistent field molecular orbital: SCF-MO				

9. Perspectives

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