Pyrimidine derivatives as potential corrosion inhibitors for steel in acid medium – An overview

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Abstract

Acidic environments are widely used in several industrial operations, such as oil well acidification, acid pickling, acid cleaning and acid descaling, which generally lead to serious metallic corrosion. Despite the relatively limited corrosion resistance of carbon steel, it is widely used in marine applications, chemical processing, petroleum production and refining, construction and metal-processing equipments due to its excellent mechanical properties and low cost. Out of several methods, usage of corrosion inhibitor is one of the most important techniques for controlling the corrosion. Several organic inhibitors have been tried for the corrosion inhibition of steel, out of which organic compounds with more than one hetero-atom containing pi-electrons are found to exhibit high inhibiting properties by providing electrons which interact with metal surface. However, the use of several heterocyclic inhibitors has caused negative effects on the environment because of their toxicity and non-biodegradability. In this context, pyrimidine derivatives are found to attract great interest due to their environmentally benign properties. In this article, it is aimed to review the usefulness of pyrimidine derivatives for the corrosion inhibition of steel in acid medium.

Key words: *pyrimidine; corrosion inhibitor; steel; acid medium.*

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1. Introduction

Pyrimidine is a heterocyclic aromatic organic compound containing two nitrogen atoms at positions 1 and 3 of the six-member ring. The chemistry of pyrimidine derivatives plays an important role in the field of medicine, agrochemicals and in many biological processes. Several pyrimidine derivatives exhibit a diverse array of biological and pharmacological activities including anticonvulsant, antibacterial, antifungal, antiviral and anticancer

properties [1]. This broad spectrum of biochemical targets has been enabled by the synthetic versatility of pyrimidine, which has allowed derivatisation of the ring nitrogens and C2/C4/C5/C6 carbon positions [2]. Pyrimidine derivatives constituted many well-established marketed drugs such as Uramustine, Piritrexim, Isetionate, Tegafur, Floxuridine, Fluorouracil, Cytarabine and Methotrexate *etc.* Moreover, Pyrimidine skeleton (mainly uracil, thiamine and cytosine) are essential part in many natural products such as nucleic bases, vitamins, enzymes, chlorophyll, hemoglobin and hormones [3, 4]. The wide variety of biological activities observed for these compounds turned pyrimidine derivatives as environmentally benign compounds. The requirement for good corrosion inhibitor, i.e., organic compounds which can donate electrons to unoccupied *d*-orbital of metal surface to form coordinate covalent bonds and can also accept free electrons from the metal surface by using their anti-bonding orbital to form feedback bonds, is also fulfilled by pyrimidine molecule. Hence pyrimidine derivatives are expected to be excellent corrosion inhibitors at industrial level, not only due to their efficiency but also due to their non-toxic nature [1].

2. Pyrimidine derivatives as corrosion inhibitors for steel

2.1. Metal

Steel is most important, multi-functional and most adaptable of materials. It is widely used in construction, marine applications, chemical processing, metal- processing equipment, and petroleum production and refining due to its excellent mechanical properties and low cost. It is considered as “green” product as it is entirely recyclable. The corrosion resistance of various steel samples including mild steel, cold rolled steel, N80 steel, austenitic stainless steel, stainless steel 304 and stainless steel 904L by using pyrimidine derivatives has been reviewed.

2.2. Medium

Acidic environments are widely used in several industrial operations, such as oil well acidification, acid pickling, acid cleaning and acid descaling [5]. The acidic content on metal is generally leads to serious metallic corrosion. Different concentrations of acids like hydrochloric acid, sulphuric acid, phosphoric acid and nitric acid have been utilized to analyze the corrosion inhibition of steel by pyrimidine derivatives in acidic medium.

2.3. Methods

The simplest way of measuring the corrosion rate of a metal is to expose the sample to the test medium and measure the weight loss of the material as a function of time. Even though it has less accuracy, it gives the preliminary data of corrosion rate. The other methods including potentiodynamic polarization, gravimetric method, electrochemical impedance spectroscopy, electrochemical frequency modulation *etc.* have been utilized to analyze the

corrosion inhibition of steel samples by pyrimidine derivatives [6]. The scanning electron microscope is used to analyze the formation of a protective film on the metal surface by the addition of inhibitors. Atomic force microscopy is also used to generate an image of the metal surface, hence concluding the adsorption of inhibitor.

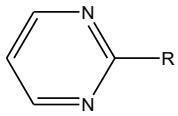
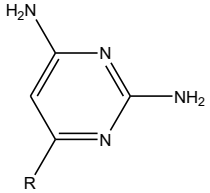
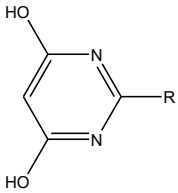
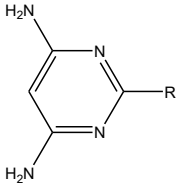
2.4. Corrosion inhibitors

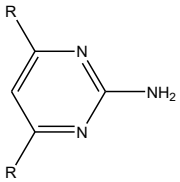
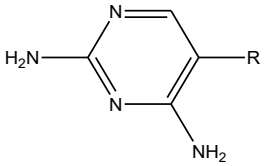
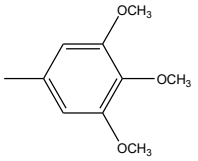
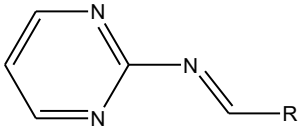
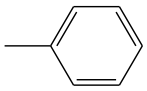
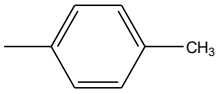
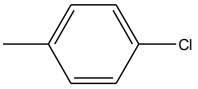
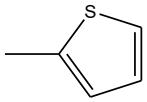
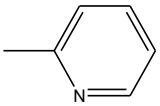
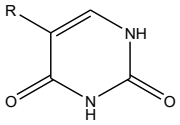
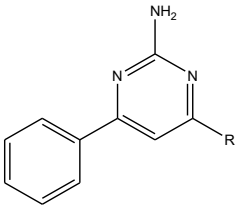
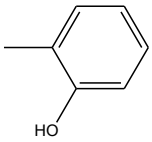
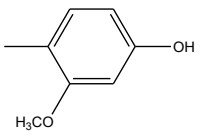
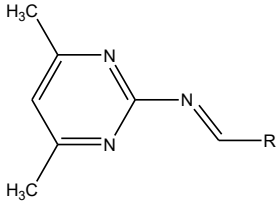
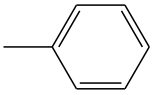
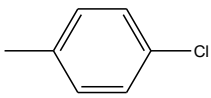
Numerous pyrimidine derivatives have been synthesized and studied their suitability for corrosion inhibition of variety of steel samples in acidic medium. The effect of many pyrimidine derivatives namely, 2-aminopyrimidine, 4,6-dihydroxypyrimidine, 2,4-diaminopyrimidine, 2,4-diamino-6-hydroxypyrimidine, 2,4,6-triaminopyrimidine, 4,6-diamino-2-mercaptopyrimidine [7, 8], 2,6-dimethylpyrimidine-2-amine, *N*-Benzylidene-4,6-dimethylpyrimidine-2-amine and 2-[(3,6-dimethylpyridimine-2-ylimino)methyl]-4-nitrophenol [9] in 2 M HCl; thymine, uracil, thymidine and uridine [10], 4,6-dihydroxy-2-mercaptopyrimidine [11], 5-(3,4,5-trimethoxybenzyl)pyrimidine-2,4-diamine [12], benzylidene-pyrimidin-2-yl-amine, (4-methyl-benzylidene)-pyrimidine-2-yl-amine and (4-chloro-benzylidene)-pyrimidine-2-yl-amine [13], 4-((4,6-dimethylpyrimidin-2-ylimino)-methyl)chlorobenzene, 4-((4,6-dimethylpyrimidin-2-ylimino)methyl)-*N,N*-dimethylaniline, 4-((4,6-dimethylpyrimidin-2-ylimino)methyl)phenol [14], ethyl (2-amino-5-methyl[1,2,4]-triazolo[1,5-*a*]pyrimidin-7-yl)acetate, ethyl (5-methyl[1,2,4]triazolo[1,5-*a*]pyrimidin-7-yl)-acetate [15], 5-phenyl-10-((3*R*,5*S*,6*R*)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2*H*-pyran-3-yl)-9,10-dihydropyrido[2,3-d:6,5-d´]dipyrimidine-2,4,6,8(1*H*,3*H*,5*H*,7*H*)-tetraone, 5-(4-nitrophenyl)-10-((3*R*,5*S*,6*R*)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2*H*-pyran-3-yl)-9,10-dihydropyrido[2,3-d:6,5-d´]dipyrimidine-2,4,6,8(1*H*,3*H*,5*H*,7*H*)-tetraone, 5-(4-tolyl)-10-((3*R*,5*S*,6*R*)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2*H*-pyran-3-yl)-9,10-dihydropyrido[2,3-d:6,5-d´]dipyrimidine-2,4,6,8(1*H*,3*H*,5*H*,7*H*)-tetraone, 5-(4-hydroxy-phenyl)-10-((3*R*,5*S*,6*R*)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2*H*-pyran-3-yl)-9,10-dihydropyrido[2,3-d:6,5-d´]dipyrimidine-2,4,6,8(1*H*,3*H*,5*H*,7*H*)-tetraone [16], D-glucose derivatives of dihydropyrido-[2,3-d:6,5-d′]-dipyrimidine-2,4,6,8(1*H*,3*H*,5*H*,7*H*)-tetraone [17] and 3-(2-(4-(hydroxymethyl)-1*H*-1,2,3-triazol-1-yl)ethyl)-2-methyl-6,7,8,9-tetra-hydropyrido[1,2-a]pyrimidin-4-one [18] in 1 M HCl; 2-amino-pyrimidine [19], 6-methyl-4-morpholin-4-yl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester, 6-methyl-4-morpholin-4-yl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester, 6-methyl-4-morpholin-4-yl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid hydrazide, 6-methyl-4-morpholin-4-yl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid hydrazide [20] in 0.5 M HCl; 2-((1*E*)-2-aza-2-pyrimidine-2-ylvinyl)-thiophene, 2-((1*Z*)-1-aza-2-(2-pyridyl)vinyl)pyrimidine, 2-((1*E*)-2-aza-2-(1,3-thiazol-2-yl)vinyl)thiophene, 2-((1*Z*)-1-aza-2-(2-thienyl)vinyl)benzothiazole [21] in 0.1 M HCl; pyrimidine, 2-aminopyrimidine, 2-hydroxypyrimidine hydrochloride, 2-mercapto-pyrimidine, 2,4-diaminopyrimidine, 2,4,6- triaminopyrimidine, 2,4-diamino-6-hydroxy-pyrimidine and 2,4-diamino-6-meracaptopyrimidine [7], *N*-(pyrimidin-2-ylcarbamothioyl)-

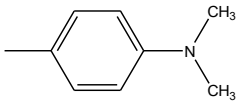
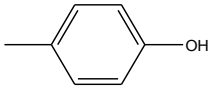
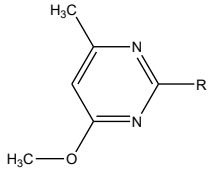
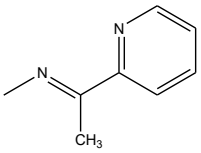
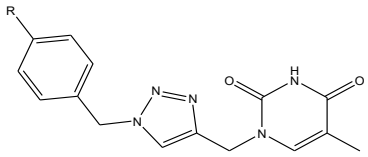
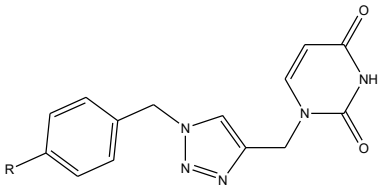
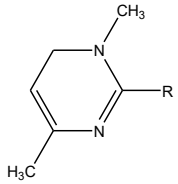
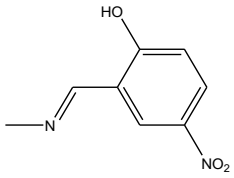
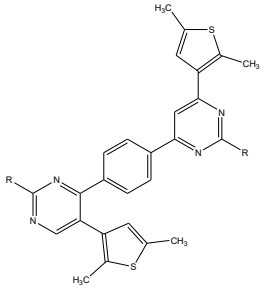
benzamide [22], 7-methoxypyrido[2,3-*d*]pyrimidin-4-amine and 4-amino-7-methoxy-pyrido[2,3-d]pyrimidin-2(1*H*)-one [23], 5-(4-methoxyphenyl)-1,3,5,6,8-pentahydro-7-thioxo-pyrimido[4,5-*d*]pyrimidine-2,4-dione, 5-phenyl-1,3,5,6,8-pentahydro-7-thioxo-pyrimido[4,5-d]pyrimidine-2,4-dione, 5-(4-methoxyphenyl)-1,3,5,6,8-pentahydro-pyrimido[4,5-d]pyrimidine-2,4,7-trione and 5-phenyl-1,3,5,6,8-pentahydro-pyrimido[4,5-*d*]pyrimidine-2,4,7-trione [24] in HCl: 4,6-diphenyl-3,4-dihydropyrimidine-2(1*H*)-thione, 4-(4-methylphenyl)-6-phenyl-3,4-dihydropyrimidine-2(1*H*)-thione and 4-(4-methoxy-phenyl)-6-phenyl-3,4-dihydropyrimidine-2(1*H*)-thione [25], 5-(2,5-dimethylthiophen-3-yl)-4-(4-(6-(2,5-dimethylthiophen-3-yl)-2-hydroxypyrimidin-4-yl)phenyl)pyrimidin-2-ol, 5-(2,5-dimethylthiophen-3yl)-4-(4-(6-(2,5-dimethylthiophen-3-yl)-2-mercaptopyrimidin-4-yl)phenyl)pyrimidin-2-thiol [26], thiazolo-pyrimidine derivatives [27], aminopyrimidine derivatives [28] in 1.0 M sulphuric acid, (4-methoxy-6-methyl-pyrimidin-2-yl)-(1-pyridin-2-yl-ethylidene)-amine [29], 1-(7-methyl-5-morpholin-4-yl-thiazolo[4,5-d]pyrimidin-2-yl)-hydrazine [30], 2-aminopyrimidine and 2,4-diaminopyrimdine [31] in 0.5 M sulphuric acid, 2-amino-4,6-dimethyl pyrimidine [32] in neutral medium has been studied for the corrosion inhibition of carbon steel. Similarly, several pyrimidine derivatives have been studied for the corrosion inhibition of other variety of steel samples. 5-Benzoyl-4-(4-carboxphenyl)-6-phenyl-1,2,3,4-tetrahydro-2-iminopyrimidine, 5-benzoyl-4-tolyl-6-phenyl-1,2,3,4-tetrahydro-2-thioxopyrimidine in 1 M HCl [33] and 5-benzoyl-4-(substituted phenyl)-6-phenyl-3,4-dihydropyrimidine-2(1*H*)-(thio)ones in 0.5M H_2SO_4 [34] for the corrosion inhibition of austenitic stainless steel; 5-styryl-2,7-dithioxo-2,3,5,6,7,8-hexahydropyrimido[4,5-d]-pyrimidin-4(1*H*)-one and 5-(2-hydroxyphenyl)-2,7-dithioxo-2,3,5,6,7,8-hexahydropyrimido[4,5-d]-pyrimidin-4(1*H*)-one in 15% HCl [35] for N80 steel corrosion; 1,5-diallyl-1*H*-pyrazolo[3,4-d]-pyrimidine [36] in 1 M H_3PO_4 for 904L stainless steel; 2-hydroxypyrimidine, 2-mercaptopyrimidine in 1 M HCl [37], 2-chloropyrimidine, 2-hydroxypyrimidine, 2-bromopyrimidine, 2-aminopyrimidine and 2-mercaptopyrimidine in 0.1 M HNO_3 [38] for cold rolled steel; 4-(4′-methylphenyl)-6-(phenyl)-3,4-dihydropyrimidine-2(1*H*)-thione and 4-(4′-methoxylphenyl)-6-(phenyl)-3,4-dihydro-pyrimidine-2(1*H*)-thione in 2.0 M H_2SO_4 [39] for stainless steel 304 have been studied by using various techniques (Table 1). Studies reported that the adsorption of the pyrimidine derivative on steel surface mainly depends on its physico-chemical properties, electronic density of donor atom and possible interaction of its π-orbitals with d-orbitals of the surface atom. The results showed that the inhibition efficiency of the investigated compounds was found to depend on the concentration and the nature of the inhibitors. The efficiency of the inhibitors increases with the increase in the inhibitor concentration but decreases with a rise in temperature. Polarization results indicated that majority of these compounds behave as mixed type inhibitors. However, there are some compounds which act as cathodic-type inhibitors [16, 28] and anodic inhibitors [21]. The adsorption of many of these compounds on steel surface followed Langmuir adsorption isotherm, where as few of the compounds were found to obey the Dubinin–Radushkevich adsorption isotherm [33,

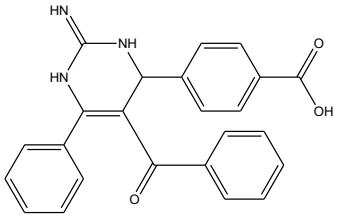
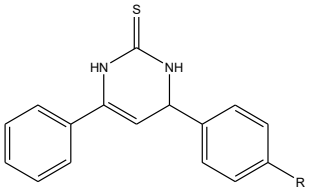
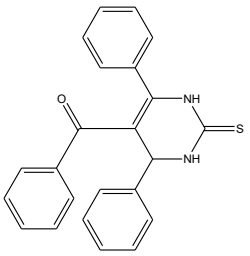
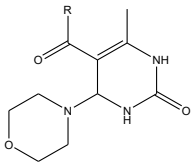
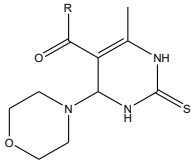
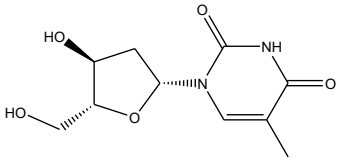
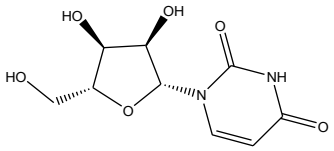
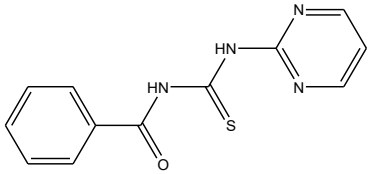
34], Frumkin adsorption isotherm [7] and Temkin's adsorption isotherm [21]. The scanning electron microscope (SEM) results showed the formation of a protective film on the metal surface in the presence of these additives. Computational studies were undertaken to provide mechanistic insight into the roles of the different substituents on the corrosion inhibition and adsorption behavior of the studied compounds.

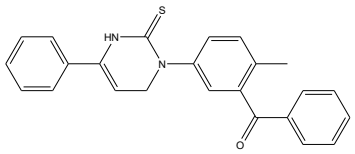
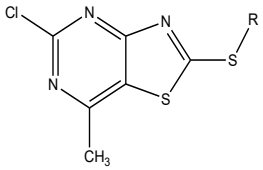
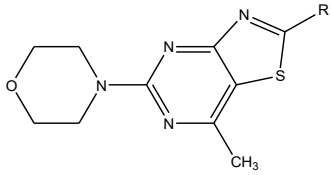
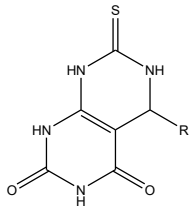
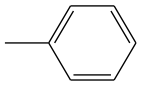
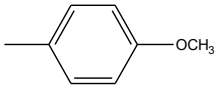
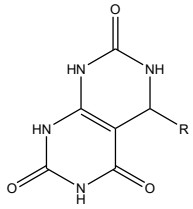
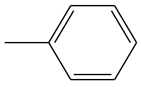
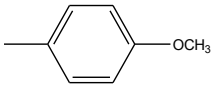
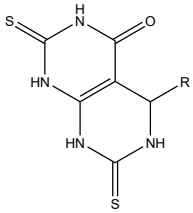
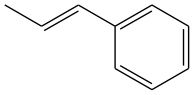
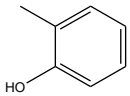
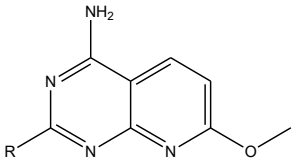
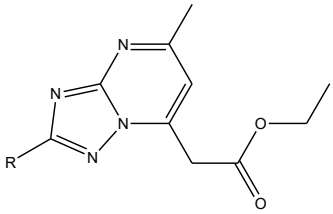
Table 1. List of pyrimidine derivatives used for the corrosion inhibition of steel samples in different acid medium.

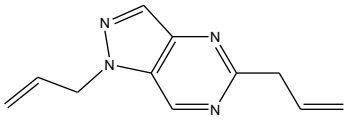
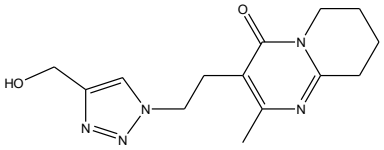
Pyrimidine Moiety	–R	Steel Sample	Medium	Reference
	–H	Carbon steel	2 M HCl	[7]
	$–NH_2$	Carbon steel	2 M HCl	[7, 8]
			0.5 M H_2SO_4	[31]
			0.5 M HCl	[19]
		Cold rolled steel	0.1 M HNO_3	[38]
	–Br	Cold rolled steel	0.1 M HNO_3	[38]
	–Cl	Cold rolled steel	0.1 M HNO_3	[38]
	–OH	Cold rolled steel	0.1 M HNO_3	[38]
			1 M HCl	[37]
	–OH·HCl	Carbon steel	2 M HCl	[7]
	–SH	Carbon steel	2 M HCl	[7]
		Cold rolled steel	0.1 M HNO_3	[38]
			1 M HCl	[37]
	–H	Carbon steel	2 M HCl	[7, 8]
			0.5 M H_2SO_4	[31]
	–OH	Carbon steel	2 M HCl	[7, 8]
	–SH	Carbon steel	2 M HCl	[7]
	–H	Carbon steel	2 M HCl	[8]
	–SH	Carbon steel	1 M HCl	[11]
	$–NH_2$	Carbon steel	2 M HCl	[7, 8]
	–SH	Carbon steel	2 M HCl	[8]

Pyrimidine Moiety	–R	Steel Sample	Medium	Reference
	$–CH_3$	Carbon steel	2 M HCl	[9]
			Neutral	[32]
	$–C_6H_5$	Carbon steel	1 M H_2SO_4	[28]
		Carbon steel	1 M HCl	[12]
		Carbon steel	1 M HCl	[13]
		Carbon steel	1 M HCl	[13]
		Carbon steel	1 M HCl	[13]
		Carbon steel	0.1 M HCl	[21]
		Carbon steel	0.1 M HCl	[21]
	$–CH_3$	Carbon steel	1 M HCl	[10]
	–H	Carbon steel	1 M HCl	[10]
		Carbon steel	1 M H_2SO_4	[28]
		Carbon steel	1 M H_2SO_4	[28]
		Carbon steel	2 M HCl	[9]
		Carbon steel	1 M HCl	[14]

Pyrimidine Moiety	–R	Steel Sample	Medium	Reference
		Carbon steel	1 M HCl	[14]
		Carbon steel	1 M HCl	[14]
		Carbon steel	0.5 M H_2SO_4	[29]
	–H	Carbon steel	1 M HCl	[40]
	–F	Carbon steel	1 M HCl	[40]
	–Cl	Carbon steel	1 M HCl	[40]
	–Br	Carbon steel	1 M HCl	[40]
	–I	Carbon steel	1 M HCl	[40]
	–H	Carbon steel	1 M HCl	[40]
	–F	Carbon steel	1 M HCl	[40]
	–Cl	Carbon steel	1 M HCl	[40]
	–Br	Carbon steel	1 M HCl	[40]
	–I	Carbon steel	1 M HCl	[40]
		Carbon steel	2 M HCl	[9]
	–OH	Carbon steel	1 M H_2SO_4	[26]
	–SH	Carbon steel	1 M H_2SO_4	[26]

Pyrimidine Moiety	–R	Steel Sample	Medium	Reference
		Austenitic stainless steel	1 M HCl	[33]
	–H	Carbon steel	1 M H_2SO_4	[25]
	$–CH_3$	Stainless steel 304	2 M H_2SO_4	[39]
		Carbon steel	1 M H_2SO_4	[25]
	$–OCH_3$	Stainless steel 304	2 M H_2SO_4	[39]
		Carbon steel	1 M H_2SO_4	[25]
		Austenitic stainless steel	0.5 M H_2SO_4	[34]
	$–OC_2H_5$	Carbon steel	0.5 M HCl	[20]
	$–NHNH_2$	Carbon steel	0.5 M HCl	[20]
	$–OC_2H_5$	Carbon steel	0.5 M HCl	[20]
	$–NHNH_2$	Carbon steel	0.5 M HCl	[20]
		Carbon steel	1 M HCl	[10]
		Carbon steel	1 M HCl	[10]
		Carbon steel	1 M HCl	[22]

Pyrimidine Moiety	–R	Steel Sample	Medium	Reference
		Austenitic stainless steel	1 M HCl	[33]
	–H	Carbon steel	1 M H_2SO_4	[27]
	$–C_2H_5$	Carbon steel	1 M H_2SO_4	[27]
	$–CH_2–C_6H_5$	Carbon steel	1 M H_2SO_4	[27]
	$–SC_2H_5$	Carbon steel	1 M H_2SO_4	[27]
	$–NHNH_2$	Carbon steel	0.5 M H_2SO_4	[30]
		Carbon steel	1 M HCl	[24]
		Carbon steel	1 M HCl	[24]
		Carbon steel	1 M HCl	[24]
		Carbon steel	1 M HCl	[24]
		N80 Steel	15% HCl	[35]
		N80 Steel	15% HCl	[35]
	–OH	Carbon steel	15%HCl	[23]
	–H	Carbon steel	15% HCl	[23]
	$–NH_2$	Carbon steel	1 M HCl	[15]
	–H	Carbon steel	1 M HCl	[15]

Pyrimidine Moiety	–R	Steel Sample	Medium	Reference
		904L Stainless steel	1 M H_3PO_4	[36]
		Carbon steel	1 M HCl	[18]

2.5 Theoretical studies

Quantum chemical calculations have been widely used to study the reaction mechanism and to interpret the experimental results as well as to solve chemical ambiguities. This is a useful approach to investigate the mechanism of reaction between the inhibitor molecules and the metal surface. The structural and electronic parameters of the inhibitor molecules can be obtained by means of theoretical calculations using the computational methodologies of quantum chemistry [41]. The adsorption mechanism and inhibition performance of several pyrimidine derivatives, namely, 6-methyl-4-phenyl-4,5-dihydropyrimidine-2-thiol, 4,6-diphenyl 4,5-dihydropyrimidine-2-thiol [42], 5-tolyl-2-phenylpyrazolo[1,5-*c*]pyrimidine-7(6*H*)-thione, 5-tolyl-2-phenylpyrazolo-[1,5-c]-pyrimidine-7(6H)-one [43], triazolopyrimidinones, triazolopyrimidine-thione [44], 5-(3-phenylallylidene)pyrimidine-2,4,6-trione, 5-(2-hydroxybenzylidene)pyrimidine-2,4,6-trione, 5-benzlidene pyrimidine-2,4,6-trione [45], 5-benzoyl-4-(4-carboxphenyl)-6-phenyl-1,2,3,4-tetrahydro-2-iminopyrimidine and 5-benzoyl-4-tolyl-6-phenyl-1,2,3,4-tetrahydro-2-thioxo-pyrimidine [46] have been investigated using density functional theory at the B3LYP/6-31G(d,p) basis set level. Quantum chemical method showed that the pyrimidine derivatives can be directly adsorbed at the steel surface on the basis of donor–acceptor interactions between π-electrons of pyrimidine and vacant d-orbitals of iron atoms. The variation in inhibitive efficiency mainly depends on the type and nature of the substituents present in the pyrimidine molecule. The calculated quantum chemical parameters related to the inhibition efficiencies are the orbital energies (EHOMO and ELUMO), Separation Energy (ELUMO–EHOMO), Dipole moment (μ), Polarizability, Hardness (η) and Softness (S). The results showed that the theoretically calculated order of ionization potential was found to be in close agreement with the experimental order. Quantitative Structure Activity Relationship (QSAR) approach was used on a composite index of some quantum chemical parameters to characterize the inhibition performance of the studied molecules. To explain the inhibition performance of the pyrimidine derivatives, their local reactivities were analyzed through Fukui functions.

Conclusions

Corrosion inhibition of steel samples in acid media by pyrimidine derivatives has been reviewed. From the above discussion, it is evident that pyrimidine derivatives are effective corrosion inhibitors against mild steel in acid medium. Weight loss, electrochemical impedance, and potentiodynamic polarization techniques were mainly used to confirm corrosion inhibition in acidic media. It has been observed that the corrosion inhibition generally increases with increase in the concentration of inhibitor. Quantum chemical calculations were helped in establishing detailed mechanisms for corrosion inhibition. Scale-up experiments for industrial applications are needed to be done so as to commercialize these pyrimidine derivatives to effectively replace the conventional chemicals currently used to control the corrosion of steel.

Acknowledgements

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