CAAP Quarterly Report

[12/31/2024]

Project Name: Multi-Compound Green Corrosion Inhibitor for Gas Pipeline: Synthesis, Optimization, and Evaluation

Contract Number: 693JK32350004CAAP

Prime University: Arizona State University

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Reporting Period: [10/2024 – 12/2024]

Project Activities for Reporting Period:

Task 1. Design and Synthesis of Multi-compound Green Inhibitors

Our team achieved significant progress in Q5 by conducting a comprehensive literature review to identify potential corrosion inhibitors. From this review, we carefully selected the most promising candidates and evaluated their performance through three detailed tests: static weight loss tests, gas-phase corrosion tests, and electrochemical analyses. These tests offered crucial insights into the inhibitors' effectiveness under various conditions. The key activities are summarized as follows:

- Task 1.1: Quick screening of green inhibitors for gas pipeline protection
 - Conducted a comprehensive literature review on green inhibitors and selected six candidates based on availability, cost, and efficiency.
 - Performed weight loss tests in three different media for all six candidates to evaluate and compare their effectiveness.
 - Conducted electrochemical tests in two different media to further assess and compare the efficiency of the six candidates.
 - Natural product-based biocorrosion inhibitor screening (GTI effort)

Task 2. Simulation-based Inhibitor Optimization in Gas Gathering and Transportation Pipelines

During this reporting period, we have made significant progress in Task 2, focusing on establishing the neural network framework for more efficient prediction on the flow regime. The key activities are outlined below:

- o 2.1: Numerical simulation of multiphase flow for inhibitor distribution in gas pipeline systems
 - Investigated key parameters affecting inhibitor particle accretion.
 - Developed a CFD-based approach to study particle-wall interaction.
- o 2.2: AI-assisted inhibitor optimization gathering and transportation pipelines
 - Built a machine learning surrogate model to predict wall accretion.
 - Compared different neural network frameworks with uncertainty quantification.

A comprehensive report detailing the tasks is provided in the appendix. Additionally, the presentation file for the quarterly report, prepared for the Technical Advisory Panel (TAP) members and PHMSA program managers, is also enclosed in the appendix.

Project Financial Activities Incurred during the Reporting Period:

For Task 1, we supported 1 RA at ASU For Task 2, we supported 1 RAs at ASU

Project Activities with Cost Share Partners:

Engaged in discussions with the Technical Advisory Panel members to solicit recommendations for our team's research activities.

Project Activities with External Partners:

Conducted regular discussions with the Technical Advisory Panel, in addition to several separate meetings and email communications with individual advisory members.

Potential Project Risks:

Nothing to report.

Future Project Work:

For Task 1:

- Finalizing the screening process for green inhibitors for gas pipeline protection.
- Enhancing corrosion protection efficiency of selected green inhibitors through chemical modification.
- Verifying the compatibility of selected green inhibitors with industry standards and performance requirements

For Task 2:

- Continue the investigation of Neural Networks modeling to enhance the efficiency of pipe flow simulation with inhibitors
- o Include uncertainty quantification for inhibitor degradation risk assessment
- Explore potential maintenance optimization methodology to mitigate the risk of inhibitor degradation
- Collaborate with Task 1 group to revise the simulation framework with target inhibitor properties

Appendix 1 Technical Progress Description for Task 1

Task 1. Design and Synthesis of Multi-compound Green Inhibitors

1.1 Background:

In the initial phase of this project, we focused on developing eco-friendly corrosion inhibitors to address pipeline corrosion in industrial settings. Our approach utilizes abundant, renewable natural materials like citrus peels and shrimp shells as raw materials. This aligns with our commitment to sustainability, human health, and safety by creating non-toxic, bio-based inhibitors that are safe for gas pipelines. By repurposing these readily available by-products, we aim to provide cost-effective, environmentally responsible solutions to corrosion challenges, without compromising safety or regulatory standards. Our efforts support PHMSA's safety mission and work toward minimizing the environmental footprint of corrosion prevention, benefiting both industry and the environment.

During the first quarter, we conducted an extensive literature review to identify potential eco-friendly inhibitors. This stage was critical for understanding the capabilities and limitations of various natural resources as corrosion inhibitors. Additionally, we collaborated with industry leaders to ensure that our proposed methodologies met rigorous safety and compatibility standards, setting a robust foundation for subsequent experimental phases. A significant milestone in this phase was the successful extraction of pectin from orange peels, a renewable material recognized for its potential as a corrosion inhibitor.

In the second quarter, we intensified our efforts to optimize the synthesis processes and enhance the functional properties of our bio-based inhibitors. We concentrated on refining the extraction and functionalization techniques for pectin, aiming to improve its interaction with metal surfaces and thereby increase its corrosion inhibition efficiency. Concurrently, we initiated the synthesis of chitosan from shrimp shells, diversifying our portfolio of eco-friendly inhibitors. To evaluate the performance of these materials, we established rigorous corrosion testing protocols, including static weight loss measurements and electrochemical analyses, ensuring a high level of precision and reliability in our assessments.

In the fourth quarter, we tested pectin as a bio-corrosion inhibitor under various conditions to assess its potential for pipeline corrosion protection. These tests were critical in evaluating its performance across different environments, providing valuable insights into its effectiveness and limitations. Building on these findings, we explored modifications to the pectin structure to enhance its efficiency and performance, with the goal of ensuring that the bio-based inhibitor provides corrosion protection equal to or better than conventional inhibitors. Our efforts focus on maximizing the inhibitor's protective capabilities while ensuring it aligns with PHMSA's mission to maintain pipeline safety.

1.2 Quarterly Objectives

The primary goal this quarter was to identify and evaluate eco-friendly green corrosion inhibitors for gas pipeline protection. A literature review identified around 60 potential green inhibitors, including those derived from natural sources like leaves, tree bark, and other plant- and animal-based materials. These candidates were evaluated for availability, cost, and reliability, and

five were shortlisted for detailed testing in controlled media to study their corrosion inhibition under various conditions.

Efforts also focused on analyzing the functional groups in the shortlisted inhibitors, which are key to their adsorption and protective mechanisms. Characterizing these groups provided insights into their corrosion prevention properties and established a foundation for linking specific functional groups to their protective efficiency, paving the way for further research.

Task 1.1: Quick screening of green inhibitors for gas pipeline protection

1.3 Conducting a comprehensive literature review on green corrosion inhibitors for gas pipelines and selecting six candidates based on availability, cost, and efficiency.

An extensive literature review was conducted to explore the application of green corrosion inhibitors for carbon steel. To ensure reliability, the selected studies were sourced from top-ranked, peer-reviewed journals [1-53]. Table 1.1 summarizes the identified green inhibitors, their optimum efficiency in HCl corrosion media, and their respective sources.

Table 1.1 List of Identified Green Corrosion Inhibitors for Carbon Steel Pipelines and Their Properties

No.	Inhibitor	Efficiency (IE%)	Derived Source	References
1	Psidium guajava extract	98.0%	Plant	(El-hoshoudy et al., 2021)
2	Sonneratia caseolaris Leaf Extract	98.0%	Plant	(Manh et al., 2022)
3	Aeluropus lagopoides extract	97.2%	Plant	(Motawea, 2022)
4	Seaweed extract	97.0%	Plant (Algae)	(Wang et al., 2024)
5	Allium Jesdianum extract	96.18%	Plant	(Kahkesh and Zargar, 2021)
6	Onion and Garlic Leaves	96.65%	Plant extract	(Rashid et al., 2022)
7	Vanillin extract	96.04%	Plant	(Tawfik and Negm, 2016)
8	Artemisia argyi leaves extract	96.4%	Plant	(Wang et al., 2022)
9	Ruta Graveolens Essential Oil	95.97%	Plant	(Manssouri et al., 2024)
10	Garcinia livingstonei leaves extract	95.23%	Plant	(Rathod et al., 2022)
11	Portulaca grandiflora leaf	95.20%	Plant	(Fadhil et al., 2020)
12	White turnip bark extract	95.20%	Plant	(Alemnezhad et al., 2023)

13	Walnut fruit green husk extract	95.06%	Plant	(Shahmoradi et al., 2021)
14	Paprika extract	95.0%	Plant	(Kamel et al., 2021)
15	Hyalomma tick	95.0%	Animal	(Bidi et al., 2020)
16	Xanthum Gum	95%	Plant extract	(Chopda and Dave, 2023)
17	Datura stramonium plant seed extract	94.2%	Plant	(Hjouji et al., 2023)
18	Ceratonia Siliqua L seeds extract	95.30%	Plant	(Abbout et al., 2021)
19	Onion-Garlic leaves blend extract	94.19%	Plant	(Rashid et al.)
20	Pueraria lobata leaf extract	94.37%	Plant	(Wang et al., 2021)
21	Apricot pomace extract	94.60%	Plant	(Vorobyova and Skiba, 2020)
22	Nutmeg oil	94.73%	Plant	(Abdallah et al., 2021)
23	Eruca sativa seed extract	94.80%	Plant	(Gadow and Fakeeh, 2022)
24	Soybean Extract	94.25%	Plant extract	(Wan et al., 2022)
25	Date palm seed extract	94.0%	Plant	(Mohammed and Othman, 2020)
26	Cupressus arizonica fruit oil	93.0%	Plant	(Cherrad et al., 2022)
27	Garcinia indica fruit rind extract	93.0%	Plant	(Thomas et al., 2020)
28	Chitosan	92%	Shrimp shells	(Zhang et al., 2023)
29	Inula viscosa extract	92.40%	Plant	(Kouache et al., 2022)
30	Artemisia herba alba	92.0%	Plant	(Berrissoul et al., 2020a)
31	Salsola oppositifolia extract	91.86%	Plant	(Kh S and SZ, 2023)
32	Spinacia oleracea extract	91.1%	Plant	(Hameed et al., 2022)

33	Fructus cannabis protein extract	89.8%	Plant	(Liao et al., 2023)
34	Olax subscorpioidea root extract	89.7%	Plant	(James and Iroha, 2022)
35	Vigna unguiculata Coat Extract	86.7%	Plant	(Kikanme et al., 2020)
36	Cola acuminata extract	86.0%	Plant	(Mohammed et al., 2020)
37	Oestrus ovis larvae extract	86.0%	Animal (Parasite)	(Mobtaker et al., 2022)
38	Lavandula mairei extract	88.90%	Plant	(Berrissoul et al., 2020b)
39	Fucus spiralis	87.0%	Plant (Algae)	(Afrokh et al., 2021)
40	Mentha rotundifolia extract	87.0%	Plant	(Khadraoui et al., 2016)
41	Lilium brownii leaves extract	85.0%	Plant	(Zuo et al., 2021)
42	Origanum vulgare oil	85.64%	Plant	(Ihamdane et al., 2023)
43	Gelatin Extract	84.25%	Animal extract	(Haruna et al., 2018)
44	Dysphania ambrosioides essential oil	84.0%	Plant	(Daoudi et al., 2022)
45	Ammi visnaga L. extract	84.0%	Plant	(Zaher et al., 2022)
46	Propolis	79.0%	Animal (Bee)	(Rizvi et al., 2020)
47	Albumin	78.45%	Egg extract	(Vashishth et al., 2023)
48	Paederia Foetida leaves extract	73.77%	Plant	(Hossain et al., 2021)
49	Combretum indicum leaf extract	82.59%	Plant	(Neriyana and Alva, 2020)
50	Sunflower petals extract	82.7%	Plant	(Khoshsang and Ghaffarinejad, 2022)
51	Castor oil-based corrosion inhibitor	85% to 91%	Plant	(Farhadian et al., 2020)
52	Cationic gemini-surfactants based on waste cooking oil	~97%	Plant	(Khalaf et al., 2020)

53	Avocado oil-based inhibitor	99.6%	Plant	(Sotelo-Mazon et al., 2019)

From the list of identified inhibitors, our team selected six based on their availability, costeffectiveness, and reliability for rapid screening to identify the most effective candidate. Below is the list of selected inhibitors for screening.

- 1) Waste vegetable cooking oil
- 2) Vegetable oil
- 3) Chitosan
- 4) Xanthan Gum
- 5) Pectin
- 6) Gelatin

Waste cooking oil: Waste cooking oil is a complex mixture of triglycerides, fatty acids, and degraded organic compounds formed through high-temperature processing, including cracking and hydrolysis. Its key functional groups include carboxylic acids, esters, and unsaturated double bonds. Carboxylic acids and their derivatives can enhance corrosion inhibition by adsorbing onto metal surfaces and forming a protective hydrophobic barrier. Unsaturated double bonds may also contribute to surface adsorption through π -electron interactions with the metal.

Vegetable oil: Vegetable oils consist mainly of triglycerides, which are esters formed from glycerol and fatty acids. The functional groups present include ester groups, carboxyl groups (from free fatty acids), and unsaturated bonds (in unsaturated fatty acids). The carboxyl groups and ester linkages can adsorb onto the metal surface, forming a protective film that prevents corrosion. The unsaturated double bonds may also contribute to the adsorption process, enhancing the inhibition efficiency.

Chitosan: Chitosan is a polysaccharide derived from chitin, consisting of glucosamine and N-acetylglucosamine units. Its primary functional groups include amino $(-NH_2)$ and hydroxyl (-OH) groups along the polymer backbone. The amino groups are especially effective in corrosion inhibition, as they can donate lone electron pairs to the metal surface, forming stable coordination bonds. This adsorption creates a protective layer, shielding the metal from corrosive agents.

Xanthan gum: This high-molecular-weight polysaccharide is composed of glucose, mannose, and glucuronic acid residues. Its functional groups include hydroxyl (-OH), carboxylic acid (-COOH), and acetyl groups. The carboxylic acid groups play a key role in corrosion inhibition by adsorbing onto the metal surface and forming a barrier that reduces interaction with corrosive species. Additionally, the hydroxyl groups may contribute to film stability through hydrogen bonding with the metal surface.

Pectin: A polysaccharide composed of galacturonic acid units, with some esterified carboxylic groups. The key functional groups include carboxylic acid (-COOH), methyl ester (-COOCH₃), and hydroxyl groups (-OH). The carboxylic acid groups, both free and esterified, play a vital role

in corrosion inhibition by forming strong bonds with the metal surface, thereby creating a protective layer. The hydroxyl groups also contribute to surface interaction, enhancing inhibitor performance.

Gelatin: This protein, derived from collagen, contains amino acids with functional groups such as amine (-NH₂), carboxylic acid (-COOH), and imidazole groups (from histidine residues). The amine and carboxylic acid groups are highly effective in corrosion inhibition, coordinating with the metal surface to form a durable protective film that minimizes metal exposure to corrosive environments. Additionally, the imidazole groups, when present, can further enhance adsorption through strong interactions with the metal.

Table 1.2 summarizes the key functional groups present in the selected green inhibitors, highlighting their potential roles in corrosion inhibition mechanisms.

Pectin	Chitosan	Xanthan gum	Gelatin	Cooking oil	Waste cooking oil
Carboxyl groups (-COOH)	Amino groups (-NH2)	Carboxyl groups (-COOH)	Amino groups (-NH2)	Ester groups (in triglycerides) (-COOR)	Ester groups (in triglycerides) (-COOR)
Hydroxyl groups (-OH)	Hydroxyl groups (-OH)	Hydroxyl groups (-OH)	Carboxyl groups (-COOH)	Unsaturated fatty acids	Unsaturated fatty acids
Ester groups (-COOR)		Acetyl groups (-COCH3)	Hydroxyl groups (-OH)		carboxyl groups
Methoxyl groups (-OCH ₃)			Amide groups (-CONH)		

Table 1.2 Key Functional Groups in Selected Green Inhibitors

1.4 Conducting weight loss tests in three different media to compare the efficiency of all six candidates

1.4.1 Weight Loss Test in Gas Concentrated Medium

During natural gas transmission, temperature fluctuations, particularly during cooling, can cause certain gas components, such as water vapor, butane, and propane, to condense. This results in the formation of liquid droplets that settle on the inner walls of the pipeline, contributing to gas pipeline corrosion. To replicate these conditions in a controlled environment, a beaker containing an A36 metal coupon in 30 mL of tap water is sealed with a rubber stopper. A vacuum pump is used to evacuate air from the beaker, creating a low-oxygen environment. Once the air is removed, nitrogen and carbon dioxide are injected into the beaker to simulate the low-oxygen conditions typically found inside a gas pipeline. Of the remaining 50 mL of headspace in the beaker, 45 mL is purged with nitrogen (N₂) gas to create an inert atmosphere, while 5 mL of carbon dioxide (CO₂) is introduced to mimic the presence of acidic gases commonly found in gas pipelines. This setup effectively simulates the condensation and gas composition conditions encountered during gas transmission, providing valuable insights into the processes leading to gas pipeline corrosion. The metals are weighed before and after the tests to calculate the corrosion weight loss. Figure 1.1 illustrates the steps involved in the weight loss test under gas-concentrated conditions.



Figure 1.1. Steps of the Weight Loss Test under Gas-Concentrated Conditions

Table 1. 3 Average weight loss of carbon steel in each media and inhibitor corrosion efficiency in weight loss test under gas concentrated condition

Inhibitor	Measured weight	Average	Weight	Corrosion	Inhibitor
			Loss (g)	(%)	Efficiency (%)
Control	Weight before corrosion	3.798	-0.005	-0.125	
	Weight after corrosion	3.794			
Pectin	Weight before corrosion	3.808	-0.006	-0.156	-24.65
	Weight after corrosion	3.802			
Chitosan	Weight before corrosion	3.800	-0.007	-0.181	-44.75
	Weight after corrosion	3.793			

Xanthan	Weight before corrosion	3.795	-0.002	-0.058	54.03
gum	Weight after corrosion	3.793			
Gelatin	Weight before corrosion	3.831	-0.005	-0.142	-13.61
	Weight after corrosion	3.826			
Cooking	Weight before corrosion	3.801	-0.002	-0.052	58.52
oil	Weight after corrosion	3.799			
Waste	Weight before corrosion	3.812	-0.001	-0.014	88.61
cooking	Weight after corrosion	3.811			
oil					

Table 1.3 presents the average weight loss of carbon steels in different media and the anticorrosion efficiency of each inhibitor. The gas-concentrated corrosion tests reveal varying degrees of inhibitor performance in reducing corrosion, as reflected in weight loss and inhibition efficiency. Among the tested inhibitors, waste cooking oil demonstrated the highest inhibition efficiency at 88.61%, with minimal weight loss (-0.001 g) and a corrosion rate of -0.014%. Cooking oil followed with an efficiency of 58.52%, a weight loss of -0.002 g, and a corrosion rate of -0.052%. Xanthan gum also showed promising performance, achieving 54.03% efficiency, a weight loss of -0.002 g, and a corrosion rate of -0.058%. In contrast, gelatin exhibited moderate inhibition efficiency at -13.61%, with a weight loss of -0.005 g and a corrosion rate of -0.142%. Pectin and chitosan performed poorly, with inhibition efficiencies of -24.65% and -44.75%, respectively, along with higher weight losses of -0.006 g and -0.007 g and corrosion rates of -0.156% and -0.181%. The control sample, without any inhibitor, showed a weight loss of -0.005 g and a corrosion rate of -0.125%, serving as a baseline for comparison. These results establish waste cooking oil as the most effective inhibitor, with cooking oil and xanthan gum also exhibiting potential for corrosion mitigation under gas-concentrated conditions. Figure 1.2 visually compares the corrosion of carbon steels in each medium to their original state.



Figure 1.2 Comparison in inhibitor anti-corrosion efficiency after one week of performing the gas concentrated tests

1.4.2 Static Weight Loss Tests in NaCl

The experiments were conducted over one week to evaluate corrosion behavior. To minimize oxygen exposure and maintain consistent conditions, the beakers were placed in a fume hood. Before immersion, each steel coupon was precisely weighed to record its initial mass. After the exposure period, the coupons were retrieved and thoroughly cleaned to remove corrosion products. This process involved scrubbing under running water with a bristle brush, followed by acetone cleaning. The coupons were then dried in acetone to eliminate residual moisture before being reweighed to determine their final mass. Weight loss—calculated as the difference between the initial and final mass—served as the primary metric for assessing corrosion. This allowed for a quantitative comparison of the inhibitors' protective effects, particularly pectin, in the test solutions. The study used harsh environments to identify the most effective inhibitors under extreme conditions. Table 1.4 presents the average weight loss of carbon steels in different media and the anti-corrosion efficiency of each inhibitor in the NaCl solution.

Inhibitor	Measured weight	Average	Weight	Corrosion	Inhibitor	
			Loss (g)	(%)	Efficiency (%)	
Control	Weight before corrosion	3.819	-0.016	-0.428	-	
	Weight after corrosion	3.802				
Pectin	Weight before corrosion	3.803	-0.005	-0.143	66.66	
	Weight after corrosion	3.798				
Chitosan	Weight before corrosion	3.801	-0.010	-0.259	39.48	
	Weight after corrosion	3.792				
Xanthan gum	Weight before corrosion	3.793	-0.004	-0.104	75.76	
	Weight after corrosion	3.789				
Gelatin	Weight before corrosion	3.808	-0.004	-0.104	75.79	
	Weight after corrosion	3.804				
Cooking oil	Weight before corrosion	3.826	-0.008	-0.203	52.54	
	Weight after corrosion	3.818				
Waste	Weight before corrosion	3.827	-0.003	-0.072	83.10	
cooking oil	Weight after corrosion	3.824				

Table 1.4 Average weight loss of carbon steel in each media and inhibitor corrosion efficiency in weight loss test in 3.5% NaCl solution

The static weight loss results in 3.5% NaCl media provide a clear comparison of the corrosion inhibition performance of the tested inhibitors. Each inhibitor was evaluated using three A36 carbon steel coupons, measuring weight loss before and after corrosion. Waste cooking oil proved to be the most effective inhibitor, achieving the highest inhibition efficiency of 83.10%, with the lowest weight loss (-0.003 g) and the lowest corrosion rate (-0.072%). Gelatin and xanthan gum also demonstrated strong performance, with inhibition efficiencies of 75.79% and 75.76%, respectively, both resulting in minimal weight losses (-0.004 g) and corrosion rates (-0.104%). Pectin followed with a solid inhibition efficiency of 66.66%, a weight loss of -0.005 g, and a corrosion rate of -0.143%, confirming its effectiveness in reducing corrosion. Cooking oil exhibited moderate inhibition, with an efficiency of 52.54%, a weight loss of -0.008 g, and a corrosion rate of -0.203%. Chitosan, while less effective, still provided some protection, achieving an inhibition efficiency of 39.48%, with a weight loss of -0.010 g and a corrosion rate of -0.259%. In contrast, the control sample (without any inhibitor) exhibited the highest weight loss (-0.016 g) and the highest corrosion rate (-0.428%), establishing the baseline corrosion levels in the absence of protection. Overall, waste cooking oil emerged as the most effective inhibitor, significantly reducing corrosion in NaCl media.

1.4.3 Static Weight Loss in 1M HCl Medium

Using the same approach, the efficiency of inhibitors in preventing corrosion was assessed in the highly corrosive 1 M HCl media. Table 1.ble 1.5 presents the average weight loss observed in carbon steels and the corrosion inhibition efficiency of each inhibitor in 1 M HCl. **Table 1.5** Average Weight Loss of Carbon Steel and Corrosion Inhibition Efficiency ofInhibitors in 1 M HCl Solution (Weight Loss Test)

Inhibitor	Measured weight	Average	Weight	Corrosion	Inhibitor
			Loss (g)	(%)	Efficiency (%)
Control	Weight before corrosion	3.811	-0.056	-1.474	-
	Weight after corrosion	3.754			
Pectin	Weight before corrosion	3.819	-0.026	-0.673	54.32
	Weight after corrosion	3.793			
Chitosan	Weight before corrosion	3.811	-0.061	-1.595	-8.21
	Weight after corrosion	3.750			
Xanthan gum	Weight before corrosion	3.812	-0.048	-1.247	15.37
	Weight after corrosion	3.764			
Gelatin	Weight before corrosion	3.830	-0.039	-1.024	30.53
	Weight after corrosion	3.791			
Cooking oil	Weight before corrosion	3.829	-0.042	-1.087	26.26
	Weight after corrosion	3.787			
Waste cooking oil	Weight before corrosion	3.803	-0.016	-0.411	72.13
	Weight after corrosion	3.788			

Waste cooking oil proved to be the most effective inhibitor, achieving the highest inhibition efficiency of 72.13%, with the lowest weight loss of -0.016 g and a corrosion rate of -0.411%. Pectin also demonstrated significant corrosion mitigation, with an inhibition efficiency of 54.32%, a weight loss of -0.026 g, and a corrosion rate of -0.673%. Gelatin exhibited moderate performance, showing an inhibition efficiency of 30.53%, a weight loss of -0.039 g, and a corrosion rate of -1.024%. Cooking oil and xanthan gum displayed lower inhibition efficiencies of 26.26% and 15.37%, respectively, suggesting their limited effectiveness under these aggressive conditions. Chitosan performed poorly, with a negative inhibition efficiency of -8.21%, indicating that it exacerbated corrosion rather than preventing it.

1.5 Performing electrochemical tests in two different media to compare the efficiency of all six inhibitors

For corrosion testing and validation, the inhibitors were subjected to thorough testing in both hydrochloric acid (HCl) and sodium chloride (NaCl) media. The testing framework included electrochemical impedance spectroscopy (EIS), Tafel polarization, static weight loss measurements, and gas-concentrated tests. EIS and Tafel polarization provided essential insights into the electrochemical behavior of the inhibitors, particularly their ability to reduce corrosion currents and enhance charge transfer resistance. Static weight loss tests measured the mass loss of carbon steel samples over time, offering a direct indication of the inhibitors' efficiency in mitigating corrosion under both media.

1.5.1 Electrochemical Impedance Spectroscopy (EIS)

The interpretation of EIS data is typically facilitated using Nyquist and Bode plots, which graphically represent the impedance characteristics of the system. These plots can reveal:

- **Charge Transfer Resistance**: Related to the ease with which electrons can move across the electrode/electrolyte interface.
- **Double Layer Capacitance**: Reflects the capacitive behavior at the interface, influenced by the thickness and properties of the electrochemical double layer.
- Warburg Impedance: Indicates diffusion-controlled processes, often seen in porous coatings or corrosion layers.

1.5.1.1 Methodology for Electrochemical Impedance Spectroscopy

Electrochemical Impedance Spectroscopy (EIS) tests were conducted to evaluate the efficiency of the shortlisted corrosion inhibitors. These tests were performed in seven different media:

- Medium 1 (Control): 3.5% NaCl solution (control sample)
- Medium 2: 3.5% NaCl with 2g per liter pectin
- Medium 3: 3.5% NaCl with 2g per liter chitosan
- Medium 4: 3.5% NaCl with 2g per liter Xanthan gum
- Medium 5: 3.5% NaCl with 2g per liter Gelatin
- Medium 6: 3.5% NaCl with waste cooking oil Dip
- Medium 7: 3.5% NaCl with vegetable oil Dip

The EIS measurements utilized a standard three-electrode cell setup:

- Working Electrode: A36 steel specimen polished and brushed using sandpaper to remove oxidable layer.
- **Reference Electrode**: Saturated calomel electrode (SCE).
- **Counter Electrode**: Platinum wire.

The Electrochemical impedance spectroscopy was performed utilizing a frequency response analyzer in conjunction with a potentiostat. This setup ensured precise maintenance of the electrode potential while recording the impedance response. A summary of the specific parameters employed during the EIS tests is presented in Table 1.6.

Parameter	Value	Description
AC Signal Amplitude	10 mV	The amplitude of the alternating current signal.
Frequency Range	100 kHz to 10 mHz	The range over which impedance was measured.
Potentiostat Mode	Potentiostatic (constant potential)	Maintains a constant electrode potential during measurements.
Equilibration Time	At least 3 hours	Allows the system to stabilize before measurements.

Table 1.6 EIS Test Parameters

EIS measurements commenced following a stabilization period, allowing the electrochemical system to achieve a steady state. Impedance data were collected over the designated frequency range to encompass the full electrochemical response.

The impedance data were analyzed by fitting them to an equivalent circuit model to extract key parameters such as solution resistance (Rs), charge transfer resistance (Rct), and constant phase element (CPE). These parameters were derived from Nyquist plots, which graph the imaginary part of impedance (Z") against the real part (Z').

The equivalent circuit (Figure 1.2) used for analyzing the impedance plots consisted of:

- **R1**: Solution resistance (Rs).
- **R2**: Charge transfer resistance (Rct).
- **CPE1**: Impedance of the constant phase element.



Figure 1.2 Equivalent Circuit Used for Analyzing the Impedance Spectra

1.5.1.2 Steps for Measuring Solution and Charge Transfer Resistance

- 1) **Perform EIS Measurement**: Conduct an EIS experiment over a broad frequency range.
- 2) Analyse Nyquist Plot: Plot the Nyquist diagram and identify the intercepts and features corresponding to Rs and Rct.
- 3) Calculation of Parameters:
 - Solution Resistance (Rs): High-frequency intercept on the real axis of a Nyquist plot.
 - Charge Transfer Resistance (Rct): Represents the electron transfer resistance at the electrode-electrolyte interface.

1.5.1.3 Results:





Figure 1. 3 Nyquist Plot of EIS Test for Each Inhibitor in NaCl Solution

The x-axis represents the real component of impedance, denoted as Z' $(\Omega \cdot cm^2)$, while the y-axis represents the imaginary component of impedance, denoted as Z'' $(\Omega \cdot cm^2)$. The curves on this plot correspond to different corrosion inhibitors, with each semicircle representing a specific sample and inhibitor. In Nyquist plots, the size of the semicircles reflects the polarization resistance (Rp) of the system. Larger semicircles indicate higher polarization resistance, which is directly related to improved corrosion resistance. The more extensive the semicircle, the more effective the inhibitor is at reducing corrosion by hindering the electrochemical processes at the metal surface.

Sample	Rs (solution resistance) (Ω cm ²)	RP (Polarization resistance) (Ω cm ²)	CPE (constant phase element) (F/s)	CPE exponent (n)	Inhibition efficiency (%)
Control	4.964	1047	4.3 *10-4	0.79745	
Pectin	5.089	1072	1.96 * 10 ⁻⁴	0.7609	2.3%
Chitosan	2.825	1524.6	6.37 * 10 ⁻⁵	0.90009	31.3 %
Xanthan gum	1.7	3013	2.1 * 10 ⁻⁴	0.865	65.3 %
Gelatin	3.108	1260.1	3.5 * 10-4	0.782	16.7%
Cooking oil	1.633	3047.3	1.6 * 10-4	0.806	65.6 %
Waste cooking oil	9.7	8381.6	1.33 * 10 ⁻⁸		87.5 %

Table 1.7 EIS Results for Each corrosion inhibitor in 3.5% NaCl and Corrosion Inhibition Efficiency of Inhibitors

Table 1.7 presents the EIS results for each medium and the corrosion inhibition efficiency of the inhibitors. The electrochemical impedance spectroscopy (EIS) data in NaCl media highlight significant variations in corrosion inhibition efficiency, with polarization resistance (Rp) serving as a key indicator of inhibitor performance. Waste cooking oil demonstrated the highest polarization resistance (Rp = 8381.6 $\Omega \cdot cm^2$) and the greatest inhibition efficiency (87.5%), showcasing its exceptional ability to reduce corrosion. Cooking oil also performed well, with Rp = 3047.3 $\Omega \cdot cm^2$ and an inhibition efficiency of 65.6%. Xanthan gum exhibited similar effectiveness, achieving Rp = 3013 $\Omega \cdot cm^2$ and an inhibition efficiency of 65.3%. Chitosan showed moderate performance, with Rp = 1524.6 $\Omega \cdot cm^2$ and an inhibition efficiency of 31.3%. Gelatin and pectin displayed relatively lower performance, with Rp = 1260 $\Omega \cdot cm^2$ and 16.7% inhibition efficiency for gelatin, and Rp = 1072 $\Omega \cdot cm^2$ and 2.3% for pectin. The control sample, without any inhibitor, recorded the lowest polarization resistance, indicating the highest level of corrosion.

1.5.1.3.2 Nyquist Plot (HCL Medium)

The electrochemical tests were performed in HCL media with the same parameters and incorporating the same equivalent circuit. The A36 Carbon steel was dipped in 1M HCl solution, with the following samples produced.

- Medium 1 (Control): 1M HCL solution (control sample)
- Medium 2 1M HCL with 2g per liter pectin
- Medium 3: 1M HCL with 2g per liter chitosan
- Medium 4: 1M HCL with 2g per liter Xanthan gum

- Medium 5: 1M HCL with 2g per liter Gelatin
- Medium 6: 1M HCL with waste cooking oil Dip
- **Medium 7:** 1M HCL with vegetable oil Dip



Figure 1.4 Nyquist Plot of EIS Test for Each Inhibitor in 1M HCl Solution

The x-axis represents the real component of impedance, denoted as Z' $(\Omega \cdot cm^2)$, which provides information about the resistance to the flow of current in the system. The y-axis represents the imaginary component of impedance, denoted as Z'' $(\Omega \cdot cm^2)$, which reflects the reactive or capacitive behavior of the system. The Nyquist plot, which presents these components, is a useful tool for analyzing the electrochemical characteristics of the inhibitors, with the diameter of the semicircles correlating to the polarization resistance (Rp), an indicator of the inhibitor's effectiveness in mitigating corrosion.

The electrochemical impedance spectroscopy (EIS) results in HCl media reveal varying levels of corrosion inhibition performance among the tested inhibitors, as indicated by the polarization resistance (Rp) and inhibition efficiency. As shown in Figure 1.5 and Table 1.8, pectin emerged as the most effective inhibitor, exhibiting the highest Rp of 3003.6 $\Omega \cdot \text{cm}^2$ and an inhibition efficiency of 65.18%. Waste cooking oil followed closely, with an Rp of 2889.3 $\Omega \cdot \text{cm}^2$ and an inhibition efficiency of 63.8%. Gelatin showed moderate performance, achieving Rp of 1332.4 $\Omega \cdot \text{cm}^2$ and 21.5% inhibition efficiency. Chitosan and xanthan gum demonstrated lower effectiveness, with Rp of 1100.6 $\Omega \cdot \text{cm}^2$ and 4.96% inhibition efficiency for chitosan, and Rp of 936.12 $\Omega \cdot \text{cm}^2$ and a negative inhibition efficiency of -11.4% for xanthan gum. Surprisingly, cooking oil exhibited poor performance, with Rp of 466.6 $\Omega \cdot \text{cm}^2$ and a significantly negative inhibition efficiency of -124%. The control sample, without any inhibitor, recorded Rp of 1046 $\Omega \cdot \text{cm}^2$, providing a baseline for comparison. These results highlight pectin and waste cooking oil as the most promising inhibitors in this study for corrosion protection in HCl media.

Sample	Rs (solution resistance) (Ω cm ²)	RP (Polarization resistance) (Ω cm ²)	CPE (constant phase element) (F/s)	n	Inhibition efficiency (%)
Control	2.1	1046	9.9 *10-5	0.87	
Pectin	0.747	3003.6	5.03 *10-5	0.906	65.18
Chitosan	1.024	1100.6	6.82 *10-5	0.876	4.96
Xanthan gum	1.19	936.12	5.29 *10-5	0.876	-11.4
Gelatin	0.463	1332.4	4.13 *10-5	0.893	21.5
Cooking oil	2.83	466.6	6.57 *10-5	0.84	-124
Waste cooking oil	21.5	2889.3	1.43 *10-5	0.86	63.8

Table 1.8 EIS Results and Anti-Corrosion Efficiency of Inhibitors in 1M HCl Solution

1.5.2 Tafel Polarization

1.5.2.1 Equipment Setup and Preparation

For the Tafel polarization test, a controlled electrochemical setup was utilized, typically comprising a potentiostat, a three-electrode cell, and software for data acquisition and analysis. The three-electrode system consisted of a working electrode (the metal under test), a reference electrode, and a counter electrode.

1.5.2.2 Stabilization of Open Circuit Potential (OCP)

The metal sample was immersed in the test solution, and the system was allowed to equilibrate to the open circuit potential (OCP). This step was crucial as it established a stable baseline condition, for the electrochemical system. The OCP is the potential where the net current at the electrode surface is zero, indicating that the rates of the anodic and cathodic reactions have reached equilibrium.

1.5.2.3 Test Parameter Configuration

The configuration of the test parameters was performed through the software interface of the potentiostat. Key parameters entered included:

- **Initial Potential (Einitial)**: Set 10 mV negative relative to the OCP. This was the starting point for the potential sweep.
- **Final Potential (Efinal)**: Set 10 mV positive relative to the OCP. This defined the endpoint of the potential sweep.
- Scan Rate: Determined to be approximately 0.125 mV/s. The scan rate was crucial for ensuring that the system did not deviate significantly from equilibrium during the test.

1.5.2.4 Execution of the Potentiodynamic Polarization Tests

Once the parameters were set, the potentiodynamic polarization test was initiated. The software controlled the potentiostat to apply a linear sweep of potential from the initial to the final set values. During this sweep:

- The potential was incrementally increased from Einitial to Efinal.
- The current response of the system was continuously measured as the potential was varied.

1.5.2.5 Data Acquisition and Plotting

The current and potential data collected during the tests were automatically recorded by the software. This data was used to generate the Tafel plot, which graphed the potential (E) on the Y- axis versus the logarithm of the current density (log I) on the X-axis. The Tafel plot was essential for analyzing the electrochemical behavior of the metal under the test conditions

1.5.2.6 Identification of Linear Regions and Extrapolation

The Tafel plot typically exhibited linear regions corresponding to the anodic and cathodic branches. These regions were critical for the analysis as they reflected the kinetics of the oxidation and reduction reactions. Using the software:

- The linear portions of the anodic and cathodic curves were identified.
- These linear regions were extrapolated back to their intersection at the corrosion potential (Ecorr).

1.5.2.7 Calculation of Corrosion Current Density (icorr)

The intersection points of the extrapolated anodic and cathodic lines provided the corrosion current density (icorr), which is a critical parameter directly related to the corrosion rate of the metal. Using specialized software, icorr was converted into the corrosion rate by applying predefined constants and material properties, such as the metal's equivalent weight (EW) and density. Subsequently, the corrosion rate (CR) of the corrosion inhibitor were calculated using the following formulas:

$$CR = \frac{I_{corrK EW}}{\rho A} \tag{1.1}$$

1.5.2.8 Results:1.5.2.8.1 Tafel Polarization Tests in 3.5% NaCl Medium

- Medium 1 (Control): 3.5% NaCl solution (control sample)
- Medium 2 : 3.5% NaCl with 2g per litre pf pectin
- Medium 3: 3.5% NaCl with 2g per litre chitosan
- Medium 4: 3.5% NaCl with 2g per litre Xanthan gum
- Medium 5: 3.5% NaCl with 2g per litre Gelatin
- Medium 6: 3.5% NaCl with waste cooking oil Dip
- Medium 7: 3.5% NaCl with vegetable oil Dip





Table 1.9 Tafel Polarization Results and Anti-Corrosion Efficiency of Various Green Inhibitors

 in 3.5% NaCl Solution

Sample	Ecorr (mV)	Icorr (μA/cm²)	CR (mmpy)	Inhibition efficiency (%)
Control	-683.5	22.6	0.261	
Pectin	-616.7	14.2	0.164	37.2
Chitosan	-499.5	19.6	0.2266	37.2
Xanthan gum	-701.1	8.22	0.951	63.6
Gelatin	-653.8	9.84	0.1138	13.3
Cooking oil	-670.1	5.584	0.06457	75.3
Waste cooking oil	-452.5	2.94	0.034	87.0

The corrosion testing results highlight significant variations in inhibition efficiencies based on the corrosion current density (I_{corr}), where a lower Icorr value correlates with better corrosion protection. As shown in Figure 1.6 and Table 1.9, waste cooking oil emerged as the most effective inhibitor, demonstrating the highest inhibition efficiency of 87.0%, with the lowest Icorr of 2.94 μ A/cm² and a corrosion rate (CR) of 0.034 mm/y. This positions it as the top-performing inhibitor. Cooking oil followed closely with an inhibition efficiency of 75.3% and an I_{corr} of 5.584 μ A/cm², showing strong corrosion mitigation. Xanthan gum showed a moderate inhibition efficiency of 63.6%, while pectin and chitosan achieved more modest efficiencies of 37.2%. Gelatin exhibited the least effective performance, with an inhibition efficiency of just 13.3%. The control sample, without any inhibitor, exhibited the highest I_{corr} of 22.6 μ A/cm², underscoring the notable corrosion protection provided by the inhibitors, especially waste cooking oil and cooking oil.

1.5.2.8.2 Tafel Polarization Tests in 1M HCl Medium

- Medium 1 (Control): 1M HCl solution (control sample)
- Medium 2: 1M HCl with 2g per litre pectin
- Medium 3: 1M HCl with 2g per litre chitosan
- Medium 4: 1M HCl with 2g per litre Xanthan gum
- Medium 5: 1M HCl with 2g per litre Gelatin
- Medium 6: 1M HCl with waste cooking oil Dip
- Medium 7: 1M HCl with vegetable oil Dip



Figure 1.6 Tafel Plots of Various Inhibitors Displaying Anodic and Cathodic Currents in 1M HCl Solution.

Sample	E _{corr} (mV)	Icorr (µA/cm²)	CR (mmpy)	Inhibition efficiency (%)
Control	-453.05	18.94	0.219	
Pectin	-480.6	7.4	0.0856	60.93
Chitosan	-480.3	17.3	0.20005	8.66
Xanthan gum	470.5	21.32	0.2465	12.57
Gelatin	-493.6	15.1	0.17746	20.3
Cooking oil	-474.0	25.5	0.2949	-34.6
Waste cooking oil	-417.3	9.2	0.1064	51.42

Table 1.10 Tafel Polarization Results and Anti-Corrosion Efficiency of Various Green Inhibitors

 in 1M HCl Solution.

The Tafel polarization results in HCl media indicate varying levels of corrosion inhibition efficiency among the tested inhibitors, with corrosion current density (I_{corr}) serving as the primary indicator of performance. As shown in Figure 1.7 and Table 1.10, pectin emerged as the most effective inhibitor, achieving the highest inhibition efficiency of 60.93%, with a significantly reduced Icorr of 7.4 μ A/cm² and a corrosion rate (CR) of 0.0856 mm/y. Waste cooking oil also showed strong performance, with an inhibition efficiency of 51.42%, an Icorr of 9.2 μ A/cm², and a CR of 0.1064 mm/y. Gelatin exhibited moderate corrosion inhibition, with an efficiency of 20.3% and an Icorr of 15.1 μ A/cm². Chitosan and xanthan gum demonstrated relatively low inhibition efficiencies of 8.66% and 12.57%, respectively, with higher Icorr values indicating weaker corrosion protection. Surprisingly, cooking oil performed poorly, exhibiting a negative inhibition efficiency of -34.6% and the highest Icorr of 25.5 μ A/cm², indicating a tendency to exacerbate corrosion. These results underscore pectin and waste cooking oil as the most promising inhibitors for mitigating corrosion in HCl media.

1.6 Natural Product-based Biocorrosion Inhibitor Screening (GTI's Efforts)

In another experiment, we exploited several natural products and enzymes to identify candidate inhibitors with the potential to coat the surface of gas-transporting pipelines and to inhibit general corrosion. The substances were obtained from commercial sources or produced in the laboratory. Screening and preliminary corrosion inhibitory activities were tested using 1 M HCl solution in the presence of carbon-steel beads. The beads are C1018-based carbon steel materials, having the same composition as the C1018 carbon steel coupons routinely used for corrosion monitoring in oil and gas industries. They have high surface area to volume ratio of exposure to corrosive environments than the coupons and are ideal for screening of large number of inhibitors in a small volume. This reduces both the cost and the time spent in using coupons for screening large number of inhibitors. Once the screening is done, we will use the coupons to test the best candidate. The use of HCL as an aggressive corrosive chemical was selected with the assumption that the inhibitors performing well in this condition will likely be the best candidate inhibitors for gas-transporting pipeline conditions.

1.6.1 Identification of Green Corrosion Inhibitors

1.6.1.1 Products from Commercial Sources

A total of 15 natural products were obtained from commercial sources. The products were selected based on the presence of bioactive molecules such as amines, alkaloids, flavonoids, tannins, saponins, or essential oils and also based on their availability for mass production. The lists of these compounds are shown in Table 1.11

Table 1.11 Commercially obtained natural products as candidate green corrosion inhibitors.

Active compounds	Source
α-Amylase from Bacillus sp.	Sigma Aldrich
Protease from bovine pancreas	Sigma Aldrich
Lipase from wheat germ	Sigma Aldrich
Pectin	Sigma Aldrich
L-(+)-Arabinose	Sigma Aldrich
Epoxide hydrolase from Rhodococcus rhodochrous	Sigma Aldrich
Pectinase from Aspergillus	Sigma Aldrich
Surfactin	Sigma Aldrich
Acylase I from porcine kidney	Sigma Aldrich
Gramicidin from Bacillus aneurinolyticus	Sigma Aldrich
Resveratrol	Fisher Scientific
Pterostilbene	Fisher Scientific
Putrescine	Fisher Scientific
Spermine tetrahydrochloride	Fisher Scientific
Tyramine	Fisher Scientific

1.6.1.2 Laboratory-produced Products

Feedstock for laboratory-produced products were selected based on literature indicating the presence of diverse groups of known and unknown functional groups or bioactive molecules used for various purposes, as shown in Figure 1.8. The selected feedstocks include plant leaves (*Moringa oleifera* and *Eucalyptus* sp.), a blend of food waste, microalgae culture (*Chlorella* sp.), fungi cultures (*Phanerochaete chrysosporium and Penicillium chrysogenum*), and bacterial culture (*Pseudomonas putida*) extract.





1.6.2 Preparation and Extraction of Natural Products/enzymes

Moringa powder and Eucalyptus leaves were obtained from commercial sources and used as feedstocks. Eucalyptus feedstock was prepared by grinding/shredding fresh leaves to increase the surface area for extraction efficiency. Microalgae, fungi, and bacterial extracts were obtained from a crude lysate of cultures or supernatants that were grown in specific growth media. The fungi and bacterial cultures were grown in potato dextrose and Luria-Bertani (LB) broth, respectively, while the microalgae culture was grown in algae media (Bristol media) amended with carbon dioxide. After a specific growth period (three days for fungi, two days for bacteria, and one week for microalgae), the cultures were harvested by centrifugation at 8,000 rpm for 10 minutes, washed twice with phosphate buffer solution (pH 7.4), and lysed using ultrasonication. Unbroken cells were removed by centrifugation at 10,000 rpm for 40 minutes and cell-free lysates were used for corrosion inhibitor testing. For bacteria culture, the cell-free supernatant and the crude lysate (crude enzyme) were used for corrosion testing. The bioactive compound extraction procedure from the culture supernatant is indicated below. Food waste samples were artificially created using blends of processed and unprocessed foods collected from groceries in the western suburbs of Chicago. The samples included meat (cooked fish, cooked and uncooked chicken, and uncooked bacon), cooked and uncooked vegetables/tubers (broccoli, cauliflower, cabbage, cucumber, carrot, lettuce, spinach, tomato, potatoes, onion, and peppers), bread, cooked rice, potato chips, beans, fruits (orange, banana, watermelon, and avocado), and fast-food wrapping papers. The samples were chopped and blended using a blender to create a slurry of food.

The active compounds were extracted from the processed feedstocks using aqueous or solvent extraction methods. As shown in Figure 1.9, The aqueous soluble fractions were extracted by mixing 20 grams of the samples in deionized water at the ratio of 1:5 (w/v) and stirring for 4 hours at room temperature. The soluble fractions were separated from solids by filtration and directly used for corrosion inhibitor testing. For solvent extraction, the procedures were mainly focused on acid-base manipulation to extract compounds, such as alkaloids or amines, which are the major functional groups involved in corrosion inhibition. The ground feedstocks (20 gram) were resuspended in 2% hydrochloric acid solution at the ratio of 1:5 (w/v). This protonates the amine-containing compounds, which are water-soluble in acidic conditions. The solution was stirred for 4 hours at room temperature and filtered using filter paper to remove the solid residues. The clarified solution was made basic by raising the pH to 9-11 using NaOH to recover the compounds in their free base form. The basified mixture was then transferred to a separatory funnel, and diethyl ether was added to recover the organic solvent-soluble fractions. Diethyl ether was then evaporated, and the resulting solid was used for corrosion inhibitor testing after resuspending in water.



Food waste-acid food waste-water Moringa-water Moringa-acid Eucalyptus-acid Eucalyptus-water

Figure 1.9 Images showing acid-soluble and aqueous soluble feedstock solutions before (top images) and after (bottom images) filtration.

1.6.3 Corrosion Inhibitor Testing (GTI's Efforts)

To evaluate the corrosion inhibitory activities of candidate inhibitors, carbon steel (C1018) ball bearings (Grainger, hardness C60 to C67, Grade 200) were used in microtiter plates. Because of their small size (55.0 \pm 0.3 mg, \emptyset = 0.238 \pm 0.001 cm, A =0.178 cm2) and increased surface area of exposure, these ball bearings were ideal for large-scale screening in small volume in microtiter plates [54, 55]. Beads were pretreated according to the National Association of Corrosion Engineers (NACE) protocol RP0775-2005, which involved sanding the beads using sandpaper by rolling them between two sheets of grit size 220 or 300 sandpaper for several minutes. The beads were then rinsed in isopropyl alcohol and left to dry overnight under air stream. Beads were sorted into pairs and weighed. Corrosion inhibitory activities were performed in 24well plates containing 2 mL of 1 M HCl solution in deionized water and 1,000 ppm of the inhibitors. Bead pairs (110 mg) without the inhibitors were used as controls. Triplicate wells containing two beads per well were used for each sample. The microtiter plate wells were sealed with microtiter sealing films, covered with lids, and incubated under anaerobic conditions in a Coy anaerobic hood filled with 10% CO2 in Nitrogen. The plates were incubated at 30°C for 12 days. At the end of the incubation period, the bead pairs were removed from the microtiter plates and cleaned by sonicating in a 15% HCl solution containing 5 g/L of corrosion inhibitor 1,3-di-n-butyl-2 thiourea (DBT) for 2 minutes, sonicating in 1 M NaHCO3 for 2 minutes, submerging in deionized water, and sonicating in isopropyl alcohol for 2 minutes. The bead pairs were allowed to dry under an air stream and weighed to obtain final weights.

1.6.4 Microscopic Imaging

Carbon steel beads that showed the highest and lowest weigh loss corrosion were selected for microscopic imaging. The cleaned beads were imaged using the Hitachi S-3500N Scanning Electron Microscope (SEM) to visualize their morphological differences. The beads were held inside the SEM vacuum chamber using double-sided tape attached to the holder. The images were captured at a magnification of 35X

1.6.5 Results and Discussions

1.6.5.1 Corrosion Inhibitor Screening

Bead weight loss of more than 40% was observed for most of the inhibitors in the presence of 1M HCl. HCl is an aggressive corrosive chemical, and any inhibitor that shows resistance to this chemical will be considered the best candidate inhibitor for real pipeline conditions. The average weight changes in the bead pairs after 12 days of incubation ranged from a weight loss of 34-66 mg (Figure 1.10). The highest weight loss (66 mg) was observed in the presence of resveratrol. Resveratrol is a natural phenol or polyphenol and a phytoalexin (stilbenoid or allelochemical) produced by several plants (grapes, blueberries, raspberries, mulberries, and peanuts) in response to injury or when the plant is under attack by pathogens, such as bacteria or fungi. It has been considered a nutraceutical chemical with several therapeutic effects [56, 57]. The reason for the loss of corrosion inhibitory activity of this substance is likely due to the absence of an amine functional group on the compound. An amine or amino (–NH₂) group of compounds serves as a site for interaction with the metallic surface and behaves as a water-repellent to the inhibit corrosion through coordination of bonding [58]. The lowest weight loss was observed in the presence of Moringa leaves organic extract (34 mg) followed by putrescine (40 mg). Moringa extract contains several bioactive compounds, and several reports indicate the corrosion inhibitory activity of the extracts with varying efficiencies [59-61]. Putrescine is the most common polyamine present in almost all organisms, including plant tissues, and it plays a major role in biotic and abiotic stress responses [62, 63]. Although putrescine has two amine functional groups, its role as a corrosion inhibitor is not known. The present study highlighted the importance of putrescine as a candidate green corrosion inhibitor.



Figure 1.10 Changes in weight of bead pairs in 1M HCl solution in the presence of natural products. Each bead pair was weighed after the cleaning process, and the average weight change was graphed.

1.6.5.2 SEM Images of Beads

Beads that showed higher and lower weight losses were selected for SEM imaging and compared with the control, to which the inhibitors were not added. Imaging of the beads indicated aggressive corrosion induced by the HCl solution (Figure 1.11) confirming the weight loss data. Severe morphological impacts were observed in beads without an inhibitor (control) and in the presence of resveratrol. The impacts were visible from distortion of the moon-like structure of beads in the presence of effective inhibitors or unexposed beads. In agreement with the weight loss corrosion data, the presence of some of the inhibitors minimized the corrosive impact of the HCl solution. Inhibitors that minimized these impacts include food waste organic extract, *P. putida* organic extract, Moringa organic extract, putrescine, and protease. The corrosion inhibitory activities observed with these natural products under such an aggressive condition suggested that

they are likely the best candidates for inhibition under fluid and gas conditions observed in gastransporting pipelines. Future research will focus on using different concentration gradients of the selected products at lower concentrations (less than 1,000 ppm) and determining their inhibitory activities in HCl solution. The best candidates for this will be putrescine and Moringa organic extracts, as these showed the lowest weight loss corrosion. The lowest concentrations that showed inhibitory activities will be determined and used for coupon-weight loss and electrochemical testing in brine solution that mimic the natural gas fluid constituents.



Figure 1.11 Morphological changes of beads in 1M HCl in the presence or absence of candidate green corrosion inhibitors after 12 days of incubation.

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<u>Task 2. Simulation-based Inhibitor Implementation Optimization in Gas</u> <u>Gathering and Transportation Pipelines</u>

1. Introduction

1.1 Background

Current operational gas pipelines inevitably suffer damage from accumulation of liquid containing corrosive substances like CO_2 and H_2S at lower places. Besides, another type of pipe corrosion called top of the line corrosion (TLC), which is generally caused by condensation of corrosive vapor on the top pipe wall [64]. This introduces the necessity of protection for the gas pipeline.

During the first quarter, we developed a simulation framework for optimizing green corrosion inhibitors in gas pipelines. A review of CFD methods guided initial model creation, focusing on straight pipeline geometries and key parameters like inhibitor concentration and shear stress. Early simulations provided insights into inhibitor distribution and identified potential corrosion-prone areas.

In the second quarter, significant advancements were made in simulating green corrosion inhibitors for gas pipelines. A Fourier Neural Operator (FNO) model was developed to predict wall shear stress (WSS) based on pipeline roughness, providing key insights into the degradation mechanisms of inhibitor films. Multi-fidelity data integration using a Convolutional Neural Network (CNN) was also explored, enabling accurate predictions of fluid dynamics parameters with reduced computational demands. These efforts laid a strong foundation for optimizing inhibitor application and improving pipeline protection.

In the third quarter, we further developed the FNO-based surrogate model for predicting Wall Shear Stress (WSS) by improving its adaptability to unseen roughness shapes. Uncertainty quantification, incorporating both aleatoric and epistemic uncertainties, was introduced to enhance prediction reliability. Additionally, a multi-fidelity approach was implemented, integrating low-fidelity (2D) and high-fidelity (3D) data to achieve accurate predictions with reduced computational costs. Progress was also made in establishing an inhibitor degradation model, linking WSS and time to inhibitor performance, providing insights into flow-induced degradation mechanisms.

In the fourth quarter, the focus was on refining latent space models for efficient temporal flow field predictions, leveraging an autoencoder and FNO for improved accuracy and computational efficiency in flow regime prediction. The multi-fidelity approach was further developed, combining low-fidelity (2D) and high-fidelity (3D) simulations to enhance predictive accuracy while reducing computational costs. These advancements provided critical insights into

the performance and degradation of green inhibitors under dynamic pipeline conditions, contributing to the project's goal of sustainable corrosion prevention.

The above research aims to establish a predictive model applicable to pipeline flow fields considering inhibitor degradation based on the experimental results of corrosion inhibition performance (Task 1). For the practical usage of corrosion inhibitors, another more important point is their application approach.

Currently, the batch application is widely used for inhibitor coating, as shown in Figure 2.1. This process leverages specially designed devices known as pipeline pigs to navigate the pipeline that excels in expunging liquids and solids from the pipeline while concurrently accelerating the concentration of inhibitors to promptly address any sudden increases in corrosive activity. Despite these advantages, this method may prove incompatible with pipelines that possess complex geometrical configurations or operate under certain environmental constraints.



Figure 2.1: Illustration of batch application for coating of inhibitor film.

Another method called 'continuous application' has the potential to be used to compensate for the above shortcomings. Through a portable chemical injection system, it ensures a steady and uninterrupted supply of corrosion inhibitors [65]. This strategy sustains a continuous presence and consistent concentration of the inhibitor, making it the ideal choice when constant protection is required in stable conditions. However, the continuous injection may lead to significant financial commitments owing to the costs associated with system setup and ongoing maintenance. Thus, alternating both methods may provide a balance and optimized outcomes. At this point, some critical issues appear, such as how to evaluate the efficacy of continuous injection application, how to optimize the functionality of inhibitor for different applications and how to optimize the frequency and dose to assure the protection reliability.

In this study, we utilized computational fluid dynamics (CFD) simulations to explore the optimization of inhibitor injection schemes, aiming to enhance the efficiency of corrosion inhibitor usage. As an initial framework for investigating inhibitor distribution after injection, a simplified 2D straight gas pipeline model with a length of 6 meters was simulated in ANSYS Fluent using the discrete phase model (DPM). This model tracked the behavior of inhibitor particles within the pipeline. The simulation employed a flat-fan atomizer to generate a spray of inhibitors, represented as a continuous stream of particles with varying diameters. The accretion of particles on the lower wall (measured in kg/m) served as an indicator of inhibitor deposition at specific locations. Adjustments to parameters such as the injection flow rate and the inlet velocity of the continuous phase were evaluated for their impact on deposition efficiency.

It is essential to acknowledge that the current simulation significantly diverges from realworld scenarios mainly in two aspects. On one hand, long-distance transportation should be considered in actual inhibitor injections, whereas the simulated pipeline in this study is only 6 meters long. On the other hand, while both the upper and lower walls of pipelines are susceptible to corrosion, the current simulation only considers the lower wall. These simplifications were deliberately introduced to focus on developing a basic methodology and clarifying the workflow so that future work can conveniently expand the scope to include more realistic conditions, ensuring closer alignment with practical applications.

Although CFD provides the reference for practical applications, it is nothing less than hard work to simulate every segment in a pipeline. In such cases, machine learning (ML) provides an ideal solution, as it can leverage historical data and simulation results to predict inhibitor usage patterns without the need to simulate every segment of the pipeline explicitly. By training surrogate models on existing data, ML can significantly reduce computational overhead while maintaining accuracy and efficiency in optimization. In the completed study, several types of Bayesian neural network (BNN) models are compared in prediction performance with uncertainty quantification, where the distribution of wall accretion was set as the prediction target.

1.2 Objectives

The main objective of this research is to construct an AI-enhanced simulation framework for optimizing the utilization of corrosion inhibitors in the pipeline, applying the continuous application. While the optimal strategy in practice would involve a combination of batch and continuous applications, the current research focuses on continuous application due to its higher associated uncertainties. The continuous application introduces complexities in predicting the wall accretion of inhibitor particles, necessitating CFD simulation and AI-enhanced modeling to forecast inhibitor behavior and optimize injection parameters accurately. The batch application has existing guidelines and experiences, and we will use them in the future optimization framework.

A key aim is to accurately simulate inhibitor injection in CFD using DPM, providing reliable initial observation of conditions of the continuous application.

The research also seeks to build a surrogate model in predicting wall accretion of inhibitor particles, which is considered as the index of injection performance. A well-trained surrogate model can significantly reduce computational overhead while maintaining accuracy and efficiency in optimization.

By achieving these objectives, the simulation project aspired not only to contribute to improving the longevity and safety of pipelines but also to demonstrate a scalable and efficient model for conducting simulations that traditionally require significant computational efforts from engineering design and analysis to research and development in fluid mechanics.

2. Methodology

2.1 CFD simulation for continuous application

2.1.1 Simulation setup

To develop a basic framework and clarify the workflow of studying continuous applications in the pipeline, a 6m-length 2-D pipe with a diameter of 0.5m is simulated in ANSYS Fluent, as shown in Figure 2.2. With the utilization of DPM, detailed settings are described below:

- Meshing Properties:
 - *General size:* The general size of grids affects the accuracy of the flow field in the upper area. In the currently considered low-speed steady flow, the flow solution can still converge even when the general size is in a relatively large value (up to 20 mm).
 - *Inflation layer:* Grid inflation is beneficial to improve the gradient computation of near-wall flow regime. For the studied case without large gradient changes, two inflation layers are enough to optimize the quality of meshing.
- Phase Properties:
 - *Continuous phase:* Methane gas is considered as the only continuous phase with the density of 0.656 kg/m³ and the viscosity of 0.01 mPa·s (25° C).
 - *Discrete phase:* Inhibitor injection is simulated by the flat-fan atomizer in DPM. Inhibitors are regarded as inertia oil-like particles with the density of 770 kg/m³ and the viscosity of 50 mPa·s (25° C).
- Solution Properties:
 - \circ *Viscous model:* The viscous model is related to the exchange of momentum, energy, and concentration among fluid media, which influence flow dynamics and computational WSS results. The k- ω model is used to simulate flow viscous.
 - *Discrete phase model:* DPM provides calculation of particle injection and interaction with the continuous phase. The involved erosion model is opened to record particle properties on the pipe wall.
 - *Particle injection:* In DPM, the flat-fan atomizer is used to simulate particle injection in this case. Figure 2.3 gives the illustration of this type of atomizer with the parameters of virtual origin, center origin, orifice width and dispersion angle. Here, the orifice width controls the particle diameter within a certain range in each injection.
 - *Boundary condition:* This term usually contains a velocity inlet and a pressure outlet for better control of the initial flow rate, so does this study. The upper and lower boundaries are set to "wall film" for DPM calculation, which are suitable to describe

the behavior of liquid films that form when particles, droplets, or liquid streams interact with solid surfaces.

• *Solution method*: The "Coupled" method is applied that solves momentum and continuity equations in a tightly coupled manner. This can accelerate the convergence of the solution significantly.



Figure 2.3: Illustration of the flat-fan atomizer in Fluent.

2.1.2 Data generation

The optimization of corrosion inhibitor injection is mainly achieved by adjusting case parameters, such as the settings of atomizers, fluid properties, and pipeline geometry mentioned. To determine the impact of each considered parameter under various pipe cases based on limited CFD simulations, the idea of neural networks is adopted to leverage historical data and simulation results to predict inhibitor usage patterns without the need to simulate every segment of the pipeline explicitly. In the current study, only the orifice width for the inhibitor injection, flow rate of the atomizer, and inlet velocity of the continuous phase are selected in different values as the network input for simplification, which also shows more complex effects on wall accretion that is set as the network output as well as the prediction target.

The training dataset is constructed by sampling the three input parameters, each defined within a specified range, with values taken as an arithmetic sequence. The ranges of the three parameters, including their upper and lower bounds and the common difference, are detailed in Table 2.1. Each parameter has 11 evenly spaced values, resulting in $11 \times 11 \times 11 = 1331$ total combinations for the training samples. In each sample, particle accretion of the lower bound of the pipe segment from x=1.2m to x=4m is extracted as output, including 160 grid points for each sample, as illustrated in Figure 2.4. For the testing dataset, the input parameters are randomly sampled within the same ranges as the training dataset. A total of 200 test samples are generated to evaluate the model.





Tuble 2.1. Runges of the input parameters			
	Orifice width (m)	Flow rate (kg/s)	Inlet velocity (m/s)
Lower bound	1×10 ⁻⁷	1×10 ⁻³	5.0
Upper bound	2×10-7	1×10 ⁻³	0.5
Common difference	1×10 ⁻⁷	2×10 ⁻³	10.0

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Note: the flow rate characterizes the injection rate of particles, while the inlet velocity describes the continuous phase

In this case, each sample is output after 210 calculation time steps, which is representative in the status of accretion amount. This can be illustrated by Figure 2.5 that shows the comparison of accretion under different calculation time steps. It can be seen that the accretion basically conforms to proportional relationship as time steps increase by the same difference.



Figure 2.5: Comparison of accretion under different calculation time steps.

2.2 AI-enhanced inhibitor accretion prediction

2.2.1 Illustration of model training

The architecture of a neural network has a significant impact on its ability to predict particle accretion under varying pipeline conditions. In this study, three different neural network frameworks are investigated: fully connected neural networks (FCNNs), Deep Operator Networks (DeepONets), and Fourier Neural Operators (FNOs). As shown in Figure 2.6, these models differ

in their architectures and learning approaches, which can influence both their predictive accuracy and their ability to generalize to new conditions.



Figure 2.6: Illustration of different networks.

Besides, to more clearly estimate the reliability of predictions, Bayesian uncertainty quantification is incorporated into all three frameworks, focusing on aleatoric uncertainty (AU). This type of uncertainty accounts for inherent noise and measurement inaccuracies in the data. The loss function used to model AU is as follows:

$$Loss = \frac{1}{N} \sum_{i=1}^{N} \left[\frac{1}{2} \exp(-\sigma) \| y_i - \bar{x} \|^2 + \frac{1}{2} \sigma \right]$$
(2.1)

Where is the number of samples; y_i represents the ground truth values for the *i*-th sample; \bar{x} is the mean value of the predictions for the *i*-th sample and obtained from one branch of the network; σ is the standard deviation of the predictions, obtained from the second branch of the network. Figure 2.7 illustrates the generation of \bar{x} and σ in the FCNN as the example, where the two branches are denoted by "FCNN1" and "FCNN2" with the same framework but different sets of parameters. In the loss function of AU, the term $\frac{1}{2}\exp(-\sigma)||y_i - \bar{x}||^2$ scales the prediction error based on the uncertainty, allowing the model to focus less on noisy samples, while the regularization term $\frac{1}{2}\sigma$ prevents the model from overestimating uncertainty.



Figure 2.7: Illustration of generating the mean value and standard deviation for AU analysis.

2.2.2 Testing results and discussion

Figure 2.8 depicts the prediction uncertainty of the three networks in testing samples. Within the prediction range (x=1.2 to x=4.0), y values of the figure reflect the uncertainty of each grid point, which is characterized by standardized uncertainty, expressed as follow:

$$U = \frac{1}{N} \sum_{i=1}^{N} \frac{1.96\sigma_i}{\bar{x}}$$
(2.2)

Where N = 200 is the number of testing samples; based on 95% CI = $\bar{x} \pm 1.96\sigma$, $1.96\sigma/\bar{x}$ denotes the half-standardized uncertainty interval. From the figure we can see certain fluctuation as the x value changes. This conforms to the trend of uncertainty in certain samples, as shown in Figure 2.9 for example, in which the uncertainty region is of approximate width along the prediction range. The standardized uncertainty can be equal to the relative magnitude between the mean value and the standard deviation. Thus, standardized uncertainty is in the similar trend as mean values in each sample. Nevertheless, standardized uncertainty can clearly present the reliability of the model in predicting a set of testing samples. For example, the point (2.5, 0.14) in Figure 2.8 illustrates the maximum prediction error at x = 2.5m can be regarded as 14% deviating from the mean value.



Figure 2.8: Standard deviation of predicted accretion under different networks.



Figure 2.9: Prediction result of a sample using FCNN.

Besides, in view of prediction differences among the three networks, FCNN gives the smallest uncertainty. This is understandable. Although DeepONet and FNO show much more potential in many cases, predicting accretion amount in such a short distance may be too simple to use neural operators to map the relationship, while their introduced complexity would lead to larger uncertainty. In this case, the accretion of all samples approximates the blue curve shown in Figure 2.9 with noise-like fluctuation. In other words, FCNN is enough to capture the relationship between input and output. Nonetheless, for future studies involving long-distance transfer of inhibitor particles, the distribution of accretion may be more complicated, resulting in the inapplicability of FCNN.

3. Future research

The current study established a basic framework for predicting the distribution of inhibitors after injection using the surrogate model so that pipe technicians can make the inhibitor-protection scheme more efficiently, which can be the time-dependent reliability variation curves for pipe protection combining the knowledge of inhibitor degradation, as shown in Figure 2.10 for schematic illustration. We will search for literature data on inhibitor degradation properties and use synthetic data for methodology demonstration if no such data is available. Future additional testing is needed for experimental measurements and validation. At this point, two types of applications can be combined more effectively to promote better pipeline protection measures.



Figure 2.10: Time-dependent reliability variation.

The next step's work will be focus on studying the accretion model in long distance transfer based on a more complex pipeline, in which the size of injected particles can be adjusted by changing the flow rate and the orifice width. Figure 2.11 shows the particle distribution in the pipe when setting the orifice width to 2×10^{-8} , leading to smallest particles that are potential to transfer to longer distance. Besides, the effect of geometry changes such as bending angle and pipe diameter on particle accretion to build applicable inhibitor transfer model for various pipe segments.



Figure 2.11: Time-dependent reliability variation.

By adjusting injection parameters with the surrogate model, the work in the year 2025 will further propose the most cost-effective pipeline protection strategy to reduce corrosion risks and improve the uniformity of inhibitor distribution.

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