# CAAP Quarterly Report

**[12/28/2023]**

***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**: [09/2023 – 12/2023]*

## Project Activities for Reporting Period:

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

During this reporting period, we have made significant progress in Task 1, focusing on the design and synthesis of green inhibitors. The key activities are outlined below:

- 1.1: Quick Screening of Green Inhibitors for Gas Pipeline Protection
  - A comprehensive literature review was conducted to identify potential candidates of green inhibitors suitable for gas pipeline protection.
  - Engaged with the industry advisory board to gather insights on industry standards regarding the compatibility and safety of green inhibitors.
- 1.2: Synthesis and Characterization of Green Inhibitors from Renewable Feedstock
  - Explored various methods for converting renewable feedstock into green inhibitors tailored for gas pipeline protection.
  - Developed an experimental protocol for converting citrus peel into pectin, identified as a promising green inhibitor.
  - Successfully synthesized the initial pectin samples derived from orange peels.
- 1.3: Corrosion Testing for Verification and Validation
  - Conducted a thorough review of corrosion testing methods, with ongoing development of testing protocols.

Task 2. Simulation-based inhibitor optimization in Gas Gathering and Transportation Pipelines

The primary activity of this task is to develop an AI-augmented simulation framework for gas-water-inhibitor multi-phase flow, aiming to optimize the physical properties of corrosion inhibitors, such as viscosity and density, as well as their application parameters, including injection location, speed, volume, and gas pressure. This simulation tool will enable an in-depth analysis of the distribution and accumulation of inhibitors in gas pipelines under complex multiphase flow conditions. An AI-augmented computational fluid dynamics (CFD) framework is used to simulate this process, offering efficient analysis and optimization, fusing multiple fidelity models.

Subsequently, the framework will assess pipeline corrosion risk and inhibitors' effectiveness across diverse operational scenarios, incorporating intricate pipeline designs and environmental variables. The ultimate objective is to analyze these numerical results to identify the most effective parameters for inhibitor deployment, providing crucial insights for formulating robust and efficient corrosion control strategies.

**Project Financial Activities Incurred during the Reporting Period:**

For Task 1, we supported 1 RA at ASU

For Task 2, we supported 1 RA at ASU

**Project Activities with Cost Share Partners:**

PIs are working with their academic time cost shared by the university.

**Project Activities with External Partners:**

Regular discussions with the technical advisory panel and several individual meetings with advisory members.

**Potential Project Risks:**

Nothing to report.

**Future Project Work:**

For Task 1:

- 1.1: Quick Screening of Green Inhibitors for Gas Pipeline Protection
    - Finalize the candidates of renewable feedstock to be investigated in this project.
    - Summarize the industry standards regarding the compatibility and safety of green inhibitors.
- 1.2: Synthesis and Characterization of Green Inhibitors from Renewable Feedstock
    - Optimize the experimental protocol developed in Q1.
    - Determine the physical and chemical properties of orange pectin.
    - Explore the synthesis of chitosan-based inhibitors from shrimp shells.
- 1.3: Corrosion Testing for Verification and Validation
    - Develop testing protocols for the verification and validation of the synthesized green inhibitors.

For Tasks 2:

In the forthcoming quarter, our main emphasis will be centered on the advancement and integration of AI-enhanced Computational Fluid Dynamics (CFD) simulations. This focus aims to significantly enhance the precision and efficiency of our simulation processes. Alongside this, we will be dedicating substantial efforts towards optimizing the implementation of corrosion inhibitors. This dual approach is expected to yield a more comprehensive and nuanced understanding of multiphase flow dynamics in pipeline systems, and enable the development of more effective strategies for inhibitor deployment, thereby improving overall pipeline integrity and performance.

**Potential Impacts to Pipeline Safety:**

The proposed study will mitigate internal corrosion risk by developing environmentally friendly inhibitors and optimizing their performance.

# Appendix

# Task 1. Design and Synthesis of Green Inhibitors

**Background and Objectives in the Current Quarter**

**Background**:

Corrosion in pipelines poses a substantial challenge to the integrity and efficiency of transportation systems for fluids and gases. The search for environmentally sustainable and effective corrosion inhibitors has intensified in recent years, leading to the development of green inhibitors as a promising solution. Green inhibitors, derived from renewable sources, offer an eco-friendly alternative to conventional inhibitors, aligning with the global shift toward sustainable practices.

Traditionally, corrosion inhibitors have often been derived from petroleum-based compounds, raising concerns about environmental impact and resource depletion. In response to these challenges, researchers have turned their attention to green inhibitors sourced from renewable materials, such as agricultural by-products, plant extracts, and waste biomass.

The synthesis of green inhibitors involves a multi-faceted approach. Initially, a thorough literature review is conducted to identify suitable candidates with inhibitive properties. This involves exploring various organic compounds and extracts known for their corrosion-inhibiting capabilities. Additionally, engagement with industry advisory boards ensures alignment with industry standards and the compatibility of green inhibitors with existing pipeline materials and fluids.

The next crucial step in the synthesis process is the conversion of renewable feedstock into effective inhibitors. Methods for transforming natural resources, such as citrus peels, into inhibitors with corrosion-resistant properties are explored. Experimental protocols are developed to guide the synthesis process, ensuring reproducibility and scalability.

In the specific context of pipeline corrosion protection, the utilization of green inhibitors becomes paramount. These inhibitors not only exhibit corrosion inhibition properties but also contribute to sustainable practices by utilizing waste materials. One notable example involves the conversion of citrus peel into pectin, a substance identified for its corrosion-inhibiting potential.

As research progresses, emphasis is placed on the thorough characterization of synthesized inhibitors to understand their chemical composition and structural properties. This includes advanced analytical techniques to validate the inhibitive performance of green inhibitors under simulated corrosion conditions.

**Objective**: The primary objective of this quarter is to survey the literature to identify potential candidates for green inhibitors, to establish synthesis protocols for extracting active constituents from renewable feedstock (plant extracts, bio-based wastes, and microbial enzymes), and to establish testing methods for verification and validation. The other objective of this task is to consult with the industry advisory board on industry standards on the compatibility and safety of green inhibitors. During the project kickoff meeting, the program manager, Dr. Zhongquan Zhou mentioned the MRP reviewer panels' comments on our proposal and suggested we investigate this subject.

**Task 1.1**: Quick Screening of Green Inhibitors for Gas Pipeline Protection

- Conducted a comprehensive literature review to identify potential candidates of green inhibitors suitable for gas pipeline protection.

Conducting a comprehensive literature review was a key step in our project of developing green inhibitors tailored for gas pipeline protection. This extensive exploration involved investigating a vast body of existing research and scholarly works to identify potential candidates with inhibitive properties. The objective was to discern promising organic compounds and extracts known for their corrosion-resistant capabilities, with a particular focus on those derived from renewable sources. By synthesizing knowledge from diverse scientific publications, we aimed to gain insights into the latest advancements, challenges, and trends in the field of green inhibitors for corrosion protection.

The literature review not only facilitated the identification of potential inhibitor candidates but also provided a holistic understanding of the various mechanisms and factors influencing corrosion inhibition. This knowledge base proved instrumental in guiding subsequent research activities and refining our approach to the synthesis of green inhibitors. Furthermore, insights garnered from the literature review informed our decisions regarding the selection of inhibitor candidates that not only demonstrated robust inhibitive properties but also aligned with the principles of sustainability and environmental consciousness. As we move forward with our research, the outcomes of this comprehensive literature review serve as a crucial reference point for shaping the direction and focus of our investigation into innovative solutions for gas pipeline corrosion protection.

We aim to rapidly assess a diverse range of green inhibitors derived from plant extracts, characterized by a polar hydrophilic functional group and a non-polar hydrophobic tail. The hydrophilic functional groups encompass hydroxyl, carbonyl, carboxyl, amino, sulfhydryl, phosphate groups, among others, while the non-polar hydrophobic tail consists of alkyl chains of varying lengths. Additionally, we will explore the potential of microbial enzymes, such as Gramicidin, surfactin, and lactonase, as green inhibitors within this project. The expeditious screening process will leverage an electrochemical approach that integrates linear polarization resistance and electrochemical impedance spectroscopy.

By subjecting the metal surface to this electrochemical method, we anticipate observing changes such as increased polarization resistance or impedance, coupled with a reduction in corrosion current upon the application of the inhibitors. These alterations will serve as quantifiable metrics to rank the performance of various green inhibitor candidates swiftly. The most promising inhibitors identified through this initial screening will progress to a more detailed evaluation in subsequent tasks, namely **Tasks 1.2** and **1.3**, ensuring a focused investigation into their efficacy and potential for gas pipeline protection. This strategic screening methodology allows us to efficiently identify and prioritize top-performing green inhibitors for further scrutiny and development.

In **Task 1.1**, our investigation has highlighted the efficacy of organic compounds containing nitrogen, oxygen, and/or sulfur as formidable industrial corrosion inhibitors. These synthetic organic inhibitors exhibit the capability to create a protective layer between the metal surface and the corrosive environment, thereby slowing down the process of metal disintegration through an adsorption mechanism. However, a significant drawback lies in the often-exorbitant cost and toxic nature of these synthetic counterparts. The disposal of such industrial corrosion inhibitors further compounds environmental concerns, necessitating a shift toward more sustainable practices.

Recognizing the escalating demand for environmentally friendly alternatives, there is a growing inclination toward green-based inhibitors. These inhibitors, derived from sources like plant extracts and microbial enzymes, present a compelling solution. Their inherent non-toxic nature positions them as preferable options compared to their commercial counterparts. Notably, plant extracts and microbial enzymes are regarded as green and sustainable materials due to their natural and biological properties. These compounds demonstrate the ability to effectively inhibit the corrosion of metals and alloys. Among these, the leaves stand out as a particularly advantageous source, as they boast an abundance of phytochemicals—active components synthesized by the plant—mimicking the performance of commercial inhibitors. This shift toward green and sustainable materials reflects a conscientious effort to address both environmental and economic considerations in the realm of corrosion inhibition.

**Table 1**. Examples of bio-based corrosion inhibitors to be investigated in this project.

| Plant or Source | Active Constituent | Solvent & extraction method | Metal to Protect | Corrosive Environment | Corrosion Inhibition Efficiency (%) | Inhibitor Concentration |
|---|---|---|---|---|---|---|
| Citrus peel | Pectin | HCl and ethanol | Mild steel | 1M HCl | 94.2 at 45 °C | 2 g $L^{-1}$ |
| Shrimps shell waste | Chitosan | NaOH | Carbon steel | 1M HCl | 88.5 at 25 °C | $10^{-5}$ M |
| Plantago ovata | Polysaccharide (galaturonic acid) | Water | A1020 carbon steel | 1M HCl | 94.4 at 45 °C | 1 g $L^{-1}$ |
| Rhododendron schlippenbachii | Polyphenolic compounds | Methanol | Low carbon steel | 1M $H_2SO_4$ | 94.2 at 30 °C | 600 ppm |

Building on the screening results from **Task 1.1**, we propose the production of four bio-based corrosion inhibitors, as detailed in **Table 1**. The primary objective is to optimize polarization resistance and minimize corrosion current, aiming for robust protection of pipelines.

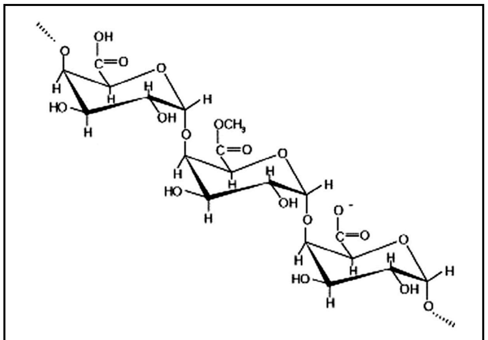

**Fig. 1**. Molecular structure of pectin

To extract pectin, we will employ a systematic process using fresh citrus peels obtained from citrus *unshiu marcovitch*, sourced from a local citrus producer in Mesa, Arizona. The first step involves vacuum freeze-drying the peels, followed by grinding them into a powder (50 mesh). Subsequently, a two-step pectin extraction method, utilizing diluted NaOH assisted by a combination of ultrasound and pressure, will be employed to process the dry citrus peel powder. The resultant natural pectic polysaccharides, primarily comprising homogalacturonan, rhamnogalacturonan I and II, and xylogalacturonan, possess a molecular structure illustrated in **Fig. 1**.

Key functional groups such as OH-, C=O, and C-O in pectin are pivotal in generating an attractive force for its adhesion to the metal surface. This mechanism effectively prevents reactive fluids from directly contacting the metal surface, thereby enhancing the inhibitor's capacity to safeguard against corrosion in pipeline systems. The careful extraction and utilization of pectin from citrus peels highlights our commitment to leveraging sustainable and effective green corrosion inhibitors for enhanced pipeline protection.

The synthesis of nitrogen-containing green inhibitors from biomass presents a highly desirable yet challenging endeavor. In our approach, we will craft these inhibitors using chitosan derived from shrimp shells, along with cinnamyl aldehyde, vanillic aldehyde, citral, and anisaldehyde. Chitosan, sourced from shrimp shells collected in local restaurants, serves as a widely distributed but recyclable green resource, albeit with a high production cost. Its distinct molecular structure positions chitosan derivatives as effective and environmentally friendly corrosion inhibitors for oil and gas pipelines. The molecular structures of the four inhibitors, depicted in **Fig. 2**, will be meticulously synthesized following established procedures.

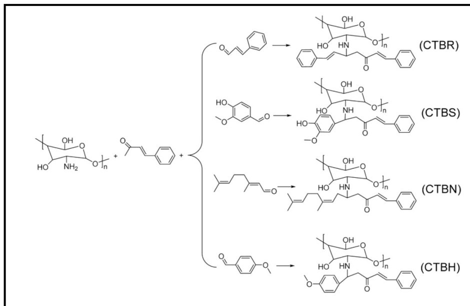


**Fig. 2**. Synthetic route to four inhibitors

Carbohydrate polymers, known for their chemical stability, biodegradability, and eco-friendliness, stand out as key macromolecules in corrosion inhibition. Derived from Plantago husk, these polymers offer an inexpensive, renewable, and abundantly available alternative. The hydroxyl group (OH) and heteroatom oxygen in polysaccharides facilitate their adsorption onto metal surfaces, contributing to corrosion prevention. The extraction process involves soaking Plantago husk in distilled water for 48 hours, followed by boiling to release mucilage. After filtration to remove insoluble husks, an equal volume of acetone is added to precipitate the polysaccharide, which is then dried, powdered, and stored.

For biodegradable green inhibitors derived from *Rhododendron schlippenbachii*, rich in phenolic compounds, a modification in the extraction process is proposed. The traditional methanol extraction method will be replaced with water as the solvent, and the leaf extracts will undergo purification before application to metal surfaces. Initial studies indicate a noteworthy 94.2% corrosion inhibition efficiency when applying 600 ppm of this green inhibitor to low-carbon steel specimens. This comprehensive approach underscores our commitment to exploring sustainable and effective green inhibitors, leveraging diverse biomass sources and extraction methods for enhanced corrosion protection.

- Engaged with the industry advisory board to gather insights on industry standards regarding the compatibility and safety of green inhibitors.

We have contacted Dow Chemicals and Baker Hughes regarding the industry standards regarding the compatibility and safety of green inhibitors and are waiting for their reply.

**Task 1.2**: Synthesis and Characterization of Green Inhibitors from Renewable Feedstock

- Explored various methods for converting renewable feedstock into green inhibitors tailored for gas pipeline protection.

The extraction of pectin from citrus peel involves a crucial and meticulous process to yield high-quality pectin with optimal properties. Various extraction methods have been employed, each with its advantages and considerations. Here is a comparison of common extraction methods used for obtaining pectin from citrus peel:

**Table 2**. Summary of Experimental Methods for Extracting Pectin from Citrus Peels

| Method | Method Description | Pros | Cons |
|---|---|---|---|
| Conventional Acid Extraction | The citrus peel is subjected to acid hydrolysis using mineral acids such as hydrochloric acid or sulfuric acid. | This method is relatively straightforward and has been widely used in the industry for its efficiency. | It may result in a lower yield of pectin due to the potential degradation of pectin molecules during prolonged exposure to high temperatures and acidic conditions. |
| Enzyme-Assisted Extraction | Enzymes, particularly pectinase, are employed to break down the cell wall structures, facilitating the release of pectin. | This method is considered gentler, preserving the structural integrity of pectin and potentially yielding pectin with better functional properties. | Enzyme extraction may be time-consuming and might require optimization of enzyme concentrations and incubation periods. |
| Microwave-Assisted Extraction | The application of microwave energy accelerates the extraction process by promoting the breakdown of cell walls. | It is known for its rapid extraction, reduced solvent usage, and potential preservation of pectin structure. | Optimization of microwave parameters is crucial, and there may be concerns about the potential degradation of pectin under certain conditions. |
| Ultrasound-Assisted Extraction | Ultrasonic waves aid in the disruption of cell walls, facilitating the release of pectin. | It is recognized for its efficiency, reduced extraction time, and potential to yield pectin with improved physicochemical properties. | Optimal conditions, including frequency and amplitude, need to be carefully adjusted to avoid potential degradation. |
| Combined Methods | Some studies combine different extraction techniques, such as enzyme-assisted extraction followed by conventional acid extraction, to leverage the advantages of each method. | Combining methods can enhance extraction efficiency and pectin yield while mitigating the drawbacks of individual techniques. | The process complexity and increased resource requirements may be considerations. |

In conclusion, the choice of extraction method for pectin from citrus peel depends on factors such as desired pectin properties, efficiency, and scalability. Researchers often explore multiple methods to optimize conditions and enhance the overall extraction process, ensuring the production of high-quality pectin for various industrial applications.

- Developed experimental protocols for the conversion of citrus peel into pectin, identified as a promising green inhibitor.

An experimental protocol was established for extracting pectin from orange peels using a simple acid extraction method. As shown in **Fig. 3**, a 9-step experimental procedure was developed and applied to extract pectin from orange peels. This experimental protocol will be validated and improved in future quarters to optimize the pectin extraction process.

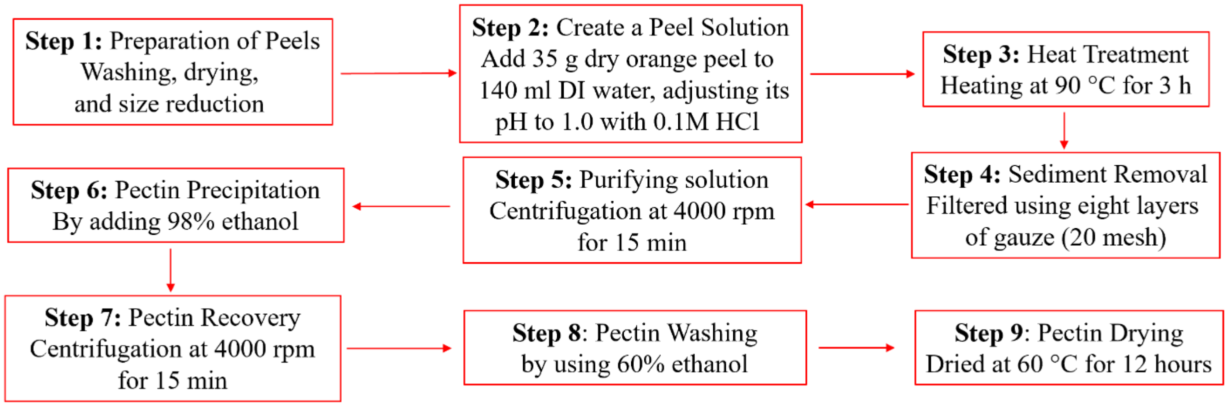


**Fig. 3**. Experimental protocol for extracting pectin from orange peels.

- Successfully synthesized the initial pectin samples derived from orange peels.

Following the test protocol shown in **Fig. 3**, we successfully synthesized a raw pectin sample from orange peels. Some images of the orange peel, extraction reaction, and solid residue sample are shown in **Fig. 4**. The pectin solution (not shown in this figure) is being dried. The chemical composition of the extracted pectin will be determined with FT-IR and NMR in the next quarter.

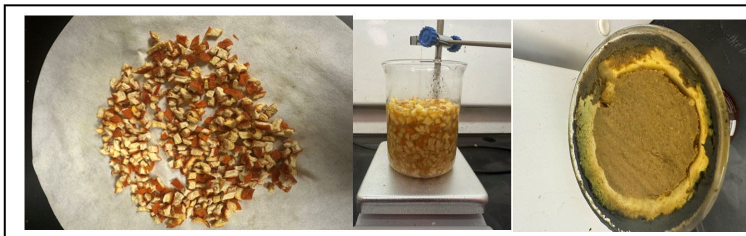

**Fig. 4**. Images of orange peels after size reduction and drying (left), orange peel extraction (middle), and solid residue (right).

**Task 1.3:** Corrosion Testing for Verification and Validation

- Conducted a thorough review of corrosion testing methods, with ongoing development of testing protocols.

Corrosion testing methods employing green inhibitors have become pivotal in the pursuit of sustainable corrosion mitigation strategies. Various techniques are employed to assess the effectiveness of these environmentally friendly inhibitors in protecting gas pipelines from corrosion. The following table compares the test methods that can be utilized to evaluate the performance of green inhibitors.

**Table 3**. Summary of Analytical Methods for Evaluating Green Inhibitors

| Method | Method Overview | Advantages | Considerations |
|---|---|---|---|
| Electrochemical Methods | Potentiodynamic polarization, electrochemical impedance spectroscopy, and linear polarization resistance are commonly employed for their sensitivity in detecting changes at the metal interface. | Electrochemical methods provide real-time data, allowing for the quantitative assessment of corrosion parameters, including polarization resistance and corrosion current density. | Proper interpretation of electrochemical data requires a comprehensive understanding of the inhibitor's impact on the corrosion kinetics. |
| Weight Loss Measurements | Weight loss tests involve exposing metal specimens to corrosive environments with and without inhibitors and measuring the mass loss over time. | It offers a straightforward and cost-effective means of quantifying corrosion rates. | Environmental factors and variability in specimen geometry may influence the accuracy of weight loss measurements. |
| SEM and XRD | SEM and XRD are utilized for morphological and structural analyses of corroded surfaces, providing insights into the protective mechanisms of green inhibitors. | These techniques offer valuable information on the nature of corrosion products and inhibitor film formation. | SEM and XRD are often employed in conjunction with other quantitative methods for a comprehensive corrosion assessment. |
| Salt Spray Testing | Salt spray tests simulate aggressive corrosive environments to evaluate the protective efficacy of green inhibitors. | These tests provide accelerated corrosion conditions, allowing for the rapid assessment of inhibitor performance. | The correlation between accelerated testing and real-world performance should be carefully considered. |
| Microbiologically Influenced Corrosion (MIC) Testing | MIC tests assess the ability of green inhibitors to mitigate corrosion induced by microbial activity. | Relevant for applications where microbial corrosion is a significant concern, such as in pipelines and marine environments. | MIC testing involves the integration of microbiological techniques, necessitating specialized expertise. |

In summary, the selection of a corrosion testing method for green inhibitors depends on the specific requirements of the application and the desired level of detail in the corrosion assessment. Integrating multiple methods often provides a more comprehensive understanding of the inhibitive performance of green corrosion inhibitors in diverse environments.

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

## 1. Introduction

### 1.1 Background

In the realm of gas pipeline systems, the integrity of pipelines is paramount, not only for the efficiency of transportation but also for environmental and safety reasons. One of the significant challenges in maintaining pipeline integrity is the occurrence of corrosion, a phenomenon that can lead to substantial financial losses and safety hazards. This research delves into two primary types of corrosion that plague gas pipelines: flow-induced corrosion and erosion-corrosion.

Flow-induced corrosion is primarily attributed to the fluid dynamics within the pipeline, where multiple phases of matter - gases, liquids, and occasionally solid particles - interact with the inner walls. This interaction often results in the disintegration of the protective inhibitor layer, leaving the metal surface vulnerable to corrosive agents. Erosion-corrosion, on the other hand, is a more complex form, where the mechanical action of moving fluids and particles exacerbates the corrosion process.

Understanding the distribution and behavior of these different phases within the pipeline system is crucial for a comprehensive evaluation of corrosion risk. The presence and dynamics of each phase—be it gaseous (natural gas, corrosive gases like CO2 and H2S), liquid (water), or solid (sulfur particles)—can significantly influence the rate and severity of pipeline corrosion.

Wall shear stress serves as a key metric for assessing the impact of multiphase flow on corrosion inhibitor films. Figure 1 depicts how the flow of gas or liquid exerts wall shear stress, adversely affecting the protective efficacy of inhibitor films on pipeline walls. This type of stress generates a velocity gradient within the inhibitor layer, with higher gradients increasing the likelihood of tearing the protective layer. Such damage leaves the pipeline wall unprotected and vulnerable to corrosive environments. Therefore, the stability of the corrosion inhibitor film under fluid flow is evaluated using wall shear stress as a pivotal reference, highlighting the critical relationship between flow dynamics and the integrity of corrosion protection.

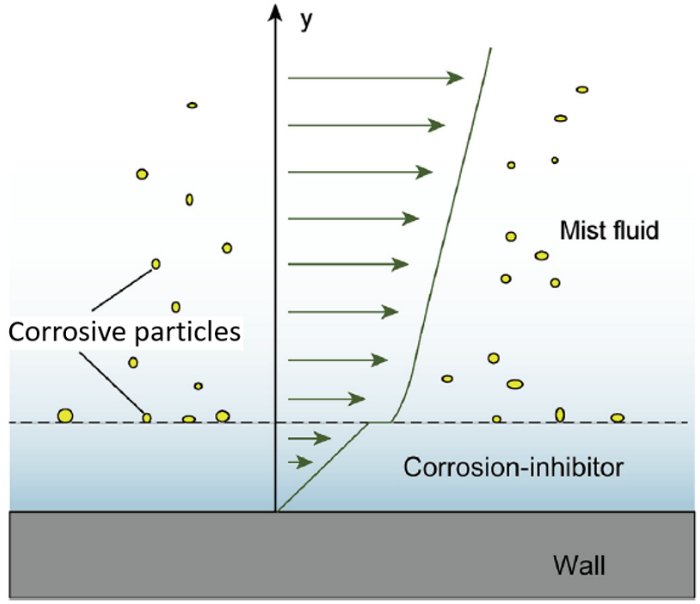

Figure 1 Effect of multiphase flow on the corrosion inhibitor film and the distribution of velocity gradients within the film.

The primary focus of this paper is to assess the efficacy of corrosion inhibitors in such complex environments using advanced Computational Fluid Dynamics (CFD) simulations. Corrosion inhibitors are chemicals introduced into the pipeline to form a protective film on the metal surface, thus mitigating the corrosive impact of the internal environment. However, the performance of these inhibitors is not solely dependent on their chemical properties; it is also significantly influenced by the flow dynamics within the pipeline, which is a function of the flow dynamics of the multi-phase system.

Our CFD simulations aim to replicate the transportation conditions of natural gas pipelines, taking into account the multiphase nature of the internal flow. By varying parameters such as the volume fractions of different phases, flow velocities, pressures, and temperatures, alongside considering different pipeline geometries, we strive to create a comprehensive picture of the conditions under which inhibitors operate. These simulations are designed to offer insights into how efficiently inhibitors can protect various sections of the pipeline under a range of operational scenarios.

The outcomes of this study are expected to contribute significantly to the development of more effective strategies for pipeline protection, enhancing the longevity and safety of these critical components in the energy infrastructure.

### 1.2 Objectives

The current progress is to employ CFD methods to model the dynamics of multiphase flow within gas pipelines, which serves as the benchmark results for the future AI-augmented computing framework. This includes simulating the flow of natural gas, water, corrosive gases, and solid particles under various operational scenarios to mimic real-world pipeline conditions.

A key aim is to evaluate the efficiency of corrosion inhibitors in different pipeline environments. The study will analyze how varying flow rates, pressures, temperatures, and pipeline geometries influence the performance and distribution of these inhibitors.

The research also seeks to identify areas within the pipeline most prone to flow-induced corrosion and erosion-corrosion using an efficient AI-augmented computing framework. It should be noted that there are existing CFD studies for pipeline flow simulation, and our objective and focus is on the development and verification of AI-augmented computing for efficient and accurate simulation.

Additionally, the study aims to optimize the deployment of corrosion inhibitors. This involves determining effective strategies for their injection and distribution, thereby enhancing the overall protective capacity of these inhibitors.

In a subsequent phase, the research intends to use the insights gained from these simulations to develop enhanced corrosion prevention strategies. This will contribute to improving the longevity and safety of pipelines, addressing a critical need in the energy infrastructure sector.

## 2. Methodology

In tackling the complexities of multiphase flow in natural gas pipelines, the application of CFD models is indispensable. CFD theory employs computational power to resolve the partial differential equations governing fluid flow. This approach facilitates a deeper understanding of fluid dynamics by analyzing flow fields and other physical characteristics.

### 2.1 Meshing and Modelling

The ANSYS software is employed for physical modeling and mesh generation in pipeline systems. A structured grid was chosen due to its ability to deliver high-quality solutions with smaller cells. Figure 2 provides an example of a 3D straight pipeline mesh.

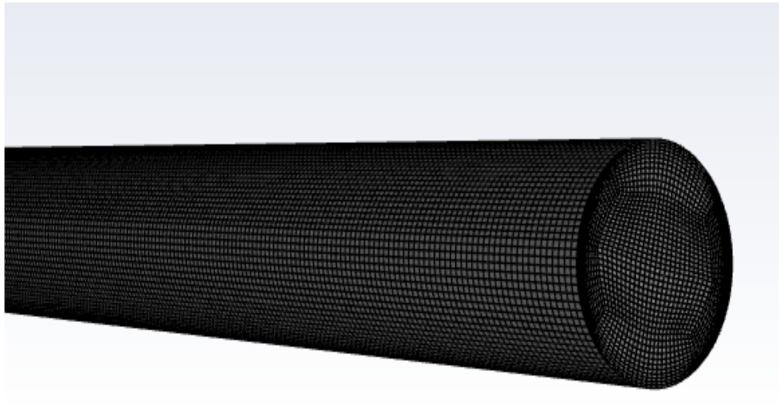

Figure 2. Example of the pipeline mesh.

### 2.2 Experimental Setup

In our comprehensive analysis of the multiphase system within gas pipelines, a variety of parameters are meticulously considered to ensure a thorough understanding of the dynamics at play. These parameters are categorized into three primary groups: Pipeline Properties, Flow Properties, and Operational Conditions.

- ***Pipeline properties***
    - ***Geometry****:* The shape, size, and layout of the pipeline, including length, diameter, and the presence of bends or junctions, which influence flow dynamics and potential corrosion sites.
    - ***Material****:* The type of material used for pipeline construction, such as steel or composite materials, which determines its resistance to corrosion and mechanical stress.
    - ***Roughness****:* The internal surface texture of the pipeline, affecting flow turbulence and the adherence of inhibitor films.
- ***Flow Properties:***
    - ***Gas****:* The properties of the natural gas being transported, including its composition, density, and viscosity.
    - ***Water****:* The presence and characteristics of water within the pipeline, crucial for understanding corrosion risks and inhibitor interactions.
    - ***Inhibitor****:* The chemical properties of the corrosion inhibitor, its interaction with other phases, and its efficacy in different conditions.
    - ***Corrosive gases****:* The concentration and behavior of corrosive gases like CO2 and H2S, which significantly contribute to pipeline corrosion.
    - ***Sloid particles****:* The characteristics of solid particles such as sulfur, including their size, concentration, and abrasive qualities.
- ***Operational Conditions:***

- ***Pressure***: The operational pressure within the pipeline, which influences the behavior of gas and liquid phases and the effectiveness of the inhibitor.
- ***Temperature***: The temperature inside the pipeline, affecting fluid properties, chemical reactions, and the performance of the corrosion inhibitor.
- ***Flow rate***: The velocity of the flow within the pipeline, which impacts shear stress, erosion potential, and inhibitor distribution.
- ***Inhibitor injection rate***: The rate at which the corrosion inhibitor is introduced into the pipeline, crucial for maintaining optimal protection.
- ***Inhibitor thickness***: The thickness of the inhibitor layer on the pipeline's interior, a factor critical to its protective ability.
- ***Inhibitor concentration***: The concentration of the inhibitor in the pipeline, affecting its ability to prevent corrosion.

## 2.3 Physical Models

In this study, we address a fluid dynamic system characterized by incompressible and Newtonian fluid properties. The behavior of such a fluid is governed by the Navier-Stokes equations, which are fundamental to fluid mechanics. These equations are presented as follows:

$$\nabla \cdot u = 0 \tag{1}$$

$$\rho\left(u\frac{\partial u}{\partial t} + u \cdot \nabla u\right) = -\nabla p + \mu \nabla^2 \mathrm{u} \tag{2}$$

To effectively resolve the Navier-Stokes equations within the realm of Computational Fluid Dynamics (CFD), a variety of numerical methods are available. These include the finite difference method, finite element method (FEM), boundary element method, finite volume method, and finite analysis method. Among these, the FEM is particularly noteworthy for its high accuracy and adeptness in managing complex boundary conditions.

The application of FEM is bolstered by the use of sophisticated software platforms such as ABAQUS, ANSYS, and MSC. ANSYS, in particular, stands out due to its comprehensive and flexible suite of modules that are well-suited to a wide range of engineering applications. Within the scope of gas-water two-phase flow analysis using ANSYS, the careful selection of specific models, particularly those for turbulence and multiphase flow, is vital.

The realm of turbulence modeling has seen extensive research, revealing distinct advantages for various models. The realizable k-ε equation, for instance, is favored for its optimal blend of computational efficiency and accuracy, proving especially effective in scenarios involving rotating and separation flows. In terms of multiphase flow analysis, ANSYS offers several model options, such as the Volume of Fluid (VOF), Euler, and mixture models. The VOF model, in particular, is highly proficient at tracking interface separation phenomena in gas-liquid two-phase flows, a conclusion well-supported by existing literature.

Table 1 Comparative analysis of turbulence models.

| Model | Characteristic | Applicable |
|---|---|---|
| Standard k-ε | Moderate calculation and high precision | Fully turbulent |
| RNG k-ε | | Transient or streamline bending flows |
| Realizable k-ε | | Rotary or separation flows |
| k-ω | Moderate calculation and precision | Wall bound or free shear flows |
| Large eddy Simulation (LES) | Large calculation and high precision | Vortex flow |
| Reynolds stress model (RSM) | High precision | Strong vortex or hurricane flows |

### 2.4 Results

#### 1) Straight Pipeline Simulation

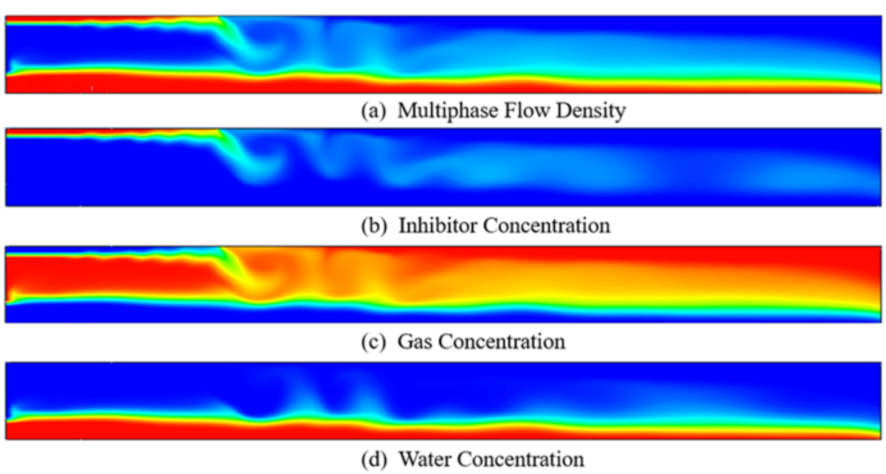

Figure 3: Illustration of the numerical simulation depicting corrosion inhibitor distribution. (Brighter areas represent higher concentrations or densities.)

The flow dynamics of a gas-water-inhibitor mixture within pipeline systems exhibit considerable variation under different operational conditions. This phenomenon is illustrated in the preliminary 2D flow simulation depicted in Figure 3. Here, the pipeline's flow field is represented as a three-phase amalgamation of gas, water, and the corrosion inhibitor, with the latter being introduced from the pipeline's top. A notable observation from the simulation is the tendency of the inhibitor to initially align along the pipeline's upper section before gradually descending towards the bottom, influenced by gravity. Over time, a decrease in the inhibitor's concentration at the top is observed, consequently heightening the risk of top-of-line (TOL) corrosion.

The simulation also sheds light on how varying the flow rate impacts the inhibitor's behavior. An increase in the flow rate appears to decelerate the inhibitor's downward movement, thus offering enhanced protection to the pipeline's upper wall. Concurrently, an escalation in gas flow and turbulence is observed to diminish the water concentration, effectively mitigating the risk of bottom-of-line (BOL) corrosion. Therefore, the simulation suggests that elevating both the gas flow rate and turbulence could serve as a strategic measure to safeguard both the upper and lower sections of the pipeline against corrosion.

Building upon these insights, the proposed study aims to develop advanced 3D simulation models. These high-fidelity models are intended to provide a more detailed and nuanced understanding of the complex interactions within the gas-water-inhibitor system under varying operational scenarios, thereby enabling more effective corrosion prevention strategies in pipeline systems.

**2) Inclined Pipeline Simulation**

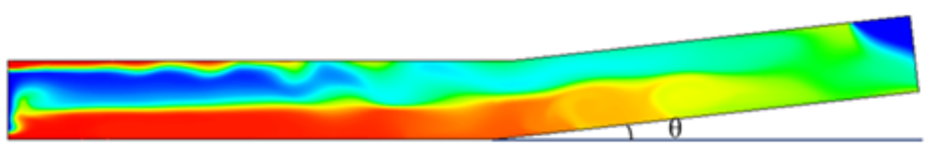


Figure 4: Illustration of the numerical simulation depicting corrosion inhibitor distribution in inclined pipeline.

Prior simulation research has provided key insights into the factors influencing the distribution of corrosion inhibitors in pipeline systems. Critical variables such as gas flow rate, filling rate, pipe inclination, and the size of particles have been identified as major contributors to how corrosion inhibitors are dispersed within pipelines. The complexity of pipeline geometry, particularly in gathering pipelines and certain segments of transportation pipelines, plays a pivotal role in altering the distribution and efficacy of these inhibitors.

A striking example of this is illustrated in the preliminary study showcased in Figure 4. This study highlights the significant effect of even a slight inclination, denoted as angle θ, on the distribution of the three-phase flow - consisting of gas, water, and inhibitors - within pipeline systems. Such inclinations are a common feature in gathering pipeline systems and serve as a testament to the nuanced impact of pipeline geometry on flow dynamics. This understanding underscores the need for thorough analysis and tailored strategies in corrosion inhibitor deployment, particularly in pipeline systems with complex geometries or variable operational conditions.

### 3) Complex Pipeline Simulation

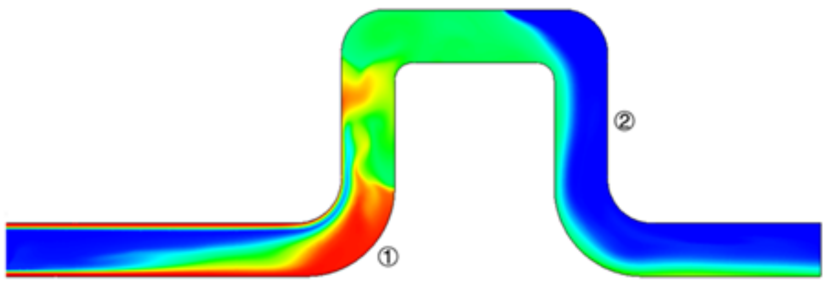


Figure 5: Illustration of the numerical simulation depicting corrosion inhibitor distribution in horse-shoe bent pipeline.

Figure 5 presents a compelling illustration of the complexities in pipeline design and their implications for corrosion control. A notable example is the horseshoe bend in the pipeline, commonly encountered when navigating around obstacles. This specific design feature can lead to the accumulation of water at the first joint, referred to as location 1, potentially resulting in bottom-of-line (BOL) corrosion. The accumulation of water at this juncture not only poses a risk to the pipeline's integrity but also disrupts the effective transport of both gas and corrosion inhibitors. Consequently, this leads to an uneven distribution of the inhibitor, particularly evident after the second joint, designated as location 2. In this area, the top section of the pipeline, or the top-of-line part, suffers from a lack of adequate inhibitor protection.

Interestingly, the presence of an inclination in the pipeline's design can have a dual effect. On one hand, it contributes to a more uniform distribution of contents within the pipeline, which is beneficial for protecting the upper section of the rear pipe. On the other hand, this same inclination can inadvertently promote the accumulation of water in the front pipe, thereby elevating the risk of BOL corrosion.

This nuanced interaction between pipeline geometry, fluid dynamics, and corrosion prevention underscores the importance of carefully selecting the parameters for corrosion inhibitors. Such selection is crucial in ensuring effective corrosion prevention, particularly in pipeline systems with complex geometries or varying operational conditions. It highlights the need for a tailored approach in designing and implementing corrosion prevention strategies, taking into account the unique characteristics and challenges of each pipeline system.

## 3. Future Direction

The use of traditional Computational Fluid Dynamics (CFD) methods, while effective, often encounters limitations in terms of time efficiency and precision, especially when dealing with complex geometrical structures in pipeline systems. To address these challenges, we propose the integration of a cutting-edge approach: the Physics-Informed Neural Network (PINN). This method represents a significant advancement in the application of deep learning to solve supervised problems that are heavily reliant on both empirical data and the fundamental governing equations, such as partial differential equations (PDEs).

PINN stands out from traditional finite element methods by directly incorporating PDEs and initial/boundary conditions as constraints within the model framework. Figure 6 illustrates the architecture of PINN, which comprises an input layer represented by blue nodes, multiple hidden layers depicted as orange nodes, and an output layer shown as pink nodes. The input layer is responsible for feeding the model with spatial-temporal data that encapsulate the dynamics within the flow field. In contrast, the output layer focuses on generating predictions for crucial variables like velocity and pressure distribution in the context of multiphase flow.

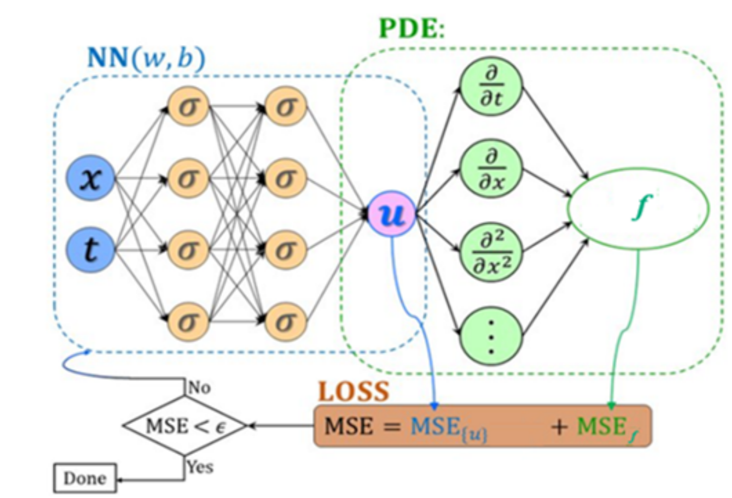


Figure 6: Architecture of the physics-informed neural network (PINN)

A key aspect of PINN is its unique loss function, which is composed of two components: $MSE_u$ and $MSE_f$. $MSE_u$ evaluates the agreement between the model's predictions and the initial/boundary conditions, whereas $MSE_f$ enforces the constraints of the PDEs on the neural network. The computation of $MSE_f$ involves deriving the model's predictions (indicated by green nodes) with respect to the input variables and then comparing these derivatives against those stipulated by the

PDEs. The process of minimizing this loss function effectively integrates the principles of fluid dynamics into the model's predictions.

The application of physics-informed neural networks facilitates the efficient optimization of key parameters within pipeline systems, including the location, rate, and angle of inhibitor injection. This optimization, when combined with variables such as flow rate and pipeline geometry, significantly enhances the effectiveness of corrosion inhibitors. Consequently, this approach not only improves the efficacy of inhibitors but also plays a crucial role in reducing the risk of corrosion, thereby contributing to the preservation and longevity of the pipeline system’s integrity.

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

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## Main Objectives and Goals

- Engineer sustainable inhibitors from renewable feedstocks.
- Perform AI-based simulation for optimal inhibitor deployment.
- Establish evaluation metrics and implement maintenance optimization.
- Validate the proficiency guided by technical advisory panel.

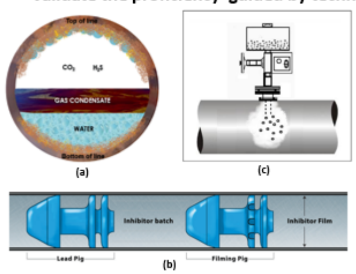


Figure 1: (a) Illustration of BOL and TOL corrosions; (b) batch and (c) continuous applications of inhibitor [1].

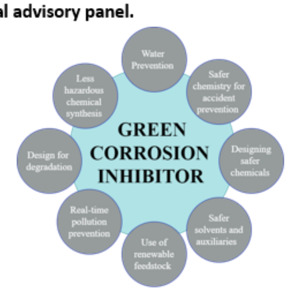


Figure 2. Green corrosion inhibitor.

## Project Approach/Scope

- Design and Synthesis of Multi-compound Green Inhibitors;
- Simulation-based Inhibitor Implementation Optimization in Gas Pipelines;
- Inhibitor evaluation and maintenance scheduling based on inspection.

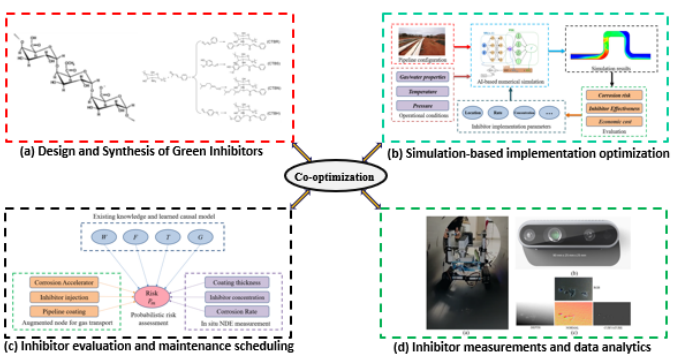


Figure 3. Schematic illustration of the co-optimization of proposed tasks [2].

## Expected Results or Results to Date

- We anticipate that the combined efficacy of multi-compound green inhibitors will be validated in real-world condition.
- AI-based simulations are expected to reveal the performance of the inhibitor under various operational scenarios.
- The outcomes will also provide guidance on further improvements of the inhibitors as per the recommendations of the technical advisory panel.

Table 1. Examples of bio-based corrosion inhibitors to be investigated in this project [3].

| Plant or Source | Active Constituent | Solvent & extraction method | Metal to Protect | Corrosive Environment | Corrosion Inhibition Efficiency (%) | Inhibitor Concentration |
|---|---|---|---|---|---|---|
| Citrus peel | Pectin | HCl and ethanol | Mild steel | 1M HCl | 94.2 at 45 °C | 2 g $L^{-1}$ |
| Shrimps shell waste | Chitosan | NaOH | Carbon steel | 1M HCl | 88.5 at 25 °C | $10^{-5}$ M |
| Plantago ovata | Polysaccharide (galaturonic acid) | Water | A1020 carbon steel | 1M HCl | 94.4 at 45 °C | 1 g $L^{-1}$ |
| Rhododendron schlippenbachii | Polyphenolic compounds | Methanol | Low carbon steel | 1M $H_2SO_4$ | 94.2 at 30 °C | 600 ppm |

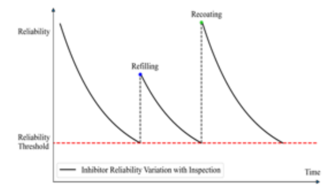


Figure 4. Schematics for time-dependent inhibitor reliability with maintenance.

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