CAAP Annual Report

Date of Report: *09/31/2023*

Prepared for: *U.S. DOT Pipeline and Hazardous Materials Safety Administration*

Annual Period: **From** *(10, 1,2022)* **to** *(10, 01, 2023)*

Contract Number: *693JK32250007CAAP*

Project Title: *Accelerating Transition towards Sustainable, Precise, Reliable Hydrogen Infrastructure (Super-H2): Holistic Risk Assessment, Mitigation Measures, and Decision Support Platforms*

Prepared by: Zhibin Lin (PI), Kevin Wang, Jace Anderson, Hong Pan

Contact Info.:

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Table of Contents

Section A: Business and Activities

(a) Contract Activities

- Contract Modifications: N/A
- Educational Activities:
  - Student mentoring:

1) Li Shang, a Ph.D. student in civil Engineering at North Dakota State University worked on the project starting the 1st quarter of this project.
   Student internship: N/A

2) Mohsin Ali Khan, a Ph.D. student in civil Engineering at North Dakota State University worked on the project starting the 2nd quarter of this project.
   Student internship: N/A

3) Zahoor Hussain (partially working with Dr. Ying Huang's CAAP project), a Ph.D. student in civil Engineering at North Dakota State University worked on the project starting the 2nd quarter of this project.
   Student internship: N/A

4) Xuanyu Zhou, a Master student in civil Engineering at North Dakota State University worked on the project starting the 2nd quarter of this project.
   Student internship: N/A

5) Allison Fleck, a undergraduate student in civil Engineering at North Dakota State University worked on the project starting the 2nd quarter of this project.
   Student internship: Associated with pipelines and water in Summer 2023

6) Wentao Ma, a Ph.D. student in Department of Aerospace and Ocean Engineering, Virginia Tech worked on the project starting the 1st quarter of this project.
   Student internship: N/A

7) Noah Eilers, a undergraduate student in the Department of Aerospace and Ocean Engineering, Virginia Tech worked on the project starting the 2nd quarter of this project.
   Student internship: N/A

  - Educational activities:

1) In the summer of 2023 and fall 2023, Dr. Lin (PI) and his team organized the engineering series for high-school girls (about 4-6 students) and introduced engineering structures, including pipelines, to the students. This series will continue this fall and next spring semester.

2) In the summer of 2023, Prof. Wang (Co-PI) served as an instructor in Virginia Tech's C-Tech^2 summer camp. He offered four interactive lectures to a total of 70-80 high school students. C-Tech^2 offers high school students an opportunity to learn about college life--from residence halls to classrooms and everything in-between. It provides access to information and technology necessary to best prepare the students for their future studies. The C-Tech² program targets rising junior and senior high school girls. (https://eng.vt.edu/ceed/ceed-pre-college-programs/c-tech2.html).

3) Since 08/2023, Prof. Wang (Co-PI) has been serving as the chairperson of the Diversity Equity and Inclusion (DEI) Committee of the Aerospace and Ocean Engineering Department at Virginia Tech. Through collaboration with the National Society of Black Engineers (NSBE), Prof. Wang has organized a Pre-College Initiative (PCI) event for middle and high school students interested in engineering.

- Career employed: N/A

- Others: N/A

- Dissemination of Project Outcomes:

  - Publications (+ advised student, * corresponding author)

1) Wentao Ma+, Xuning Zhao, Shafquat Islam, Aditya Narkhede, **Kevin Wang***, "Efficient solution of bimaterial Riemann problems for compressible multi-material flow simulations," ***Journal of Computational Physics***, Volume 493, 2023,112474. https://doi.org/10.1016/j.jcp.2023.112474. (Acknowledged this grant support)
2) Li Shang+, Zi Zhang+, Fujian Tang, Qi Cao, Hong Pan+, **Zhibin Lin*** (2023) "CNN-LSTM Hybrid Model to Promote Signal Processing of Ultrasonic Guided Lamb Waves for Damage Detection of Metallic Pipelines." ***Sensors***; *23*(16), 7059; https://doi.org/10.3390/s23167059 (Acknowledged this grant support)
3) Ali Zar, Zahoor Hussin+, Muhammad Akbar, Bassam A. Tayeh, **Zhibin Lin** * (2023) " A vibration-based approach for detecting arch dam damage using RBF neural networks and Jaya algorithms." ***Smart Structures and Systems***, accepted (Acknowledged this grant support)
4) Xingyu Wang +, **Zhibin Lin*** (2023) " A Novel High-Performance Coating with Hybrid Nanofiller Reinforcement for Superior Self-Cleaning, Anti-Icing, and Corrosion Resistance Properties ." ***Journal of Building Engineering***, accepted (Acknowledged this grant support)
5) Hong Pan+, Xingyu Wang+, Imtiaj Nahin Ahmed+, Nguyen Tam, Yan Zhang, Trung Le; **Zhibin Lin*** (2023) " Current Knowledge Gaps in Understanding Corrosion/Erosion Threats, Assessment Methodologies, and Mitigation Strategies for Pipelines" ***ASCE Pipelines 2023 Conference***, Las San Antonio, Texas (Acknowledged this grant support)
6) Mohsin Ali Khan+ Hong Pan+, Kevin Wang; **Zhibin Lin*** (2024) "Opportunity and

Risk in repurposing natural gas pipeline network for hydrogen transport", ***ASCE Pipelines 2024 Conference,*** Calgary, AB, Canada.

7) Mohsin Ali Khan+ Hong Pan+, Kevin Wang; **Zhibin Lin*** (2024) "Step Towards Sustainable Transportation of Hydrogen: Structural Integrity Assessment of Pipeline Steels in Hydrogen Environment", ***19th Pipeline Technology Conference*****,** Berlin, Germany.
8) Mohsin Ali Khan+ Hong Pan+, Kevin Wang; **Zhibin Lin*** (2023) "Are we ready for hydrogen: A comprehensive evaluation of existing energy pipeline infrastructure for its transport", ***Conference on Computational Science***, October 18, 2023, Fargo, ND (poster).
9) Xingyu Wang +, Danling Wang, Ying Huang, **Zhibin Lin*** "Advancements in Emerging MXene-Integrated Nanocomposite Coatings:: Unraveling Defect-Free Microstructure for Superior Tribological, Mechanical, and Anti-Aging Features." ***Progress in Organic Coatings***, under review (Acknowledged this grant support)
10) Li Shang+, Zi Zhang+, Fujian Tang, Qi Cao, Hong Pan+, **Zhibin Lin*** "Deep Learning Enriched Automation in Damage Detection for Sustainable Operation in Pipelines with Welding Defects under Varying Embedment Conditions." ***Computation***; under review (Acknowledged this grant support)

- Citations of The Publications: N/A
- Others

(b) Financial Summary

- Federal Cost Activities:
    - PI/Co-PIs/students involvement: During the first year period, the research team, including PI Dr. Lin, Co-PIs Dr. Wang, Dr. Pan, and Mr. Anderson, and involved students meet regularly bi-weekly. Each PI also supervised their own team to work the tasks accordingly.
    - Materials purchased/travel/contractual (consultants/subcontractors): Co-PI Mr. Anderson from EERC is planning and designing the testbed for accelerated testing of pipelines in the hydrogen environment, which includes the material supply.
- Cost Share Activities:
    - Cost share contribution: The Match fund from NDSU for this project is coming from faculty academy hours of NDSU (Dr. Lin) and Virginia Tech (Dr. Wang), and several Ph.D. students' RA tuition waivers.

The cost breakdown during the first year period in each category according to the budget proposal is shown in Table 1. Note that due to delay of budget from two Co-PIs (i.e., Virgina Tech and EERC), the information below could be different to actual expense.

Table 1 Cost breakdown during the reporting period (first year)

Category	Amount spent during the first year
Personnel	
Faculty	$10400
Postdoc	$40,800
Students (RA and UR)	$18,500
Benefits	$24,015
Operating Expenses	
Travel	$0
Materials and Supplies	$0
Recharge Center Fee	$0
Consultant Fee	$0
Subcontracts	Subawards issued
Indirect Costs	$93,515

(c) Project Schedule Update

- Project Schedule:

Table 2. Schedule of the proposed project and progress.

Tasks (Milestones)	Year 1				Year 2				Year 3			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 1 (Milestone 1)	√											
Task 2 (Milestone 2)	√	√	√	→								
Task 3 (Milestone 3)		√	√	√								
Task 4 (Milestone 4)		√	√	√								
Task 5 (Milestone 5)												
Task 6 (Milestone 6)												
Task 7 (Milestone 7)	√	√	√	√								

√ Finished, → Ongoing.

Task 2 involves the development of decision and recommendation models. Due to the current absence of experimental and simulation datasets, our focus has shifted to collecting and curating literature data. Consequently, this aspect of the project has been delayed. However, it will not impact the progress of other tasks significantly, as these tasks primarily involve providing evidence and data for refining the Task 2 model. Once we establish the risk assessment framework in Task 2, we will only need to update the model parameters based on the outcomes of the remaining tasks.

- Corrective Actions: N/A

(d) Status Update of the 4th Quarter Technical Activities

- Task 2.1: Develop risk assessment model for pipeline under hydrogen effects.

  In this quarter's research period, our focus has been on assessing fractural-related aspects. The current study was performed to assess the structural integrity of X52 and X70 pipeline steels under the hydrogen environment, with specific consideration given to the semi-elliptical cracks in the longitudinal direction. The crack size varies under specific boundary conditions and pressure loads as shown in Figure 1 . Utilizing the Finite Element Method (FEM), stress intensity factors along the crack front is determined and compared with those calculated using the analytical approach outlined in the existing standards. As such, the fracture toughness of X52 and X70 steel is determined through CTOD tests (conducted in the literature) to create a specific Failure Assessment Diagram based on the existing standard as shown in Figure 2. The established diagram is used to assess the acceptability of the cracks under the hydrogen environment. Thus, the presented FAD curves are used as reference for the crack assessment in the existing pipeline infrastructure, which will eventually give the signal of safe/not-safe condition.

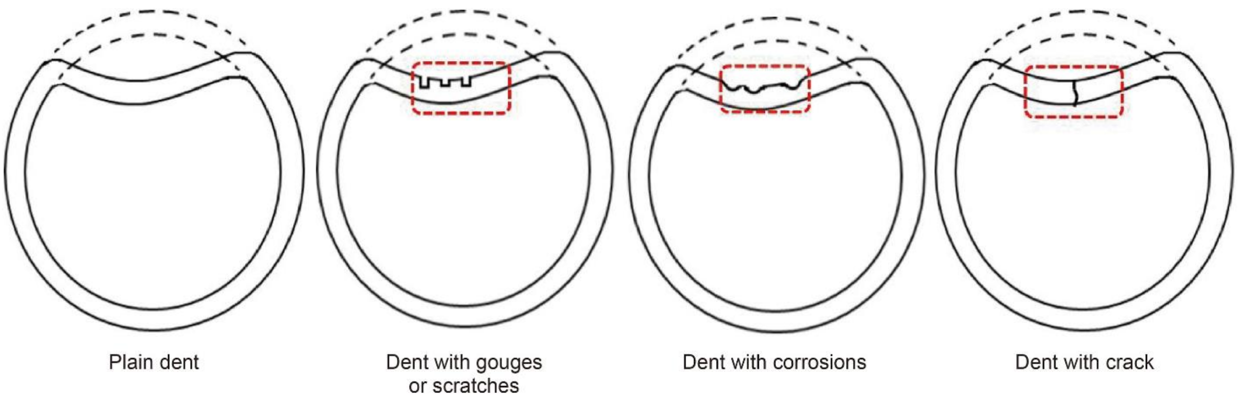


Figure 1. Graphical representation of various dent-defect configurations that can be seen on pipelines.

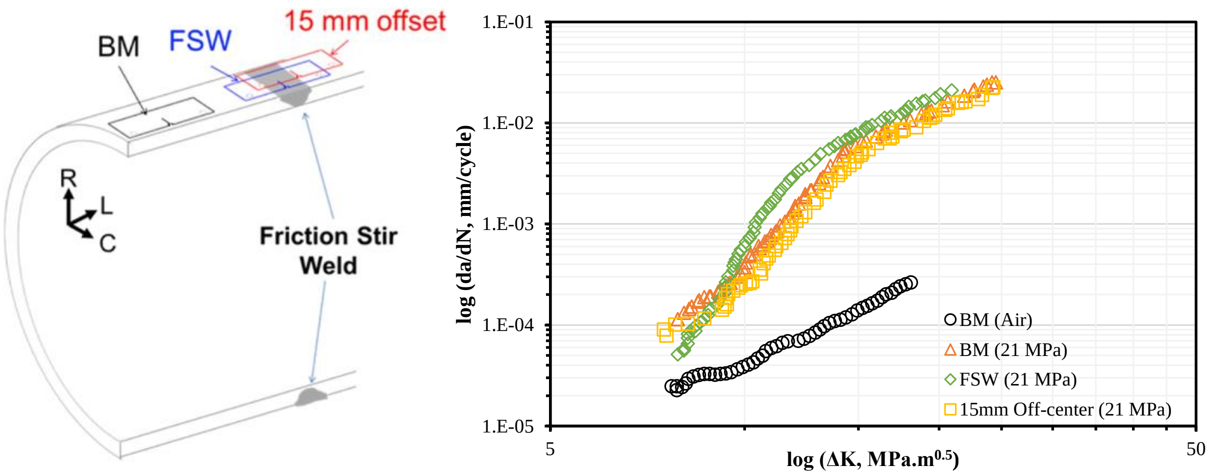


Figure 2. (a) Diagram representing the orientation of test sample with respect to pipeline, (b) da/dN versus ΔK plot for X52 pipeline steel under 21 MPa hydrogen pressure and frequency equals to 1 Hz.

- Task 2.2: Develop mitigation measures and modification/upgrading strategies for repurposed pipelines.

  During this quarter, our primary focus is on validating the effectiveness of a specialized coating designed to mitigate the effects of hydrogen. We are conducting an in-depth literature review to assess the viability and impact of this coating method.

- Task 3.1: Design of near real-world testbed for pipelines transporting pure hydrogen/hydrogen blends to simulate accelerated field conditions in a realistic environment.

  During this quarter, our design discussions centered around selecting the pipeline material, which might be influenced by its availability. The initial choice was API 5L X52; however, obtaining the required small quantity has posed challenges. After consulting with experienced members of the EERC specializing in pipeline infrastructure, alternative materials suitable for natural gas transmission, such as ASTM A106 SCH40 carbon steel or ASTM A53 SCH40 carbon steel (though primarily intended for on-site distribution), were considered. Ideally, the EERC prefers to adhere to the original plan of using API 5L.

- Task 4.1: Understanding of long-term hydrogen impacts on materials and welding requirements in realistic environments through experimental study

  During this quarter, we have kept coding the atomic scale simulations and documented the new features added to the solver in our user manual. The added materials are shown below.

23 Generation of lattices and particles

23.1 Definitions and assumptions

This component was originally implemented in the DMD (Diffusive Molecular Dynamics) solver for hybrid atomistic-continuum analysis of mass transport and material deformation [86, 87, 88]. It was originally implemented only for the FCC lattice. In 2023, the DMD code was revamped to support arbitrary lattice structures and polycrystals, and renamed to A2C ("atomistic-to-continuum"). The fundamental routines for lattice, site, and particle creation are also included in M2C for future use. The input parameters are named to be somewhat similar to those in LAMMPS (`https://docs.lammps.org/lattice.html`), but more user-friendly.

The basic concepts about lattices, sites, and particles (e.g., atoms, ions, molecules) can be found in Tadmor and Miller [89] (Chapter 3), and many other books. We try to use algorithms that are applicable to all lattice structures, rather than getting into the details of specific lattice structures. For example, when constructing shells of neighbors, we just apply a sorting algorithm, instead of implementing lattice-specific formulas.

A lattice is an infinite space filling arrangement of points/particles in a regular pattern. What we refer to as "sites" are the locations in space that *can* be occupied by particles, defined relative to a lattice. In other words, these are locations that are relevant to our analysis. In practice, they often include interstitial sites. The particles themselves can be atoms, ions, or molecules. They have mass and volume, and generally are not allowed to overlap. Note that the way we define a "lattice structure" is slightly different from (and more general than) the conventional approach that considers *crystal* = *lattice* + *basis* [89].

Each lattice structure (or *crystal*) is defined uniquely by the following parameters.

- **Lattice vectors**: $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$, in (x, y, z) coordinates, define the unit cell. The magnitude of the three vectors are the lattice spacing in the three directions. This unit cell does not need to be the primitive (i.e. smallest) unit cell. Once the lattice vectors are determined, the lattice angles are given by

$$\alpha = \cos^{-1}\left(\frac{\boldsymbol{b}\cdot\boldsymbol{c}}{\|\boldsymbol{b}\|_2\|\boldsymbol{c}\|_2}\right). \tag{629}$$

$$\beta = \cos^{-1}\left(\frac{\boldsymbol{a}\cdot\boldsymbol{c}}{\|\boldsymbol{a}\|_2\|\boldsymbol{c}\|_2}\right). \tag{630}$$

$$\gamma = \cos^{-1}\left(\frac{\boldsymbol{a}\cdot\boldsymbol{b}}{\|\boldsymbol{a}\|_2\|\boldsymbol{b}\|_2}\right). \tag{631}$$

- **Lattice origin**: The (x, y, z) coordinates of lattice site $(0, 0, 0)$.
- **Lattice sites**: The locations (in lattice coordinates) that *can* be occupied by particles. Multiple sites can be defined within each unit cell. Each site is defined by (l_a, l_b, l_c), with each coordinate in $[0,\ 1)$. Associated with each site in the unit cell, there is a *material number* (0,1,2,...). This allows different subsets of sites to be treated differently, for example, occupied by different types of particles.
- **Domain**: The domain (Ω) of each lattice structure is a geometry that includes all the lattice sites involved in the analysis. It is defined by first defining a number of regions, each one being a set in $\mathbb{R}^3$, namely S_0, S_1, S_2, ..., S_n, then applying set operations

$$\Omega \equiv \mathbb{R}^3 \circledast S_0 \circledast S_1 \circledast \cdots \circledast S_n, \tag{632}$$

where $\circledast$ is either $\cap$ or $\cup$. Note that the order of the sets in the above definition is fixed, and it matters.

Each region can be one side of a plane (excluding the plane itself), the interior or exterior of a parallelepiped, cylinder-cone, or cylinder-with-spherical-caps (excluding the surface). Note that boxes, cylinders, cones, and spheres are special cases of the above mentioned geometries.

One of the regions can be defined using a user-specified script, through dynamic linking. In this case, it can have any geometry.

For each region, the operator $\circledast$ in front of it and the subscript i must be specified in order to uniquely determine the set operations ((632)).

- **Minimum spacing**: $d_{\min}$ is the minimum spacing between sites in this lattice structure and any other lattice structures. The default value is smallest one among a_0, b_0, and c_0.

Note that we have avoided explicit mentioning of specific lattice types, such as FCC, BCC, and specific interstices such as octahedral and tetrahedral. They are naturally accommodated in our definitions.

Multiple lattice structures can be specified in the same way. They can even overlap, except that lattice sites that violate the minimum spacing will be removed.

TODO: Currently, lattice structures are not parallelized. All the processor cores store all the lattice sites. This can be improved in future.

23.2 Domain creation

The solver is capable of generating samples that involve multiple lattice structures (e.g., polycrystals). The entire simulation domain (i.e., the material sample) may consist of multiple lattice domains. The solver first constructs the individual lattice domains, then erases the "conflicting" sites in between based on $d_{\min}$.

When constructing a lattice domain, we first go over all the user-specified geometric regions (i.e. S_i) to find a bounding box that is aligned with the lattice vectors $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$. Here, it is noteworthy that all the geometric objects supported by the code (except for planes) are convex. Therefore, any box that contains the vertices of the object contains the entire object. For spheroids, cylinder-cones, and cylinder-with-spherical-caps, we first create an intermediate bounding box aligned with their own axes, as shown in Figure 49. Then, the final bounding box is defined to be the smallest box that is aligned with the lattice vectors, and contains all the vertices of the intermediate bounding box. This solution is not optimal, but easy to implement and widely applicable.

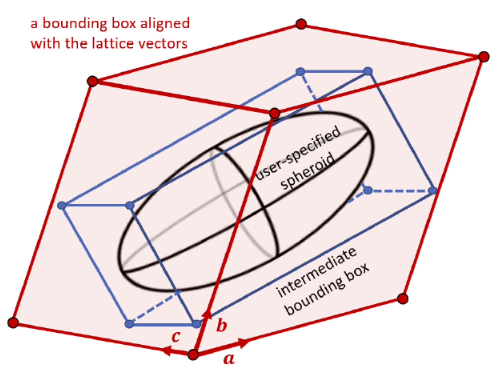


Figure 49: Generation of a bounding box aligned with lattice vectors for a spheroid.

Figure 3. The user manual for particle simulations.

Section B: Detailed Technical Results in the Report Period

1. Background and Objectives in the 1st Annual Report Period

1.1. Background

Hydrogen possesses unique characteristics that make it a versatile energy carrier, enabling the seamless integration of renewable energy sources into multiple sectors such as industrial operations, electricity generation, transportation networks, and heating systems [1-7]. The production of hydrogen involves methods such as steam methane reforming (SMR) using natural gas and coal gasification from fossil fuel sources. Additionally, sustainable hydrogen production methods include electrolysis, which relies on clean electricity from diverse sources such as nuclear power, renewables, or electricity derived from clean grids. Other viable techniques for hydrogen production encompass thermochemical processes like photo-electrolysis, high-temperature heat, and biomass gasification[8-13]. For a visual representation of the various hydrogen production pathways, along with their corresponding procedures and applications, please refer to Figure 1.

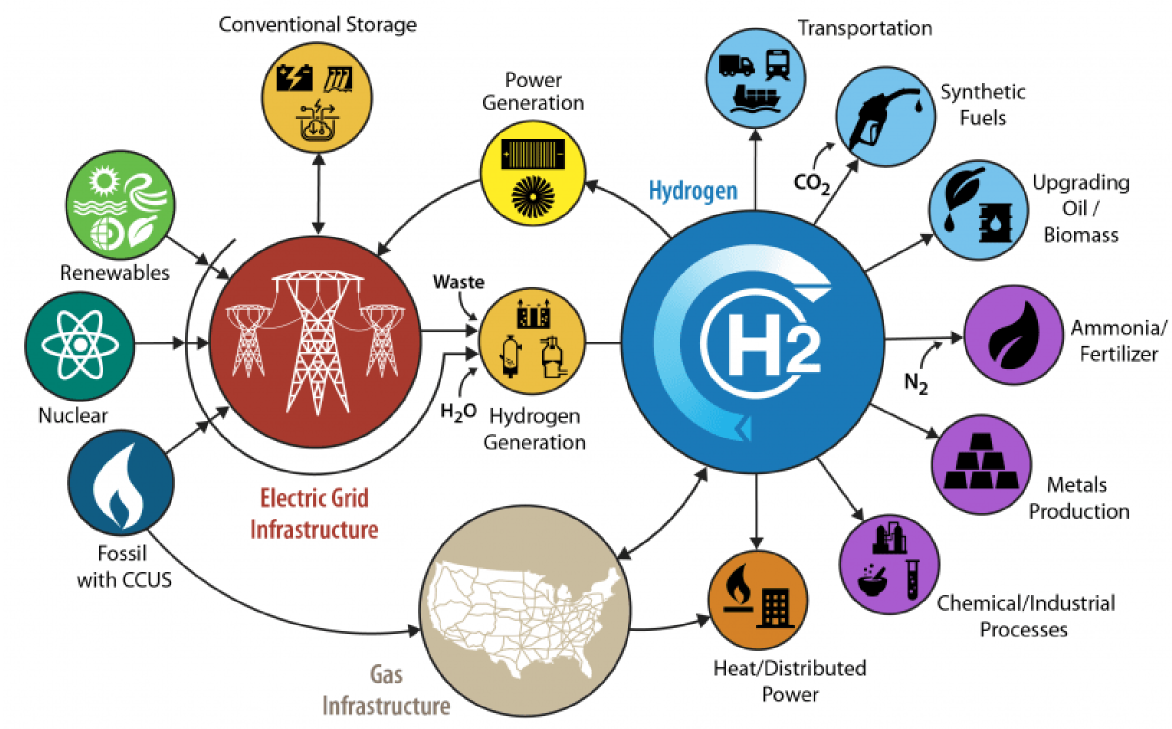


Figure 4. The DOE H2@Scale approach seeks to facilitate the implementation of widespread production of hydrogen and usage for the purpose of decarbonization.

The transportation of hydrogen and the effective utilization of existing pipelines are pivotal factors in transitioning to a green hydrogen economy. Among these considerations, evaluating the suitability of current pipelines for hydrogen transportation stands out as a crucial and primary focus.

1.2. Objectives in the 1st Annual Report Period

During the initial years of our project, we achieved several pivotal objectives as outlined in the 1st annual report period. Our primary goal was to evaluate the suitability of the existing pipeline for hydrogen transportation through a comprehensive analysis involving theoretical, simulation, and experimental approaches. The following objectives were accomplished:

a) Completed Comprehensive Literature Review on Hydrogen Suitability for Existing Pipelines (Task 1):

A thorough review of existing research was conducted, providing valuable insights into the compatibility of hydrogen with current pipeline systems. This extensive literature review served as the foundation for our subsequent analyses.

b) Successfully Collected and Curated Hydrogen-Related Fracture Testing Data (Task 2.1):

We meticulously gathered and curated a vast array of data related to hydrogen-induced fractures. This curated dataset forms the basis for our detailed analyses and decision-making processes, ensuring the accuracy and relevance of our findings.

c) Designed and Implemented an Advanced Near-Real-World Testbed for Hydrogen Effects Analysis (Task 3.1):

An innovative and sophisticated testbed was designed, replicating real-world conditions accurately. This controlled environment enabled us to conduct precise experiments, allowing for in-depth analysis of hydrogen effects on pipelines.

d) Developed Multi-Scale Simulation Models for Fundamental Understanding of Hydrogen Effects (Task 4.1, Task 4.2):

Complex multi-scale simulation models were successfully developed based on previous coding, providing a profound understanding of how hydrogen impacts pipeline integrity. Tasks 4.1 and 4.2 focused on the creation of these intricate models, allowing us to explore the intricate nuances of hydrogen behavior within the pipeline structure.

By achieving these objectives, our project has made significant strides in advancing the understanding of hydrogen transportation through existing pipelines. The completion of these tasks has laid a solid foundation for the subsequent phases of our research, positioning us at the forefront of this vital field.

1.3. Experimental Design

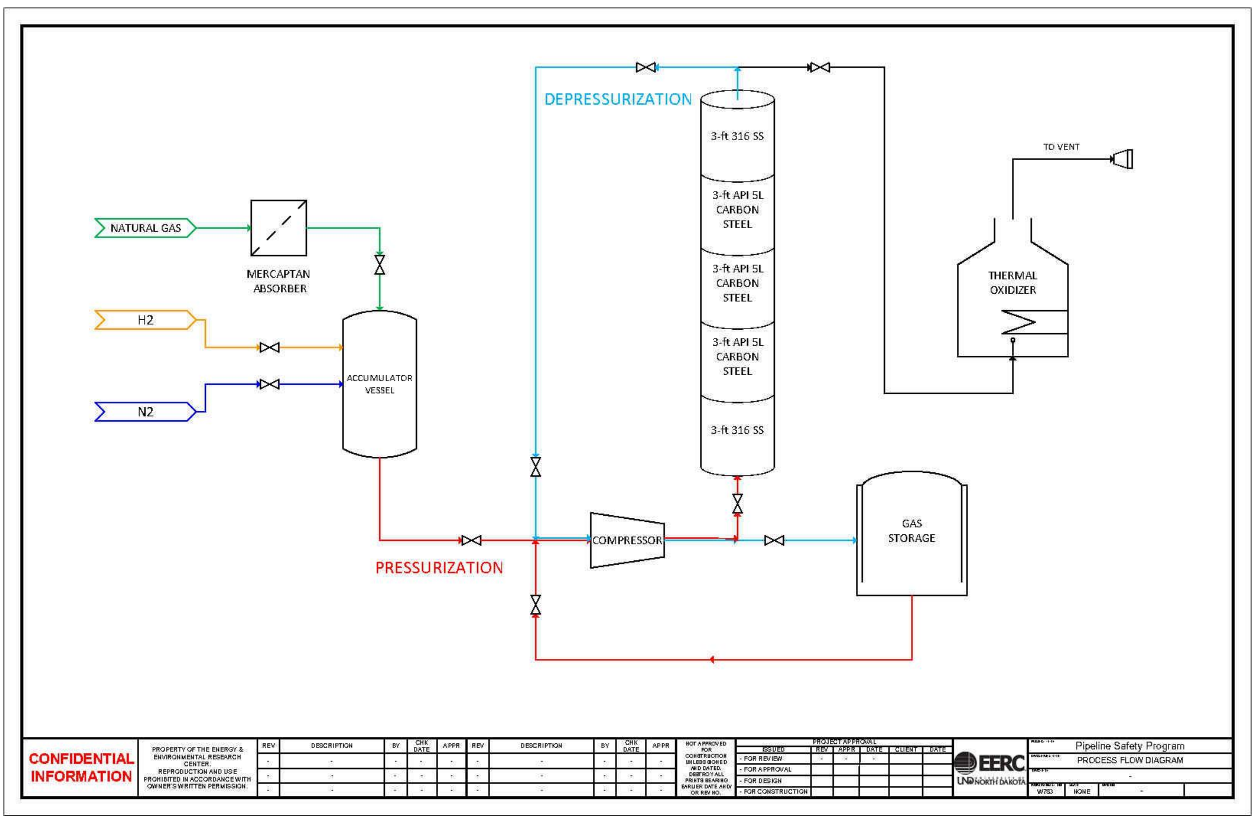
The EERC led the design of the near-real-world test, with Dr. Lin and Dr. Wang overseeing complementary coupon tastings as part of the overall design process.

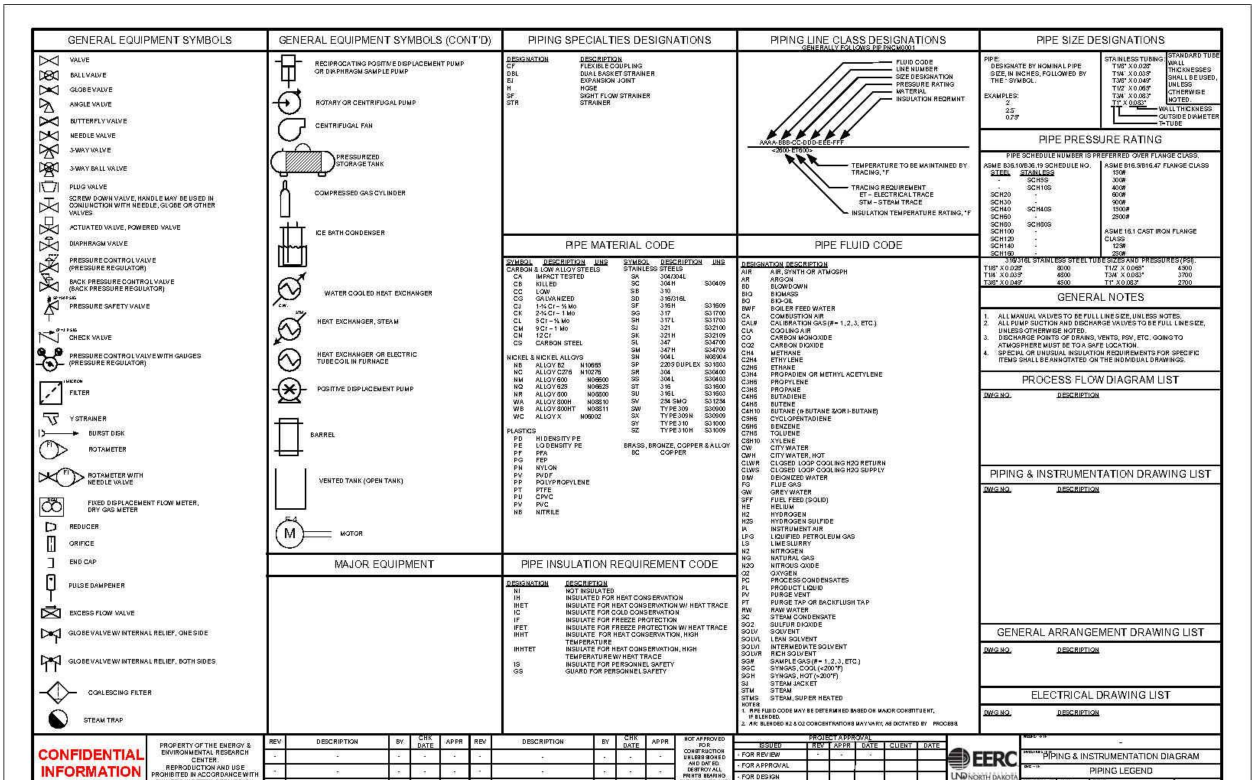
The EERC has discussed two potential siting spots for the fabrication of the pipeline. The spot has been decided upon and deconstruction and cleanup of the unused equipment in the space will begin to clear way for the new system.

An initial Hazard and Operability Analysis (HAZOP) [14] review has been done, which determined the siting was adequate, but called for some redesigning of the system itself to ensure proper recycling of the gas blend so the system won't inefficiently consume the hydrogen supply to run. Once the process and instrument diagrams (PID) and process flow diagrams (PFD) has been updated again as illustrated in Figure 5, a final HAZOP will occur.

Material purchasing will begin shortly once the sitting location is cleaned up enough to properly store the materials.

The material to be used for the pipeline is being discussed, as it may end up being a result of availability. The original plan is API 5L X52, but the availability of obtaining the small amount needed has proven difficult. After consulting with a few members from the EERC with experience in pipeline infrastructure, a suitable material used in natural gas transmission could also be ASTM A106 SCH40 carbon steel or ASTM A53 SCH40 carbon steel (however, this seems to be more for on-site distribution). If possible, the EERC would like to stick with the original plan of API 5L.





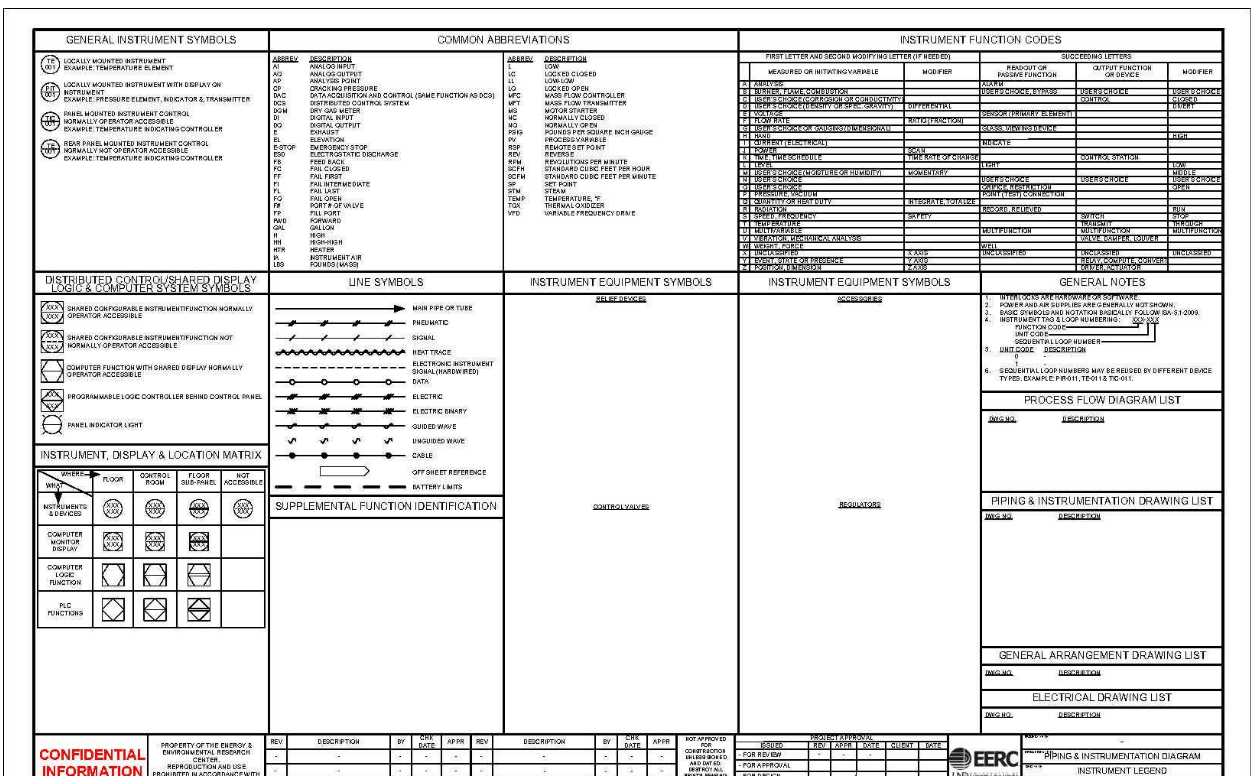


Figure 5. The PID and PFD for our testing.

1.4. Testing procedure

The main test procedure is following:

a) Pressure Cycling Testing:

i. Apply pressure cycling to the system according to predetermined cycles and pressure levels.

ii. Monitor the system's behavior under different pressure conditions.

b) Threat Scenario Induction:

i. Introduce deliberate threat scenarios one at a time.

ii. Monitor the system's response to each threat scenario, including any anomalies detected by sensors.

c) Data Collection:

i. Collect data generated during pressure cycling and threat scenario induction.

ii. Ensure that data collected includes information from individual-level sensors, NDE tools, and wireless networks.

d) Precision, Transparency, Sensitivity, and Reliability Evaluation:

i. Analyze collected data to evaluate the precision, transparency, sensitivity, and reliability of the system.

ii. Compare the system's responses to the expected outcomes based on the deliberate threat scenarios.

e) Consultation and Feedback:

i. Consult with SMEs and pipeline industry representatives to validate the system's performance and obtain feedback on its real-world applicability.

Results and Discussions

1.5. Task 1: Literature review

We have conducted a comprehensive review for hydrogen in pipeline and draft a journal paper named as: "Scientometric Based Systematical Review: Gaseous Hydrogen Transport in Existing Natural Gas Pipelines and Its Impacts on Pipe Steels.".

1.6. . Task 2: Repurposing decision platform formulation

- <u>Task 2.1: Develop repurposing related risk assessment model</u>

We have built NLP based framework to evaluate hydrogen effects as illustrated in Figure *6*, collected hydrogen effected pipeline fracture testing data as shown in Figure 7, and formulated a 3-linear function to quantify the hydrogen-based fracture curves as shown in the Figure 8.

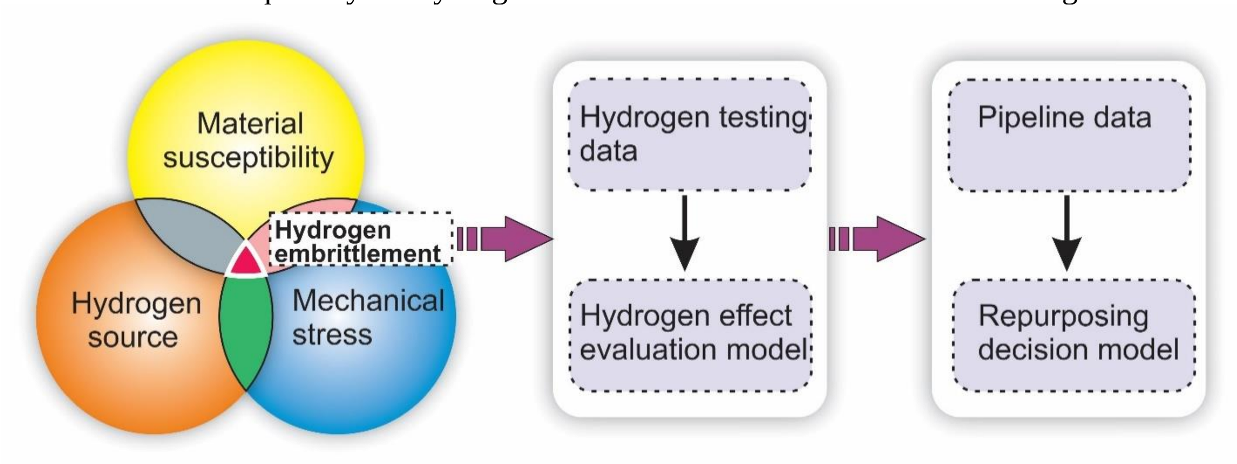


Figure 6. The Hydrogen repurposing decision model building process on the mechanical side.

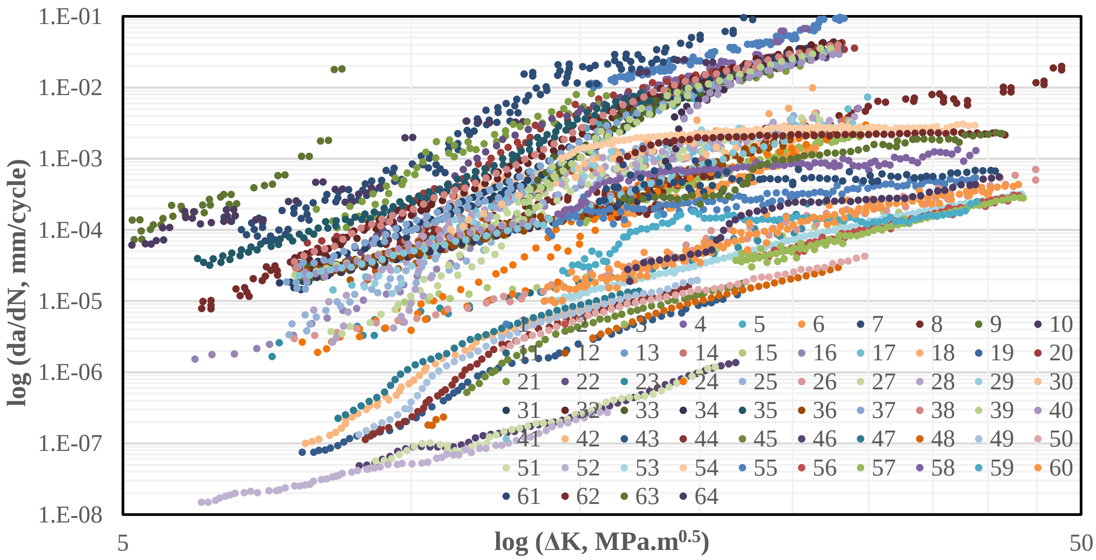


Figure 7. Fracture plot of different pipeline steel subjected to hydrogen environment.

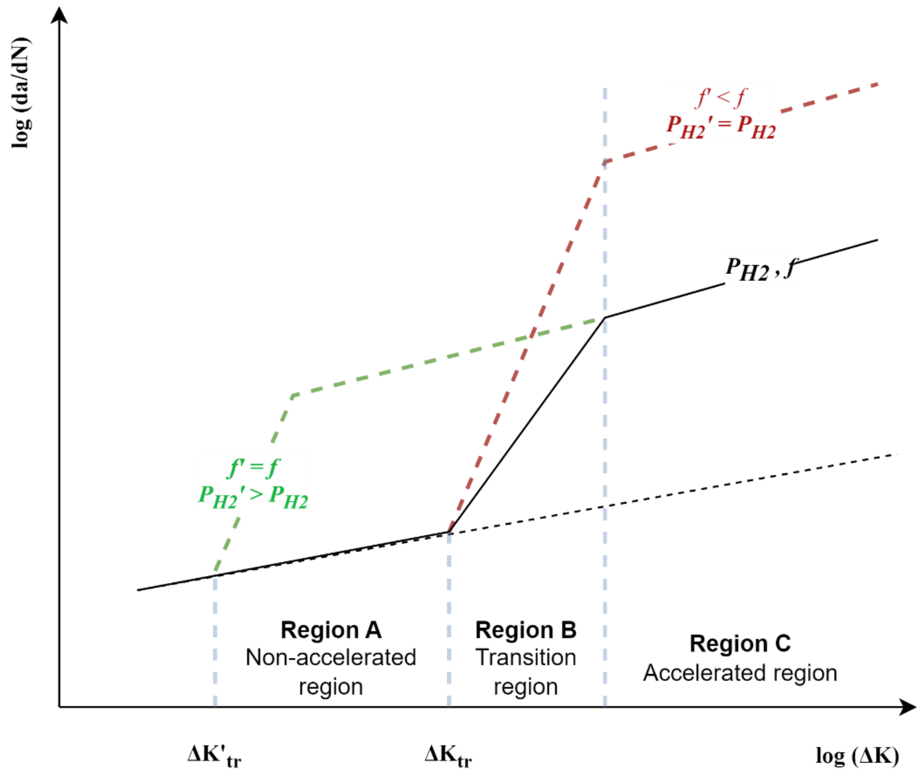


Figure 8. Generalized diagram showing trends of fatigue growth rate by the variation in the loading frequency and partial pressure of hydrogen gas

- Task 2.2: Hydrogen effects mitigation methods

To mitigate the damage of hydrogen pipeline steel, coating the interior and/or exterior surface of pipeline steel [15] is a promised method. The deployed strategy can depends on the level of degradation and risk posed to the pipeline failure. The coating is a barrier materials delay the hydrogen permeation, which will eventually decrease the risk of cracking and failure [16]. As presented in the literature, among the three different types of coating, ceramic coatings were the most preferable providing several advantages over metallic and polymeric coatings. As presented in Figure 9, ceramic coatings protect the pipeline steel from degradation, providing high strength, electrical insulation, low thermal expansion, and high thermal resistance [17]. The carbide, oxides, and nitride based ceramic coating presented their suitability as corrosion resistant at high temperature, alongside provides appealing permeability properties, which can effectively assist the hydrogen environment [18].

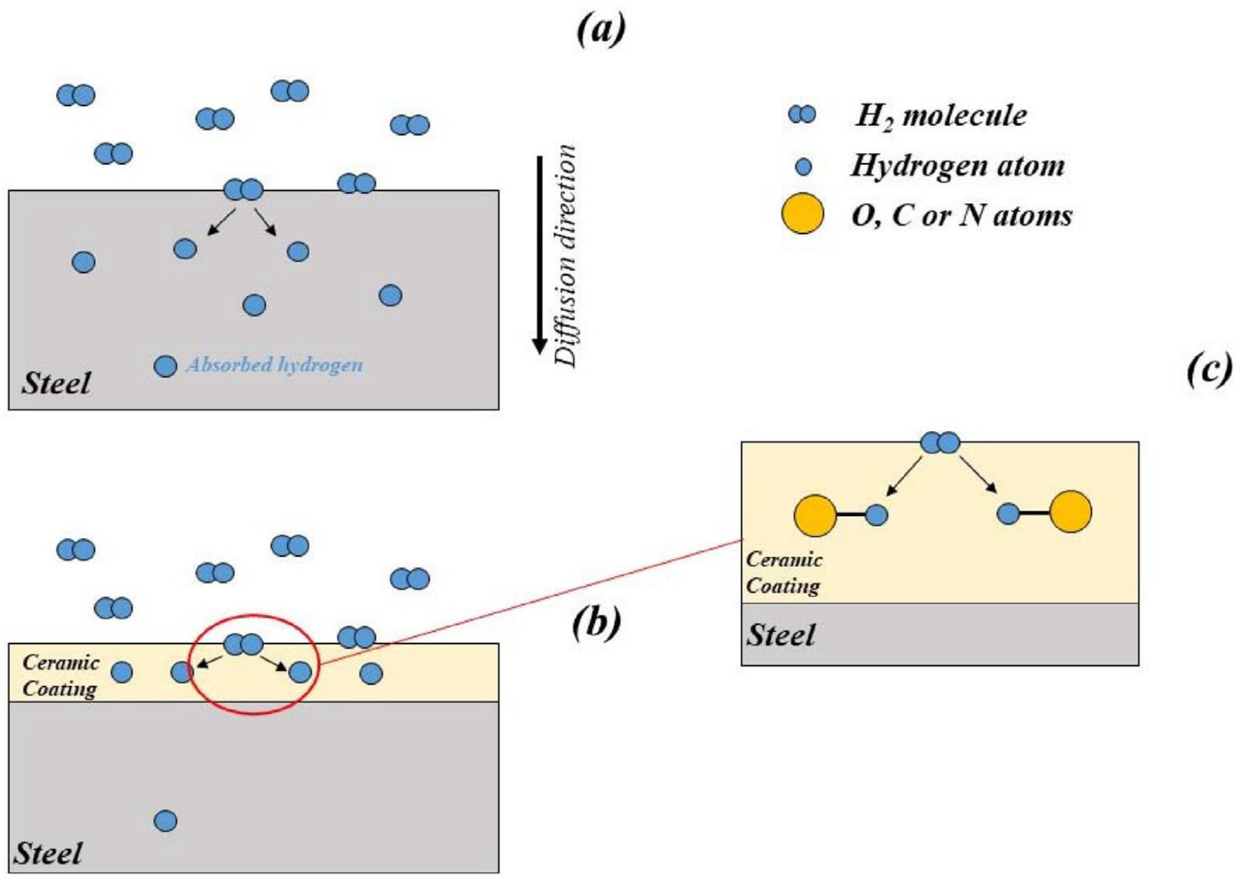


Figure 9. Mechanism of hydrogen permeation barrier using ceramic based oxide, carbides or nitride coating (a) diffusion of hydrogen before coating, (b) adsorption and dissociation in coating surface, (c) development of strong covalent bond in coating surface.

Recently, Shi et al. [10]used ion implantation and annealing method for in situ deposition of multi-layered graphene (MLG) coatings to mitigate HE of the X70 pipe steel. Different surface treatments have different mitigation effects. According to the previously study. The stacked MLG promoted the adherence of the coating and improved protection against hydrogen. Figure 10 illustrates both planar and cross-sectional images of the graphene covering that has been placed onto a Nickel substrate. The provided images illustrate MLG coating effectively covered the complete substrate and thus decreased the permeability efficiently by 48 times. Also, a 123-times reduction in diffusion was noted alongside the slow strain rate tests showing an excellent resistance against hydrogen embrittlement (HE). Furthermore, the electrochemical test indicated that MLG coating can effectively resist corrosion. Looking into the stated results, it can be deduced that graphene usage for the protection of commercial steels from HE could be a feasible solution. In the upcoming phase, we plan to authenticate our discoveries.

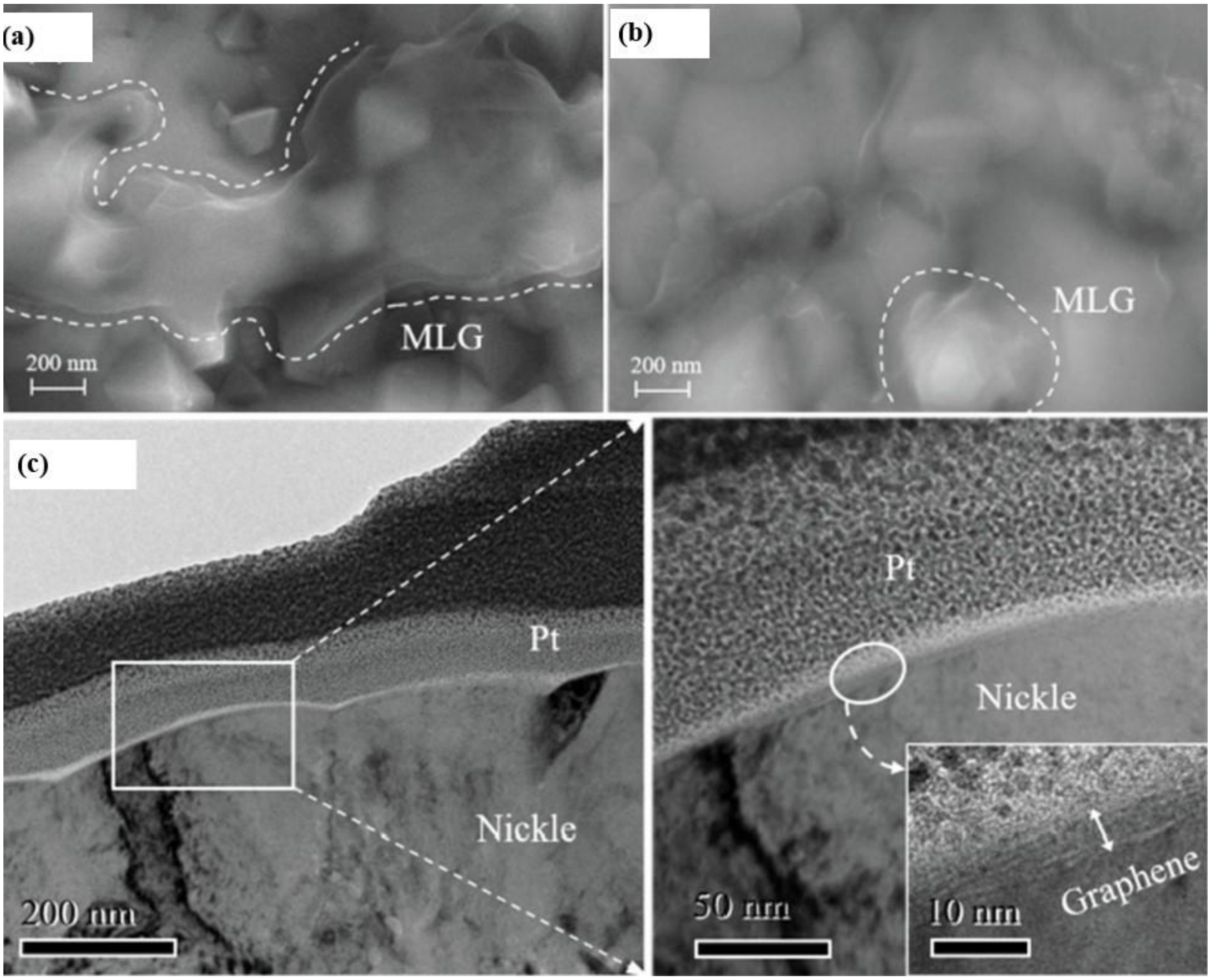


Figure 10.. **(a, b)** SEM images reflecting the Planar, **(c)** TEM images reflecting the cross section of MLG coating.

1.7. Task 3: Near real world testing

- Task 3.1: Experimental design and testing setup

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1.8. Task 4: Multi-Scale simulation

In the annual period, the Virginia Tech team has made progress in the following areas.

a) Literature review of existing models and computational methods for analyzing hydrogen embrittlement at different scales.

b) Generalization of the current DMD solver to support different lattice structures (e.g., FCC, BCC) and alloy constituents pertaining to pipeline steels; and

c) Adding the new features in the code to the user manual.

- <u>Task 2.1: Multi scale models</u>

a) Literature review

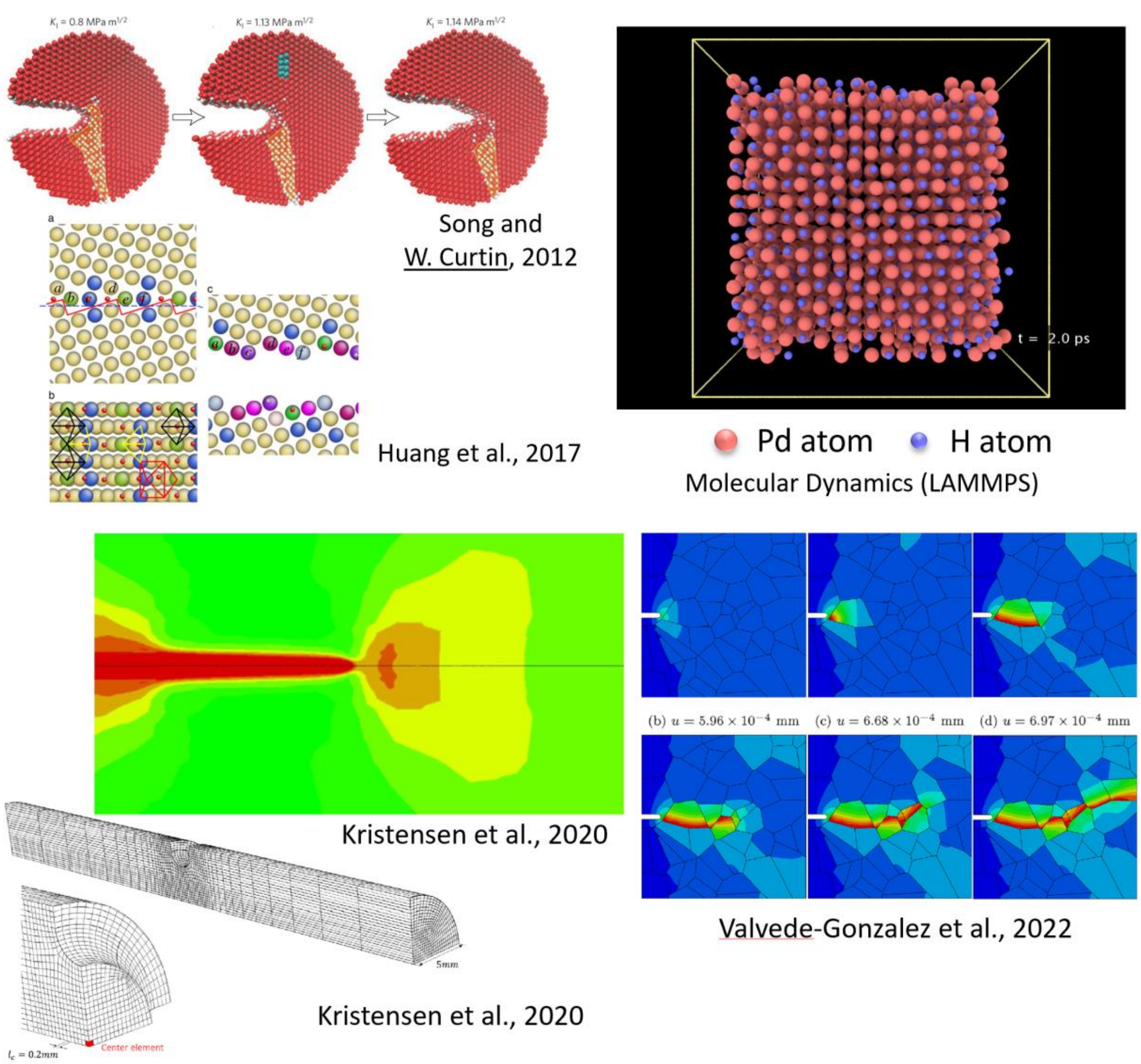
We have collected and read more than 30 research articles on hydrogen embrittlement and long-term hydrogen-induced material damage, focusing on computational models and methods at different length and time scales. We have compiled an EndNote library with these articles, and categorized them into different groups. Through the literature review, we found that most studies in the past have focused on either the atomistic scale or the continuum scale. A major limitation is that the connections between the findings obtained at these different scales are still unclear. At the atomistic scale (Figure 10 (a)), widely used methods include molecular dynamics, molecular statics [19] (i.e. neglecting thermal vibration, but retaining interatomic and chemical potentials), and crystallography. The main advantage of these methods is that they explicitly resolve individual atoms of the solute (Hydrogen) and the solvent (e.g., Iron). The fundamental questions addressed in these studies include (1) How does H influence the propagation of a crack tip at atomic scale? (2) What are the effects of atomic-scale features (e.g., impurities, defects, and grain boundaries)? The main issue of the atomistic scale methods is that the length and time scales are highly limited. As a result, direct comparison between simulation and experimental results is challenging, and rarely conducted.

At the continuum scale, popular methods include hydrogen diffusion models, material degradation models, and static mechanical equilibrium analysis (e.g., using finite element method) (Figure 10 (b)). These methods do not resolve individual atoms or molecules. But they can represent grain boundaries as internal boundaries in the computational domain. The fundamental questions addressed in these studies include (1) How does hydrogen influence the propagation of a crack in a single- or poly-crystalline material? (2) What are the effects of hydrogen pressure, material type, grain boundary, and impurities? A weakness of these continuum-scale methods is that they rely on empirical models to account for the adsorption and absorption of hydrogen. Also, comparison between simulation and experiment is rare, due to the long time scale (years) and difficulties in collecting experimental data.

2.2. Generalization of the open-source DMD solver

The DMD solver was developed to simulate the transport of hydrogen in palladium nanomaterials over a long period of time. It couples an atomistic non-equilibrium thermodynamics model with an empirical diffusion law. To model hydrogen diffusion in pipeline

(a)



(b)

Figure 11. Literature review of computational models and analysis of hydrogen embrittlement.

material (e.g., steels), the solver needs to be generalized in several aspects. First, palladium has an FCC (face-centered cubic) lattice structure, whereas steels have either the FCC or the BCC (body-centered cubic) lattice. Also, the DMD model requires an interatomic potential of the alloy as an input. Previously, we have implemented two EAM (embedded atom method) potentials for the Pd-H system. To model hydrogen diffusion in steels, new interatomic potentials need to be added to the solver.

In the reporting period, we have completed the code development needed to generalize DMD to support different lattice structures (e.g., FCC, BCC) and alloy constituents pertaining to pipeline steels. The upgraded solver, implemented in our open source code A2C, is capable of handling both single and multi-crystals, arbitrary lattice structures, and different materials (i.e., multiple interatomic potentials). It also allows the user to specify lattice defects such as voids and dislocations. The source code of A2C can be found at www.github.com/kevinwgy

Figure 12 shows the setup of a trial simulation that includes two nanoparticles with different geometry and lattice structure. One of the particles also contains two nanovoids that are not visible from this figure.

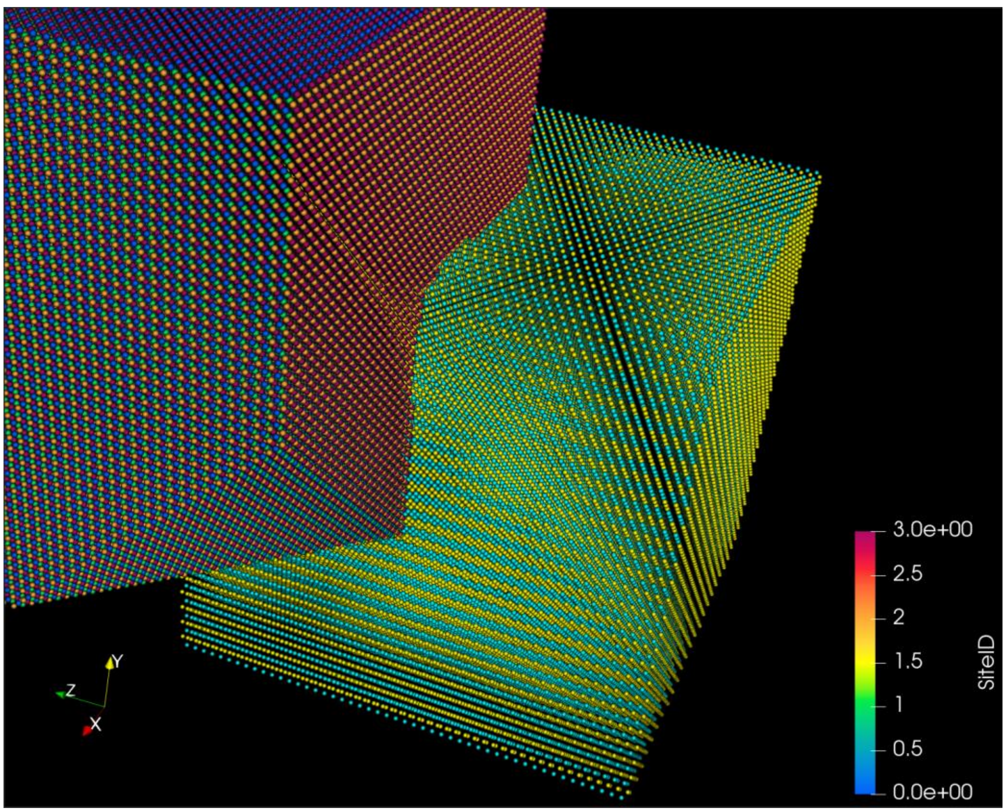


Figure 12. Screenshot of the GitHub repository of DMD.

Currently, we are modifying and extending the DMD solver to account for different lattice structures. In the next step, we will identify and implement interatomic potentials for pipeline steel materials into the solver. Then, deformation-diffusion coupled simulations can be performed to predict hydrogen absorption and the potential material damage. A screenshot of part of the input file that generated this model is shown below.

2. Future work

In the upcoming second year, our project will encompass a diverse range of activities, including experimental work, model formulation, and the development of a computational tool. Additionally, the project team will prioritize the completion of delayed tasks, specifically focusing on conducting hydrogen testing, to ensure the project remains on schedule and successfully concludes all remaining tasks. Our plan for the upcoming year involves the following research and development activities:

- Proceed with the development of a specific Failure Assessment Diagram (FAD) based on the existing standard and data, as outlined in Task 2.1 and Task 2.2.

- Continue the process of designing and selecting the most effective mitigation measures to alleviate the hydrogen effects, as specified in Task 2.2.

- Continue the construction of hydrogen test experiments, following the guidelines outlined in Task 3.1.

- Finalize the multi-scale hydrogen simulation model and conduct simulations to analyze the long-term effects, as outlined in Task 4.1.

- Work on comprehending and quantifying long-term hydrogen-induced pipe material degradation. Additionally, propose mitigation measures through micro-scale simulation, adhering to the tasks specified in Task 4.2 and Task 4.3.

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