CAAP Quarterly Report

07/01/2023

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

Contract Number: 693JK32250007CAAP

Prime University: North Dakota State University

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Reporting Period: 04/01/2023 – 07/01/2023

Project Activities for Reporting Period:

In the Quarter 1 and Quarter 2 report, Task 1 was completed and Task 2.1, 3.1 and 4.1 has started. In this quarter (Quarter 3), the research team has worked on Tasks 2.1, 2.2, 3.1, and 4.1. The summaries for the major activities that were completed during this reporting period are detailed below:

Task 2.1 Collection of hydrogen-related embrittlement fractural testing datasets and organized them based on the material property. During this reporting period, the research team (Dr. Zhibin Lin, Dr. Hong Pan, and Mohsin Ali Khan from NDSU) collected hydrogen embrittlement-related testing data and filtered it as summarized below.

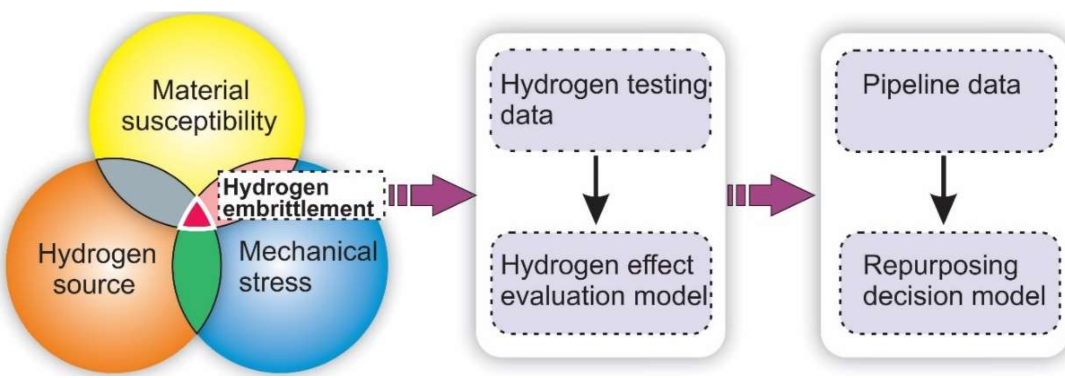


Figure 1. The Hydrogen repurposing decision model building process on the mechanical side

1) Hydrogen has a notable influence on the mechanical properties and durability of materials, especially metals. Its presence within a metal can result in a phenomenon called hydrogen embrittlement, which renders the material more susceptible to fracture and failure. In order to accurately quantify the impact of hydrogen embrittlement on the failure process, we are employing a decision model based on the process outlined in Figure 1.
2) Fracture mechanics plays a crucial role in quantifying the durability of materials and is an essential factor in estimating their service life. In our hydrogen mechanical process, we specifically consider the fatigue crack growth rate (FCGR). Generally, for metals, FCGR is expressed in the form of continuous crack (a) growth subjected to the variation in the number of load cycles (N) i.e.,

da/dN. The da/dN is commonly plotted against the primary factor i.e., stress intensity factor range ΔK. In addition, the da/dN also depends on several other factors including the load cyclic frequency (f), the waveform of applied load, stress ratio or load ratio $(R = K_{min}/K_{max})$, hydrogen gas pressure, microstructure and yield strength of the material, the temperature of the experimental chamber, and the injected impurities like oxygen, nitrogen, and Sulphur dioxide. We have collected 64 fatigue fracture testing data from different institutions as shown in Figure 2.

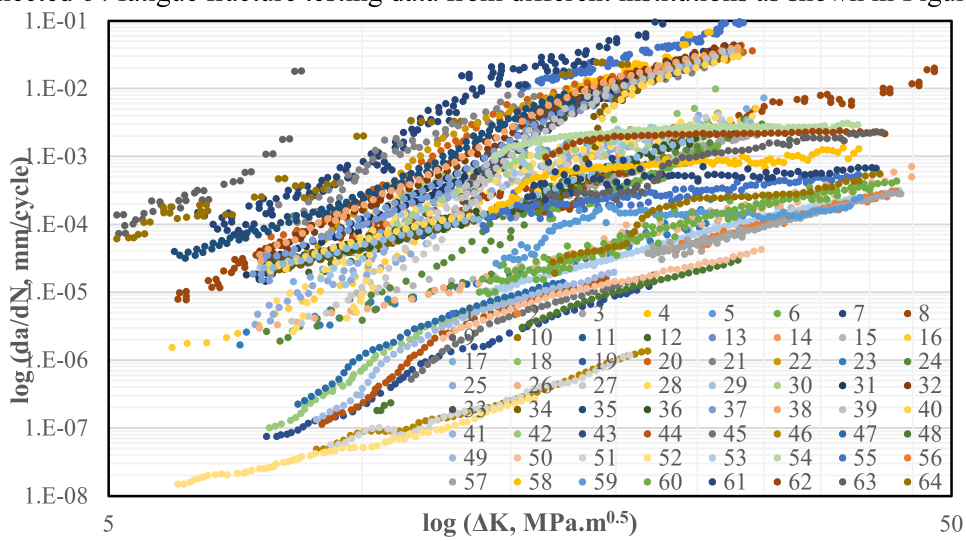
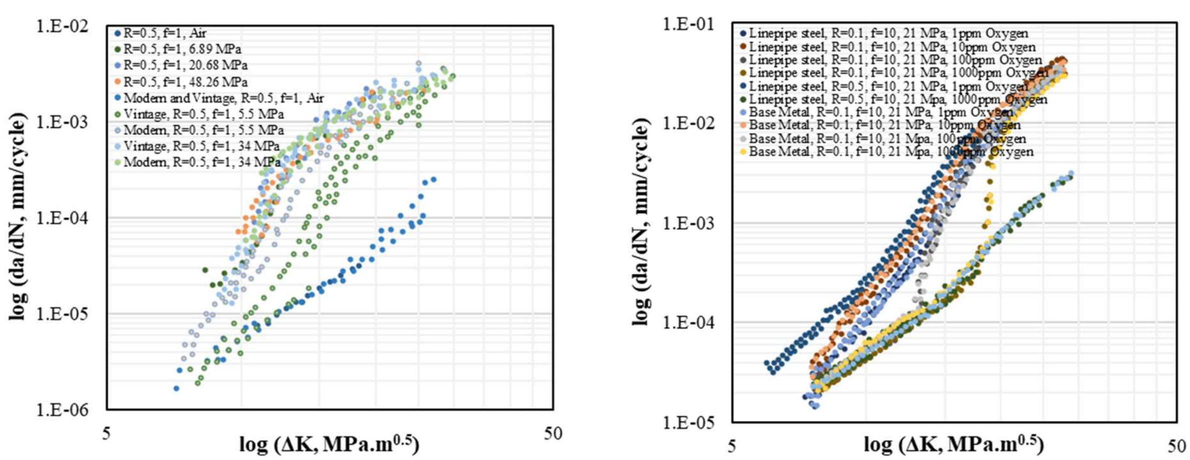


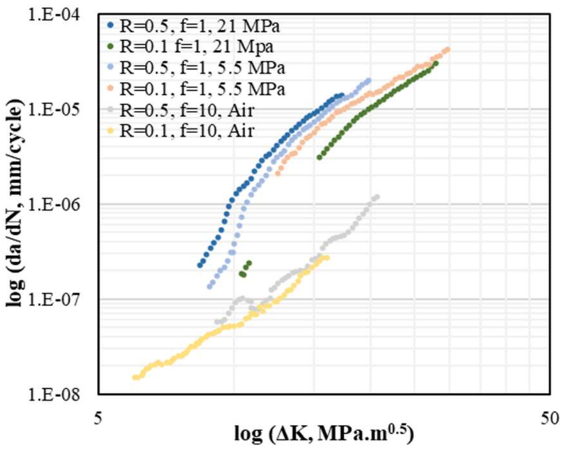
Figure 2. Fracture plot of different pipeline steel subjected to hydrogen environment (the detail of each legend is provided in Table 1)

3) To find the proper pattern behind different fracture testing, we have classified the FCGR based on different pipeline steels (e.g., X52, X60). The variation in the plots between different steel grades can be observed in Figure 2-10. The literature-derived plots indicate the higher susceptibility of the pipeline steel when subjected to a hydrogen environment. The variation of the da/dN in different ΔK regions is due to the variation in partial pressure of hydrogen, loading frequency, frequency waveform, loading ratio, temperature, and the injected impurities like oxygen and nitrogen.

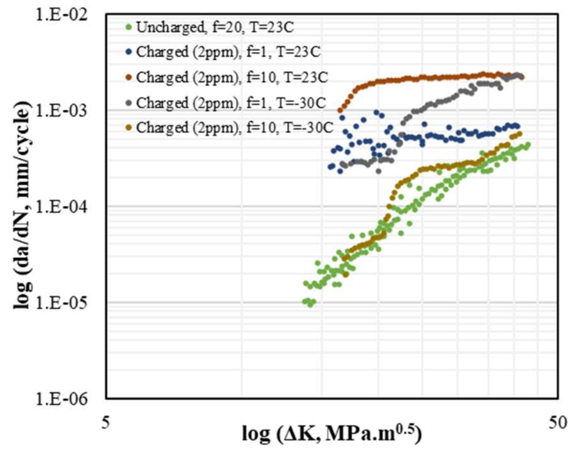


(a) FCGR plot of two different X52 pipeline steel, vintage and modern, with varying hydrogen pressure

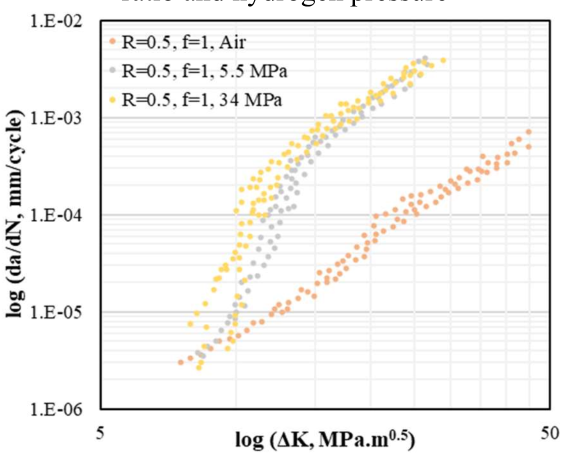
(b) FCGR plot of X52 pipeline steel and base metal with the injection of varying oxygen content, load ratio, and frequency



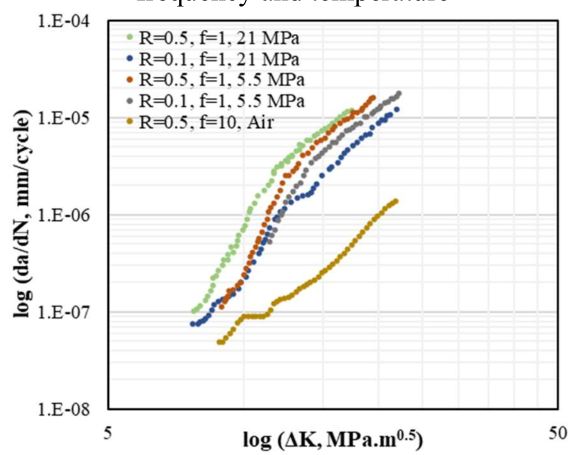
(c) FCGR plot of X60 steel with varying load ratio and hydrogen pressure



(d) FCGR plot of X65 steel with varying frequency and temperature



(e) FCGR plot of X70 steel with varying hydrogen pressure



(f) FCGR plot of X80 steel with varying load ratio and hydrogen pressure

Figure 3. FCGR plot of X80 steel with varying load ratio and hydrogen pressure

Task 2.2 Build a unified prediction model to quantitatively evaluate hydrogen embrittlement effects. During this reporting period, the research team (Dr. Zhibin Lin, Dr. Hong Pan, and Mohsin Ali Khan from NDSU) try to determine the hydrogen effects and quantify the relations between hydrogen effects and fracture curves.

1) As illustrated in Figure 4, the FCGR mainly for metallics is split into three different zones corresponding to three different stages of crack propagation i.e., Stage I (low ΔK region), stage II (intermediate ΔK region), and Stage III (higher ΔK region). In stage I, below the threshold (ΔK_{th}), the fatigue crack is inactive, indicating that the crack tip extension in the initial cycles is minute and the crack length is usually a few micrometers. Stage I can be prolonged using microstructure interfaces. Stage II indicates the prominent Paris's regime, the region of plasticity incorporates several grains, leading to lower microstructure reliance, which permits the use of a continuum approach to fracture driving force as a function of ΔK. In the mentioned region (10-6 to 10-4 mm/cycle), fracture propagation exhibits a pattern of power-law, generally modeled using the Paris Equation 1.

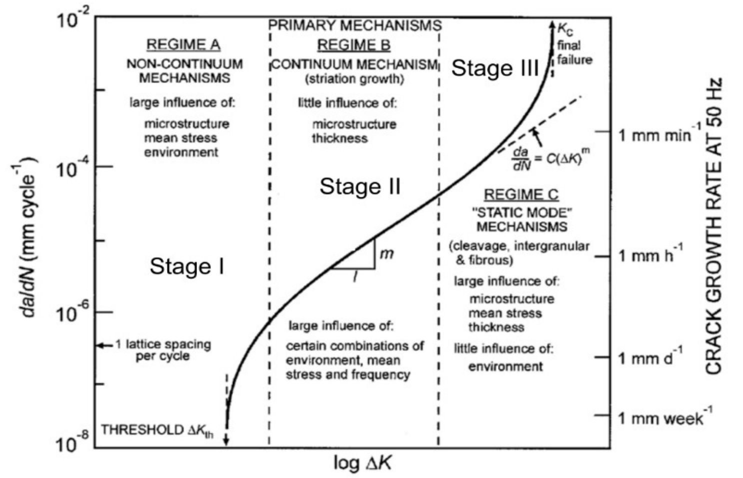


Figure 4. A typical illustration of the crack growth rate in different stages using the log-log plot of variation in fatigue crack growth rate (da/dN) against stress intensity factor ranges in metallic structure.

$$\frac{\mathrm{da}}{\mathrm{dN}} = \mathrm{C}(\Delta\mathrm{K})^{\mathrm{m}} \qquad (1)$$

where C and m are used to denote the materials constants. C is the intercept and m is the slope of the regression line of the log-log plot of da/dN vs ΔK. Without the presence of hydrogen, Stage II exhibits trans-granular fracture propagation, namely pipeline steels made of ferritic material. Lastly, stage III represents the occurrence of rapid crack propagation once the K_{max} reaches critical stress intensity (K_{IC}) considering plane strain provision.

2) The injection of hydrogen gas in the existing pipelines is widely recognized for accelerating ΔK. Therefore, to accurately determine the fatigue-related life span of pipelines used to transport gaseous hydrogen, it is essential to study and research in what manner the hydrogen-induced accelerated fatigue is affected by the partial pressure of hydrogen, loading frequency, frequency waveform, loading ratio, the temperature so on, as well as to comprehend the root cause of acceleration mechanisms. Typically, as illustrated in Figure 5, in the Paris region, a comparison of the FCGR plots produced for a gaseous hydrogen environment with those obtained for a similar material investigated in the air or an inert environment reveals the presence of three separate zones, which shows the curve plot. Note that the boundaries of the illustrated regions are significantly influenced by factors such as loading frequency and hydrogen gas pressure, as depicted in Figure 6. The crisp of findings based on these regions is provided below, which corresponds with the information presented in Figure 5.

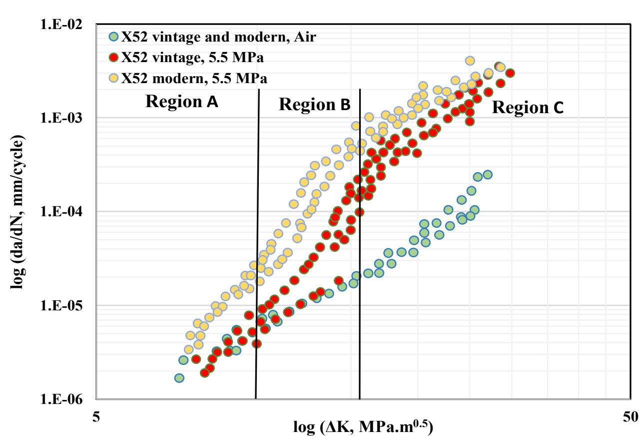


Figure 5. Variation of FCGR for vintage and modern steel pipeline for frequency 1Hz and load ratio 0.5.

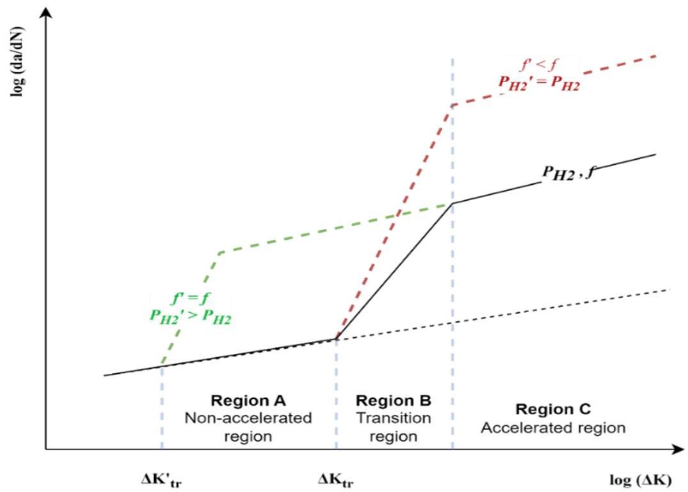


Figure 6. Generalized diagram showing trends of FCGR by the variation in the loading frequency and partial pressure of hydrogen gas.

According to ASME CC2938, the FCGR can be expressed as:

$$\frac{da}{dN} = C\left(\frac{1 + C_H R}{1 - R}\right)\Delta K^m \tag{2}$$

where R is the stress or load ratio. This equation modified the original equation (1) by emphasizing the effect of R. Similarly, In this research, we will change these equations according to the piecewise linear relations in different regions as illustrated in Figure 6 to formulate unified fracture crack growth equations which will become critical support for your repurposing models as shown in Figure 1

Task 3.1 Preparing the near real-world testbed for hydrogen testing: During this reporting period, the research team (Mr. J. Anderson from EERC) has discussed two potential sitting spots for the fabrication of the pipeline. The spot will be decided once the team has finished a HAZOP of the system design. The progress on EERC for this reporting period is summarized below:

1) A team was put together to begin official designs and planning of the fabrication of the pipeline.
2) A process flow diagram (PFD) and a piping and instrumentation diagram (PID) have been developed and are ready to go into review, as demonstrated in Figure *7*.
3) The use of activated carbon or zeolite will be necessary to remove the mercaptans from the natural gas to use the storage tank on site.
4) Plans have been made to begin material purchasing upon a successful HAZOP review.
5) The design of the pipeline itself has been changed from being a loop to a straight section, with 3 middle sections that will be the variables to be tested and the end sections made of 316 SS to better withstand the effects of hydrogen and support a more durable and lasting system lifespan.

Task 4.1 Gaining an understanding of long-term hydrogen impacts: In the reporting period, the Virginia Tech team (Dr. K. Wang from Virginia Tech) generalization of current diffusive molecular dynamics (DMD) and added the new features in the code to the user manual as detailed below.

1) 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 about pipeline steels as shown in Figure 8. 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

2) 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 potential material damage.

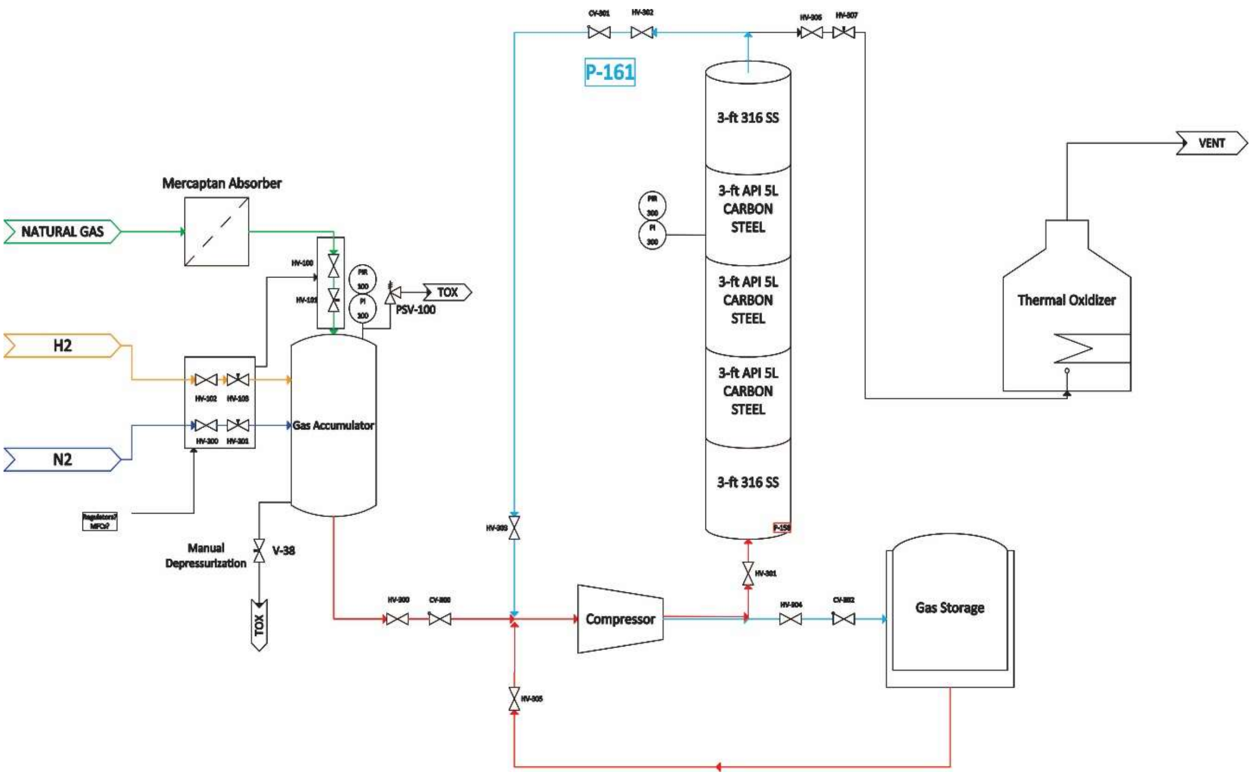


Figure 7. The designed testing PFD.

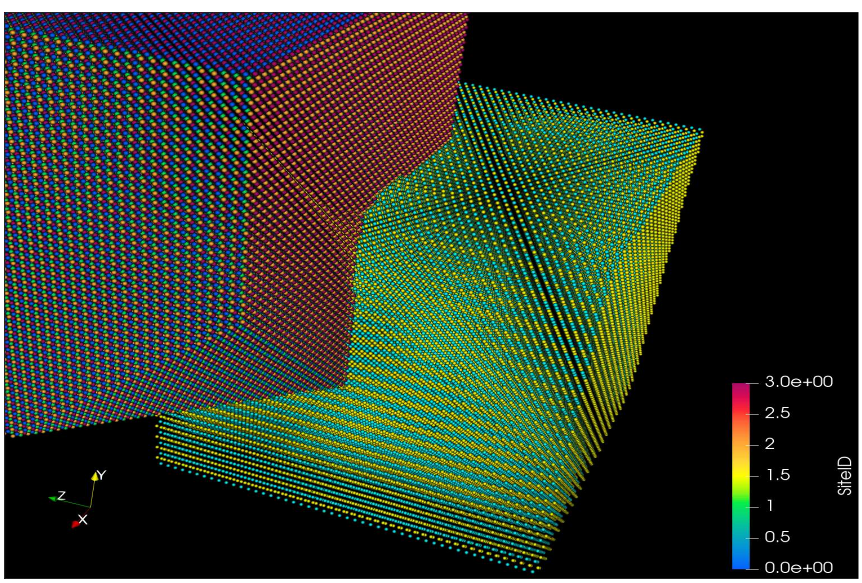


Figure 8. Screenshot of the GitHub repository of DMD.

Project Financial Activities Incurred during the Reporting Period:

The cost breakdown during the reporting period in each category according to the budget proposal is shown in Table 1.

Table 1 Cost breakdown during the reporting period (Q3)

Category	Amount spent during Q3
Personnel	
Faculty	$10200
Postdoc	$9,000
Students (RA and UR)	$9,000
Benefits	$8,910
Operating Expenses	
Travel	$0
Materials and Supplies	$0
Recharge Center Fee	$0
Consultant Fee	$0
Subcontracts	Subawards issued
Indirect Costs	$16,700

Project Activities with Cost Share Partners:

The Match fund from NDSU for this project is coming from faculty academy hours of NDSU and Virginia Tech, and two Ph.D. students' RA tuition waivers. The matching fund from Dr. Lin (NDSU) and Dr. Wang (Virginia Tech) during Q3 is estimated to be $13,341, and the students' RA tuition waiver is about $16,560, so the total amount of match is estimated at $29,9901.

Project Activities with External Partners:

During this reporting period, the research team meets regularly bi-weekly, and the sub-universities have researched as planned. Also, the research team invited Chris San Marchi from Sandia National Laboratories to present his works on pipeline-related hydrogen effects.

Potential Project Risks:

No potential risks were noticed during this reporting period.

Future Project Work:

In the next quarter, the research team will continue working on Tasks 2.2, 3.1, and 4.1, and expand the work onto Task 2.2 as planned.

Potential Impacts on Pipeline Safety:

The collected FCGR datasets can be expanded to a hydrogen fracture benchmark dataset with further clearing and collection. The benchmark datasets are critical for the public and researchers to mine more knowledge and models to guild the design and repurposing of pipelines.