6TH QUARTERLY REPORT - PUBLIC
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Validating Non-Destructive Tools for Surface to Bulk Correlations of Yield Strength, Toughness, and Chemistry

Reporting Period
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PROJECT OBJECTIVES AND REPORT SUMMARY

Project Objectives

The deliverables of this project will facilitate the use of non-destructive surface testing: micro-indentation, micro-machining, in situ chemistry, and replicate microscopy analysis as accurate, efficient, and cost-effective tools for material property confirmation.

This work will provide benefits to pipeline safety, energy continuity, and integrity assessment programs since the developed techniques and models and validated testing technology will not require a line to be taken out of service or destructively cut out samples from the in-service pipeline.

The results of this project will also be applicable to pending DOT/PHMSA regulations that require operators to backfill their material property records for grandfathered pipeline segments and/or those that do not have adequate material records.

Report Summary

During the sixth project quarter the following items were completed (see the **Technical Status** section for greater detail):

Task 2 - Develop Project Database and Pipeline Sample Library

- GTI completed the Project Pipeline Sample Library (Milestone Number **M11**) and this is included in this quarterly report in **Appendix A.**
- During the quarter the first half (35 of 70) of the project pipe sample data set was sent to ASU to start more in depth and "second generation" modeling efforts beyond the 20-pipe sample calibration set that was sent to ASU earlier in the project.

Task 3 – Develop and Execute Testing Matrix

- GTI completed a quality control review of the MMT NDE report and data and addressed on issue with the grain size data reporting which was subsequently resolved by MMT.
- Lab-based (destructive) testing continued during the quarter as scheduled, and GTI is working on the last dozen pipe samples and hopes to have these completed within the next quarter or two.
- Once these destructive tests are done GTI will select 30 samples for destructive Charpy toughness testing and also MMT NDTT non-destructive toughness testing noted above. The NDTT testing is the last of the NDE testing remaining for the project.

Task 4 – Data Analysis and Model Development and Optimization (see Appendix B)

- This quarter's work included a semi-parametric Gaussian Process regression applied to predict the yield strength of pipes and compared with the traditional linear regression.
- A detailed report of this quarter's modeling efforts and results is presented in **Appendix B** of this report.

Task 6 – Project Management

- Submitted Milestone Item **M11** (**Appendix A** of this report) - Project Pipeline Sample Library.
- Submitted Milestone Item **M12**, the sixth project quarterly report.

Risks

- There are no current risks to scope, schedule, budget.

BUSINESS AND MILESTONE STATUS
(Project Quarter #6: 11/1/2019 to 1/31/2020)

Tasks Scheduled in this Reporting Period

Table 1 shows the project tasks performed in this reporting period. All tasks are on time or ahead of schedule.

Table 1: Lists of Tasks in this Reporting Period

Task	Scheduled Start	Scheduled Completion	Completion Status
Task 2 - Develop Project Database and Pipeline Sample Library	11/1/2018	1/31/2020	Completed
Task 3 - Develop and Execute Testing Matrix	5/1/2019 (1)	10/31/2020	Ongoing
Task 4 - Data Analysis and Model Development and Optimization	8/1/2019 (1)	1/31/2021	Ongoing
Task 6 - Project Management	8/1/2018	4/30/2021	Ongoing
- 6TH Quarter Project Report	11/1/2019	1/31/2020	Completed

(1) GTI started Tasks 3 early to allow early coordination with NDE subcontractors and service providers; ASU and GTI started work in Task 4 early to develop a framework for model experimentation and testing of model performance with the calibration data set provided early by GTI. Task 3 is additionally ahead of schedule. Task 4 is on schedule.

Milestones for Activities/Deliverables Completed

Table 2 shows the project milestones for activities/deliverables/tasks completed in this reporting period. All Milestones/Deliverables are on time or ahead of schedule.

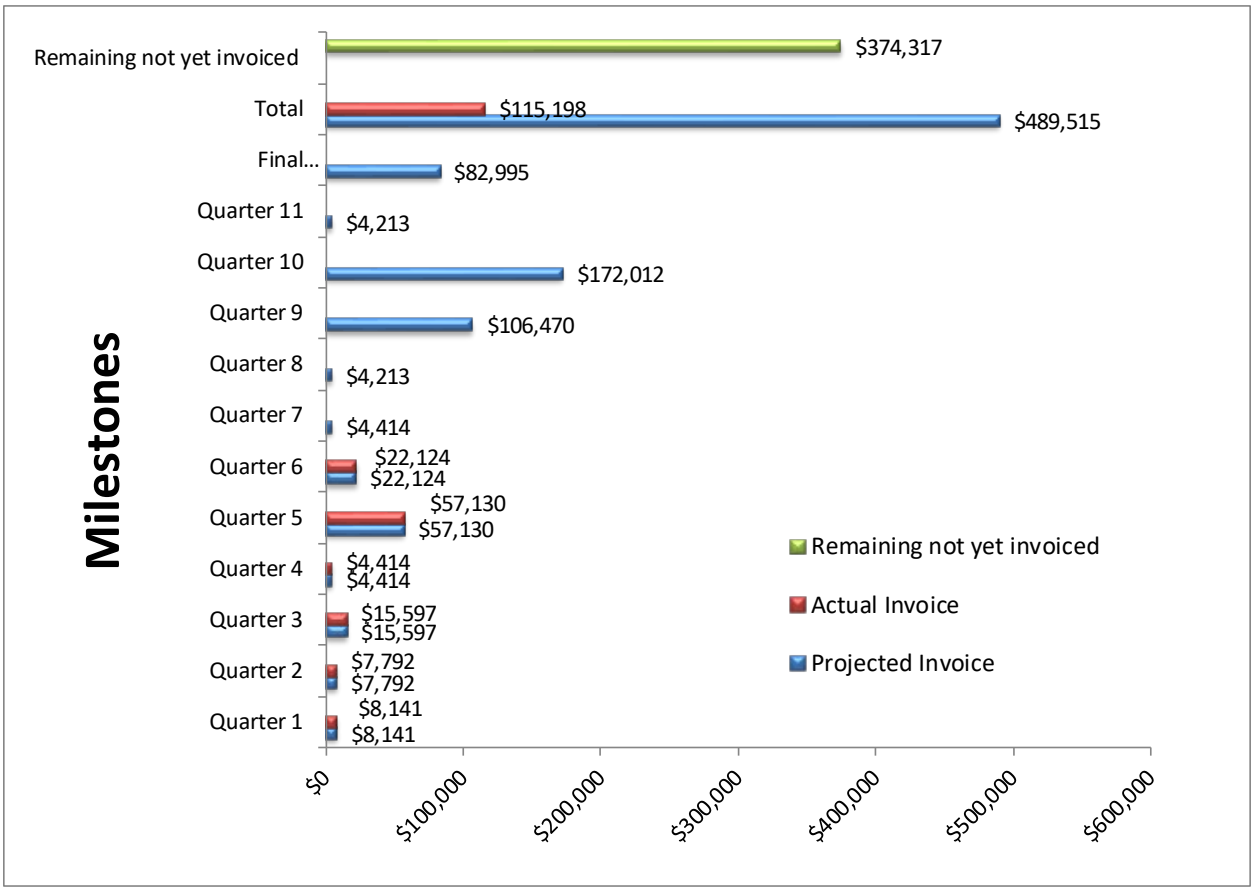
Table 2: Lists of Milestones Linked to Activities/Deliverables/Tasks this Reporting Period

Item No.	Task No.	Activity/Deliverable	Quarter No.	Scheduled Due Date	Completion Date	Payable Milestone/Title
11	2	Develop Project Database and Pipeline Sample Library	6	1/31/2020	1/31/2020	Submit Summary of Pipe Sample Library
12	6	6th Quarterly Status Report	6	1/31/2020	1/31/2020	Submit 6th quarterly report

Resource Status

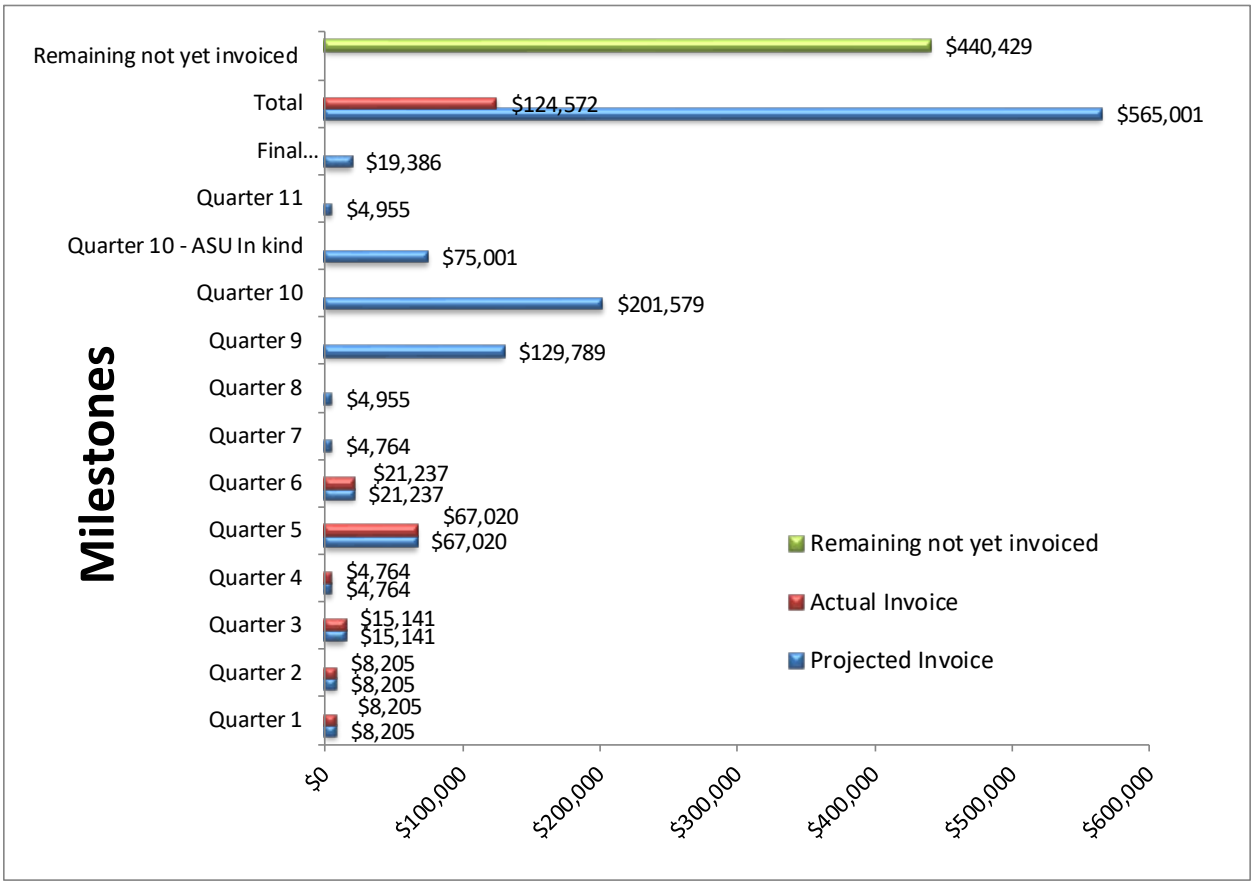
The nature of the contract for this research effort is fixed price, with clearly defined milestone/deliverable payments. Please see Figure 1 for an update on the fund status for DOT/PHMSA, and Figure 2 for the fund status of OTD and ASU.

Figure 1: Quarterly Payable Milestones/Invoices – DOT PHMSA



The sixth quarter invoice will be issued shortly after the end of the 6th project quarter.

Figure 2: Quarterly Payable Milestones/Invoices – OTD and ASU



The sixth quarter invoice will be issued shortly after the end of the 6th project quarter.

Project Risks

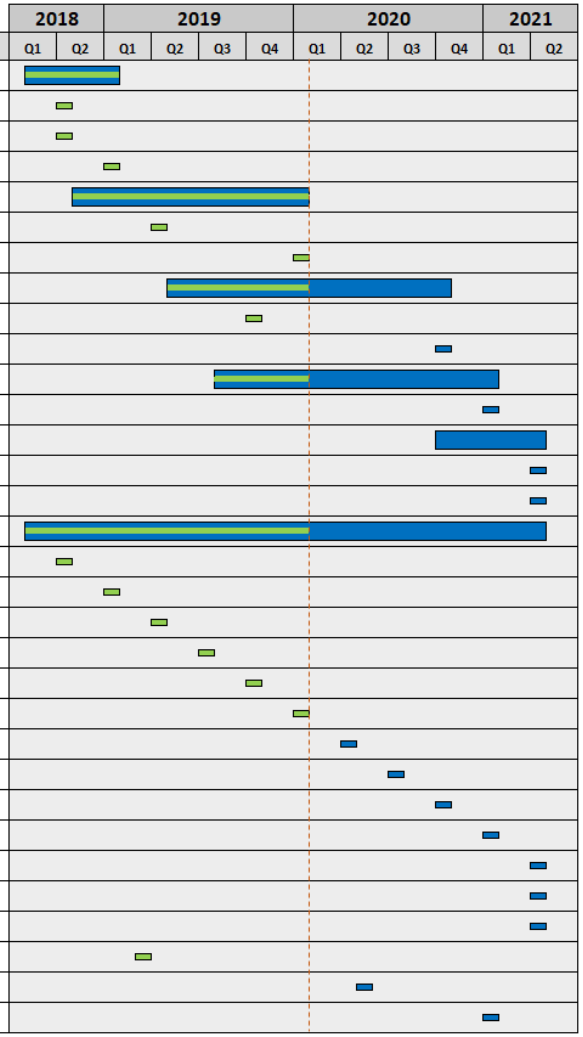
There are currently no risks to the project scope, schedule, or budget.

Schedule Update

The updated project schedule is shown in Figure 3.

Figure 3: Project Schedule

ID	Month	Task / Milestone Name	Start	Finish	% Complete
1	---	Task 1 - Form Technical Advisory Panel and Scope Confirmation	8/1/2018	1/31/2019	100%
2	1	M1 - Conduct kick-team meeting and present scope of work and objectives	10/31/2018	10/31/2018	100%
3	3	M2 - Submit final TAP list and finalize tasks and methods	10/31/2018	10/31/2018	100%
4	6	M4 - Confirmation of subcontract SOW in place	1/31/2019	1/31/2019	100%
5	---	Task 2 - Develop Project Database and Pipeline Sample Library	11/1/2018	1/31/2020	100%
6	9	M6 - Develop a project database on existing data	4/30/2019	4/30/2019	100%
7	18	M11 - Submit summary of pipeline sample library	1/31/2020	1/31/2020	100%
8	---	Task 3 - Develop & Execute Test Matrix	5/1/2019	10/31/2020	50%
9	15	M9 - Submit project testing/plan matrix	10/31/2019	10/31/2019	100%
10	27	M15 - Submit summary of executed testing plan data input into project database	10/31/2020	10/31/2020	0%
11	---	Task 4 - Data Analysis and Model Development and Optimization	8/1/2019	1/31/2021	30%
12	30	M17 - Summary of data analysis and model generation and optimization submitted	1/31/2021	1/31/2021	0%
13	---	Task 5 - Final Report and Implementation Guide	10/31/2020	4/30/2021	0%
14	33	M25 - Prepare and submit final draft report	4/30/2021	4/30/2021	0%
15	NA	M26 - Address comments and submit final report	4/30/2021	4/30/2021	0%
16	---	Task 6 - Project Management	8/1/2018	4/30/2021	50%
17	3	M3 - Submit quarterly report - Q1	10/31/2018	10/31/2018	100%
18	6	M5 - Submit quarterly report - Q2	1/31/2019	1/31/2019	100%
19	9	M7 - Submit quarterly report - Q3	4/30/2019	4/30/2019	100%
20	12	M8 - Submit quarterly report - Q4	7/31/2019	7/31/2019	100%
21	15	M10 - Submit quarterly report - Q5	10/31/2019	10/31/2019	100%
22	18	M12 - Submit quarterly report - Q6	1/31/2020	1/31/2020	100%
23	21	M13 - Submit quarterly report - Q7	4/30/2020	4/30/2020	0%
24	24	M14 - Submit quarterly report - Q8	7/31/2020	7/31/2020	0%
25	27	M16 - Submit quarterly report - Q9	10/31/2020	10/31/2020	0%
26	30	M18 - Submit quarterly report - Q10	1/31/2021	1/31/2021	0%
27	33	M19 - Submit quarterly report - Q11	4/30/2021	4/30/2021	0%
28	NA	M20 - Present at public event or publish a paper	4/30/2021	4/30/2021	0%
29	NA	M21 - Final virtual meeting	4/30/2021	4/30/2021	0%
30	NA	M22 - Peer review #1 (date TBD)	5/1/2019	5/1/2019	100%
31	NA	M23 - Peer review #2 (date TBD)	5/1/2020	5/1/2020	0%
32	NA	M24 - Peer review #3 (date TBD)	1/1/2021	1/1/2021	0%



TECHNICAL STATUS
(Project Quarter #6: 11/1/2019 to 1/31/2020)

This section provides a high-level overview of the technical activities during the reporting quarter and the status.

Additional details, reports, presentations and other support material is placed in this report's Appendix and referenced below.

Task 2 - Develop Project Database and Pipeline Sample Library

1. GTI completed the development of the project sample library. The overall library has been established with a diverse and realistic set of 70 pipeline samples.
2. GTI completed the Project Pipeline Sample Library (Milestone Number **M11**) and this is included in this quarterly report in **Appendix A**.
3. The sample library of 70 was divided into two groups of 35 pipe samples. This allows for the Task 4 modeling activities to continue model development with half the project results while the other half of the testing is being completed. Then the remaining 35 sample data set will be turned over to complete the modeling activities.
4. During this 6th quarter, the first half (35 samples) of the project pipe samples data set was sent to ASU to start the second tier modeling efforts.

Task 3 - Develop and Execute Testing Matrix

1. **MMT Testing Draft Report of Testing**
    a. GTI completed a quality control review of the report and data and addressed on issue with the grain size data reporting which was resolved by MMT.
2. **Remaining Nondestructive Testing**
    a. The NDE testing phase of the project from MMT, Frontics, and SciApps is completed with the exception of the 30 small coupons that will be tested later in the project at the MMT labs using their prototype NDTT toughness testing system.
    b. Once the destructive testing in item (3) directly below is completed, GTI will select the 30 samples to section coupons out and send to MMT for NDTT testing.
3. **Lab-Based (Destructive) Testing**
    a. This lab testing continued in Quarter 6, which included full wall tensile, hardness, chemistry, and grain size. Ongoing testing includes:
        - Full wall tensile tests per ASTM A370 with 1"-gauge length longitudinal specimens and an average of 3 specimens

- Lab GDS chemistry at 4 different depths. (0.005", 0.020", 3/4 thickness and mid thickness. Includes C, S, and P by GDS
- Bulk ICP + Bulk LECO E1019 C & S Spark Arc
- Bulk N by Leco fusion technique.
- Grain size near surface, 1/4 pt, and center for both longitudinal and transverse sections, average of 6 readings
- Average of near surface grain sizes (~0.005" deep) longitudinal and transverse specimens
- OD Rockwell B hardness after ~ 0.005" surface grind
- ID Rockwell B hardness after ~ 0.005" surface grind

b. GTI is working on the last dozen pipe samples and hopes to have these completed within the next quarter or two.

Task 4 - Data Analysis and Model Development and Optimization

A detailed report of this quarter's modeling efforts and results is presented in **Appendix B** of this report. A high-level summary of these results is presented below:

1. With the first dataset including 20 samples, semi-parametric Gaussian Process regression was applied to predict the yield strength of pipes and compared with the traditional linear regression.
2. Through doing the general case study and specific case study, it was concluded that the SGP modeling has a similar performance of linear regression model.
3. While if the dimension goes up with unchanged training set or the training set becomes smaller with unchanged dimensions, the linear regression will be slightly better than SGP regression.
4. However, the benefit of using SGP model is that the prediction confidence bound can be estimated directly which is very valuable in data analysis.
5. In addition, the SGP modeling has a great potential to achieve better predictive performance as long as having more training data.

Task 6 - Project Management

1. Submitted Milestone Item **M11** (**Appendix A** of this report) - Project Pipeline Sample Library.
2. Submitted Milestone Item **M12**, the sixth project quarterly report.

PLANS FOR FUTURE ACTIVITY
(Project Quarter #7: 2/1/2020 to 4/30/2020)

In the next quarter the project team will continue work on Tasks 3 and 4. The planned activities are listed below.

Task 3 - Develop and Execute Testing Matrix

a. Baseline (referee) lab-based testing will continue and run into the first half of 2020. This testing includes the remaining full wall tensile, hardness, chemistry, Charpy, and grain size, specifically, the tests include:
   - Full wall tensile tests per ASTM A370 with 1"-gauge length longitudinal specimens and an average of 3 specimens
   - Lab GDS chemistry at 4 different depths. (0.005", 0.020", 3/4 thickness and mid thickness. Includes C, S, and P by GDS
   - Bulk ICP + Bulk LECO E1019 C & S Spark Arc
   - Bulk N by Leco fusion technique.
   - Grain size near surface, 1/4 pt, and center for both longitudinal and transverse sections, average of 6 readings
   - Average of near surface grain sizes (~0.005" deep) longitudinal and transverse specimens
   - OD Rockwell B hardness after ~ 0.005" surface grind
   - ID Rockwell B hardness after ~ 0.005" surface grind
b. As the full-wall thickness baseline and surface-based chemical testing is completed and organized, GTI will continue the selection process for the 30 toughness coupons that will be sent to MMT for NDTT (a lab prototype surface-based toughness testing unit) calibration testing. GTI will also complete Charpy toughness testing to generate full S-curves for impact energy, lateral expansion, and %-shear failure.

Task 4 - Data Analysis and Model Development and Optimization

a. In the next quarter ASU will apply the developed Bayesian model selection, linear/nonlinear regression, and GP model to the newly obtained dataset (of 35 pipe samples) for demonstration and validation. ASU will also extend this same methodology for ultimate strength and toughness estimation.
b. GTI and ASU held several technical meetings in the last quarter and have firmed up the final modeling methods that will be used for the data analysis.
c. The Modeling Chapters that will be included in the analysis are shown in Table 3.

Table 3: Modeling Chapters Planned for Task 4 Data Analysis of Full Data Set

DOT Surface to Bulk Correlation – Modeling Chapters			
Lead	**Model #**	**Model Description**	**Abbreviation**
ASU	**1**	Parametric Ordinary Least Squares Linear Regression Models	**OLS-LR**
	2	Parametric OLS LR Model with Occam Reduction	**OR**
	3	Non-Parametric Pure Bayesian Network Model	**BNM**
	4	Semi-Parametric Gaussian Process and Semi-Gaussian Process Modeling	**GP & SGP**
	5	Bayesian Model Averaging applied to mix of OLS LR (w/ and w/out OR); BNM; and GP/SGP	**BMA**
	6	Manifold Learning Model	**MLM**
GTI	**7**	Descriptive Statistics	**DS**
	8	Causal Path Diagram with Structural Equation Modeling	**PD / SEM**
	9	Meta-Modeling	**MM**

Task 6 - Project Management

a. Submit seventh project quarterly report to DOT - Milestone Item **M13**, due 4/30/2020.

Respectfully submitted by,

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End of Quarterly Report Body

APPENDIX A – Project Pipeline Sample Library (M11)

In Table 4 below each row is a property of the pipeline sample library sample. These are the attributes about the pipe sample, generally reported at the time of submission and/or as determined by physical testing, e.g. for "chemistry grade". If a value is unknown it is stated as "Unknown" and if it was not reported it is stated as "NotReported". If additional testing is needed to determine a value it will have a place holder "TBD" for to be determined.

Table 4: Pipeline Sample Library Attribute Descriptions

Pipeline Attribute	Description of Attribute
arbitrary number	Arbitrary number from 1 to 70, not the official pipe library number
diameter nominal	Nominal diameter of the pipe in inches
wall thickness	Wall thickness of the pipe in inches without any treatment to the sample
year installed	Specifies the installation date as provided by the utilities
grade reported	Shows the steel grade as known by the utilities
steel type	Specifies the GTI estimate of steel (rimmed, capped, killed Si, killed, Al, semi-killed)
chemistry grade	States the steel grade as per SAE-ASTM
long seam type	Long seam weld type according to inspection

A series of four plots show the distribution of some of the pipeline attributes in Figure 4 to Figure 7. A small jitter was added to the plotted points if the categorical values for pairs were overlapping in these plots.

The sample set of seventy (70) pipelines has an excellent distribution of properties and along with the additional calibration set of twenty (20) pipelines will provide a diverse and realistic pipe sample set for the project, testing, and modeling.

Figure 4: Diameter vs. Wall Thickness.

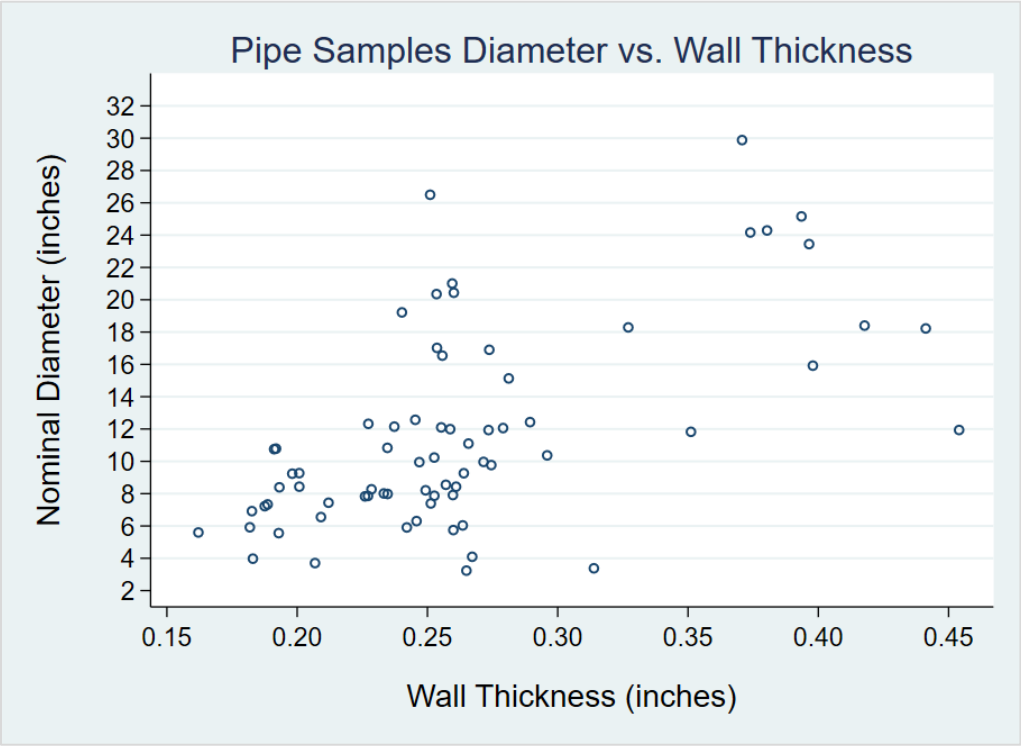


Figure 5: Steel Type vs. Long Seam Type.

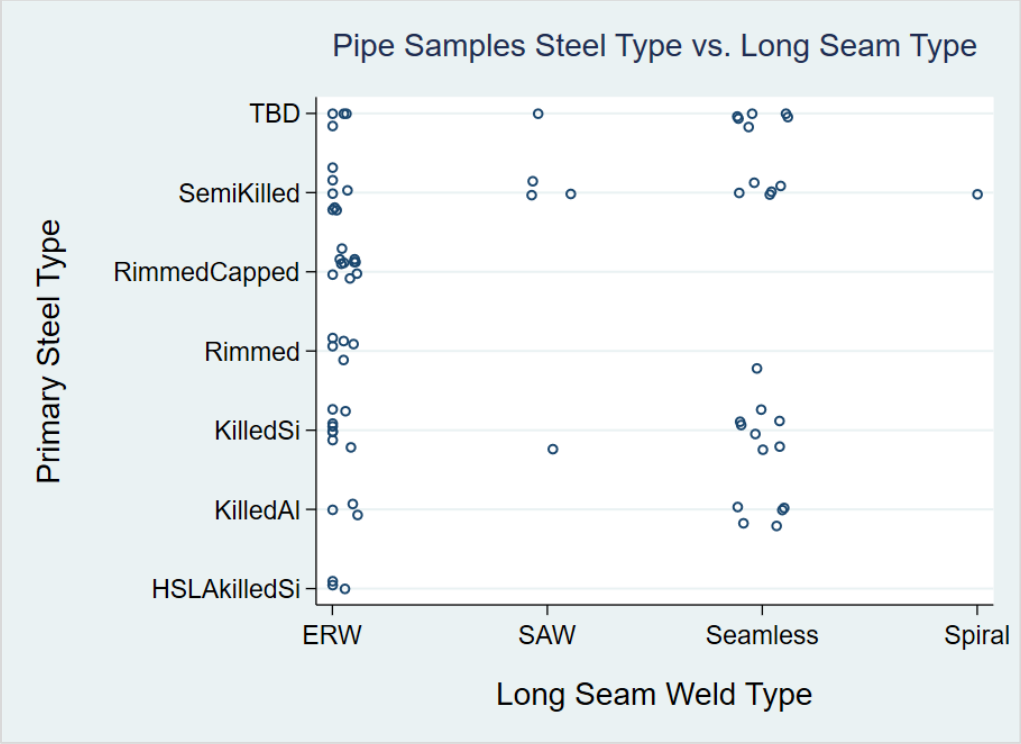


Figure 6: Year Installed vs. Pipe Grade Reported.

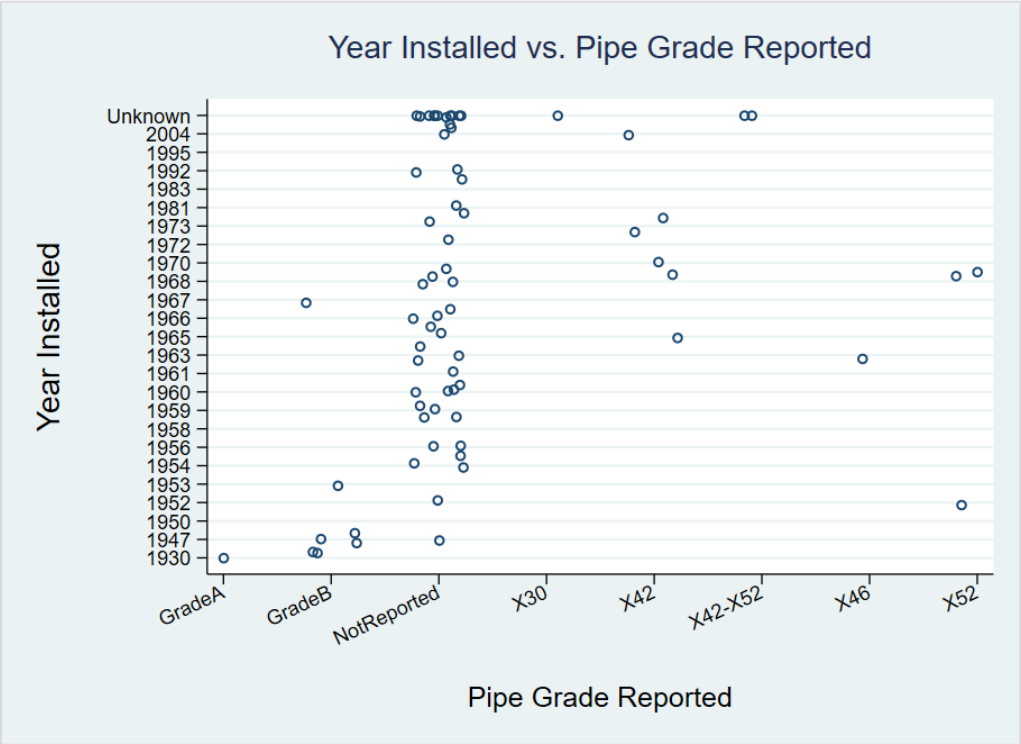
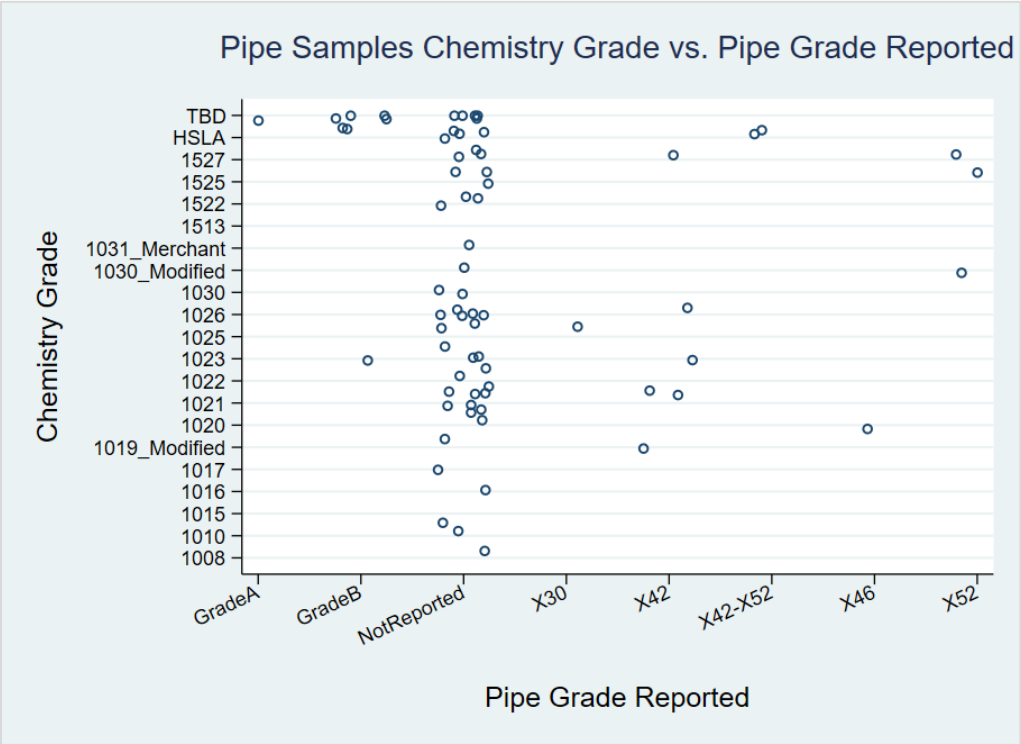


Figure 7: Chemistry Grade vs. Pipe Grade Reported.



The pipeline sample attributes are listed in Table 5 below.

Table 5: Pipeline Sample Library

arbitrary_number	diameter_nominal	wall_thickness	year_installed	grade_reported	steel_type	chemistry_grade	long_seam_type
1	4	0.19	1966	NotReported	KilledAl	1017	ERW
2	4	0.202	1959	NotReported	RimmedCapped	1021	ERW
3	4	0.263	1960	NotReported	SemiKilled	1023	ERW
4	4	0.266	1960	NotReported	SemiKilled	1023	ERW
5	4	0.319	1960	NotReported	KilledAl	1020	Seamless
6	6	0.159	Unknown	NotReported	Rimmed	1026	ERW
7	6	0.183	1965	NotReported	KilledSi	1025	ERW
8	6	0.188	1992	NotReported	KilledSi	1522	ERW
9	6	0.198	1965	NotReported	KilledSi	1025	ERW
10	6	0.203	Unknown	NotReported	RimmedCapped	1022	ERW
11	6	0.24	1960	NotReported	Rimmed	1008	ERW
12	6	0.24	Unknown	NotReported	SemiKilled	1021	Seamless
13	6	0.253	1981	NotReported	KilledAl	1022	ERW
14	6	0.261	1960	NotReported	SemiKilled	1026	Seamless
15	8	0.188	1966	NotReported	SemiKilled	1525	ERW
16	8	0.189	1958	NotReported	Rimmed	1015	Seamless
17	8	0.19	1966	NotReported	RimmedCapped	1021	ERW
18	8	0.203	1965	NotReported	SemiKilled	1525	Seamless
19	8	0.217	1947	GradeB	TBD	TBD	ERW
20	8	0.219	1947	GradeB	TBD	TBD	Seamless
21	8	0.222	1947	GradeB	TBD	TBD	Seamless
22	8	0.234	1967	GradeB	TBD	TBD	Seamless

arbitrary_number	diameter_nominal	wall_thickness	year_installed	grade_reported	steel_type	chemistry_grade	long_seam_type
23	8	0.236	1947	GradeB	TBD	TBD	Seamless
24	8	0.241	1960	NotReported	SemiKilled	1026	Seamless
25	8	0.251	1968	NotReported	Rimmed	1026	ERW
26	8	0.253	1954	NotReported	RimmedCapped	1525	ERW
27	8	0.255	1954	NotReported	RimmedCapped	1021	ERW
28	8	0.255	1968	NotReported	RimmedCapped	1020	ERW
29	8	0.255	1947	GradeB	TBD	TBD	Seamless
30	8	0.257	1968	NotReported	RimmedCapped	1021	ERW
31	10	0.188	Unknown	NotReported	TBD	TBD	ERW
32	10	0.188	1967	NotReported	TBD	TBD	ERW
33	10	0.193	1995	NotReported	KilledSi	1021	ERW
34	10	0.196	1983	NotReported	KilledSi	HSLA	Seamless
35	10	0.231	Unknown	NotReported	KilledSi	HSLA	ERW
36	10	0.247	Unknown	NotReported	KilledAl	HSLA	ERW
37	10	0.252	Unknown	NotReported	SemiKilled	HSLA	ERW
38	10	0.26	1963	NotReported	KilledAl	1525	Seamless
39	10	0.266	1963	NotReported	KilledAl	1026	Seamless
40	10	0.267	Unknown	NotReported	SemiKilled	1525	ERW
41	10	0.281	1930	GradeA	TBD	TBD	Seamless
42	10	0.302	Unknown	NotReported	KilledSi	1025	Seamless
43	12	0.23	Unknown	X42-X52	HSLAkilledSi	HSLA	ERW
44	12	0.242	Unknown	X42-X52	HSLAkilledSi	HSLA	ERW
45	12	0.251	1961	NotReported	Rimmed	1010	ERW
46	12	0.259	Unknown	NotReported	TBD	TBD	ERW
47	12	0.262	1954	NotReported	KilledAl	1030	Seamless
48	12	0.267	1965	X42	SemiKilled	1023	SAW
49	12	0.273	1956	NotReported	KilledAl	1016	Seamless
50	12	0.283	1983	NotReported	RimmedCapped	1525	ERW

arbitrary_number	diameter_nominal	wall_thickness	year_installed	grade_reported	steel_type	chemistry_grade	long_seam_type
51	12	0.353	1963	X46	KilledSi	1020	Seamless
52	12	0.461	2004	X42	KilledSi	1019_Modified	ERW
53	16	0.251	1970	NotReported	RimmedCapped	1022	ERW
54	16	0.261	1972	X42	SemiKilled	1021	ERW
55	16	0.274	1950	NotReported	KilledSi	1026	Seamless
56	16	0.281	1950	NotReported	KilledSi	1031_Merchant	Seamless
57	16	0.396	1953	GradeB	SemiKilled	1023	Spiral
58	18	0.322	1968	X42	SemiKilled	1026	Seamless
59	18	0.413	1968	X52	KilledSi	1525	Seamless
60	18	0.447	1968	X52	KilledSi	1527	Seamless
61	20	0.239	1972	X42	SemiKilled	HSLA	ERW
62	20	0.251	1973	X42	RimmedCapped	1021	ERW
63	20	0.257	Unknown	X30	Rimmed	1025	ERW
64	20	0.262	1972	NotReported	TBD	TBD	SAW
65	24	0.375	Unknown	NotReported	KilledSi	HSLA	ERW
66	24	0.383	Unknown	NotReported	KilledSi	HSLA	ERW
67	24	0.393	Unknown	NotReported	HSLAkilledSi	HSLA	ERW
68	26	0.255	1958	NotReported	SemiKilled	1021	SAW
69	26	0.392	Unknown	NotReported	KilledSi	1513	SAW
70	30	0.375	1952	X52	SemiKilled	1030_Modified	SAW

APPENDIX B – ASU Task 4 (6TH Quarter Update)

6TH QUARTER – INPUT FROM ASU
DOT Project Number: 729 (GTI 22428)
DOT Contract Number: 693JK31810003
OTD Project Number: 4.14.c.2 (GTI 22429)

Validating Non-Destructive Tools for Surface to Bulk Correlations of Yield Strength, Toughness, and Chemistry

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Abstract

Gaussian Process is one of the most popular non-parametric machine learning approach which can learn from training data directly. Unfortunately, non-parametric GP need a large amount of training data covering the state space to guarantee good predictive performance. In this research, semi-parametric Gaussian Process is proposed to predict the yield strength due to the limited training set. The input variables are selected by linear method including hardness, chemical composition Cu and Cr. Both two-dimensional (two inputs) and three-dimensional (three inputs) analysis are conducted. Then the predictive performance is compared among linear regression and semi-parametric Gaussian Process in terms of general case study and specific case study. The results show that the linear regression is slightly better than the semi-parametric Gaussian Process. As the dimension increases and the number of training data unchanged, the performance of the semi-parametric Gaussian Process would be even worse.

Introduction

Gaussian process regression has its basis in Bayesian probability theory (Bijl, 2016). The most commonly used Gaussian process is a non-parametric model, we do not have to worry about whether it is possible for the model to fit the data. Even when a lot of observations have been added, there may still be some flexibility left in the functions (Rasmssen & Williams, 2006). If more datapoints were added one would see the mean function adjust itself to pass through these points, and that the posterior uncertainty would reduce close to the observations. However, non-parametric models rely on local neighborhood training data to make predictions, thus they perform poorly when applied to regions of the state space that are not densely covered by the training dataset. This problem becomes particularly critical as the state space grows (Wu & Movellan, 2012). Since some input variables in our research are obtained surface indentation techniques which are very expensive, so it is not possible to get plenty of datapoints to cover the entire sate space. While the parametric approach can capture a great deal of prior knowledge that does not need to be learned from data. It quite necessary to combine the benefits of parametric and non-parametric approaches. Then the semi-parametric Gaussian Process seems like a better option which can combines the interpretability of parametric models with the accuracy of non-parametric models. That means considering the parametric models for the mean function, and the Gaussian Process just has to model the residual errors (Murphy, 2012).

This quarter's work focuses on the yield strength prediction using the most useful input variables based on the previous work. In this research, we use the same dataset to do both the linear regression and the semi-parametric Gaussian Process respectively. And then compare the root mean square errors of these two methods to determine the prediction performance. By analyzing the comparative results to explore the possibility and necessity of applying semi-parametric Gaussian Process to predict the yield strength of pipelines.

Gaussian Process Regression

A Gaussian Process (GP) defines a prior over functions, which can be converted into a posterior over functions once we have some observed data. In other words, it defines a distribution over the function's values at a finite, but arbitrary, set of points, say $\mathbf{x}_1, \ldots, \mathbf{x}_N$. A GP assumes that $p\big(f(\boldsymbol{x_1}), \ldots, f(\boldsymbol{x_N})\big)$ is jointly Gaussian, with mean $\boldsymbol{\mu}(\boldsymbol{x})$ and covariance $\sum(\boldsymbol{x})$ given by $\sum_{ij} = k(\boldsymbol{x_i}, \boldsymbol{x_j})$, where k us a positive definite kernel function. In our research, we use GPs for regression. Let the prior on the regression function to be a GP, denoted by

$$f(\boldsymbol{x}) \sim \mathrm{GP}(m(\boldsymbol{x}), k(\boldsymbol{x}, \boldsymbol{x}')), \tag{1}$$

where $m(\boldsymbol{x})$ is the mean function and $k(\boldsymbol{x}, \boldsymbol{x}')$ is the kernel or covariance function, i.e.,

$$m(\boldsymbol{x}) = \mathrm{E}[f(x)] \tag{2}$$

$$k(\boldsymbol{x}, \boldsymbol{x}') = \mathrm{E}[(f(\boldsymbol{x}) - m(\boldsymbol{x}))(f(\boldsymbol{x}') - m(\boldsymbol{x}'))] \tag{3}$$

For any finite set of points, this process defines a joint Gaussian:

$$p(\mathbf{f}|\mathbf{X}) = N(\mathbf{f}|\boldsymbol{\mu}, \mathbf{K}) \tag{4}$$

where $K_{ij} = k(x_i, x_j)$ and $\boldsymbol{\mu} = \big(m(x_1), \ldots, m(x_N)\big)$.

Non-parametric Gaussian Process

Note that it is common to use a mean function of $m(\boldsymbol{x}) = 0$, since the GP is flexible enough to model the mean arbitrarily well. Suppose we have a training set $D = \{(x_i,\ f_i),\ i = 1 : N\}$, where $f_i = f(x_i)$ is the noise-free observation of the function evaluated at x_i. Given a test set $\mathbf{X}_*$ of size $\mathrm{N}_* \times D$, we want to predict the function outputs $\mathbf{f}_*$. By definition of the GP, the joint distribution has the following form

$$\begin{pmatrix} \mathbf{f} \\ \mathbf{f}_* \end{pmatrix} \sim N\left(\begin{pmatrix} \boldsymbol{\mu} \\ \boldsymbol{\mu}_* \end{pmatrix}, \begin{pmatrix} \mathbf{K} & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{pmatrix} \right), \tag{5}$$

where $\mathbf{K} = \mathrm{k}(\mathbf{X},\ \mathbf{X})$ is $N \times N$, $\mathbf{K}_* = \mathrm{k}(\mathbf{X},\ \mathbf{X}_*)$ is $N \times N_*$, and $\mathbf{K}_{**} = \mathrm{k}(\mathbf{X}_*,\ \mathbf{X}_*)$ is $N_* \times N_*$. By the standard rules for conditioning Gaussians, the posterior has the following form

$$p(\mathbf{f}_*|\mathbf{X}_*, \mathbf{X}, \mathbf{f}) = N(\mathbf{f}_*|\boldsymbol{\mu}_*, \boldsymbol{\Sigma}_*), \tag{6}$$

$$\boldsymbol{\mu}_* = \boldsymbol{\mu}(\mathbf{X}_*) + \mathbf{K}_*^{\boldsymbol{T}}\, \mathbf{K}^{-1}\big(\mathbf{f} - \boldsymbol{\mu}(\mathbf{X})\big), \tag{7}$$

$$\boldsymbol{\Sigma}_* = \mathbf{K}_{**} - \mathbf{K}_*^{\boldsymbol{T}}\mathbf{K}^{-1}\mathbf{K}_*. \tag{8}$$

Semi-parametric Gaussian Process

Sometimes it is useful to use a parametric model such as a linear model for the mean of the process, as follows:

$$f(\mathbf{x}) = \beta^T \phi(\mathbf{x}) + r(\mathbf{x}), \tag{9}$$

Where $r(\mathbf{x}) \sim \mathrm{GP}\big(0,\ k(\mathbf{x},\mathbf{x}')\big)$ models the residuals. This combines a parametric and a non-parametric model and is known as a semi-parametric Gaussian Process (SGP) model.

If we assume $\beta \sim N(\mathbf{b},\ \mathbf{B})$, we can integrate these parameters out to get a new GP:

$$f(\mathbf{x}) \sim \mathrm{GP}\big(\phi(\mathbf{x})^T\mathbf{b},\ k(\boldsymbol{x},\boldsymbol{x}') + \phi(\mathbf{x})^T\mathbf{B}\phi(\mathbf{x}')\big). \tag{10}$$

Intergrating out β, the corresponding predictive distribution for test inputs $\mathbf{X}_*$ has the following form:

$$p(\mathbf{f}_*|\mathbf{X}_*,\mathbf{X},\mathbf{y}) = N\big(\bar{\mathbf{f}}_*,\ \mathrm{cov}[f_*]\big), \tag{11}$$

$$\bar{\mathbf{f}}_* = \Phi_*^T\bar{\beta} + \mathbf{K}_*^T\mathbf{K}_y^{-1}\big(y - \boldsymbol{\Phi}\bar{\beta}\big), \tag{12}$$

$$\bar{\beta} = \big(\boldsymbol{\Phi}^T\mathbf{K}_y^{-1}\boldsymbol{\Phi} + \mathbf{B}^{-1}\big)^{-1}\big(\boldsymbol{\Phi}\mathbf{K}_y^{-1}\boldsymbol{y} + \mathbf{B}^{-1}\mathbf{b}\big), \tag{13}$$

$$\mathrm{cov}[f_*] = \mathbf{K}_{**} - \mathbf{K}_*^{\boldsymbol{T}}\mathbf{K}_{\boldsymbol{y}}^{-1}\mathbf{K}_* + \mathbf{R}^{\mathrm{T}}\big(\mathbf{B}^{-1} + \boldsymbol{\Phi}\mathbf{K}_y^{-1}\boldsymbol{\Phi}^T\big)^{-1}\mathbf{R}, \tag{14}$$

$$\mathbf{R} = \boldsymbol{\Phi}_* - \boldsymbol{\Phi}\mathbf{K}_y^{-1}\big(y - \boldsymbol{\Phi}\bar{\beta}\big), \tag{15}$$

The predictive mean is the output of the linear model plus a correction term due to the GP, and the predive covariance is the usual GP covariance plus an extra term due to the uncertainty in β.

Results and Discussions

Dataset and validation steps

In this research, we use three most useful variables (Hardness, Gu and Cr) as inputs which are selected by linear method shown by previous work. The dataset with the three input variables is shown in Table 6. YS_t is the yield strength measured by tensile testing which can be seen as the benchmark of predictions. And YS_s is the yield strength got from surface indentation technique. Then the difference between YS_t - YS_s is the output. The validation follows four steps. First, draw a training set and a test set randomly. To be more specific, as shown in Table 6, there are 20 samples in total. If 5 samples were randomly selected from the dataset to be a testing set, and the rest 15 samples would work as the training set correspondingly. Second, train the SGP model and the linear model with the training set. Third, predict the output values with the testing set. Finally, analyze the results of the predictions and evaluate the predictive performance. Note that both two-dimensional (two inputs) and three-dimensional (three inputs) analysis are conducted in this research. The two inputs are hardness and Cu, and the two inputs are hardness, Cu and Cr.

Table 6: Dataset with three input variables

No.	YS_t	YS_s	diff = YS_t - YS_s	Input Variables		
				Hardness	Cu	Cr
1	52.36	54.69	-2.33	83.4	0.011	0.045
2	52.48	54.18	-1.70	82.1	0.011	0.043
3	41.30	47.67	-6.37	78.5	0.028	0.011
4	68.10	63.71	4.39	84.6	0.11	0.043
5	43.70	49.95	-6.25	75.5	0.013	0.021
6	44.66	51.28	-6.62	76.1	0.01	0.01
7	68.60	66.54	2.06	90.1	0.041	0.028
8	44.64	49.68	-5.04	81.7	0.016	0.02
9	41.02	43.02	-2.00	78.7	0.013	0.008
10	40.20	42.36	-2.16	75.3	0.009	0.006
11	47.20	49.58	-2.38	83.2	0.041	0.029
12	47.14	47.71	-0.57	83.7	0.042	0.03
13	52.96	49.82	3.14	76.7	0.09	0.02

14	50.70	51.11	-0.41	79.5	0.029	0.038
15	54.60	53.94	0.66	80.7	0.045	0.055
16	45.12	48.90	-3.78	65.5	0.08	0.03
17	40.96	47.63	-6.67	80.0	0.013	0.01
18	43.28	49.05	-5.77	74.4	0.092	0.013
19	52.24	49.87	2.37	77.0	0.038	0.02
20	57.64	56.84	0.80	86.6	0.024	0.029

General Case Study

The results of general case study are shown in Figure 8-4. There are 500 iterations have been done for each validation. The blue dots are the root mean square errors (RMSE) of linear regression and the red stars are the RMSE of SGP regression for each iteration. Similarly, the blue solid line is the average RMSE for linear regression and the red solid line is the average RMSE for SGP regression. As can be seen in figures, linear regression is slightly better than SGP regression which is different from what we expected. And numerical comparison is shown in Table 7. When the dimension goes up with the same size of training set, the performance of SGP would go even worse. That probably because the three variables we used in this research were all selected by linear method which could further lead to the dominance of linear part in the SGP model. Moreover, the size of test set is not large enough to achieve a better predictive performance.

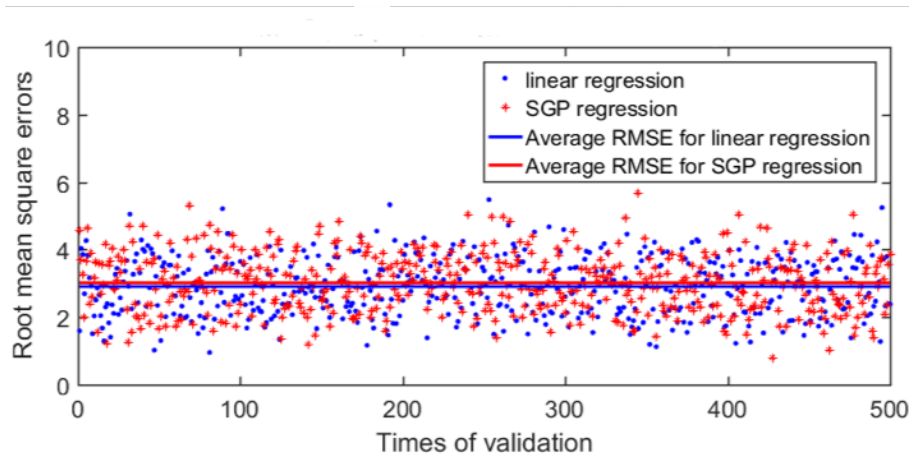

Figure 8: RMSE (2 input variables with 5 test points)

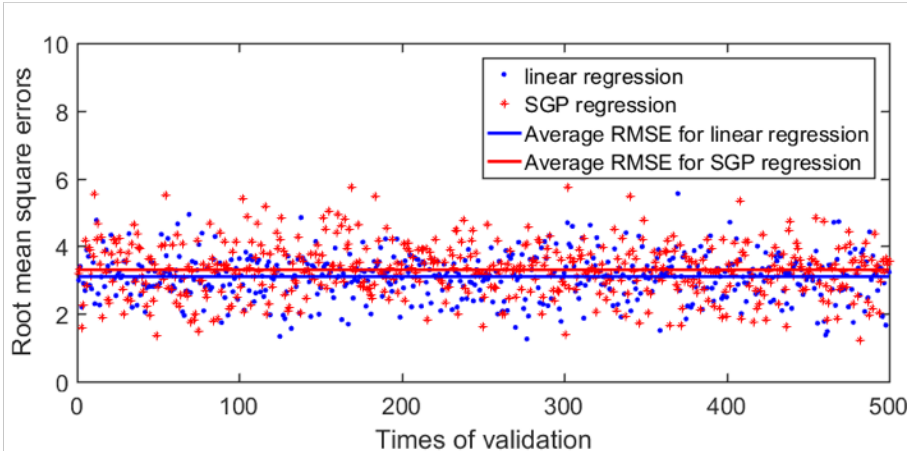

Figure 9: RMSE (2 input variables with 8 test points)

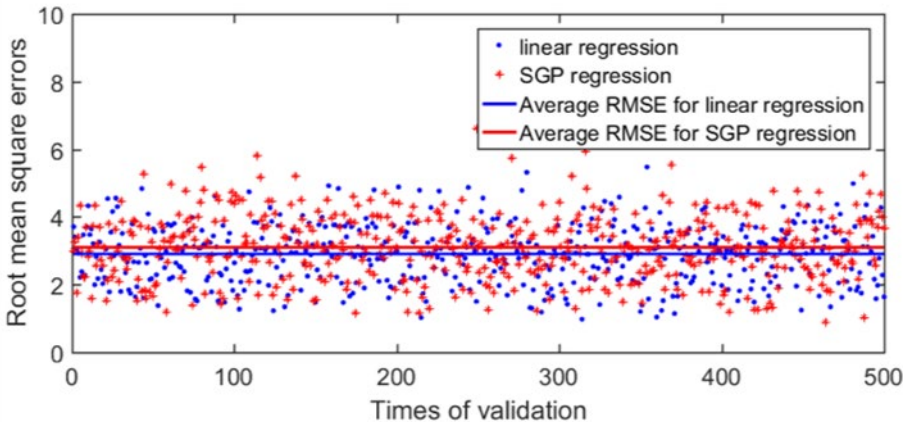

Figure 10: RMSE (3 input variables with 5 test points)

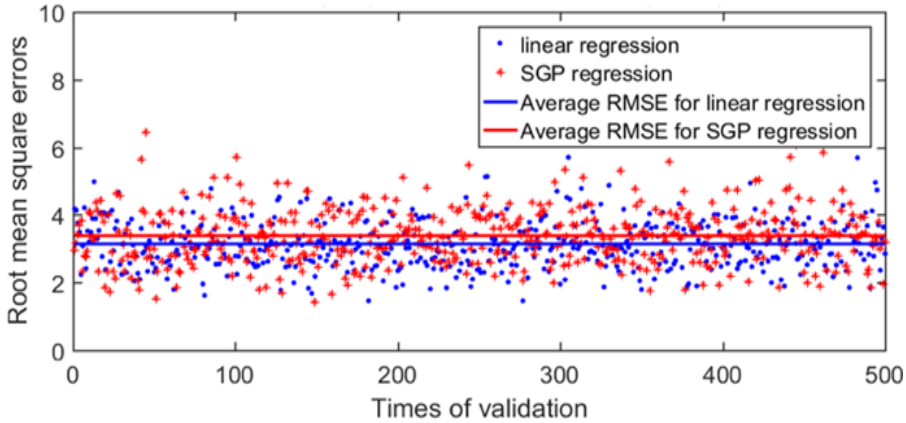

Figure 11: RMSE (3 input variables with 8 test points)

Table 7: Average root mean square errors (500 iterations)

	2 Dim_5 tests	2 Dim_ 8 tests	3 Dim_5 tests	3 Dim_8 tests
Linear	2.9065	3.1021	2.9082	3.1439
SGP	3.0184	3.3037	3.1005	3.3859

Specific Case Study

In specific case study, we use Hardness and Cu as inputs. After 15,000 iterations, the best predictions with the minimized root mean square errors of using SGP regression and linear regression have been pick up. As shown in Figure 12 and Figure 13, the blue dots are the test points of using linear regression and the red squares are the test points of using SGP regression with 95% credible interval. The best performances of linear regression and SGP regression are extremely close to each other while the linear regression would be slightly better when have less training data as shown in Table 8. In the case of 15 training points with 5 test points, the minimum RMSEs of linear regression and SGP regression are the same 0.6102. However, in the case of 12 training points with 8 test points, the minimum RMSE of SGP regression is 0.9406 which is larger than the linear regression's 0.9078. We can conclude that in the research for totally 20 samples, linear regression is slightly better than SGP regression in terms of predicting yield strength.

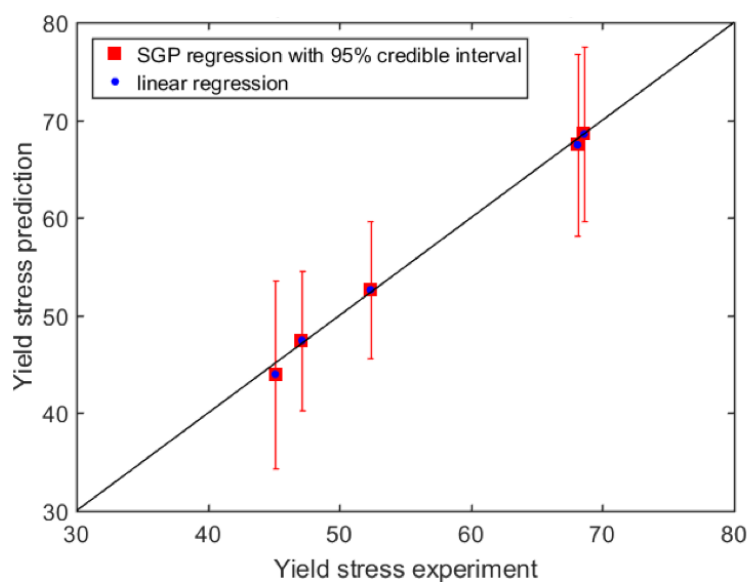

Figure 12: The Best prediction result for 5 test points

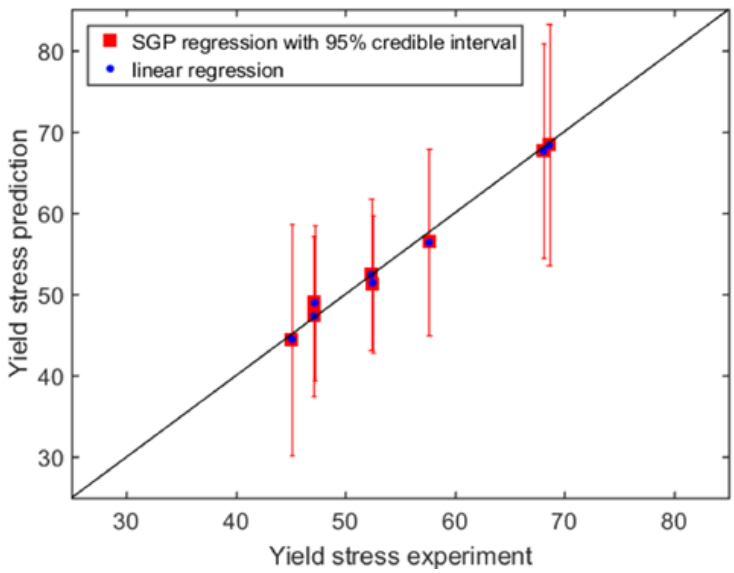

Figure 13: The Best prediction result for 8 test points

Table 8: The Best predictive performance

		Minimum RMSE	No. of data
2 Dim_5 tests	**Linear**	0.6102	[1 4 7 12 16]
	SGP	0.6102	[1 4 7 12 16]
2 Dim_8 tests	**Linear**	0.9078	[1 2 4 7 11 12 16 20]
	SGP	0.9406	[1 2 4 7 11 12 16 20]

Conclusion

In this research, with the first dataset including 20 samples, semi-parametric Gaussian Process regression is applied to predict the yield strength of pipes and compared with the traditional linear regression. By doing general case study and specific case study, it can be concluded that the SGP modeling has a similar performance of linear regression model. While if the dimension goes up with unchanged training set or the training set becomes smaller with unchanged dimensions, the linear regression will be slightly better than SGP regression. However, the benefit of using SGP model is that the prediction confidence bound can be estimated directly which is very valuable in data analysis. In addition, the SGP modeling has a great potential to achieve better predictive performance as long as having more training data.

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End of Report