Machine Learning Enhanced LIBS to Measure and Process Biofuels and Waste Coal for Gasifier Improved Operation

DOE STTR Phase II - DE-SC0022696

24 April 2024

Robert De Saro

Energy Research Company

Agenda

- Team Members
- Approach
- Objectives
- Phase I Results
- Phase II Approach
- Phase II TABA and TEA Approach

Team Members

- **ERCo**
  - R. De Saro (PI)
  - J. Craparo
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- **Lehigh University**
  - C. Romero
  - Z. Yao
  - O. Karadut
- **GTI**
  - J. Van Dyk
  - A. Soomro
  - A. Koutsostamatis
- **SpG Consulting, LLC**
  - S. Goff
- **DOE NETL Manager**
  - S. Michalik

Supporting Members

- ThermoChem Recovery International (TRI)
- SunFuel Renewables
- Appalachian Region Independent Power Producers Association (ARIPPA)
- Fulcum Bioenergy

DOE SBIR/STTR Phase II

- Office of Fossil Energy and Carbon Management
  - Topic 21 – Innovative Energy Systems
  - Subtopic f - Component Technology Advancement in Coal Waste and Biomass Gasification Systems

FECM Mission

- *..Minimize the environmental impact of fossil fuels while working towards net-zero emission. …Priority areas…include…hydrogen with carbon management…*
- Net Decarbonize Electric Utilities by 2035

The Need – Hydrogen is Environmentally Friendly

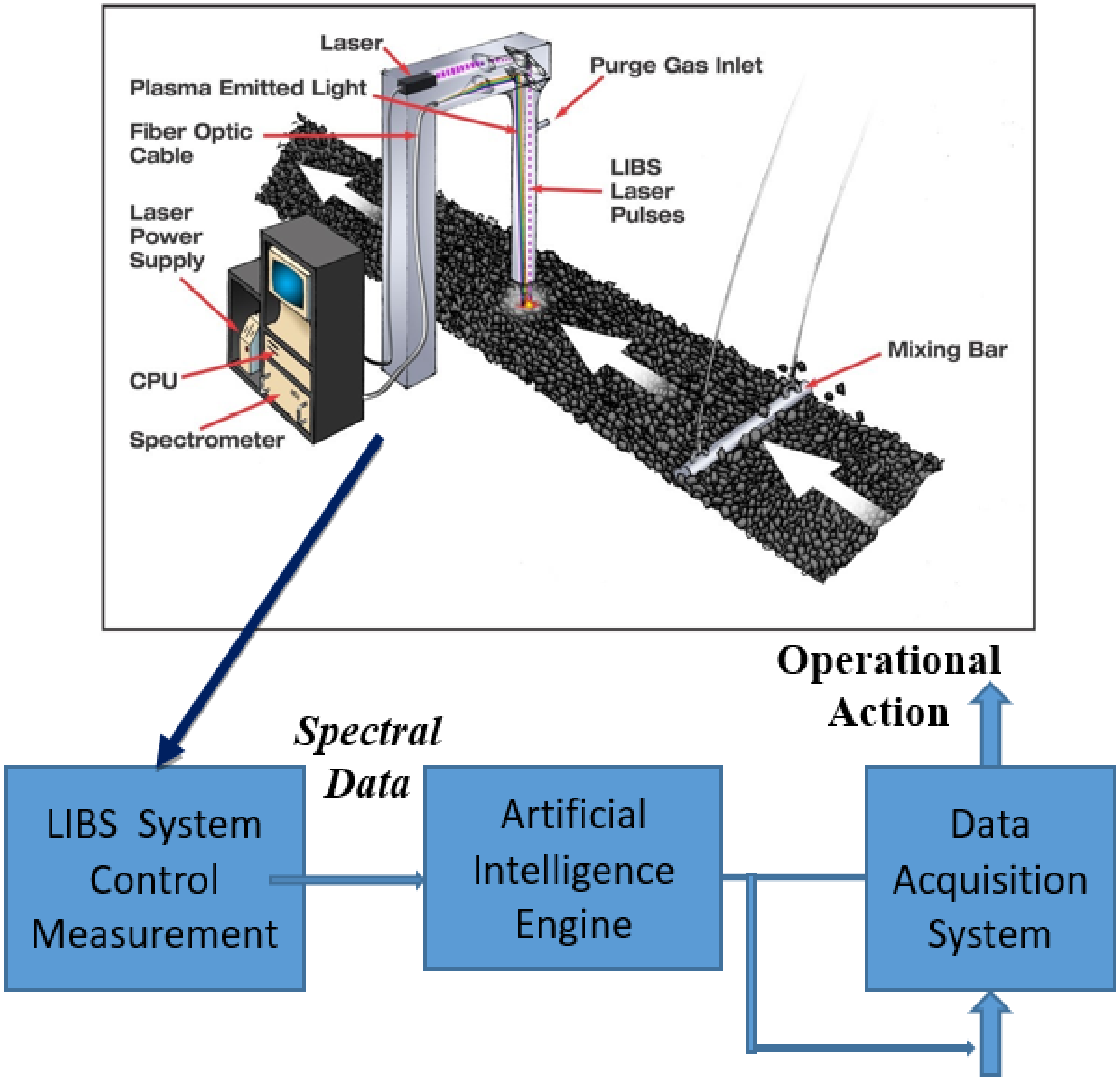
- Particularly When Produced from Biomass and Coal Wastes Through Gasification.
- It Can Be Used When Electrification is Difficult (Aircraft, Steel, Concrete, for Instance).
- But Feedstock is Highly Heterogeneous Making It Difficult to Process and
- Makes Gasification More Expensive Than It Needs To Be

The Solution

- Combine Biomass and Coal Waste to Produce Hydrogen in a Gasifier
- Measure the Feedstock to Control the Gasification Process in Real Time
- Use Machine Learning Enhanced LIBS Instrument

Project Approach

- ERCo's OnSpec™ LIBS Probe
  - Measure Elemental Spectra
  - In Real Time and In-Situ
- Lehigh
  - Machine Learning to Convert Spectra Into Actionable Parameters
  - Provide Samples, Process Feedstock for Analysis, Provide Lab Analysis.
- GTI
  - Simulator to Predict Gasifier Performance Using the ML- LIBS Results
  - Provide Gasification Technology and Know-How
  - TEA
- SpG Consulting, LLC
  - TABA


Laser
Plasma Emitted Light
Fiber Optic Cable
Laser Power Supply
CPU
Spectrometer
Purge Gas Inlet
LIBS Laser Pulses
Mixing Bar
Operational Action
Spectral Data
LIBS System Control Measurement
Artificial Intelligence Engine
Data Acquisition System

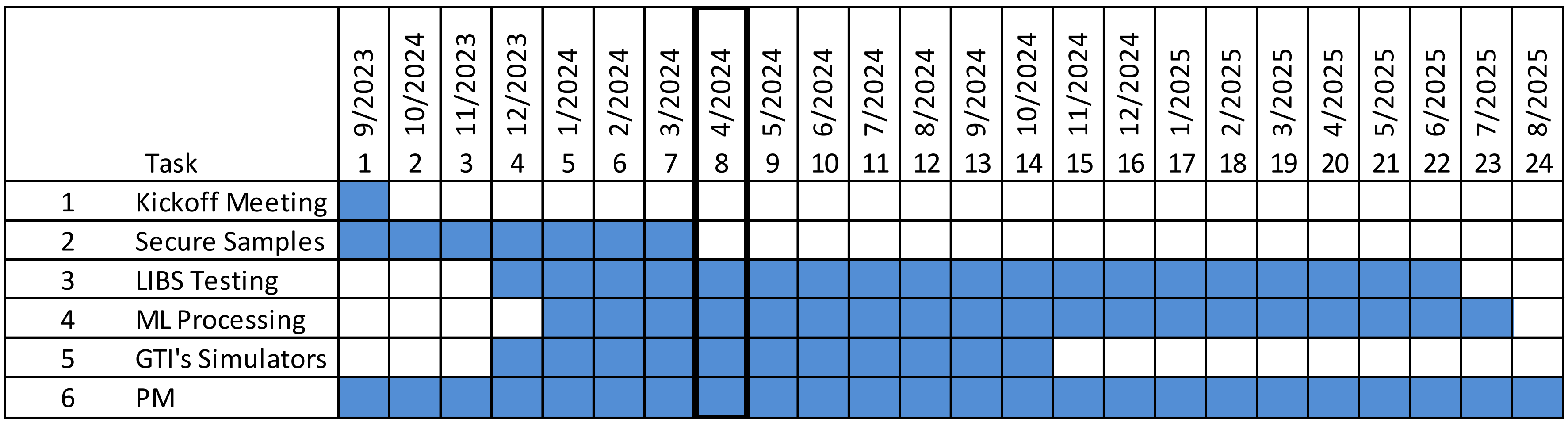
Phase I Project Objectives

- Measure *in situ* and in near real time: HHV, Ash %, C, S, Si, Al, Na, K, Ca, Fe, fusion and slagging temperatures
- Use LIBS to measure the spectra of coal wastes and biofuels provided by GTI and Dominion
- Develop ML algorithms that use the LIBS data as input to measure the properties listed above.
- LIBS-AI measurements provided online to be used to better control gasifier operation
- Achieve an accuracy and precision that will provide commercial value to GTI.

Phase II Project Objectives

- Extend the Phase I measurement success by better simulating a commercially operating gasifier. For this we will increase our testing realism by:
    - Using a commercial-ready LIBS instrument;
    - Measuring the feedstock on a moving belt, rather than on a static platform as we did in Phase I;
    - Expand the sample pool including additional types of commercial biomass and coal refuse, as well as additional blend ratios suited for gasifiers
    - Incorporate the ML algorithms into the software of our commercial-ready LIBS instrument so as to achieve real-time data display as data is taken.
- Determine the exact gasifier performance from our measurements by using the ML-LIBS data as input to GTI's gasifier simulator.

Phase II Schedule



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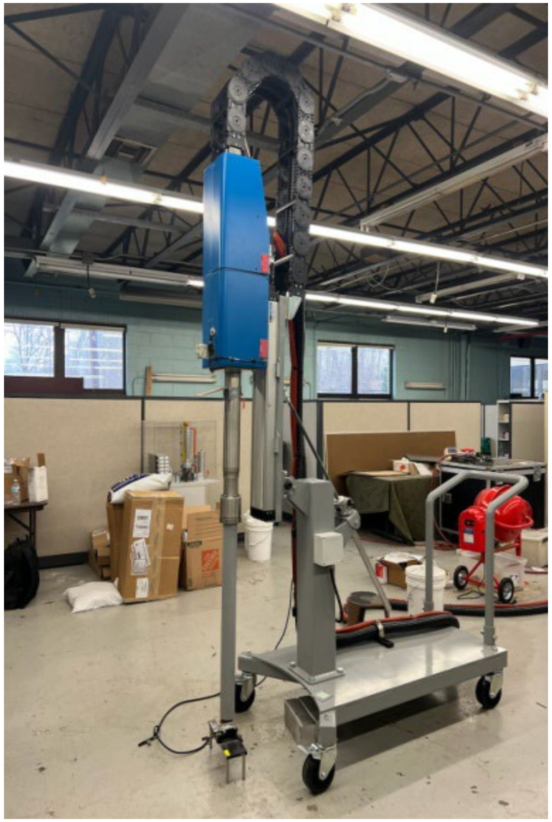
Phase II Deliverables

- Fully Automated OnSpec™ Commercial Instrument
- Single Push-Button Operation With Data Displayed In Real-Time
- Field-Capable
- Data and Conclusions
- Simulator Results
- Commercialization Feasibility and Plans

ERCo's Commercial LIBS System



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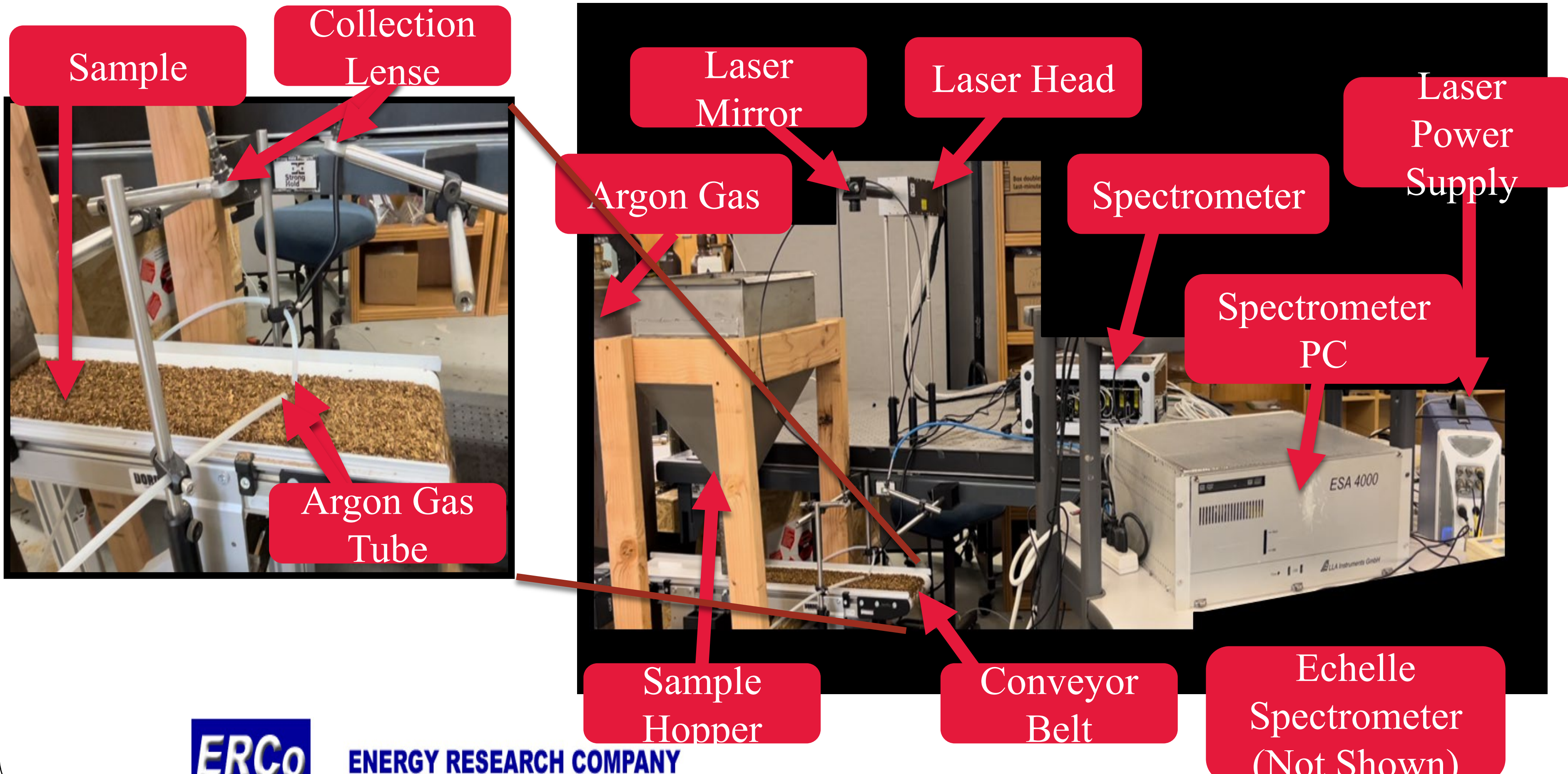
Phase I Results

ERCo's Lab System



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Phase I Results Summary

- All Project Feedstock Properties Accurately Measured
- R^2 over 0.98
- RSD Better Than 1.5% and Most Below 0.1%
- Signal to Noise Ratio of LIBS data: Excellent for all Elements
- Technical Breakthrough: We Can Get High Precision With Varied Feedstocks
- All Milestones Completed and Go/No Go Points Passed
- *Feasibility Amply Proven*

Value Proposition From Phase I Results

- Using Dynamic Control System With ML-Enhanced LIBS
- Oxygen Reduction
- Syngas Yield
- Improved Gasifier Availability
- Continual Measurements With Little Cost Per Measurement
- Payback 3.3 Months

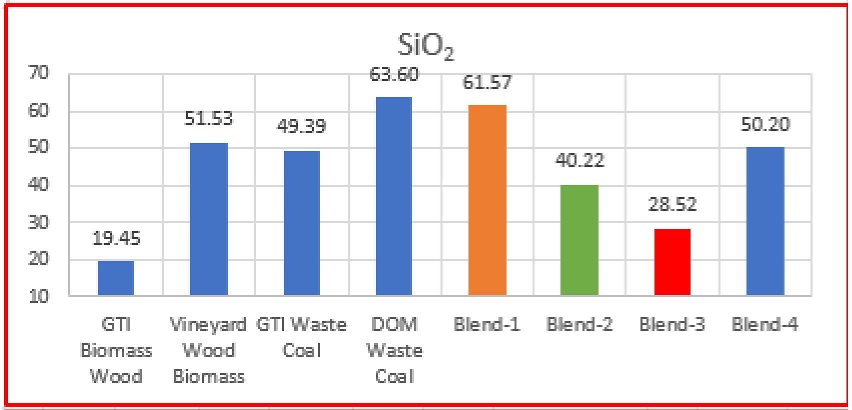
Samples Obtained

Phase I Samples Tested

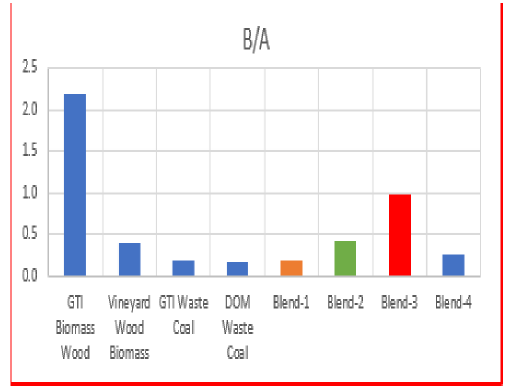
- Two Biomass as Received
- Two Coal Waste As Is
- 2 Blends**
  - Blend 1 – 25% Dominion Waste Coal, 75% GTI Biomass Wood
  - Blend 2 – 5% GTI Waste Coal, 95% GTI Biomass Wood

** *Virtual* blends made by combining data from each material.

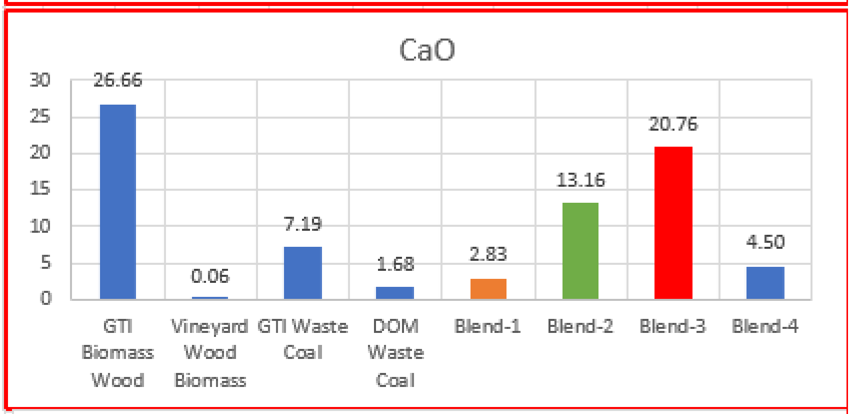
Blends



SiO_2
70
60
50
40
30
20
10
19.45
51.53
49.39
63.60
61.57
40.22
28.52
50.20
GTI Biomass Wood
Vineyard Wood Biomass
GTI Waste Coal
DOM Waste Coal
Blend-1
Blend-2
Blend-3
Blend-4



B/A
2.5
2.0
1.5
1.0
0.5
0.0
GTI Biomass Wood
Vineyard Wood Biomass
GTI Waste Coal
DOM Waste Coal
Blend-1
Blend-2
Blend-3
Blend-4



CaO
30
25
20
15
10
5
0
26.66
0.06
7.19
1.68
2.83
13.16
20.76
4.50
GTI Biomass Wood
Vineyard Wood Biomass
GTI Waste Coal
DOM Waste Coal
Blend-1
Blend-2
Blend-3
Blend-4

Analyses Completed by Certified Lab

1. Proximate analysis
2. Ultimate Analysis (C, H, N, S, O)
3. Ash composition
4. Trace element analysis
5. AFT to 2800^{o}F
6. Heating value

LIBS Results: Signal-to-Noise

Wavelength (nm)	247.86	249.77	259.94	279.52	288.15	323.45	394.4	422.67	481.05	588.99	670.78	766.49	777.47
Material/Element	**C I**	**B I**	**Fe II**	**Mg II**	**Si I**	**Ti II**	**Al I**	**Ca II**	**Zn I**	**Na I**	**Li I**	**K I**	**O I**
Wood Pellets	2522	8	105	2282	113	21	20	352	8	78	2	1423	6
Wood Chips	732	44	416	3076	218	97	38	843	29	505	17	2720	10
Wood Turnings	2367	7	77	3629	99	13	8	561	9	278	3	2248	8
Vineyard Wood	212	7	776	2389	643	414	189	976	6	353	22	1113	5
S.A. Waste Coal	311	15	1009	2736	675	458	204	579	19	253	73	460	4
Dominion Waste Coal	129	9	721	1804	525	335	131	713	6	407	107	874	4

Outcome From ML-Enhanced LIBS

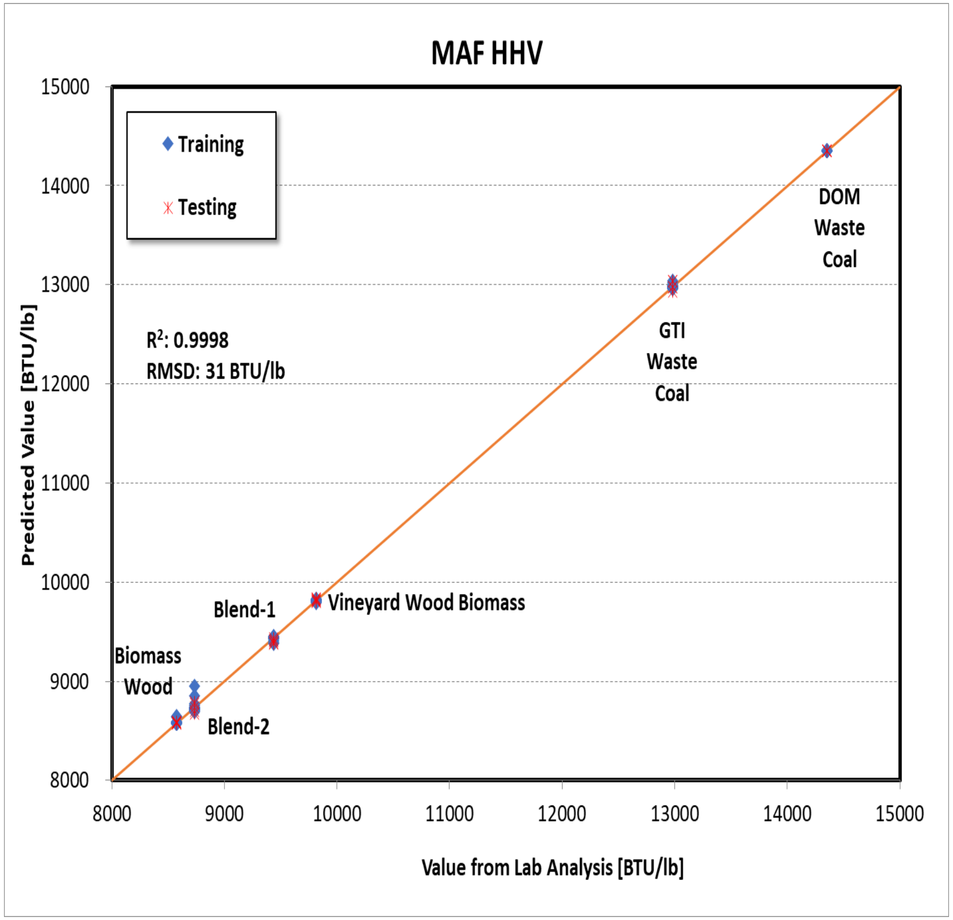
- C, S, Si, Al, Na, K, Ca, Fe, Mg, Ash
- Fusion Temperature and Heating Value

ML-LIBS Results Summary

	Target	Min	Average	Max	R^2	RMSD	CV (RMSD/Average)
1	HHV (MAF)	8576	10650	14354	0.9998	31	0.29%
2	% Ash (Dry)	0.70	18.14	45.50	0.9988	0.550	3.04%
3	% Carbon (Dry)	43.749	52.08	73.84	0.9994	0.245	0.47%
4	% Sulfur (Dry)	0.11	0.52	1.20	0.9999	0.004	0.72%
5	IDT	1251	1317	1374	0.9998	0.622	0.05%
6	SiO_2 in ash	19.45	47.63	63.60	0.9897	1.546	3.25%
7	Al_2O_3 in ash	2.62	16.84	27.59	0.9998	0.112	0.67%
8	Fe_2O_3 in ash	3.92	5.54	6.65	0.9975	0.055	0.99%
9	CaO in ash	0.06	8.60	26.66	0.9993	0.252	2.93%
10	MgO in ash	1.63	2.72	5.99	1.0000	0.011	0.39%
11	K_2O in ash	1.14	6.85	18.83	0.9994	0.145	2.12%
12	Na_2O in ash	0.25	0.53	0.80	0.9915	0.016	2.93%

CV: Coefficient of variation

MAF HHV



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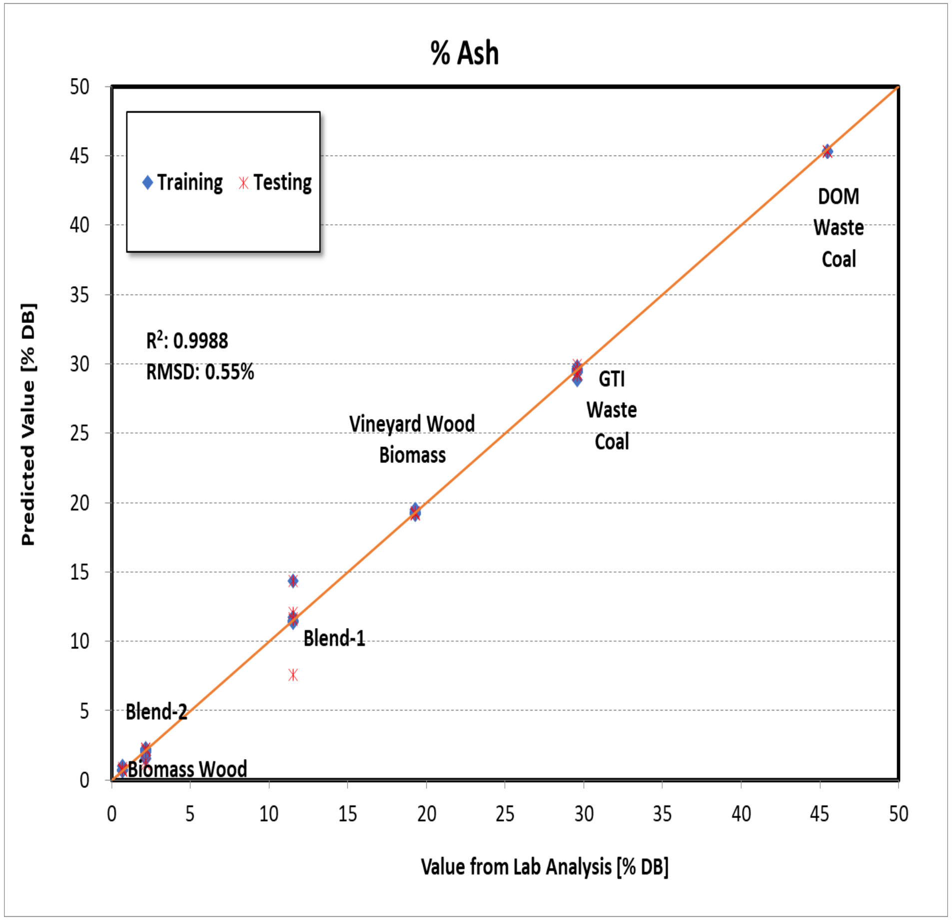
% Ash



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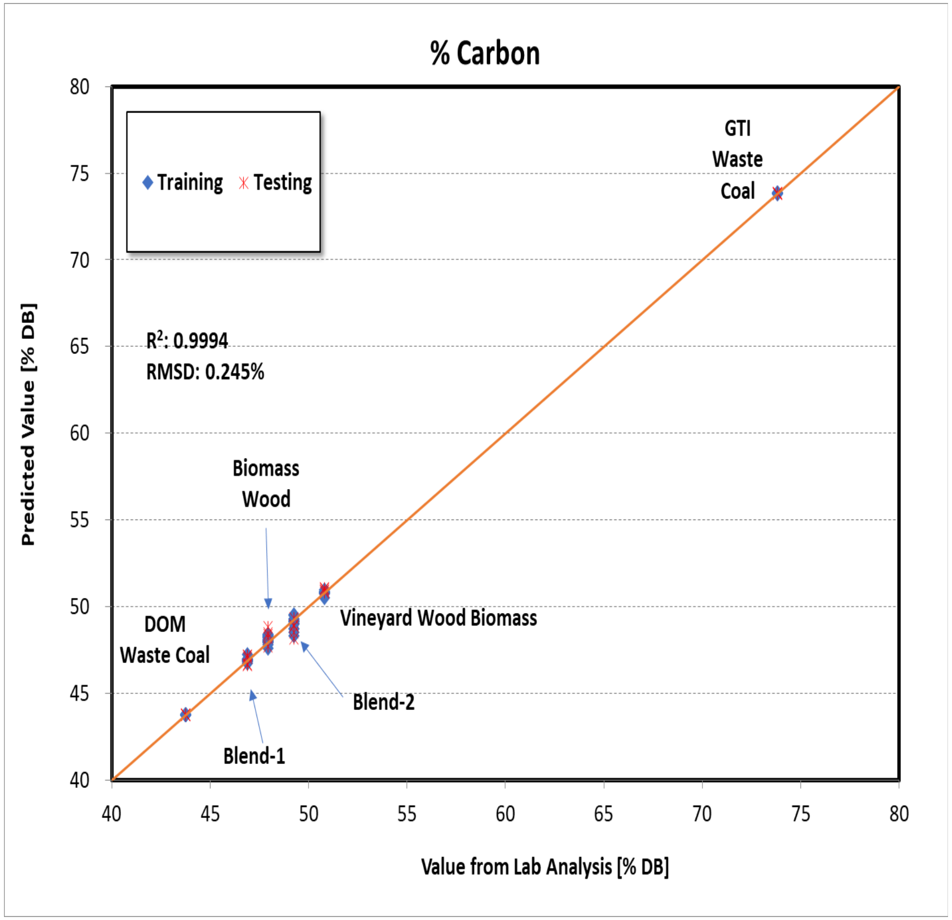
% Carbon



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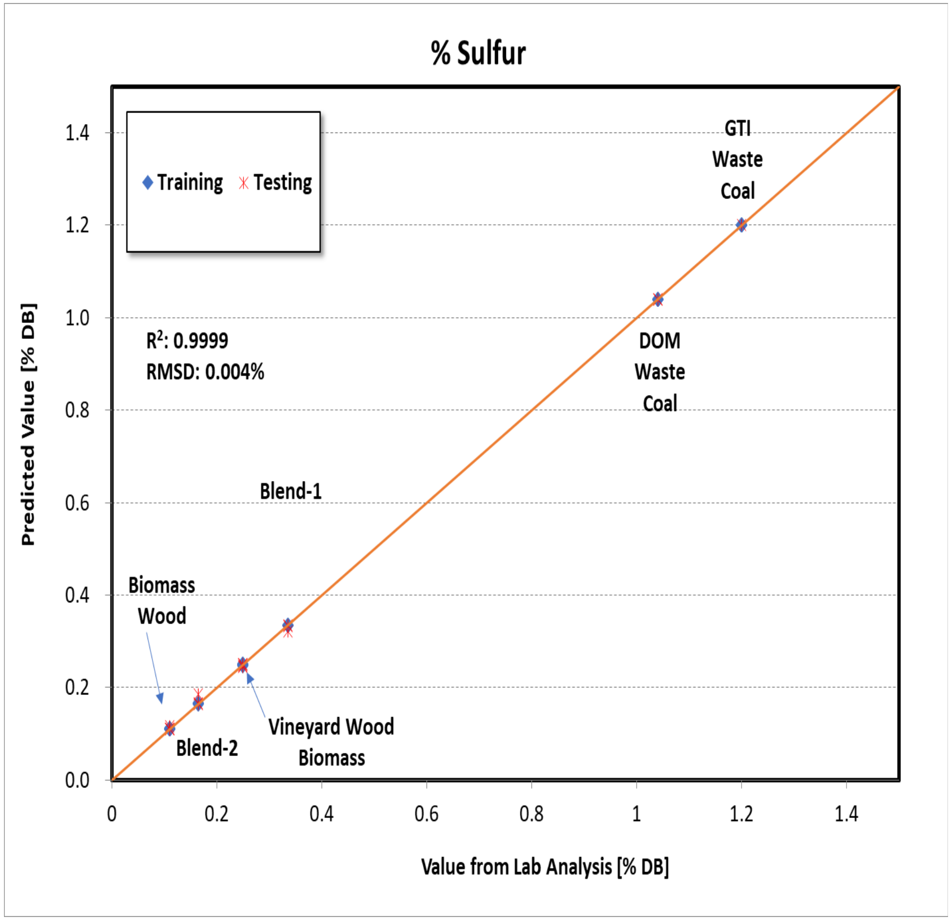
% Sulfur



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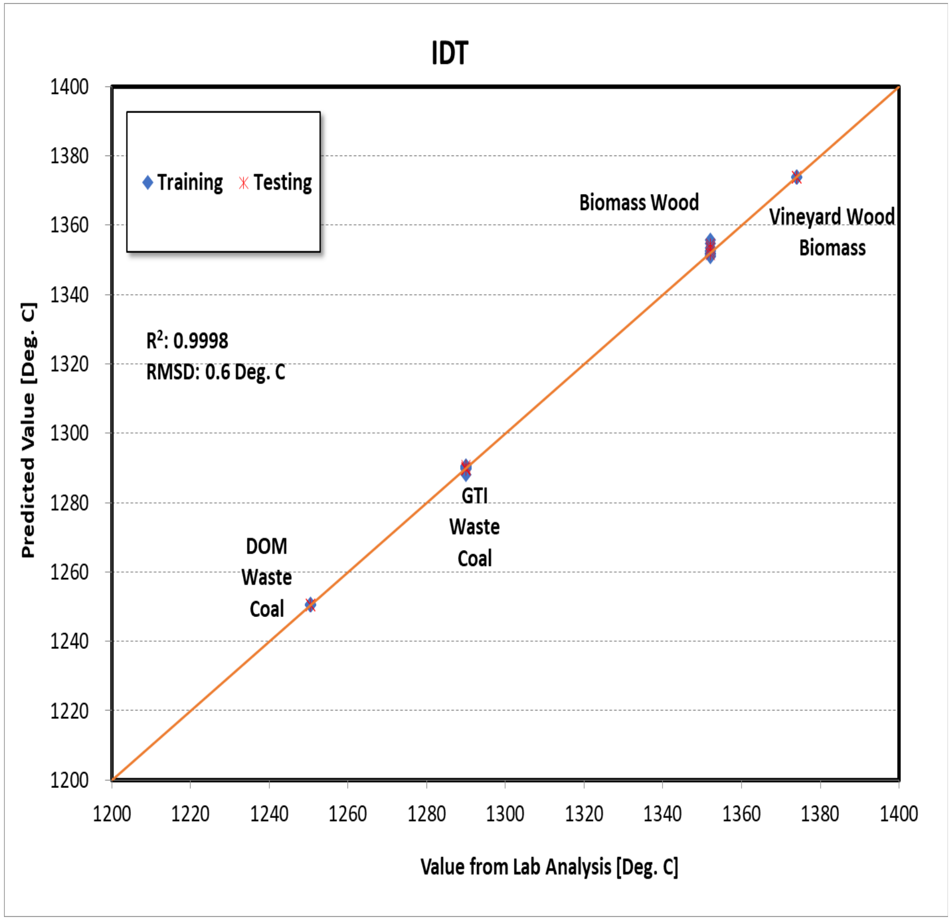
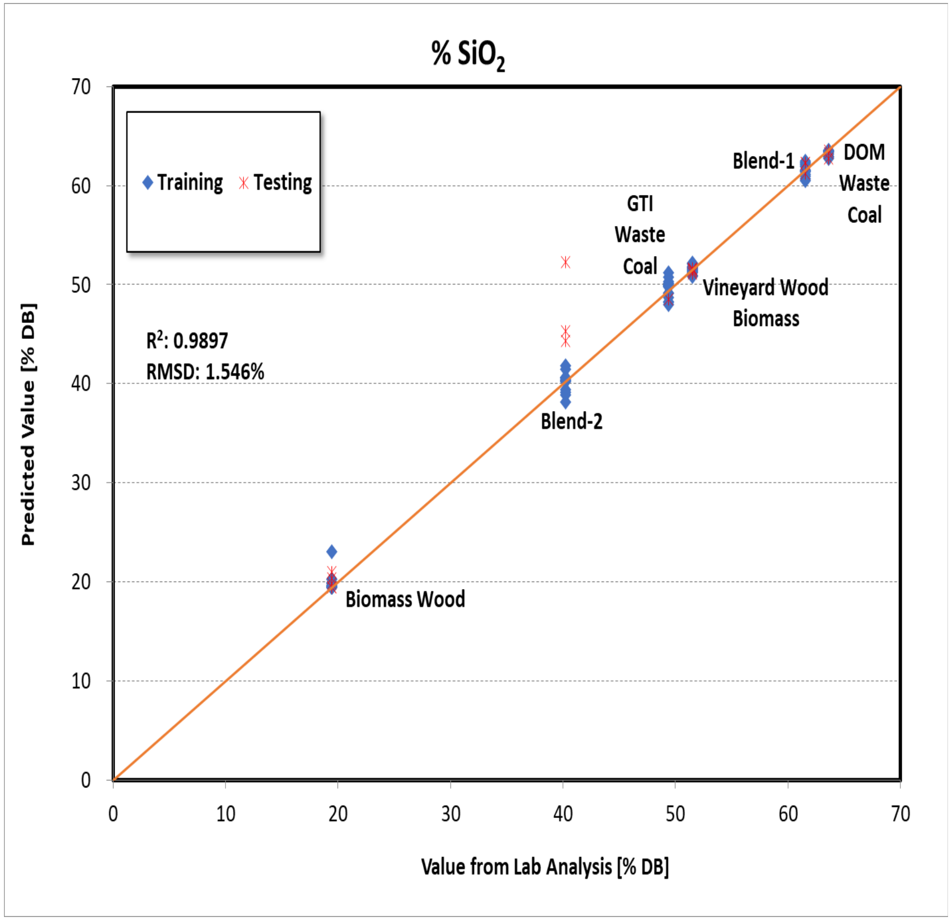
IDT



IDT
Training
Testing
Biomass Wood
Vineyard Wood
Biomass
R2: 0.9998
RMSD: 0.6 Deg. C
GTI
Waste
Coal
DOM
Waste
Coal
Predicted Value [Deg. C]
Value from Lab Analysis [Deg. C]
1200
1220
1240
1260
1280
1300
1320
1340
1360
1380
1400

$\%SiO_2$



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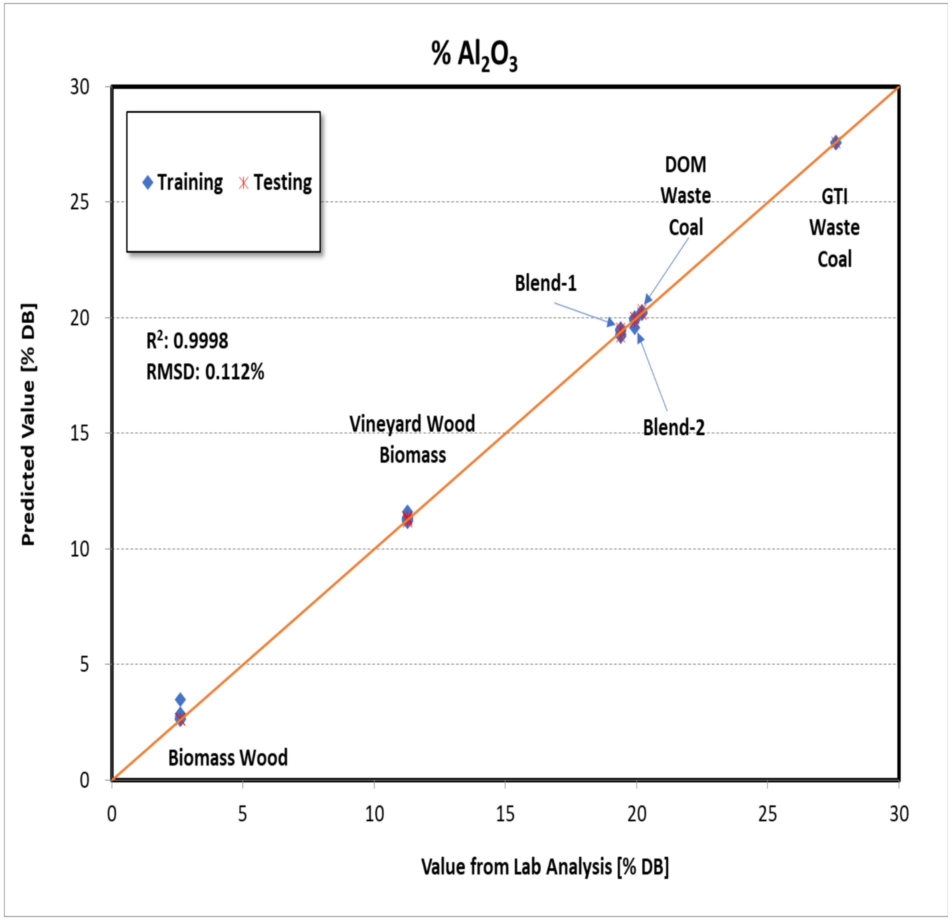
%Al_2O_3



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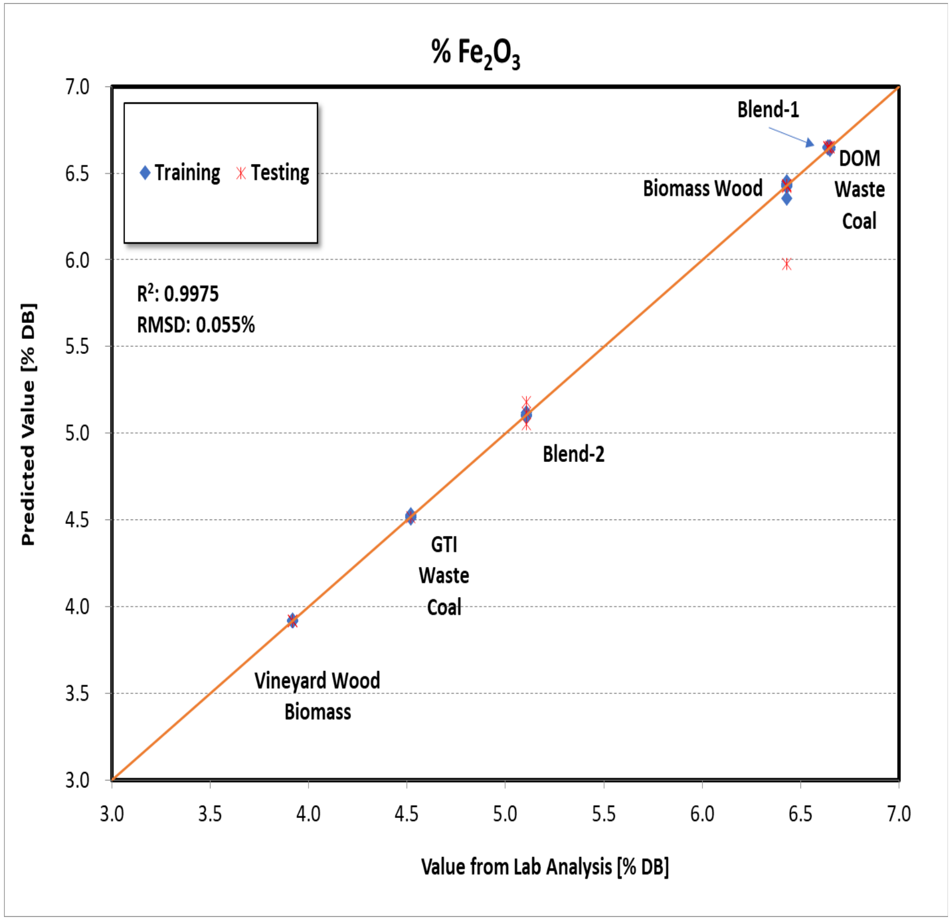
%Fe_2O_3



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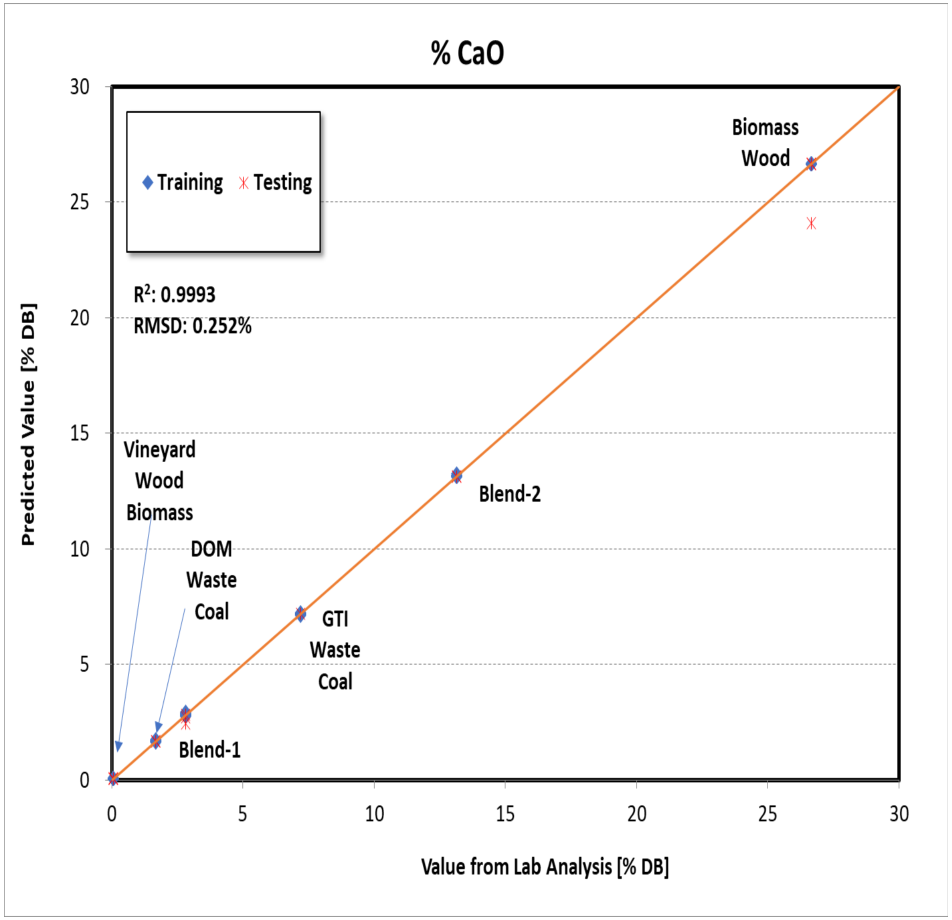
%CaO



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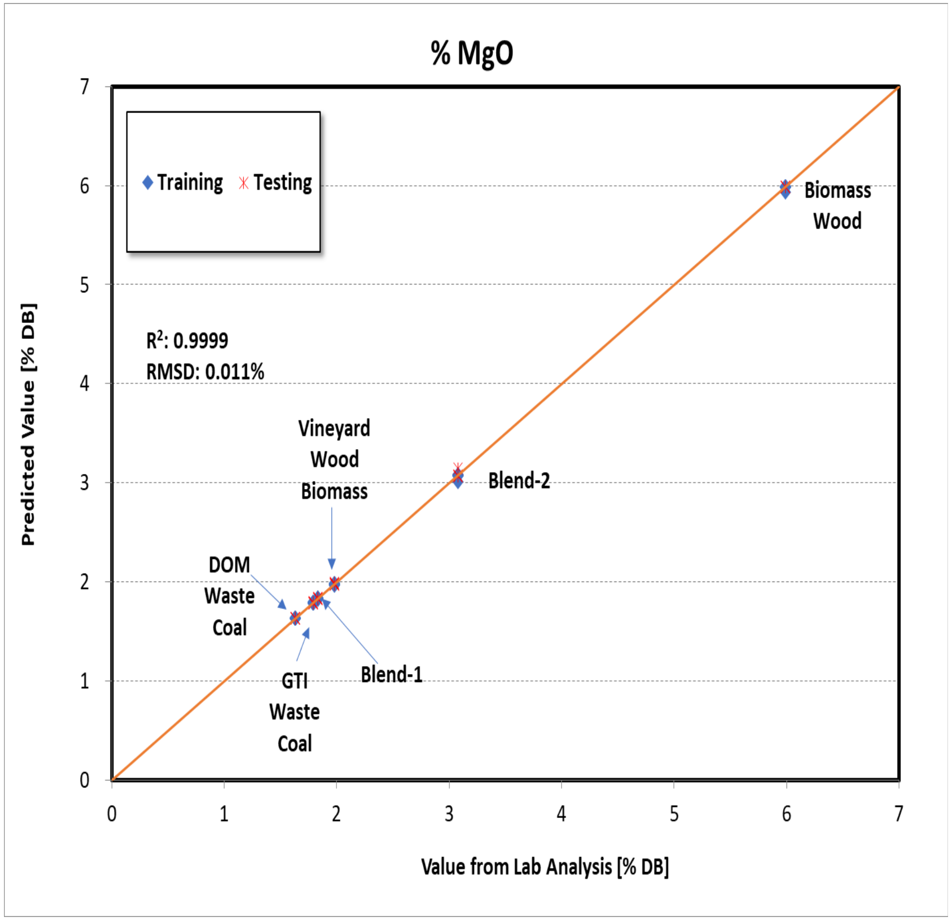
%MgO



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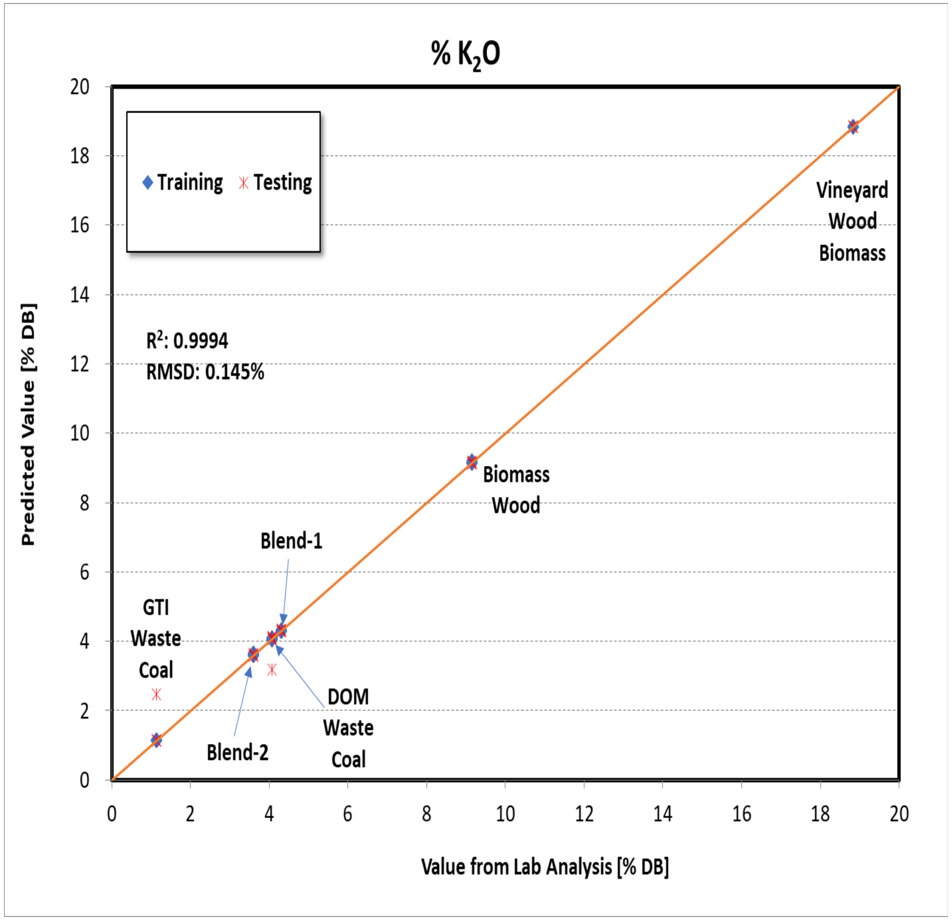
$\%K_2O$



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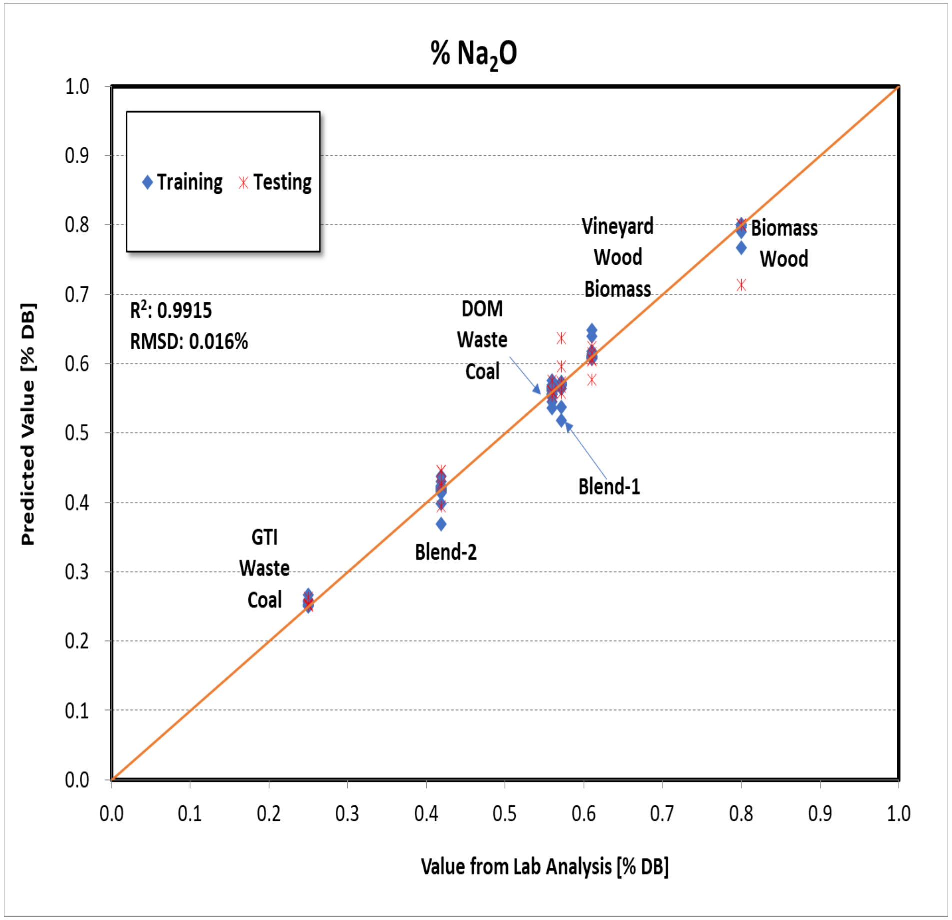
%Na_2O



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Phase II Results

Phase II Feedstocks

- 15 Feedstocks
- 2 mm and 500 Microns (0.5 mm) of Each
  - GTI Coal Waste
  - GTI Wood Pellets
  - Dominion Coal Waste
  - Three Blends of the Above
  - INL Woodchips
- Vineyard Biomass

Dominion Coal Waste

Wood Chips

Blend A – wood chips waste coal - 500 microns

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Phase II Status

- All Feedstocks Obtained and Processed to 2 mm and 500 microns
- All Independent Lab Measurements Completed
- OnSpec™ On Site
- Conveyor Belt Operational
- All Current Milestones Completed
- Currently On Schedule

GTI's Gasifier Simulator

- Determine Liquidus Temperature Based on the Ca and Si Content
- This is Important to Determine if Slagging is Possible
- Fluidized Beds Would Be Adversely Affected By Slagging and Entrained Flow Would Benefit
- Use Simulator for Feedforward Control

Commercialization Study

TABA and TEA

- TABA Will Evaluate the Market
- TEA Will Evaluate the ML-Enhanced LIBS Economic Performance on Fluidized Bed and Entrained Flow Gasifiers

Technical and Business Assistance (TABA)

- Market assessment of LIBS for gasification applications for biomass and waste coal
- Market assessment of LIBS for alternate applications for municipal solid waste and waste plastics
- TechnoEconomic Analysis of LIBS in gasification processes
  - Commercial LIBS instrument cost estimate and manufacturing plan
  - Value Proposition
- Develop commercialization plan for LIBS covering all potential markets
- Support the development of Intellectual Property to protect the LIBS technology in gasification applications

Techno-Economic Analysis (TEA)

- Determine the Impact of the ML-Enhanced LIBS technology on GTI Energy's Fluidized Bed and Entrained Gasifiers
- The system scope considered in the process simulations and techno-economic analyses shall consist of:
  - Feedstock Delivery
  - Biomass Pre-processing
  - Gasification (single gasifier train)
  - Syngas Scrubbing

Design Cases for TEA

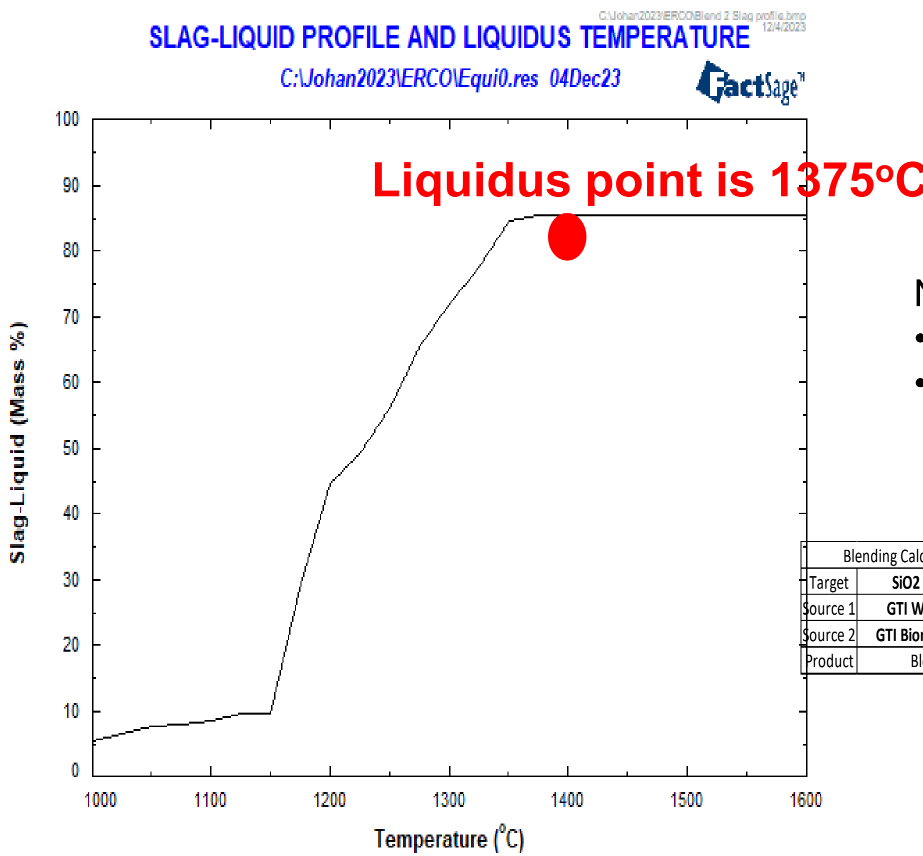
- Both Greenfield and Brownfield Scenarios Will Be Evaluated

Parameter	Greenfield Scenario				Brownfield Scenario
Gasifier Type	U-GAS		R-GAS		U-GAS
LIBS System Implemented	No	Yes	No	Yes	Yes
Feedstock (1000 STPD)	50% Biomass/ 50% Waste Coal		50% Biomass/ 50% Waste Coal		50% Biomass/ 50% Waste Coal
	100% Biomass		--		--
Total # of TEA Cases	4		2		2 (Relative difference)

TEA Methodology

- NETL's "Quality Guidelines for Energy System Studies (QGESS): Cost Estimation Methodology for NETL Assessments of Power Plant Performance".
- For the Greenfield Scenarios, the Levelized Cost of Syngas Is Calculated Using the Discounted Cash Flow Method
- For the Brownfield Evaluation, ML-Enhanced LIBS is Implemented as a Retrofit to an Existing Facility.

SLAG-PROFILE AND LIQUIDUS POINT (BLEND 2)



Next slide:

- Influence of CaO on the slag-liquid amount
- Run at liquidus of 1375°C

Blending Calculation		AR			DB					Minerals								
Target	SiO2 and CaO	Mass AR Ratio	Moisture %	% Carbon	% Ash	% V	% FC	% S	MAF HHV	SiO2	Al2O3	Fe2O3	CaO	MgO	K2O	Na2O	TiO2	B/A
Source 1	GTI Waste Coal	5%	4.50	73.84	29.60	24.9	45.5	1.20	12981	49.39	27.59	4.52	7.19	1.79	1.14	0.25	1.41	0.19
Source 2	GTI Biomass Wood	95%	6.10	47.95	0.70	82.1	17.2	0.11	8516	19.45	2.62	6.43	26.66	5.99	9.15	0.80	0.25	2.20
Product	Blend-2	100%	6.02	49.24	2.17	79.2	18.6	0.17	8679	40.22	19.94	5.11	13.16	3.08	3.59	0.42	1.05	0.41

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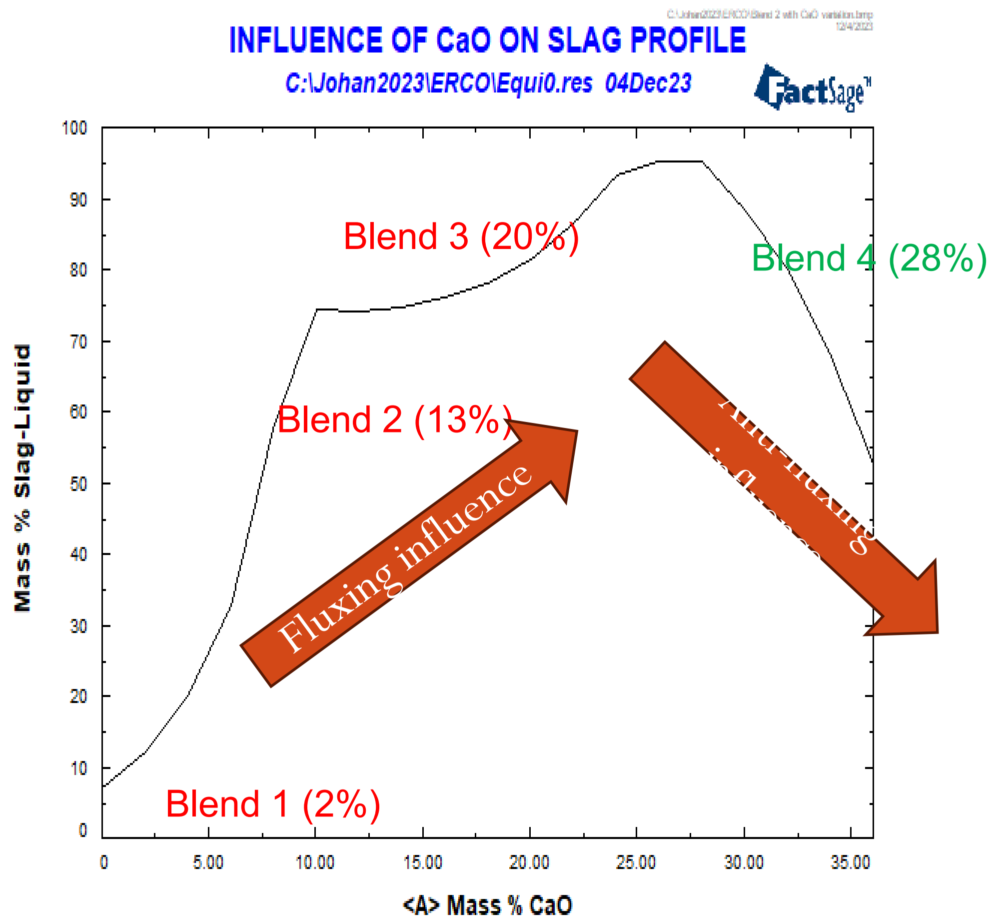
INFLUENCE OF CaO ON SLAG PROFILE



Recommendation

- 4^{th} Blend
- CaO >26.5%