Integration of LIBS with Machine Learning for Real-Time Monitoring of Feedstock in H_2 Gasification Applications

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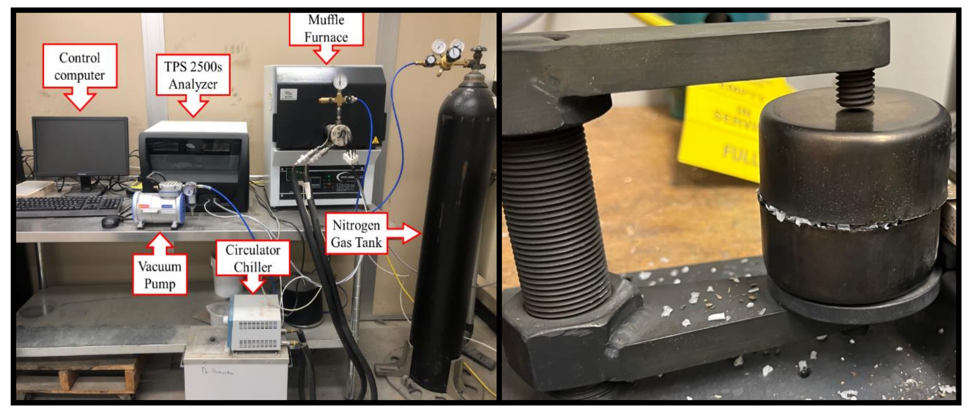
Task 2:
Material Processing and Analysis

Acquired raw materials including Northampton waste coal, corn stover from Idaho National Labs, wood chips from Burney Forest Power, and plastics from Innovative Fibers and McMaster-Carr. Prepared using an industrial shredder, coal crusher and industrial mixer. Grains a few millimeters in size were produced using this method.

6 samples were prepared.

- 4 'pure' samples: Northampton waste coal, wood chips, corn stover, and mixed plastics.
- 2 'mixed' samples: "Si-50" and "Ca-10".

Thermal conductivity analysis performed by Lehigh University using Hot Disk TPS 2500s Thermal Constant Analyzer.



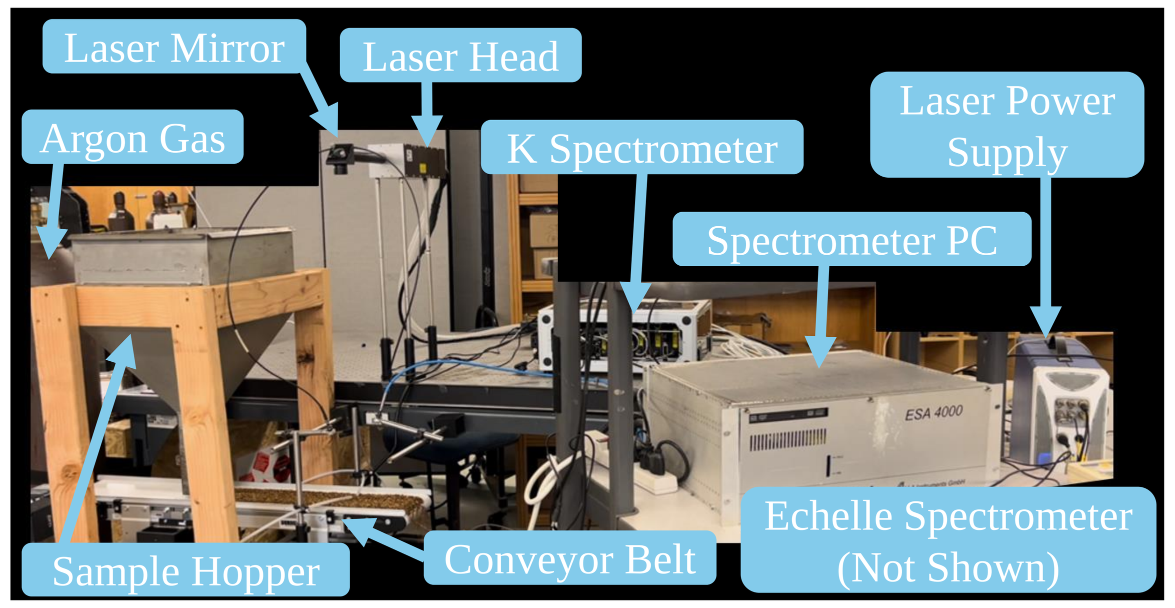
Proximate analysis, calorific value, inorganic elemental analysis, fusion temperature, viscous temperature and chloride content analyzed by G and C Coal Analytical Lab.

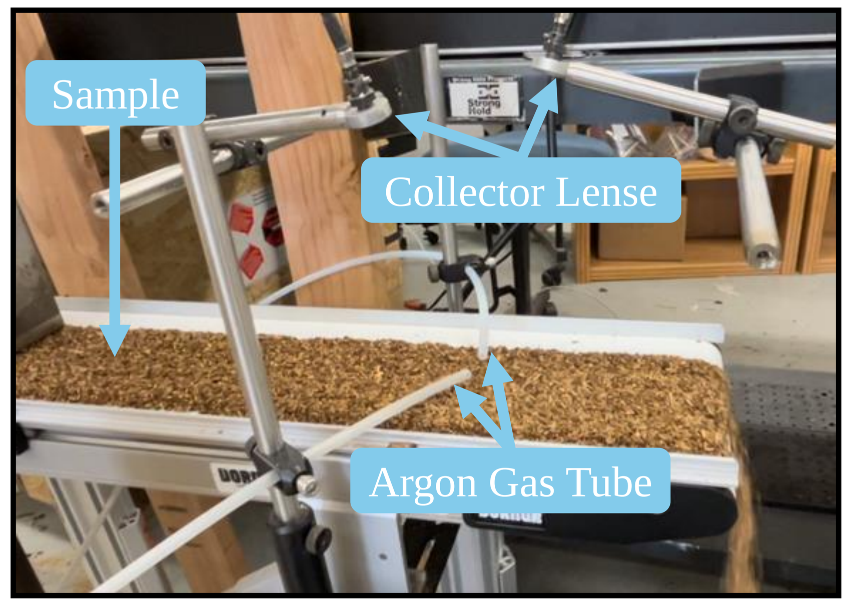
% Moisture	0.01	
% Ash	1.92	1.92
% Sulfur	0.06	0.06
B.T.U.	15,365	15,367
BTU (Moisture-ash free)	15,668	
% Volatile Matter	93.52	93.53
% Fixed Carbon	4.55	4.55
Fusing Temperature	ID: 2242 HT: 2311	ST: 2268 FT: 2335

SiO2	39.60	%
Al2O2	18.40	%
TiO2	11.60	%
Fe2O3	3.46	%
CaO	15.70	%

MgO	0.68	%
Na2O	4.55	%
K2O	3.88	%
P2O5	0.33	%
SO3	0.37	%

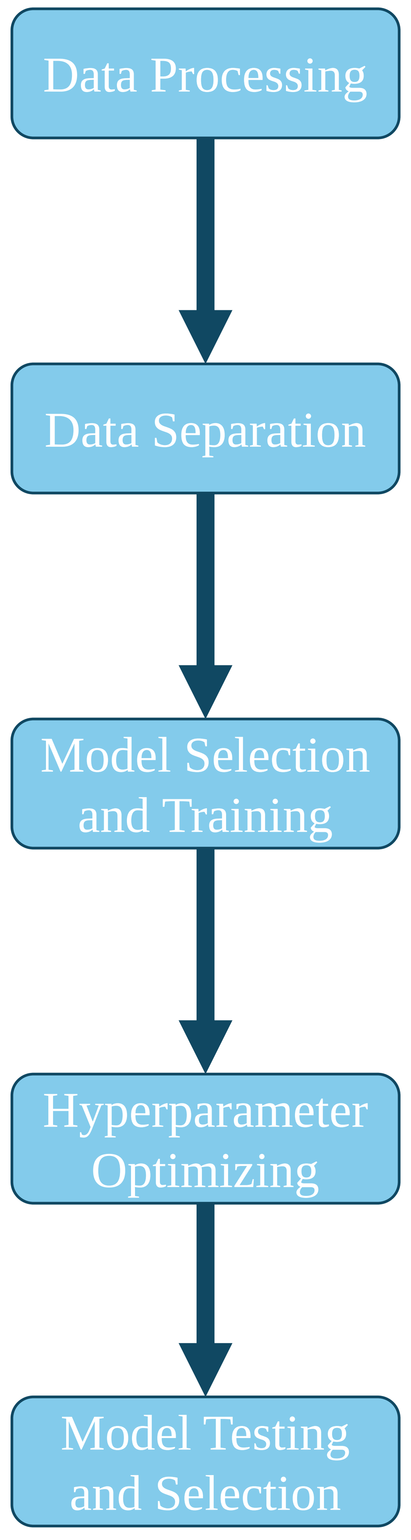
Task 3:
LIBS Lab Testing





Shown above is the set up for LIBS testing and operated as follows. Samples were feed into a hopper leading to a conveyor belt. The belt drove the material towards a laser pulsing approximately once a second. Argon gas was exhausted at the laser ablation site displacing air with inert gas and improving plasma quality. The ablation process produced a plomb of high-temperature plasma. As the plasma cooled, excited atomic electrons and ions dropped to lower excitation or ground states emitting electro-magnetic (EM) radiation. This EM radiation was collected by collector lenses and sent to the spectrometer via fiber optics. The spectrometer diffracted the radiation and split it into its component wavelengths. Two spectrometers were utilized with one focusing on potassium wavelengths. An optical detector recorded the relative intensity of light for each wavelength. Software processed and stored this information.

Task 4:
AI Modeling and Validation



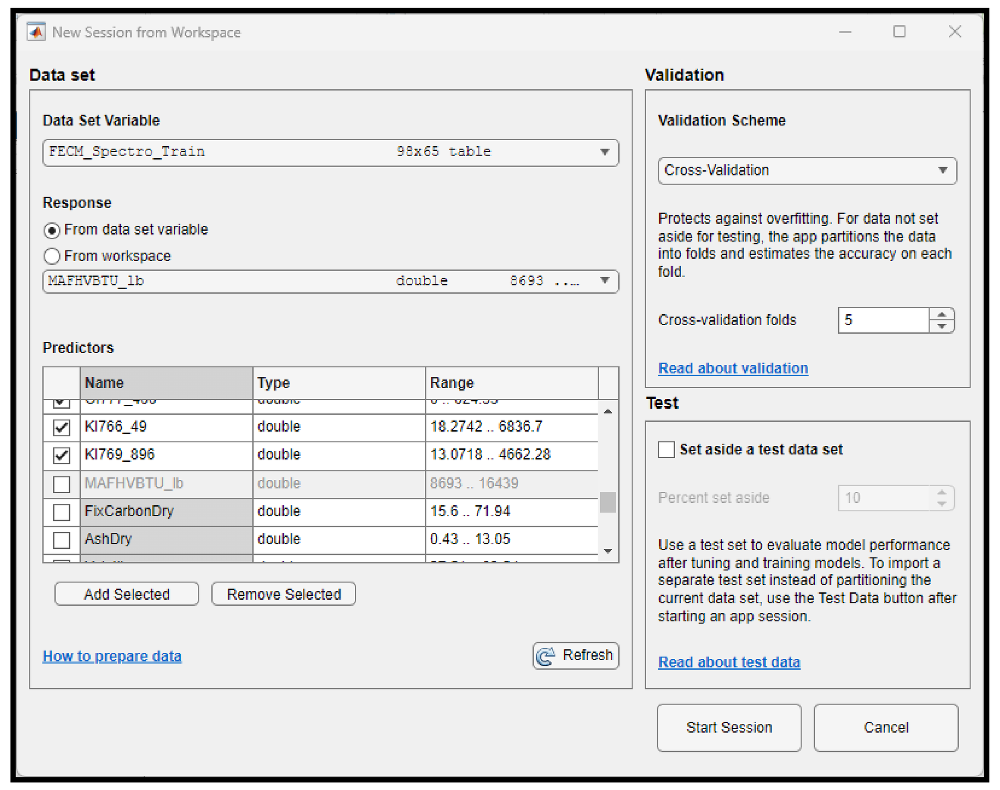
Each of the 6 samples got 20 measurements, and each measurement comprised of 800 shots. ERCo compiled, analyzed, and reduced spectral lines to a few dozen. Additionally, several spectral lines were selectively reduced for each predicated response

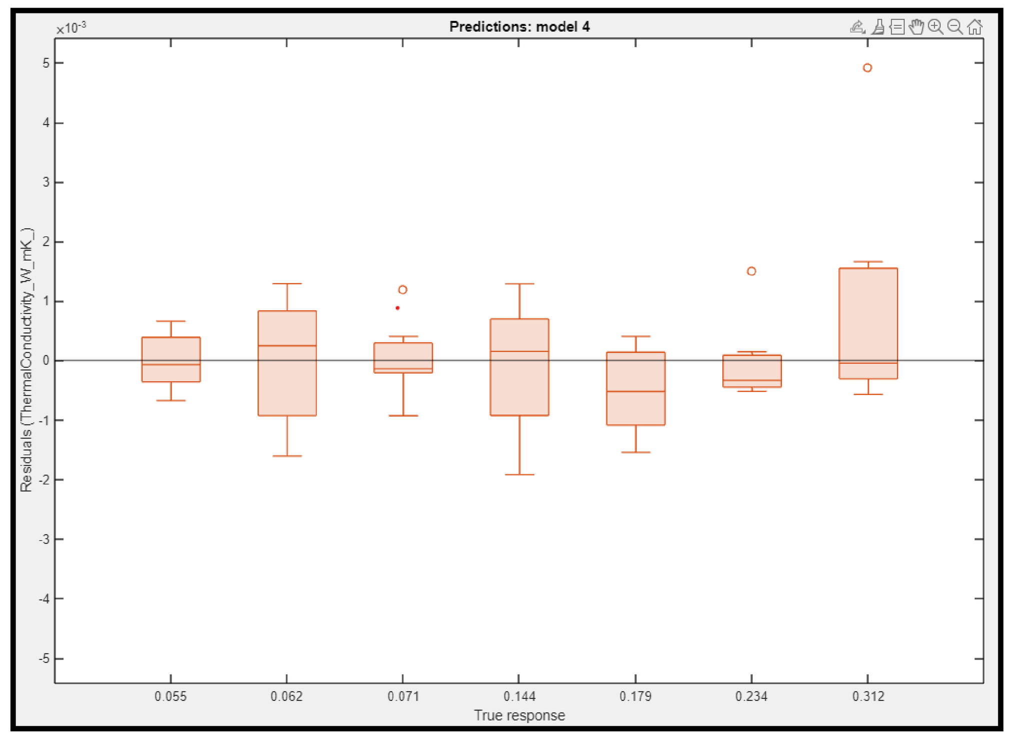
30% of the measurements were randomly selected for testing. Due to low data availability, cross-validation scheme used. Model predictors were spectral lines from LIBS data. Responses included values of proximate analysis, inorganic elemental analysis, calorific value, fusion temperature, chloride content, viscosity temperature and thermal conductivity.

MATLAB Machine Learning (ML) and Deep Learning Toolbox employed for selection and training. This toolbox offered 26 ML models. All models trained using the remaining 70% of data. Validation results were drawn on to select 1-3 models.

Each of the selected models went through an optimization process. MATLAB offers an automated optimization process that implements Bayesian, grid search or random search. Bayesian optimization was used and iterates approximately 50 times.

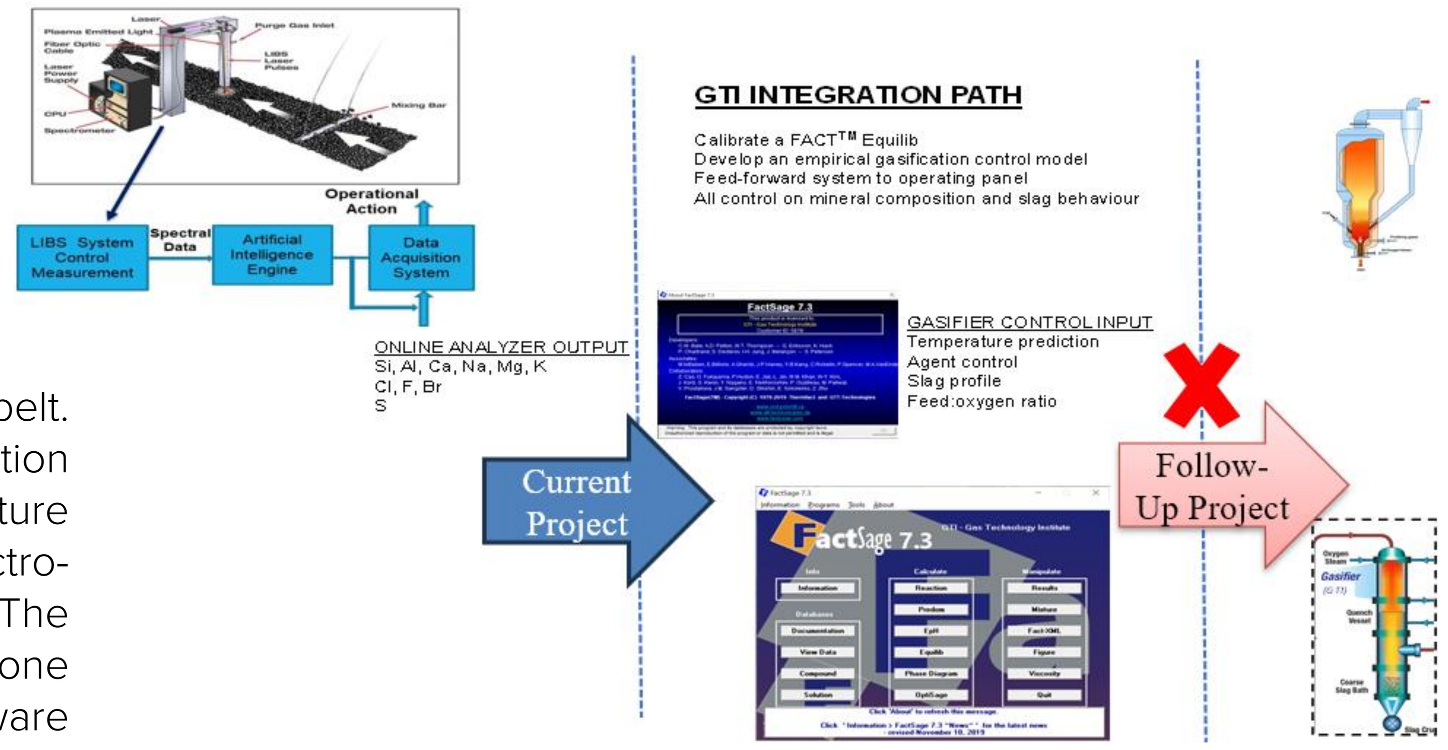
After optimization, each model was tested using the reserved test data. The models were compared using regression and residual plots as well as R-squared, root mean square error (RMSE), and mean absolute error (MAE) and other statistical parameters.





Task 5:
LIBS+ ML with Gasifier Control

- Develop phase equilibrium model predicting gasifier operational parameters (i.e. slag profile)
- Combine empirical gasifier model with phase equilibrium results enabling an input/output feed-forward gasifier control scheme



Task 6:
Technoeconomic Analysis (TEA)

- Develop simplified process-flow diagram for gasification of blended waste feedstocks for hydrogen production
- Develop Excel-based mass and energy balance
  - Gasification reactions
  - Shift reactors
  - Pressure swing adsorption (PSA) for hydrogen recovery
- Capital cost estimate of LIBS+ML online analysis merger
- Integration of mass & energy balances with budgetary economic calculations
  - Revenues
    - Hydrogen and by-product fuel sales
  - Costs
    - Feedstock purchase, oxygen & steam consumption, flux, O&M
- Enable sensitivity analyses on key parameters
  - Availability
  - Production capacity
  - Oxygen and flux consumption
  - Slag control
  - O&M costs