Developing Life Cycle Inventory for Ethanol Plants Using Machine Learning

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Introduction

- **Ethanol Production as a Pathway to Low-Carbon Energy**
  - Widely used renewable fuel, esp. in transportation sector.
  - Corn-based ethanol dominates U.S. production.
  - Produces greenhouse gases (GHGs) across its life cycle and hazardous air pollutants (HAPs) during fermentation.
    - ➢ Potential to optimize fermentation off-gas treatment: reduce GHGs while allowing slightly higher HAPs, remaining within regulatory permit limits.
- **Why Life Cycle Assessment (LCA) Matters**
  - Life Cycle Assessment (LCA) evaluates the environmental impacts of products across their full supply chain life cycle, from feedstock cultivation to fuel combustion. LCA allows comparison of alternatives and identification of key opportunities for improvement. An example of LCA comparison from a different sector is shown in Figure 1.
  - Life Cycle Inventory (LCI) a key part of LCA for tracking material, energy inputs, and emissions.
  - High-resolution LCI data is labor-intensive and often missing, esp. for dynamic processes like fermentation.
- **A Data-Driven Solution Using Machine Learning**
  - ML framework using real-time fermentation data to predict GHG emissions
  - Inputs: pH, total sugar, volume, fermentation phase (time-step variables)
  - Enables faster, scalable, and more accurate LCI generation than traditional methods

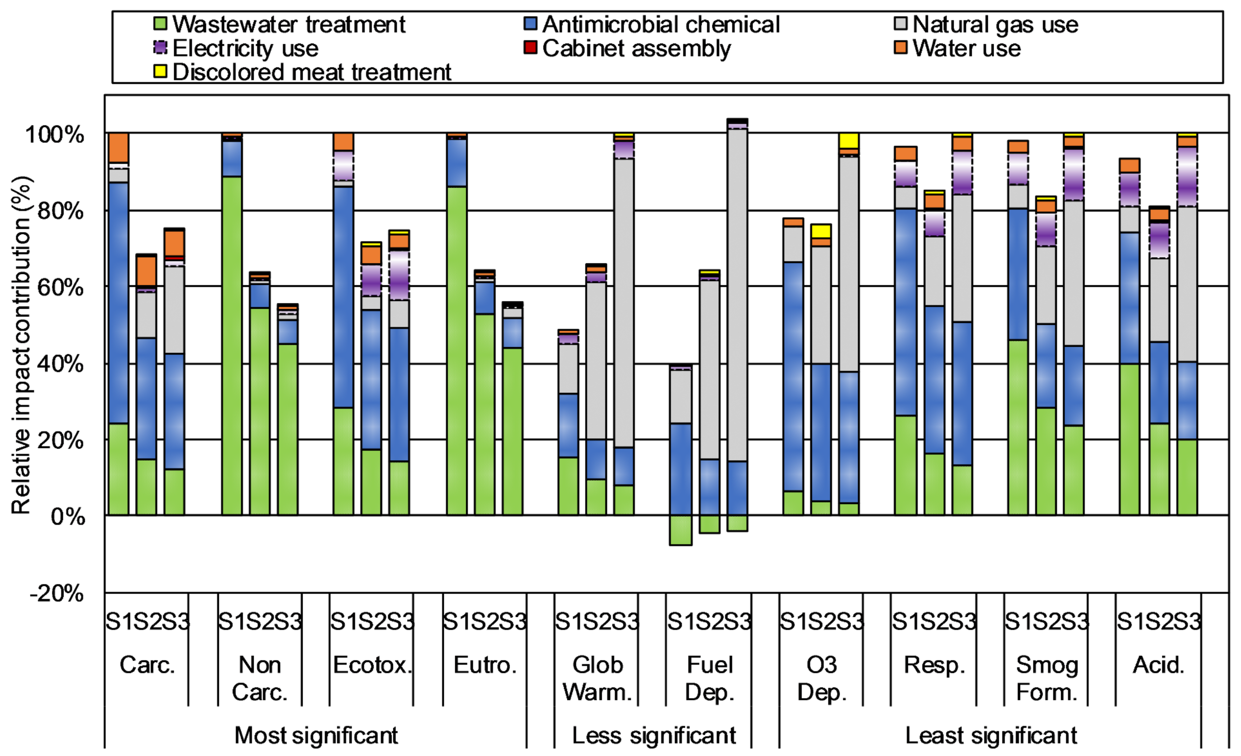

Figure 1. Example of LCA Comparison

Objectives

- Enhance environmental transparency with real-time estimation of GHG and HAP emissions.
- Support LCA of off-gas treatment trade-offs across impact categories.
- Model fermentation emissions using machine learning on real-time operational data.
- Generate LCI data from ML-based emission predictions.

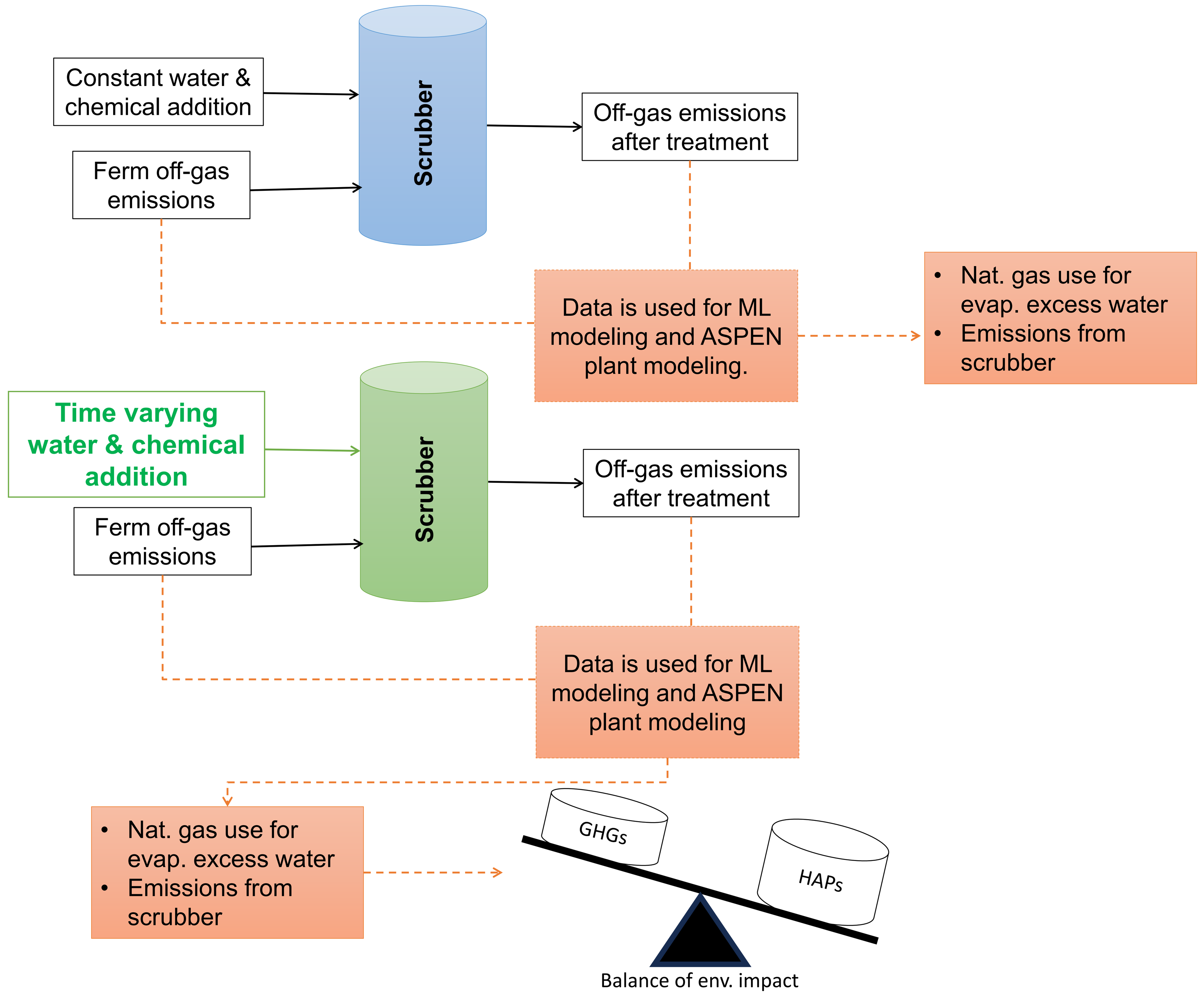

Figure 2. Infographic of the objectives

Methodology

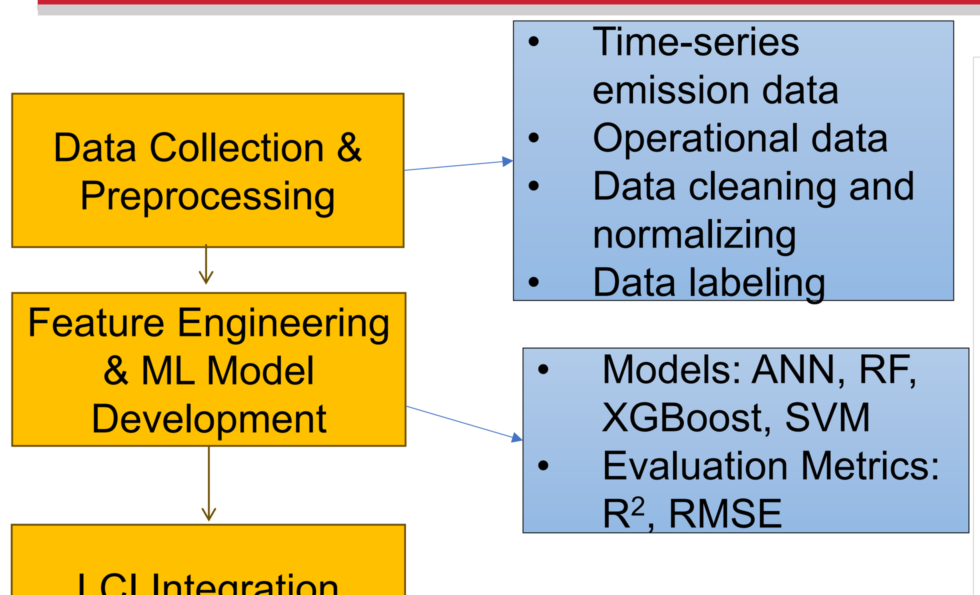

Figure 3. Modeling Framework

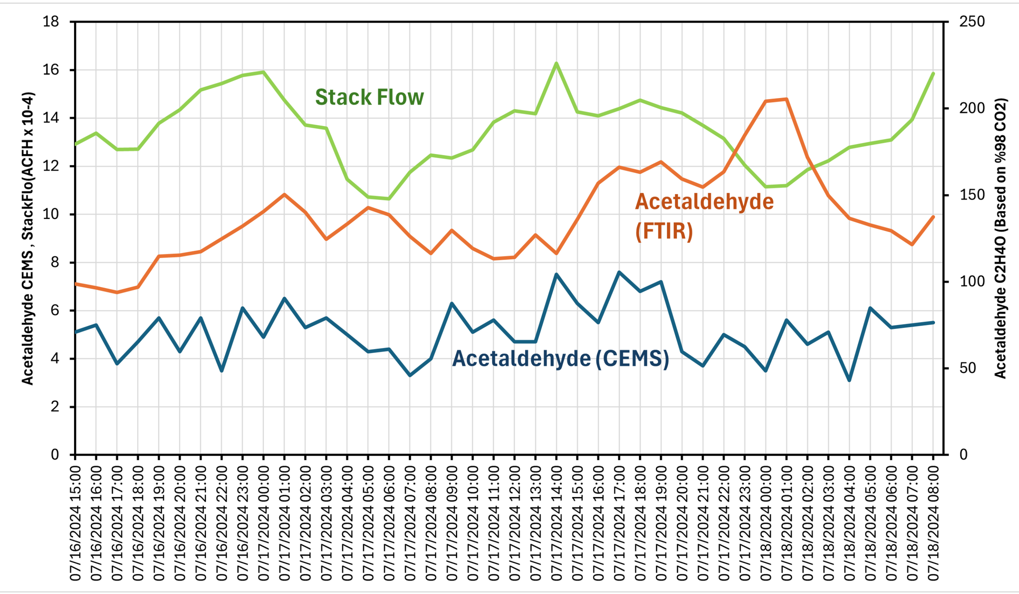

Figure 4. Example of Collected Data

Preliminary Results

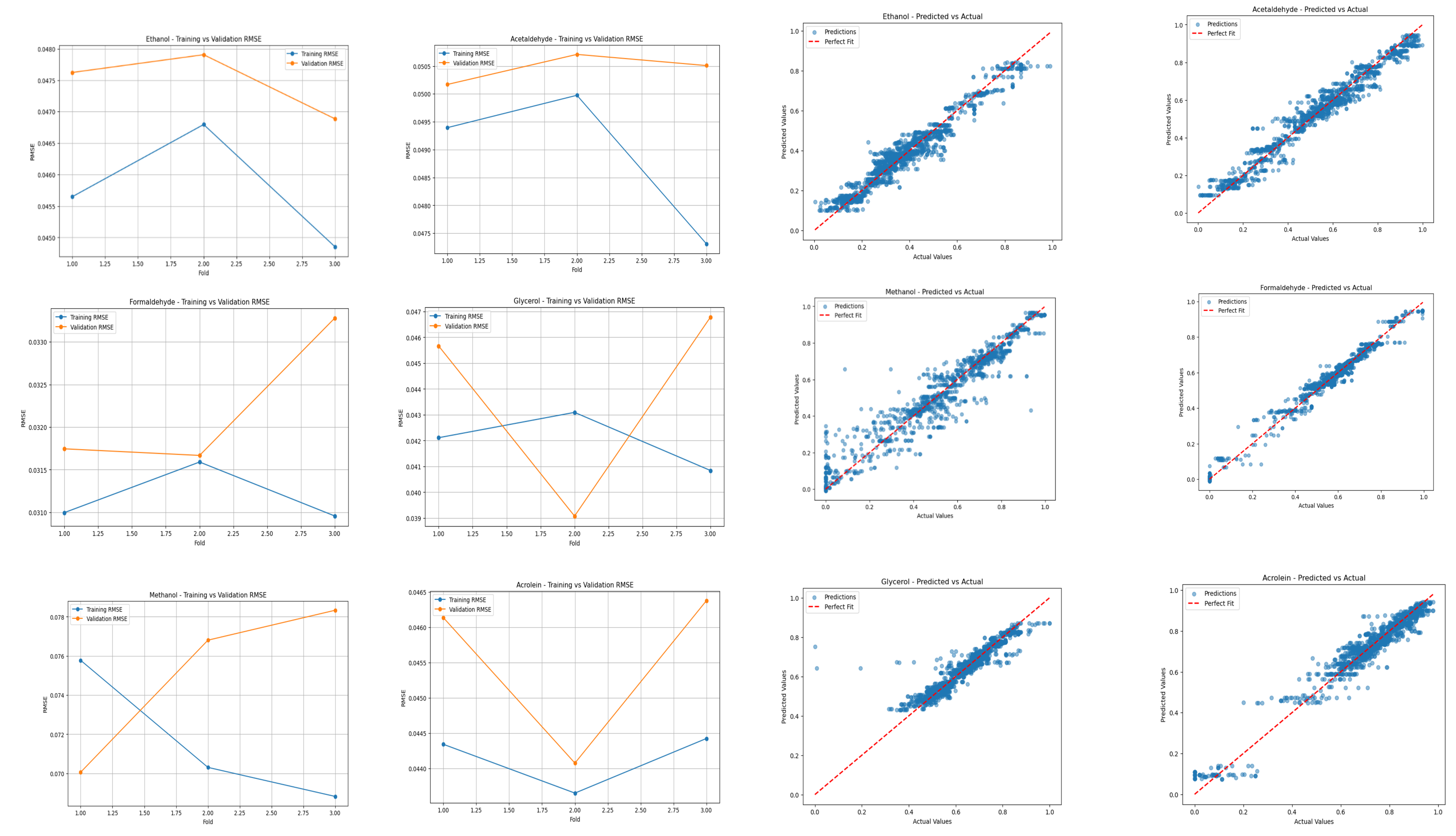

Figure 5. Preliminary results of emission modeling using XGBoost.

Anticipated Results

- Accurate CO_2 and HAP predictions using ML models (ANN, RF, XGBoost)
- Captures emission dynamics across phases (filling, fermentation, CIP)
- Identifies key drivers (pH, sugar, phase) via feature importance
- Time-step emission modeling enables high-resolution LCI data
- Generalizable pipeline across batches and similar plant setups

Potential Benefits

- Real-time estimation of GHG and HAP emissions for enhanced transparency
- ML-based modeling of fermentation emissions using operational data
- Supports LCA of off-gas treatment trade-offs across impact categories
- Enables faster, more accurate LCI generation from model predictions
- Identifies emission drivers for process optimization
- Scalable to other ethanol plants and biofuel systems
- Reduces time, cost, and expertise needed for LCA adoption

Acknowledgements

This work was supported by the Nebraska Public Power District through the Nebraska Center to Energy Sciences Research at the University of Nebraska-Lincoln.

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