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MSEL Energy Environment Health

Multi-parametric Optimization & Control

Process Synthesis and Global Optimization of Novel Ammonia Production Processes

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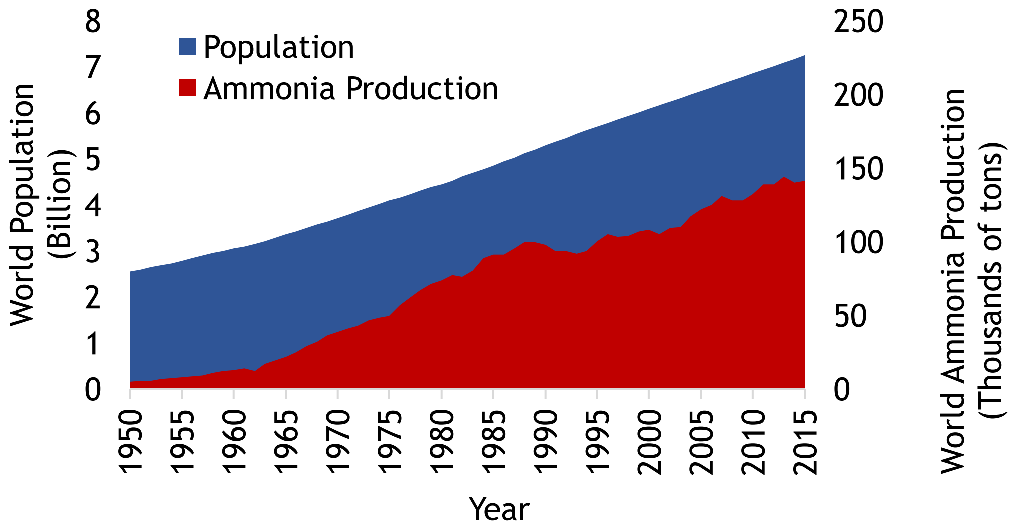
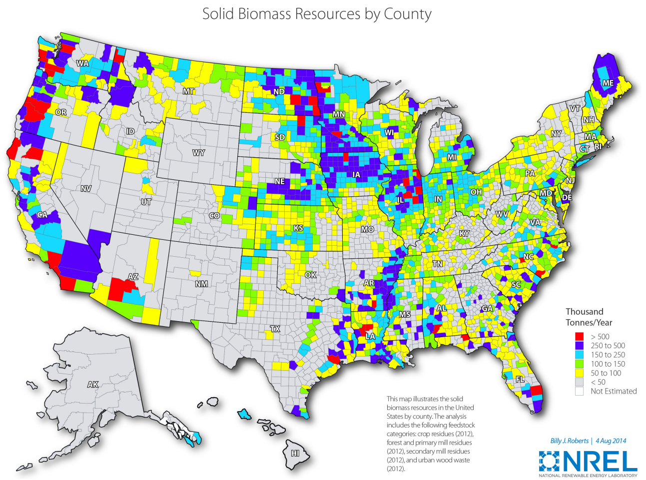
Introduction & Motivation

- World population is expected to reach 8.6 billion by 2035 and 9.4 billion by 2050 and the world GDP will double!
- Ammonia will continue to be produced and used in extensive amounts.
- Biomass is an **environmentally friendly alternative hydrogen source** to natural gas with no net CO_2 emissions





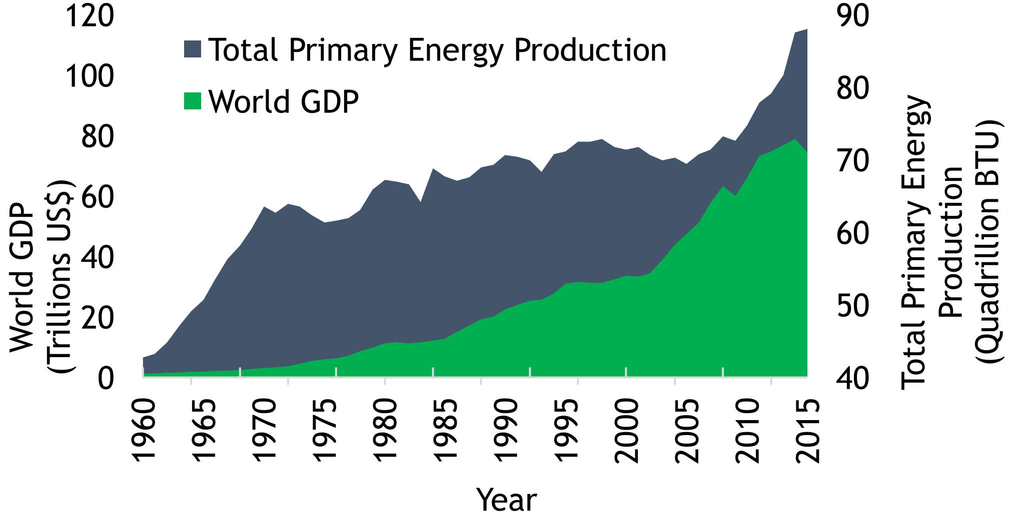
NREL Geospatial Data Science Report, 2014

US DOE, 2016 Billion-Ton Report

EIA Monthly Energy Review, Sept 2017

365 million tons/year of solid biomass was available in 2015!

Possible >1 billion tons/year will be available by 2040!



US Census Bureau, US Geological Survey, World Bank, US EIA

Aims of this Work

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Multi-parametric Optimization & Control

Aim 1: Mathematical modeling of the processes in fossil- and/or renewable fuel-based (hybrid fuel) ammonia production processes

- Develop a data-driven model for ammonia converter
- Present models for process alternatives for syngas generation, syngas cleaning, and ammonia synthesis loop sections

Aim 2: Process synthesis and global optimization of ammonia production processes

- Incorporate all process alternatives in a process superstructure with simultaneous heat, power, and water integration
- Apply global optimization methods to find the globally optimal topologies for different feedstock availabilities, greenhouse gas emission reductions, and plant scales

Ammonia Converter Modeling

Challenges of building data-driven models:

- How to find the best fitting model?
- Which terms should be included in the model?
- Overfitting?

Our solution:

- We prepared **train/validation/test** sets
- **5-fold cross-validation** approach is applied to create 5 models
- These 5 models are tested with new data (test set)
- Below are the scattered results of an example train/validation/test with 55 total points (40-10-5)

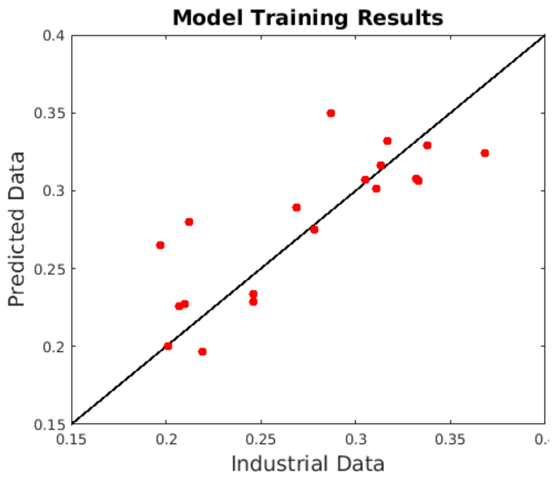
Linear model is selected!

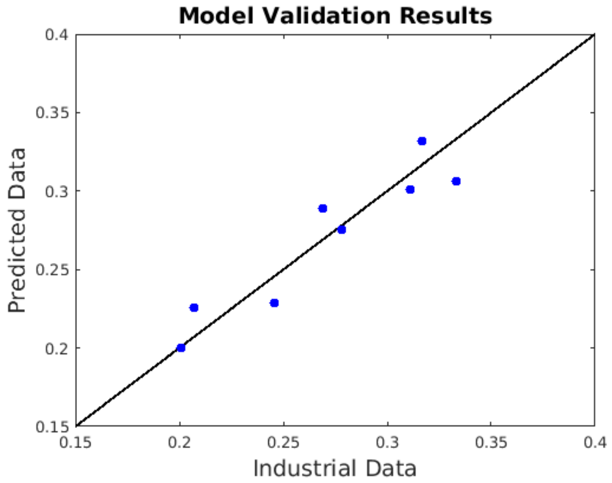
$$\text{Conversion} = \beta_0 + \sum_i \beta_i x_i$$

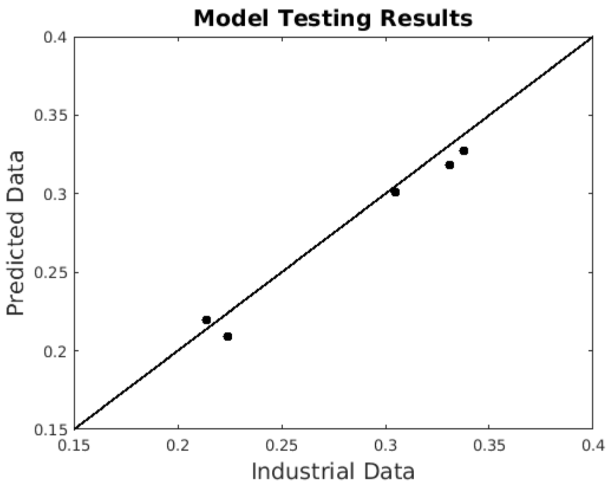
Quadratic pressure term is found to be insignificant!

Addition of quadratic terms of temperature and pressure resulted in overfitting!

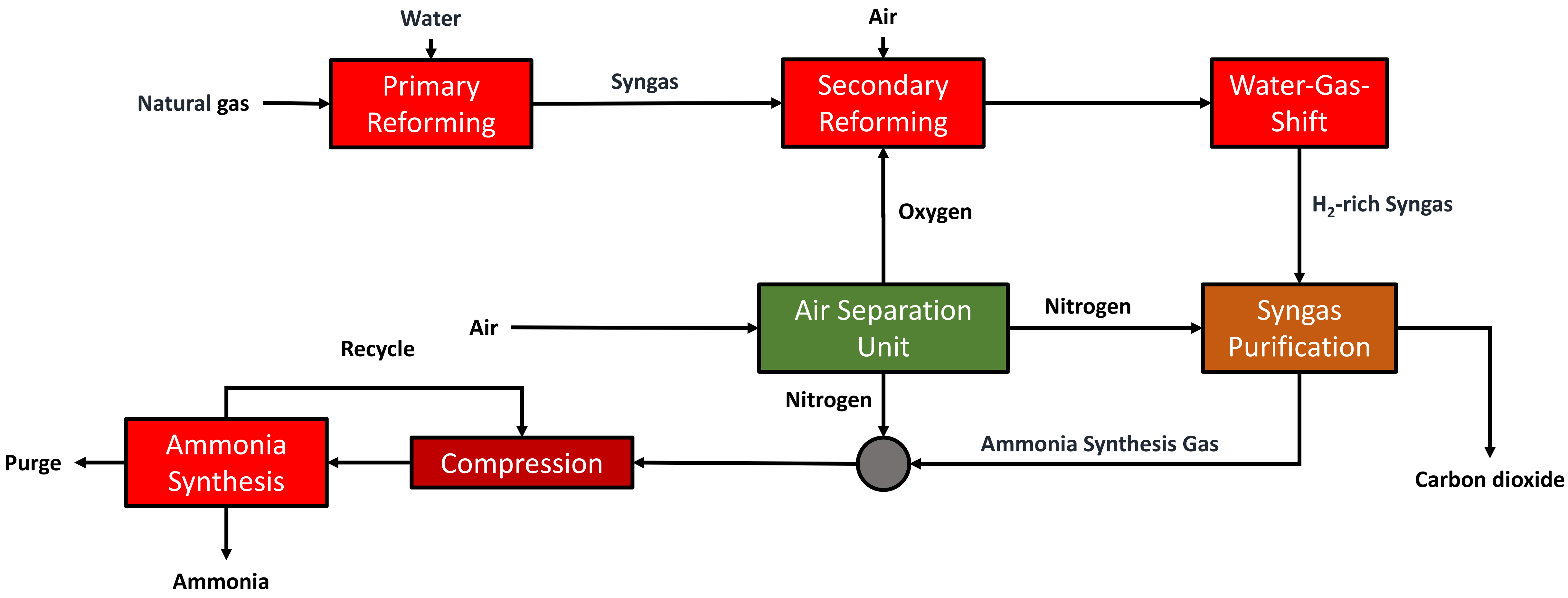
Now we can move on to the process alternatives!



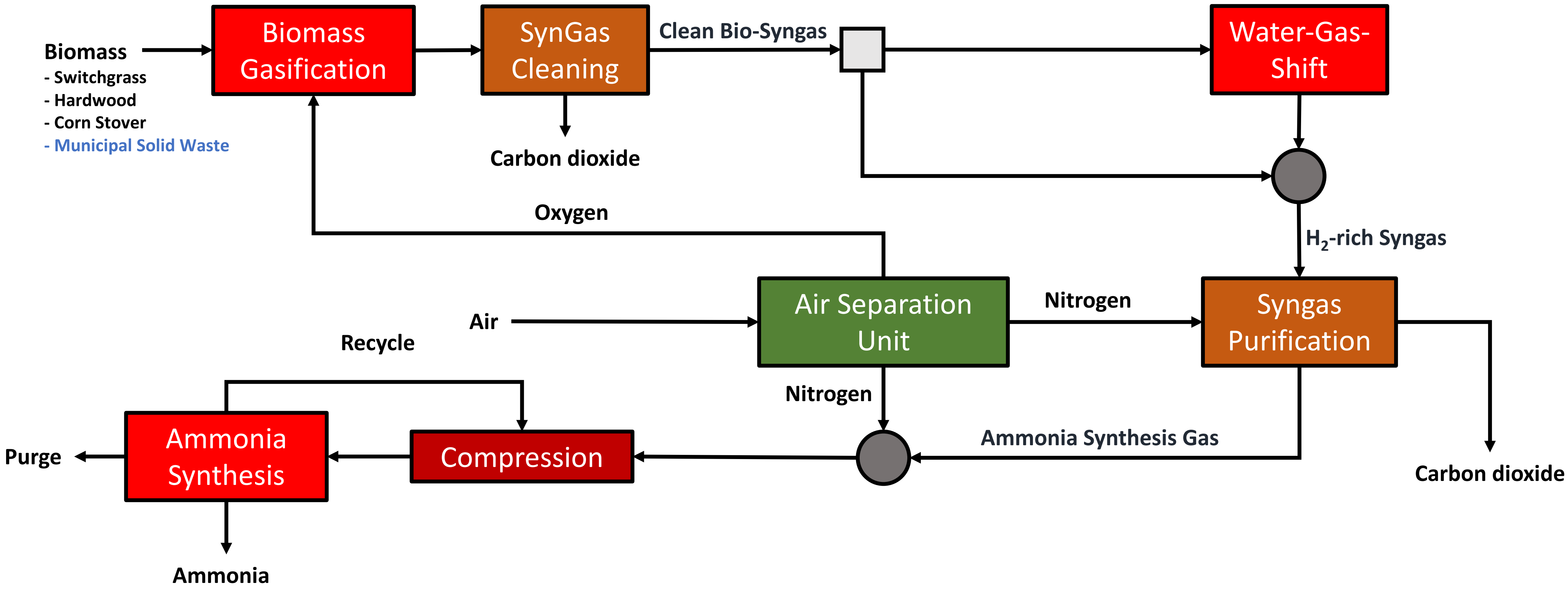




Natural Gas-Based Ammonia Production



Biomass-Based Ammonia Production



Optimization Problem

- Process synthesis problem is a **large-scale nonconvex mixed-integer nonlinear optimization (MINLP)** problem
- Binary variables are used for technology/reactor type selection
- Model includes:
  - **Mass & energy balance equations**
  - **Thermodynamic relations** (phase and chemical reaction equilibria)
  - **Simultaneous heat and power integration**
  - **Concave cost functions for calculation of unit investment costs**
- Nonlinearity comes from the following terms:
  - **Bilinear:** equilibrium reactors, splitters, flash calculations, stream compositions, etc.
  - **Trilinear and quadrilinear terms:** Thermodynamics and equilibrium calculations
- Objective function is minimizing the levelized cost of ammonia production:

$$x^{S}_{u,u_L,s} \cdot N^{T}_{u,u_L} - N^{S}_{u,u_L,s} = 0$$

$$x^{S}_{u,u',CO} \cdot {x^{S}_{u,u',H_2}}^{3} - K^{SR}_{u} \cdot x^{S}_{u,u',CH_4} \cdot x^{S}_{u,u',H_2O} = 0$$

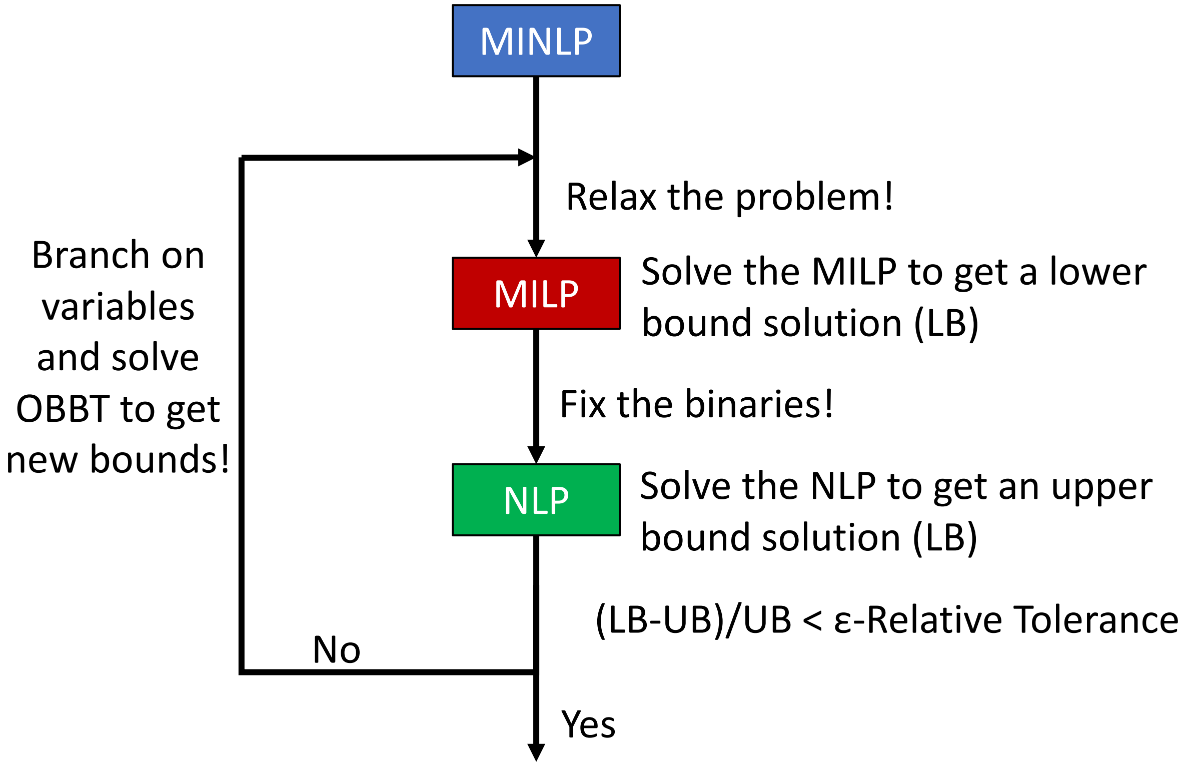
$$x^{S}_{u,u_V,s} - K^{VLE}_{u,s} \cdot x^{S}_{u,u_L,s} = 0$$

$$TDC = (1 + BOP)C_0 \left(\frac{S}{S_0}\right)^{sf}$$

$$MIN \sum_{f \in Feed} Cost_{feed} + Cost_{electricity} + Cost_{CO_2\ sequestration} - Cost_{LPG} + \sum_{u \in U_{INV}} Cost_{units}$$

Global Optimization Algorithm

- We use a tailored branch-and-bound algorithm combined with advanced term-based relaxation techniques to solve the problem to global optimality.
- Piecewise linear underestimators are used with logarithmic partitioning scheme.
- The problem is decomposed into an MILP lower bound and an NLP upper bound problem.



- Feasibility- and optimality-based bounds tightening (FFBT and OBBT) methods are used to obtain good quality bounds.
- Branching is done on the variable with the largest relaxation error.
- The aim is the get a solution within a few percent of the best possible value.

Global optimality is theoretically guaranteed!

Conclusions

- **A data-driven mathematical model is developed for ammonia converter**
- **A process superstructure is synthesized and modeled for biomass-based ammonia production and solved to global optimality**
- **Case studies showed that for single type of feedstock:**
  - Ammonia produced from hardwood type biomass had the lowest break-even price of ammonia with 50% reduction in GHG emissions being possible
  - At smaller plant size, NG-based production has lower break-even price; as the plant size becomes larger, biomass-based process has the lowest break-even price

Acknowledgements

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