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Uncertainty Analysis and ML-based Reduced Order TEA Model Development: A Case Study on HTC of Pulp and Paper Sludge

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About CanmetENERGY

- CanmetENERGY is a science and technology (S&T) branch of Natural Resources Canada and operates three labs across Canada with over 450 scientists, engineers and technicians
- CanmetENERGY-Ottawa's mission is to lead the development of energy S&T solutions for the environmental and economic benefit of Canadians

Outline

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- Identification of Key Parameters Impacting HTC Performance
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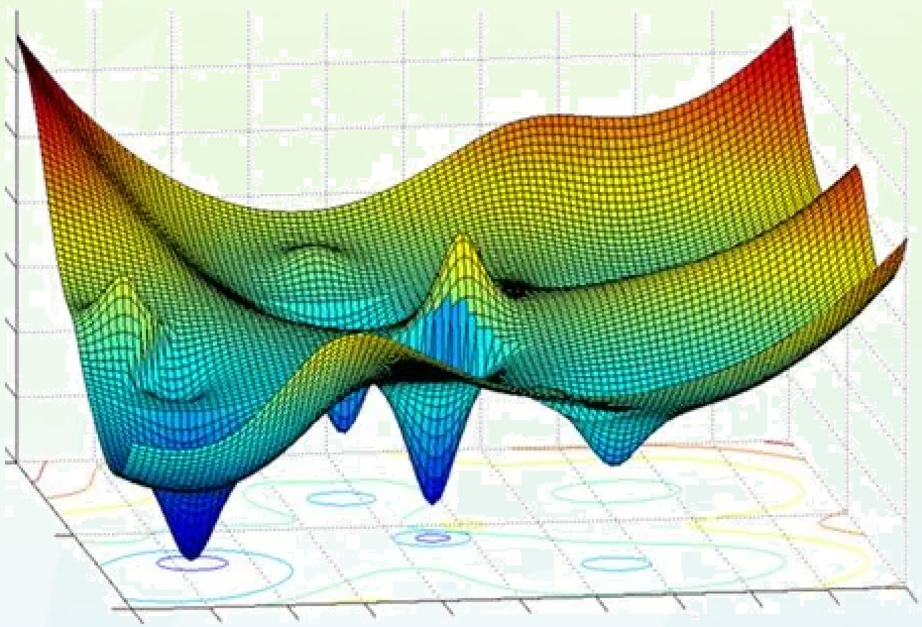
Significance of Uncertainty in Techno-Economic Analysis (TEA)

- Uncertainty analysis is important for decision-making in absence of knowledge of true values or impacts from varied inputs.
- Analysis typically involves evaluating key performance indicators (KPI) vs. a single design choice at a time while keeping others constant
- With large design spaces and many interactions, single variable uncertainy analysis represents only a tiny fraction of the design space
- Conducting sensitivity analysis in TEA of biomass conversion processes can be time-consuming and cumbersome



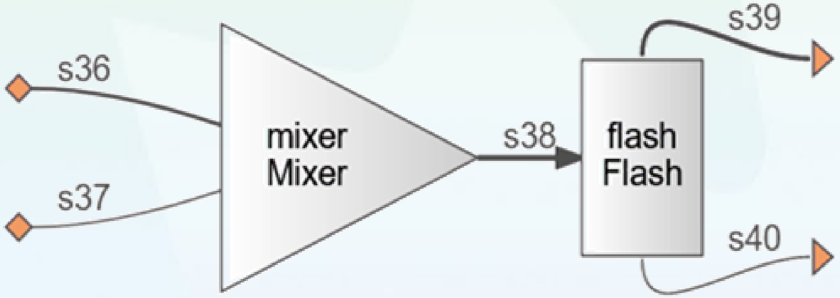
Objectives and Scope

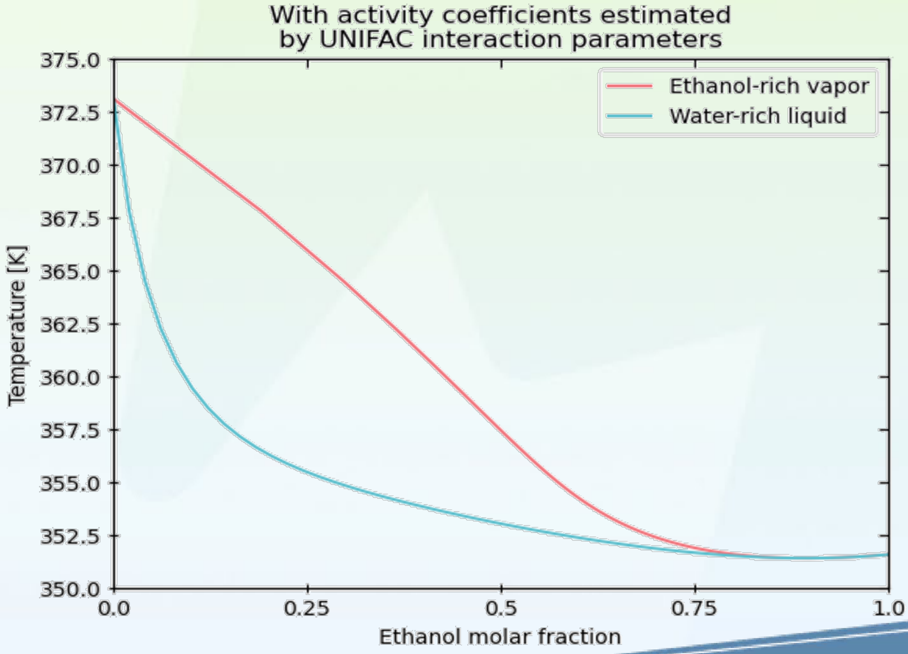
- Adoption/development of consistent, highly automated approach for biomass conversion process simulation (mass and energy balances & phase equilibrium calculations) and TEA
- Application of approach for TEA of hydrothermal carbonization (HTC) of pulp mills' primary pulp sludge
- Identification of key parameters impacting HTC performance under uncertainty
- Demonstrate application of automated TEA approach in enabling ML-based reduced-order-modeling (ROM) of biomass conversion processes

Modeling Platform Selection

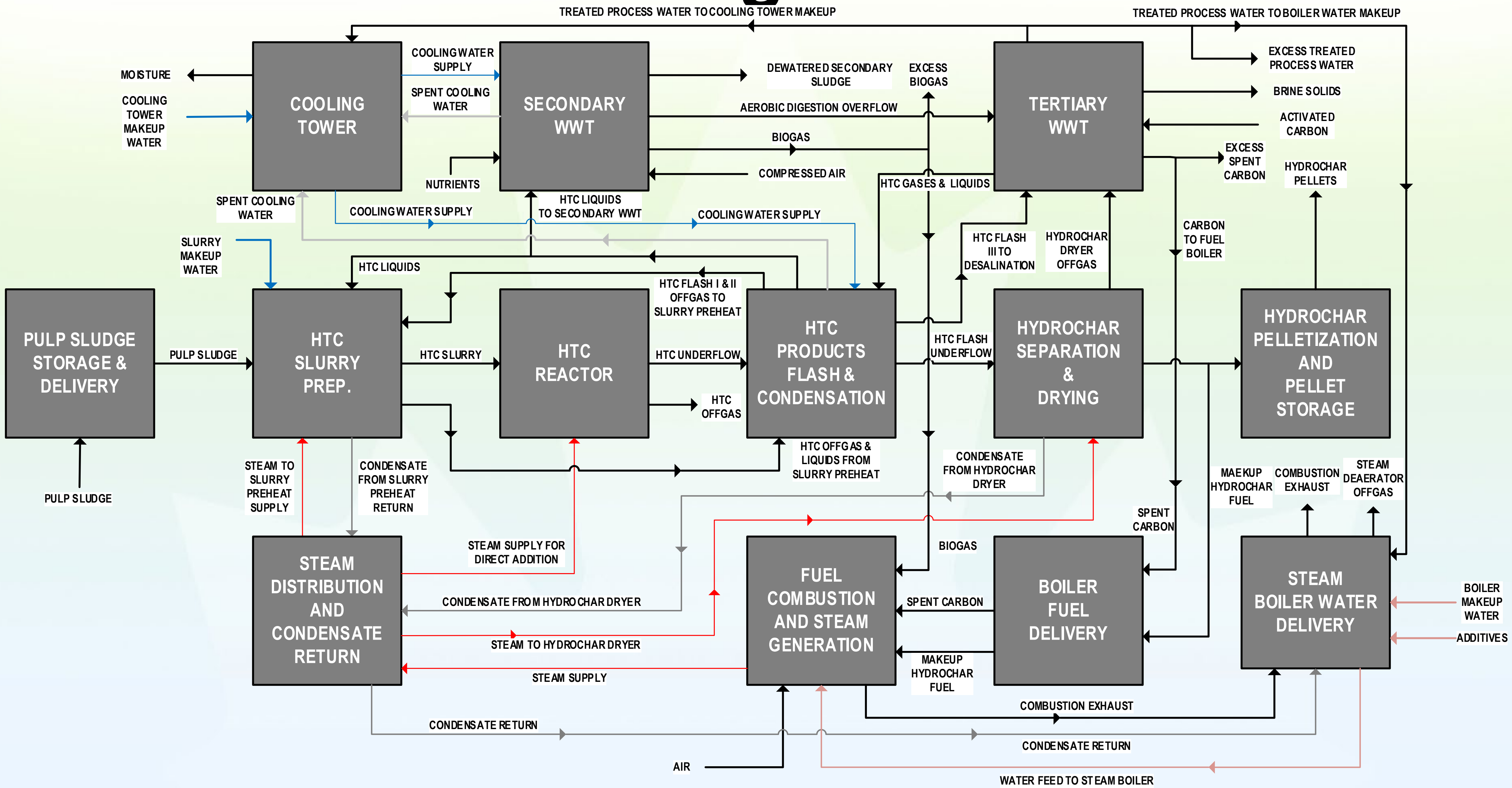
- **Bio**refinery **S**imulation and **T**echno-**E**conomic **A**nalysis **M**odules
- BioSTEAM is an open-source software based in the Python programming language
- It was developed for steady state simulation, TEA and LCA of biorefineries
- BioSTEAM may be used as a screening tool in conjunction with detailed and rigorous design of candidate optimal cases using traditional proprietary software.

```
from biosteam import *
settings.set_thermo(['Water', 'Ethanol'])
Mixer('mixer', ins=[Stream(Water=100, Ethanol=100, units='kmol/hr'),
                    Stream(Water=60, Ethanol=100, units='kmol/hr')])
Flash('flash', ins=F.mixer.effluent, T=354, P=101325)
sys = F.create_system()
sys.simulate()
sys.diagram()
```





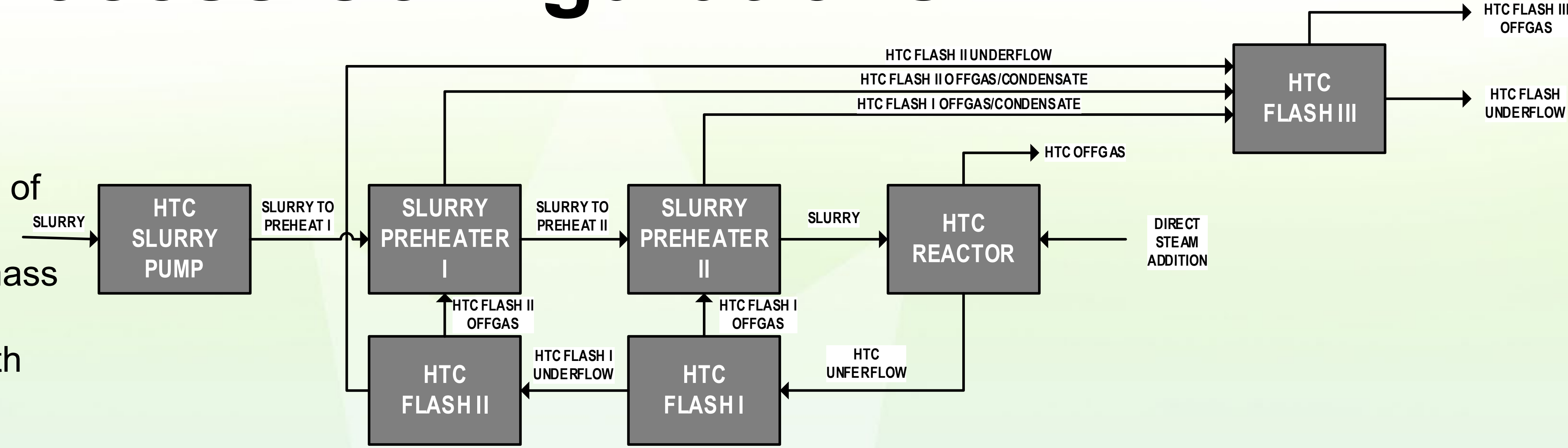
HTC Block Flow Diagram



HTC Process Configurations

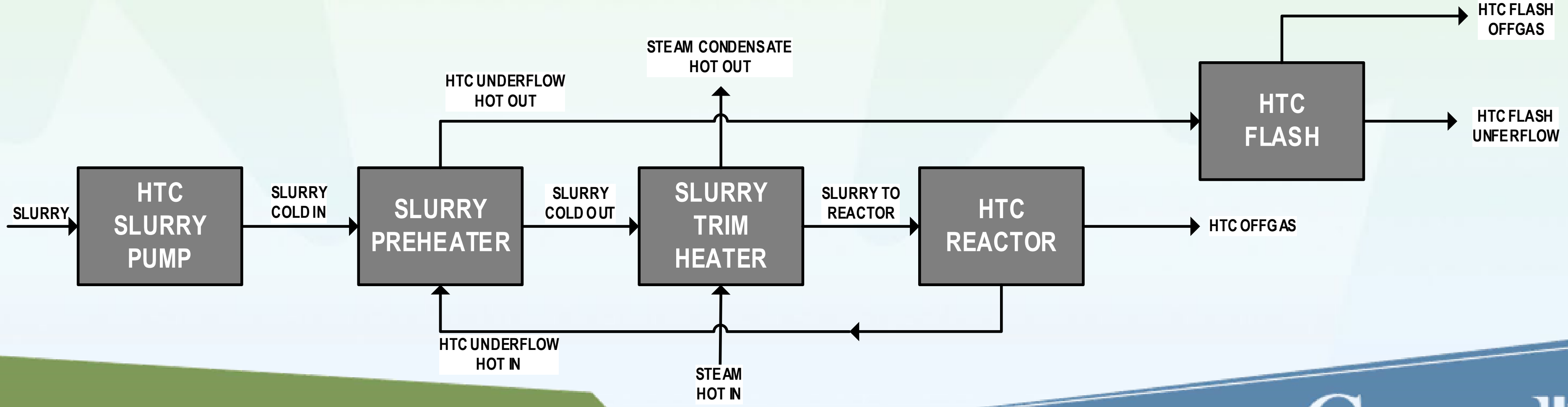
Configuration A

- Assumes difficulty of heat transfer between two biomass slurries & indirect heat exchange with slurries at high temperature



Configuration B

- Assumes no heat transfer limitations between two biomass slurries



Design Basis – Part 1

- Code for custom unit operations was developed with mass and energy balances and phase equilibrium calculations performed using BioSTEAM's engine.
- Sizing heuristics, capacity cost correlations and bare-module-factor-based costing from Turton et al. and Seider et al. were applied.
- Publicly available reports and online vendor data assuming scaling factor of 0.6 were used where costs were missing in above sources.
- Coding of HTC chemicals, process streams, units and their connectivity including process specifications (i.e. determination of flows of key streams, etc.) and reaction set formed the basis of a flowsheet
- Simulation of all units were run up to 120 iterations per case and subject to convergence marked by tolerance of component flow errors below 1% or 1 kmol/hr and temp. error of 0.10K or 0.1%

```
from bioenergy.process.stream.multiphase import *
from biosteam import Unit
import biosteam as bst
from math import pi, sqrt, ceil
from bioenergy.process.units.utilities import capacity_parallel
from bioenergy.process.units.drive import Drive
from bioenergy.process.cost.turton.purchase_cost import purchase
from bioenergy.process.cost.turton.pressure_factor import pressu
from bioenergy.process.reactions.adiabatic import adiabatic_reac

class ProcessVessel(Unit):
    _N_outs = 2
    _N_ins = 1
    _ins_size_is_fixed = False
    _units = {'Volume':'m3',
              'Diameter': 'm'}
    auxiliary_unit_names = ('agitator',)

    def _init(self,tau=10./60.,reactions=None,agitator=None,driv
        self.reactions = None
        if agitator:
            self.auxiliary('agitator', agitator, parent=self)
        self.material = material
        self.reactions = reactions
        self.tau = tau
        self.P = P

    def _run(self):
        self._meb(self.ins,self.outs)

    def _meb(self,ins,outs):
        products = rigorous_mix(ins,reactions=self.reactions,P=s
        remove_phases(products,['g'],outs[0])
        remove_phases(products,['l','s'],outs[1])
```

Design Basis – Part 2

- Experimental results from a 1L batch autoclave form the basis for HTC reaction modeling
- HTC reaction conditions: 265°C and pressures up to 1000 psig (~70 bar), 2 hours residence time
- Product yields per dry gram of pulp sludge: 0.543 g hydrochar, 0.0637 g CO_2, 0.001 g CO
- HTC liquid yields were based on optimization of elemental balances for model compounds of oxygenates with various C:H:O ratios; and speciation of N and S to heterocyclics, amino acids and common ions and water
- Pulp sludge composition (m.f.) : C : 0.54, H : 0.07, N : 0.02, O : 0.37, S : 0.004, ash : 0.04
- Hydrochar composition (m.f.) : C : 0.74, H : 0.06, N : 0.02, O : 0.18, S : 0.003, ash : 0.03
- Aerobic and anaerobic digestion cell biomass formula : $CH_{1.7}O_{0.5}N_{0.2}P_{0.02}S_{0.012}$

Typical HTC Reaction (weight-based coefficients)	Typical Anaerobic Digestion Rxn	Typical Aerobic Digestion Rxn
$pulp\ sludge, s$ $\rightarrow\ 0.0637\ CO_2, g\ +\ 0.00114\ CO, g\ +\ 0.0278\ acetic\ acid, l$ $+\ 0.0656\ furfural, l\ +\ 0.177\ H_2O, l\ +\ 0.000519\ NO_2, l$ $+\ 0.0027\ NO_3, l\ +\ 0.00135\ NH_4, l\ +\ 0.00176\ pyridine, l$ $+\ 0.00301\ sulphate, l\ +\ 0.00145\ thiophene, l$ $+\ 0.0941\ methoxyphenol, s\ +\ 0.542\ hydrochar, s$ $+\ 0.0141\ glutamic\ acid, s\ +\ 0.00343\ cysteine, s$	$0.00472\ NH3, g$ $+\ 0.568\ H_2O, l$ $+\ 0.00161\ sulphate, l$ $+\ methoxyphenol, s$ $\rightarrow 1.03\ CO_2, g$ $+\ 0.505\ CH_4, g$ $+\ 0.0351\ cell\ biomass, s$	$0.0446\ NH_3, g\ +\ 0.626\ O_2, g$ $+\ acetic\ acid, l$ $+\ 0.0147\ sulphate, l$ $+\ 0.0247\ H_2PO_4, l$ $\rightarrow 0.903\ CO_2, g\ +\ 0.48\ H_2O, l$ $+\ 0.326\ cell\ biomass, s$

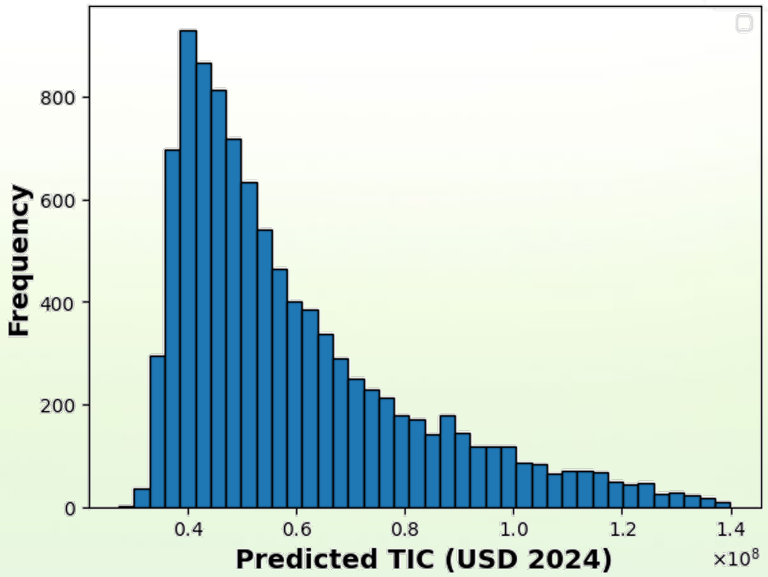
Design Basis – Part 3

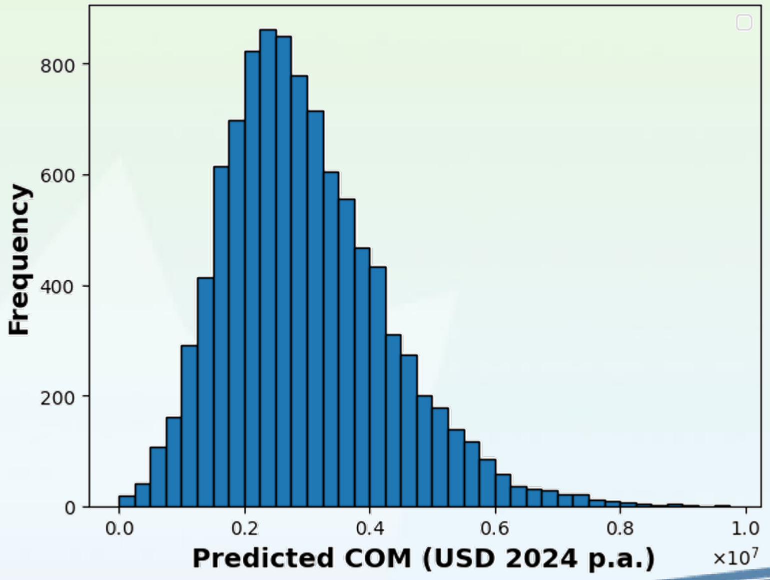
- Monte Carlo simulation with 200 varied parameters assuming rectangular distributions.
- 10000 simulations were carried out for a single pulp sludge feed rate of 2670 kg/hr dry solids
- All dollar values converted to USD for the year of 2024 assuming CEPCI of 800
- Cost of operating labour (COL): assumed 5 operating staff per 8-hour shift and typical Canadian salary within industrial sectors totaling 1.872 million USD p.a.
- Revenues are rooted in sales of hydrochar pellets at 200 USD/tonne and savings from avoidance of waste disposal costs at 90 USD/tonne of wet pulp sludge
- Cost of manufacturing (COM) follows: $0.02TIC + 1.2COL + 1.23(CUT + CWT + CRM)$, where TIC is total installed cost, CUT is cost of utilities, CWT is cost of waste treatment and CRM is cost of raw materials.
- IRR: 0.10, project duration: 10 years, depreciation: MACRS7, income tax: 20%, operating days a year 328.5, construction schedule: 40% in year -2, 60% in year -1, working capital + land: 5% TIC
- Costs of raw materials such as nutrients and activated carbon were from businessanalytiq.com.
- Cost of makeup water and electricity were 0.0002 USD/kg and 0.10 USD/kWh.

Comparison with Benchmark HTC Case Study

Parameter	This Study (most frequently observed)	IEA Task 36 (2021) HTC Case Study
TIC (USD)	40 million	35 million
CAPEX (USD/dry tonne waste p.a.)	1709	1497
COM (USD p.a.)	2.4 million	1.9 million
COL (USD p.a.)	1.9 million	<1.6 million
OPEX (USD/dry tonne of waste p.a.)	101	81

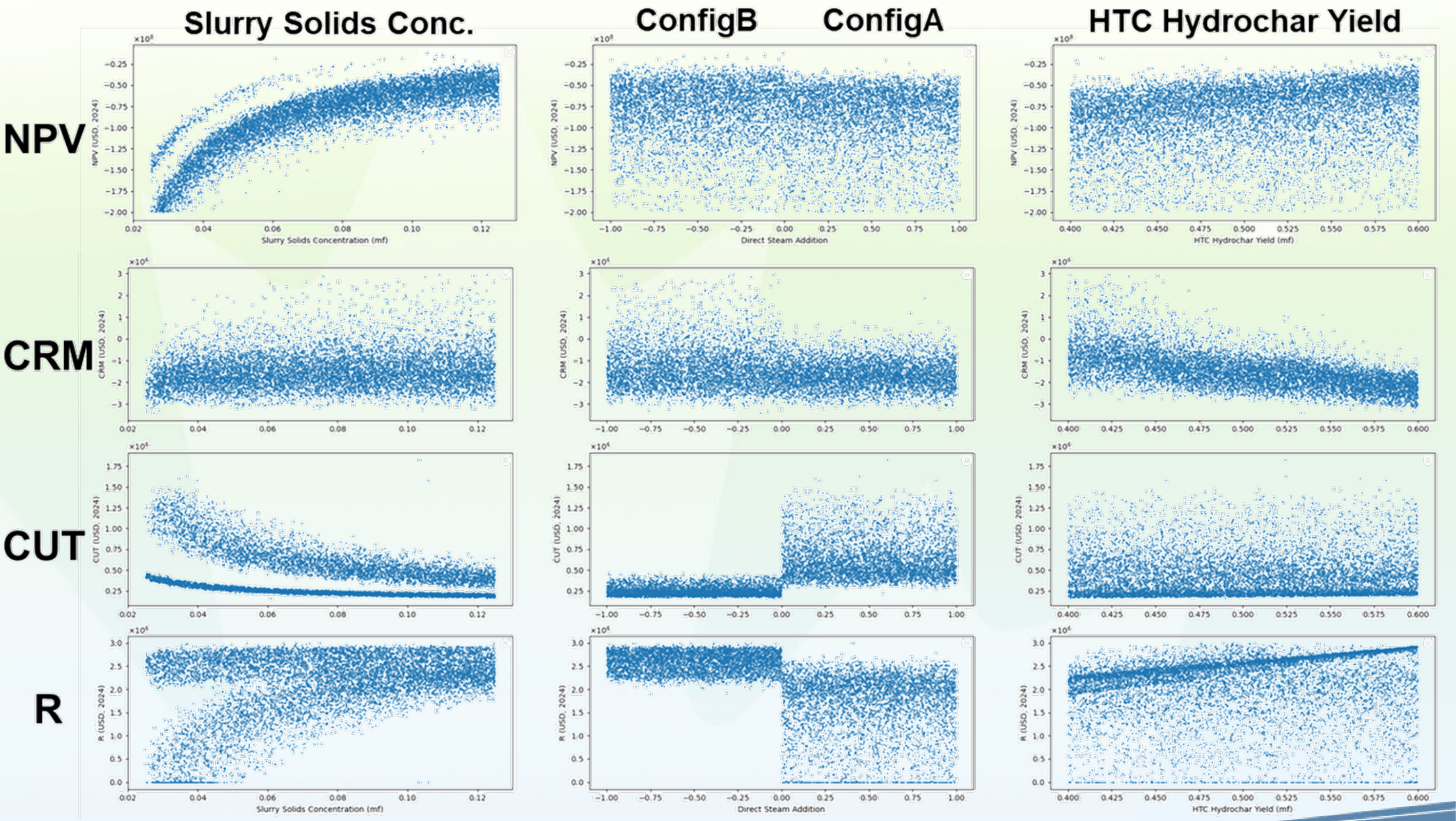
- IEA Task 36 case study uses reverse osmosis (RO) for wastewater treatment instead of secondary wastewater treatment and desalination applied here
- This study performs poorly compared to IEA case due to lower hydrochar yields and assumption in the IEA Task 36 case on revenues from RO liquids nearly matching hydrochar sales.





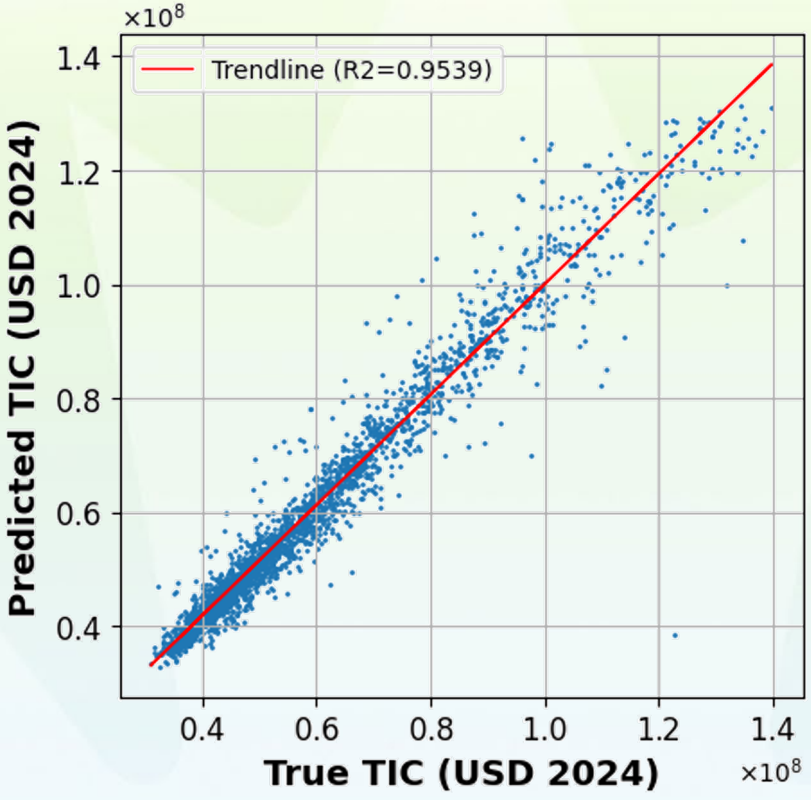
Identification of Key Parameters Impacting HTC Performance

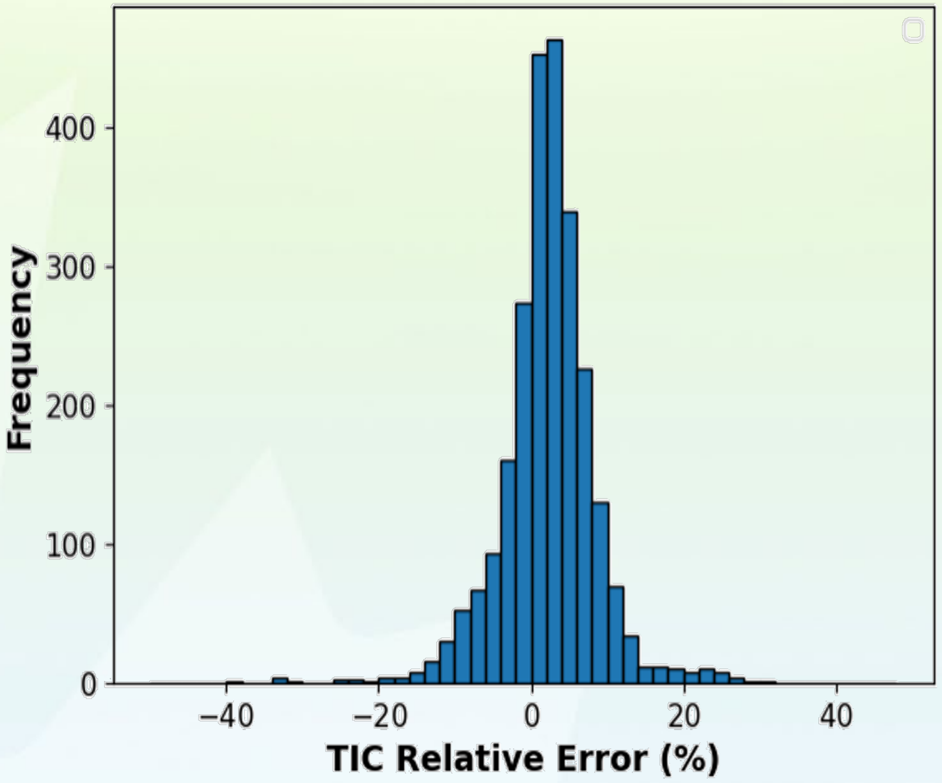
- Parameters of greatest impact on economic performance can be identified qualitatively.
- Identification of key parameters through observations of notable trends rather than non-distinct clouds
- Distinct patterns in plots arise from different configurations modeled and certain conditions fulfilled within each configuration.



ML-Based Reduced Order Model (ROM) Predictions of Total Installed Cost (*TIC*)

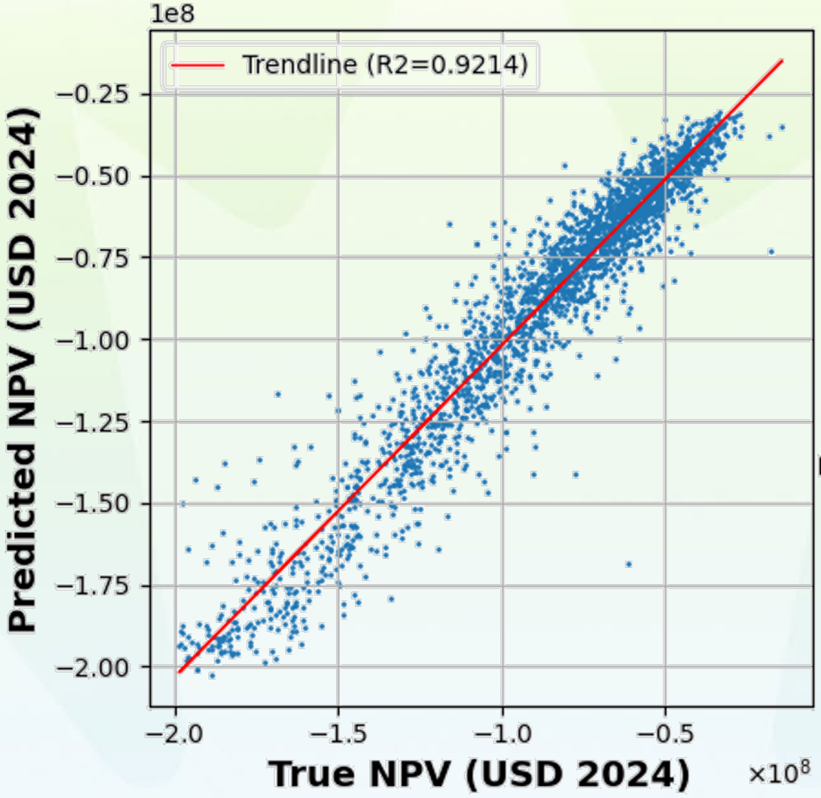
- A deep neural network (ANN) forms the basis of the ML-based ROMs shown.
- ROM with 28 scaled characteristic parameters as inputs was trained with a training dataset of 5000 cases and a validation dataset of 2500
- Plots of "True" vs. model-predicted *TIC* are derived from the remaining 2500 cases set aside and not yet seen by the model. Predictions can be generated in less than one second on a consumer-grade machine
- Majority of *TIC* estimates fall within 10% of “True” value

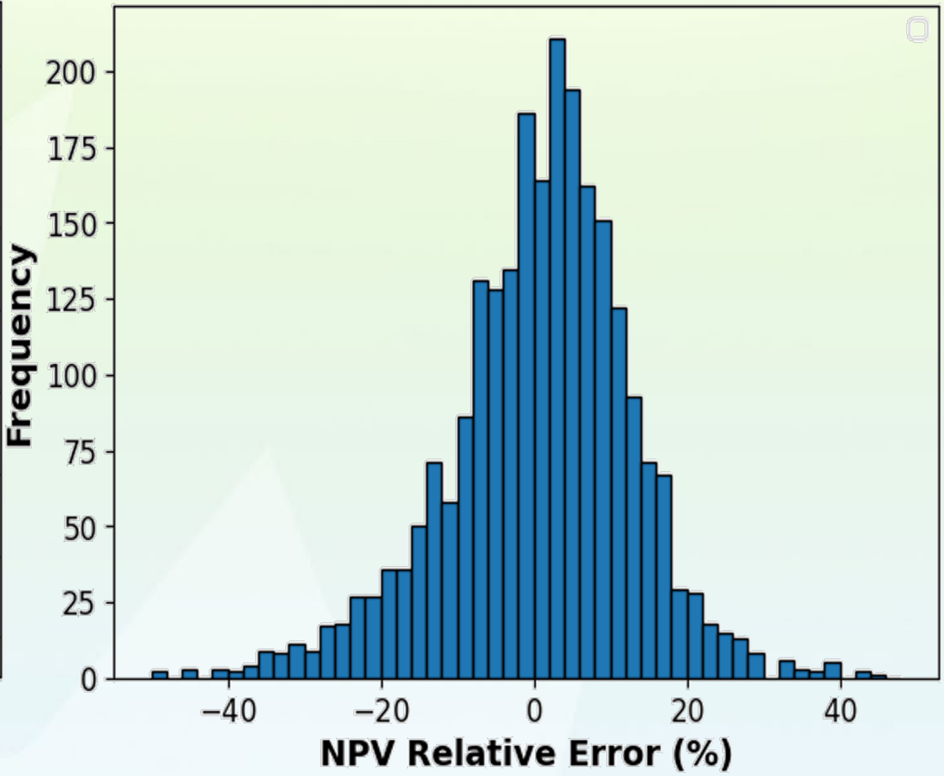




ML-Based Reduced Order Model (ROM) Predictions of Net Present Value (NPV)

- A similar ANN model was developed for NPV with different hyperparameters
- Majority of predicted NPV fall within 20% of “True” value
- The NPV model performs worst than the *TIC* model
- A larger dataset (>10000 cases) may be required to improve accuracy given just over 200 variables subject to uncertainty for the generation of the dataset from process simulation.
- Also, the model may not be tuned with the most optimal hyperparameters.





Closing Remarks

- A python-based platform, BioSTEAM, was adopted successfully for the highly automated, consistent and expeditious TEA of HTC of primary pulp mill sludge
- Predicted KPIs of economic performance from simulations compared closely to a benchmark HTC system of similar scale showcased by IEA Task 36
- Uncertainty analysis revealed HTC slurry solids concentration, feasibility of heat transfer between two biomass slurries and hydrochar yields as key factors impacting economic performance
- Large amounts of data generated from exhaustive uncertainty analysis is amenable to development of ML-based ROMs
- Future work to extend approach to various biomass conversion pathways, extension to LCA, integration with biomass mapping and application of ROMs for development of roadmaps for optimal biomass conversion process deployment in the Canadian context

Acknowledgement

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Thank you!

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