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PROCESS DESIGN AND OPTIMIZATION OF CHEMICAL PRODUCTION FROM BIOMASS FEEDSTOCKS

Department of Chemical & Biochemical Engineering

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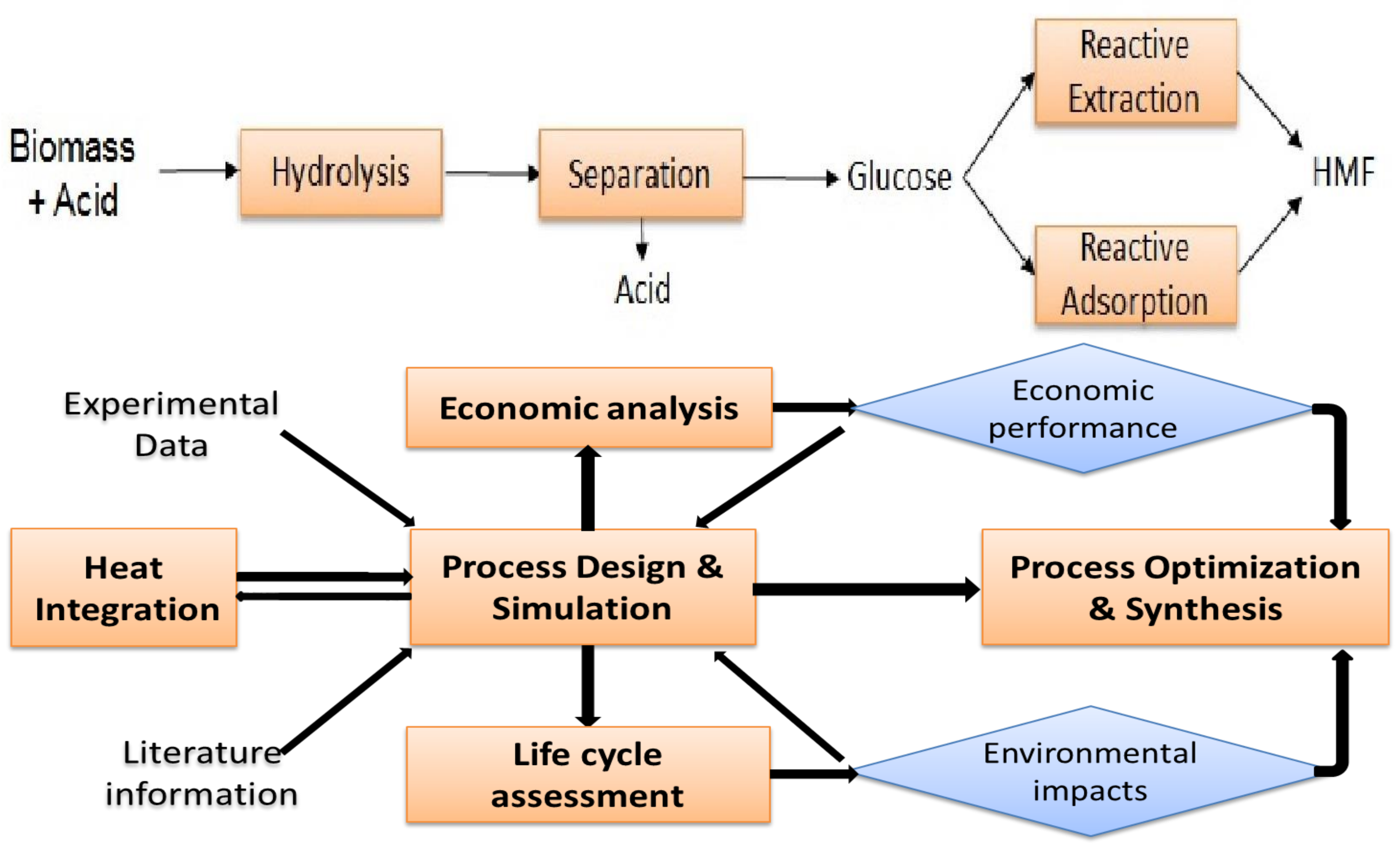
OBJECTIVE

- To investigate paths based on the non-enzymatic hydrolysis of the cellulosic and hemicellulosic fractions to produce sugar mixtures.
- To perform techno-economic and life cycle assessment to evaluate the economic and environmental performance
- To design and optimize the simultaneous production of HMF and furfural from C5 and C6 mixtures

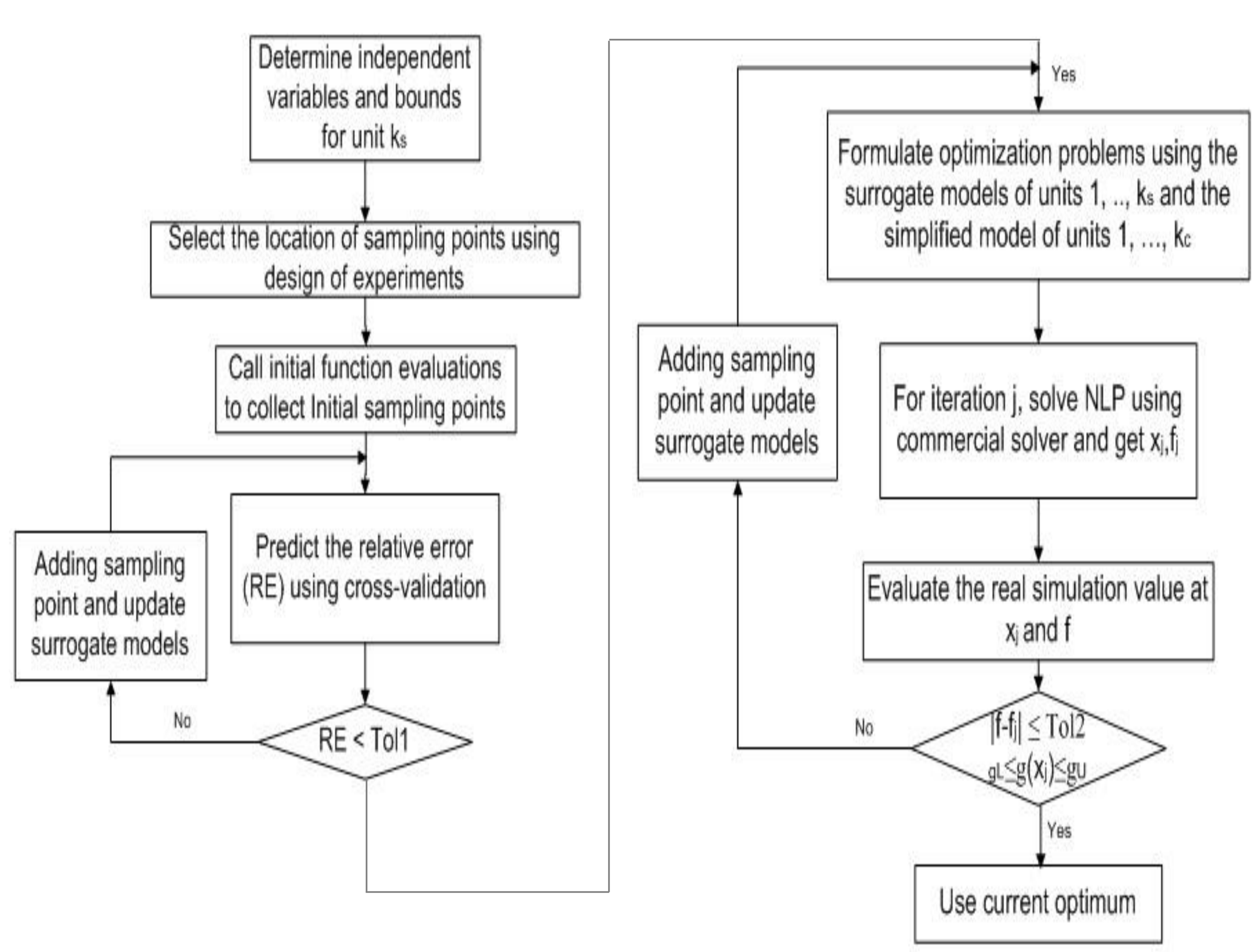
MOTIVATION

- Biomass can be processed in a biorefinery which can take advantage of different components of biomass.
- Biomass be used to produce high-volume but low value fuels as well as low-volume but high value chemicals.
- According to DOE 20% of transportation fuel and 25% of chemical will be produced from biomass in 2030.

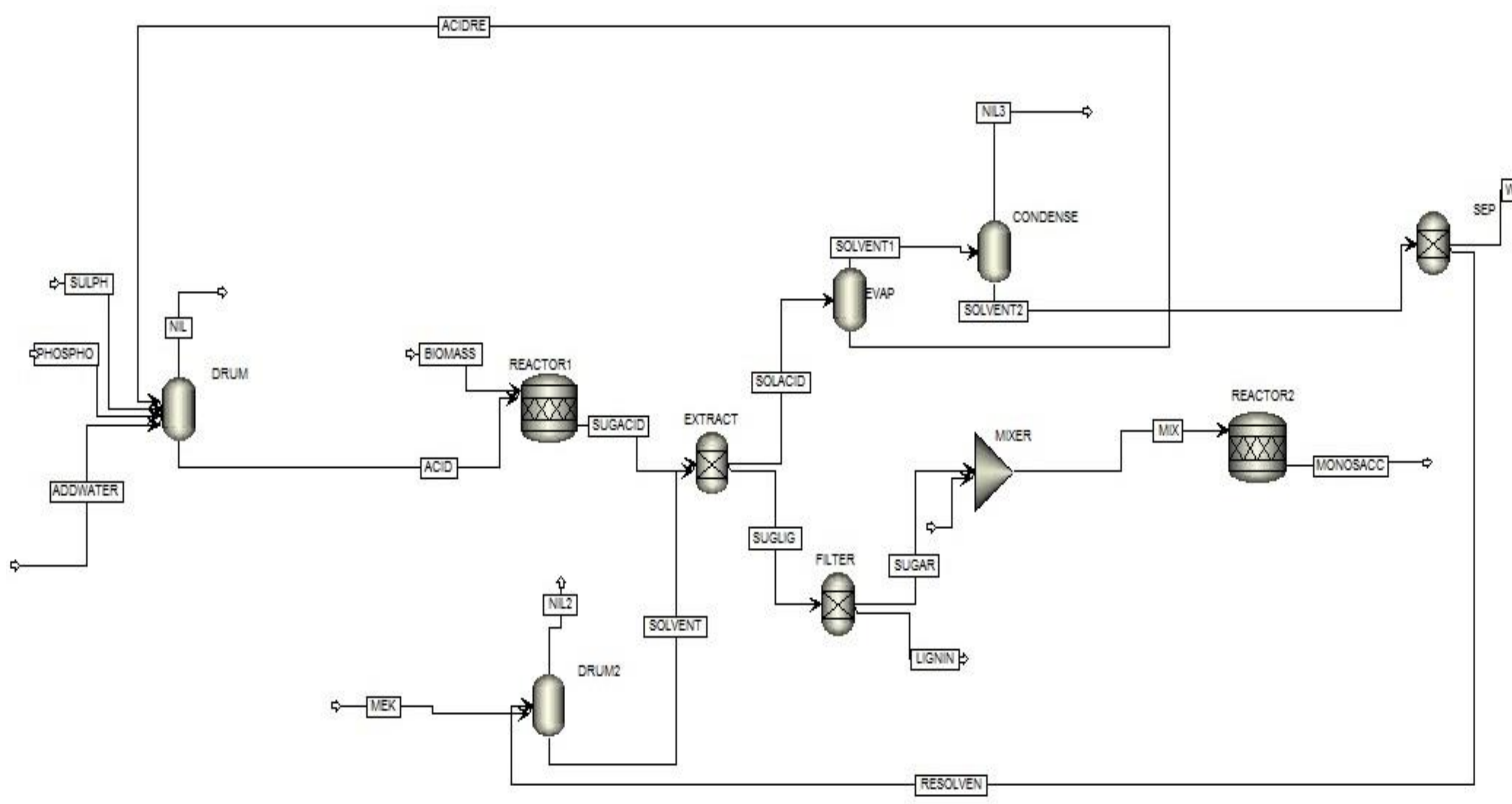
METHODOLOGY



OPTIMIZATION

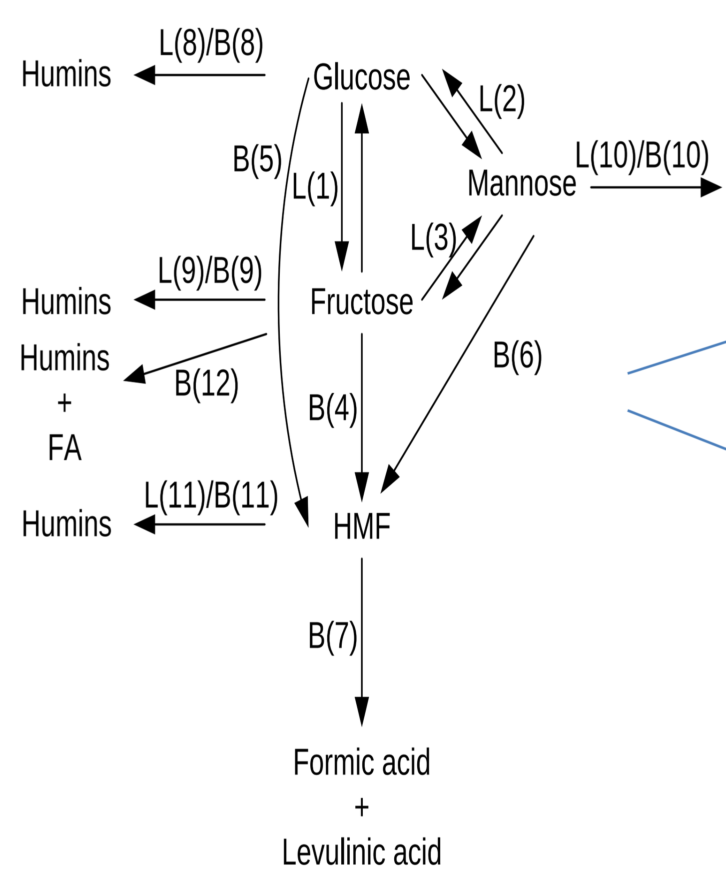


HYDROLYSIS OF BIOMASS (WEYLAND'S PROCESS)

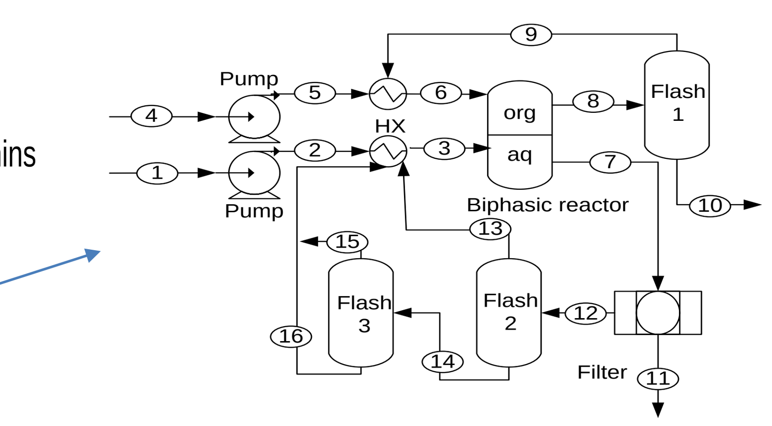


- Acid used for hydrolysis is a mixture of sulphuric acid and phosphoric acid.
- Mixture of sugar and acid is separated using solvent extraction.
- Solvent can be single or combination of at least two compounds.
- Theoretical conversion expected to be >90%.

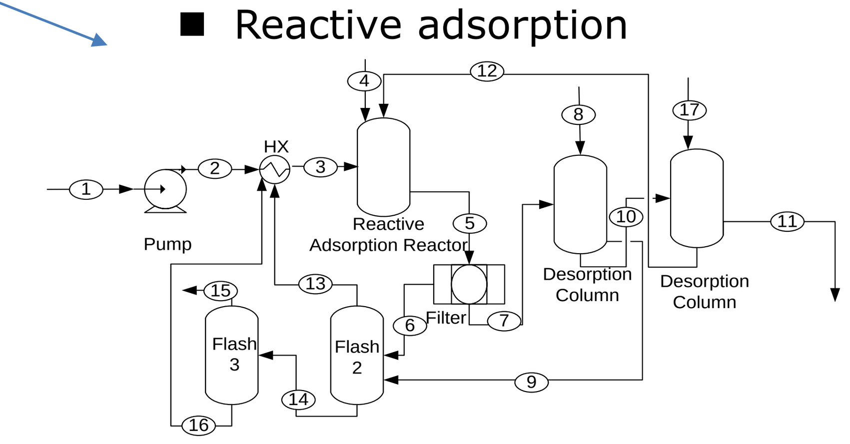
CONVERSION OF GLUCOSE TO HMF



■ Reactive extraction



■ Reactive adsorption



- Reaction and flash units are represented by kriging models

$$F_i^{out} = \hat{f}_R^{F}\left(F_{Glu}^{in}, F_{Man}^{in}, F_{Fru}^{in}, F_{HMF}^{in}, F_{LA}^{in}, F_{FA}^{in}, F_{water}^{in}, F_{CrOH^{2+}}^{in}, F_{H^+}^{in}, \tau, m\right.$$

*: is amount of activated carbon that is used in reactive adsorption

$$F_i^{out} = \hat{f}_{FL}^{F}\left(F_i^{in}, P_{FL}, Vf_{FL}, T_{feed}\right)$$

- Other units use simplified models

$$Q_{FL} = \hat{f}_{FL}^{T}\left(F_i^{in}, P_{FL}, Vf_{FL}, T_{feed}\right)$$

- Objective Function:

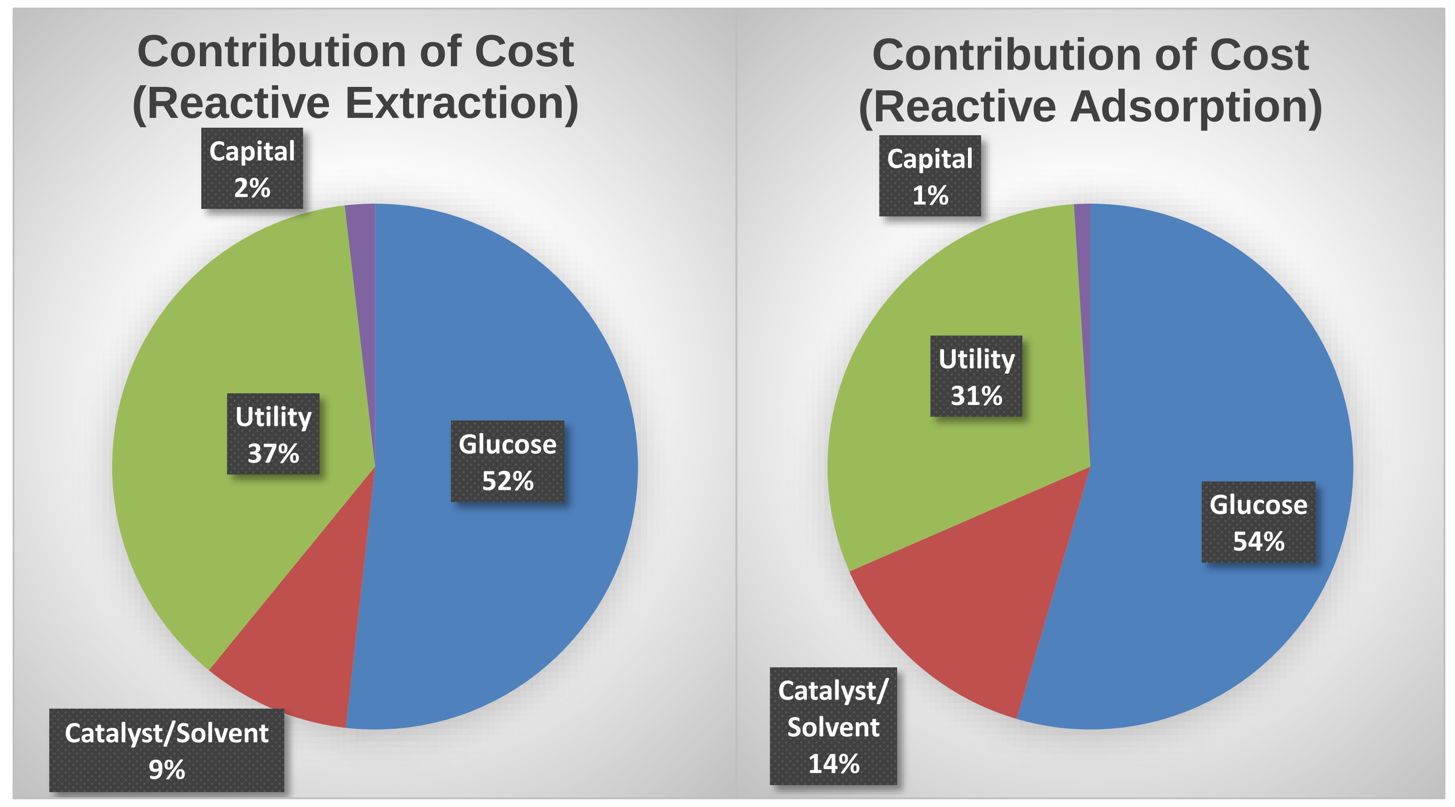
$$\frac{\sum_k R_k C_k^R + \sum_j Q_j C_j^Q + ATCC}{\sum_i P_i}$$

$$ATCC = \frac{TCC}{Project\ Life} = \frac{TDC + TIC + WC}{Project\ Life}$$

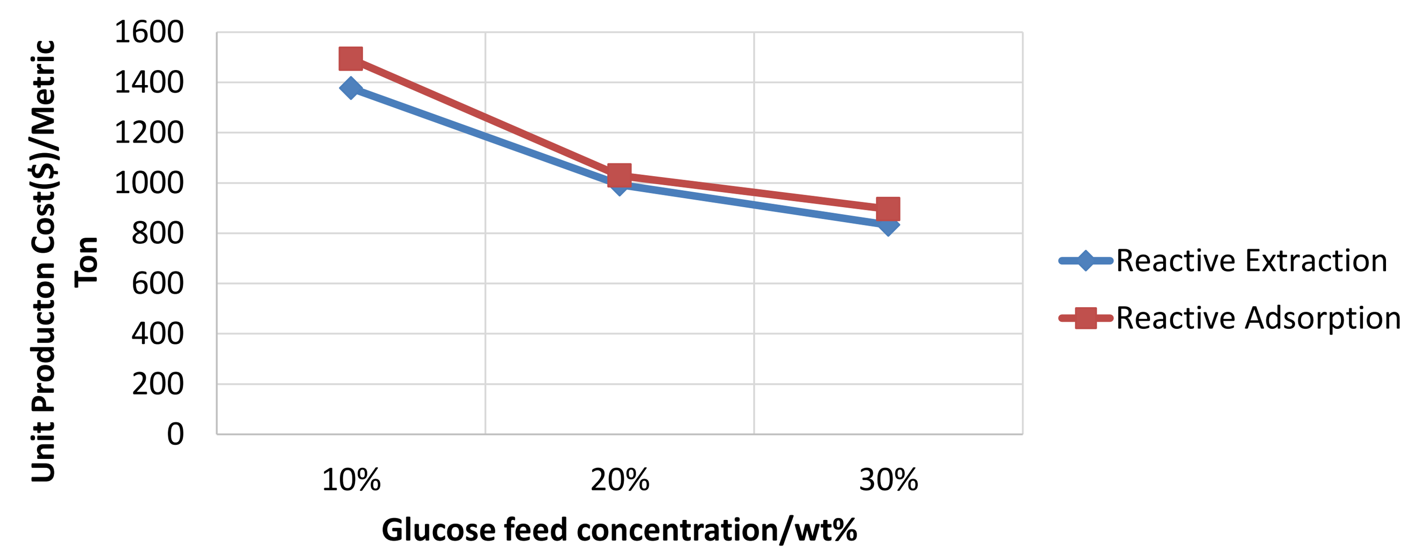
$$TDC = \sum_u TDC_u \left(\frac{CAP_u^{r}}{CAP_u^{b}}\right)^{sf}$$

OPTIMIZATION RESULTS

Optimum	Reactive Extraction	Reactive Adsorption
Reactor temperature/K	450.21	473.15
Residence time/min	16.27	27
Feed flow of glucose/mol/min	1.7555	1.7555
Activated carbon concentration/g/L	Nil	100
$P1/10^5$Pa	9	Nil
Vapor fraction of flash 1	0.6474	Nil
$P2/10^5$Pa	0.8	0.3
Vapor fraction of flash 2	0.0482	0.001
$P3/10^5$Pa	0.8	0.8
Vapor fraction of flash 2	0.2785	0.7162
Capacity /mol glucose/min	17555	17555
Feed flow of CrCl3/mol/min	0.022	0.6677
Feed flow of HCl/mol/min	0.275	2.6163



- The minimum unit production cost for Reactive Extraction is \$833/metric ton.
- The minimum production cost for Reactive Adsorption is \$896/metric ton



FUTURE WORK

- Performing techno-economic and life cycle analysis of Concentrated acid hydrolysis of Biomass to Glucose
- Adding xylose with its reaction pathway to the above model and performing optimization.
- Performing life cycle analysis of the optimized model.