Multi-objective Optimisation of Pretreatment of Sugarcane Bagasse for Bioethanol Production

Joanne Crimes

Supervisors: Prof. Duncan Fraser & Dr. Adeniyi Isafiade

Environmental & Process Systems Engineering

Chemical Engineering

University of Cape Town

South African Context

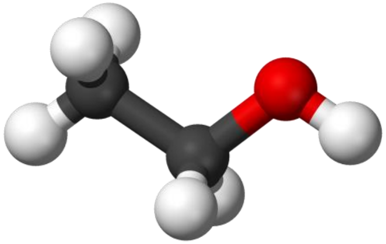
Sugarcane bagasse (SCB)

Used to produce steam

3.3 Mt/year (Lynd et al., 2003)

Project Overview

Sugarcane bagasse

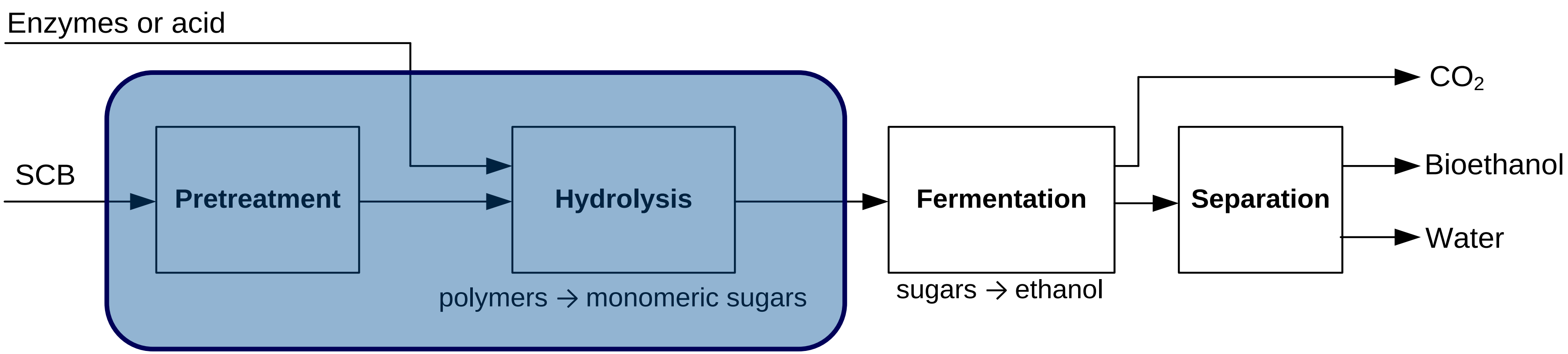


Ethanol

Lignocellulose

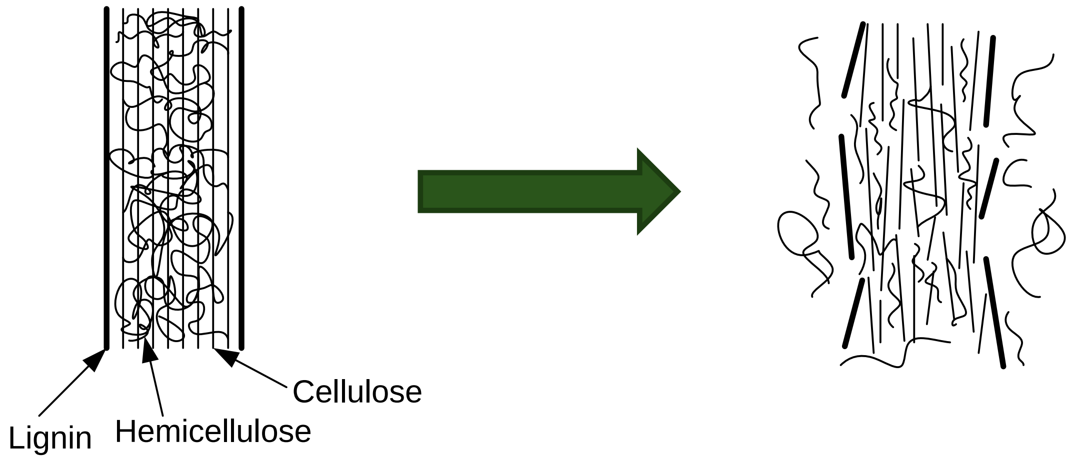
40% cellulose	(polymer of glucose, C6)
22% lignin	(aromatic polymer)
20% hemicellulose	(branched polymer of C5 & C6 sugars)

Project Overview



<u>Aim:</u> To use modelling to optimise the process flowsheet for pretreatment and hydrolysis in terms of both economic and environmental objectives.

Pretreatment



Biological, physical, chemical, physicochemical

Hydrolysis

- Breaking polysaccharides into monomers using water

$$(C_6H_{10}O_5)_n + nH_2O \rightarrow n(C_6H_{12}O_6)$$

- Enzymatic
  - pH 4.8, atm P, T of 45 – 50°C
  - May require detoxification before

- Chemical
  - Using acid, atm P, T of 180 - 230°C
  - Produce more inhibitors to fermentation

Modelling

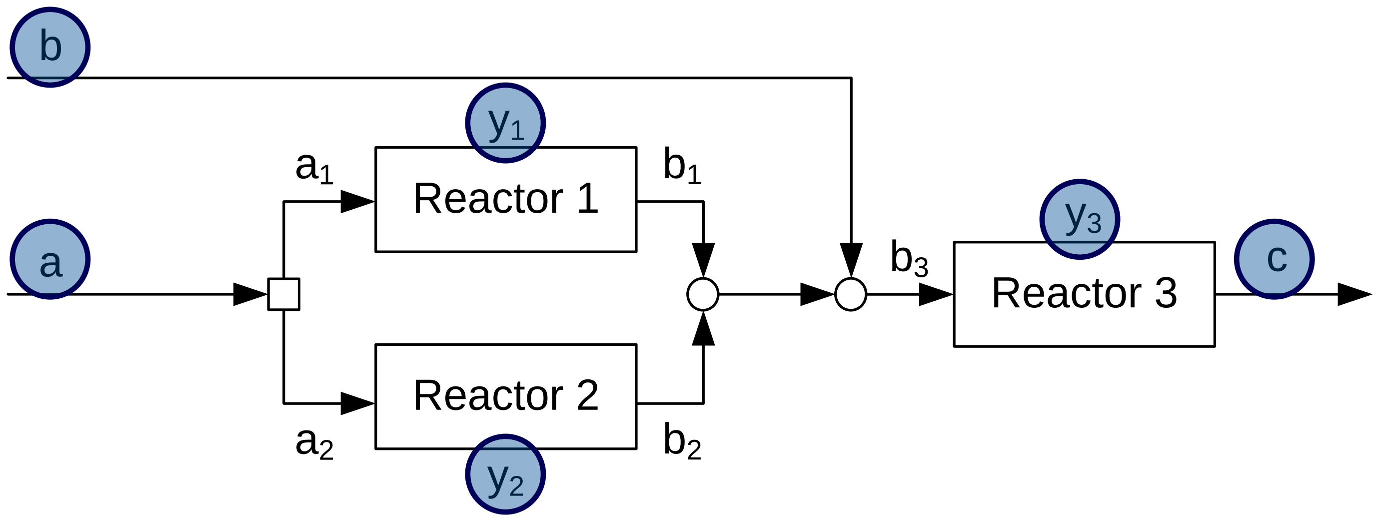
Why modelling?

- Process design is usually uses a sequential approach
- Modelling uses a simultaneous approach
  - Interactions can be taken into account and optimised

Modelling

Superstructures

Can be used to embed many possible flowsheets into one model



$$A \rightarrow B \rightarrow C$$

Modelling

General process synthesis problem formulation

$$z(y^K) = \min_x c^T y^K + f(x)$$

Such that:

$$g(x) \leq 0$$

$$h(x) = 0$$

$$A\,x = a$$

$$B\,y^K + C\,x \leq d$$

$$x \in X = \{x \mid x \in R^n, x_L \leq x \leq x_U\}$$

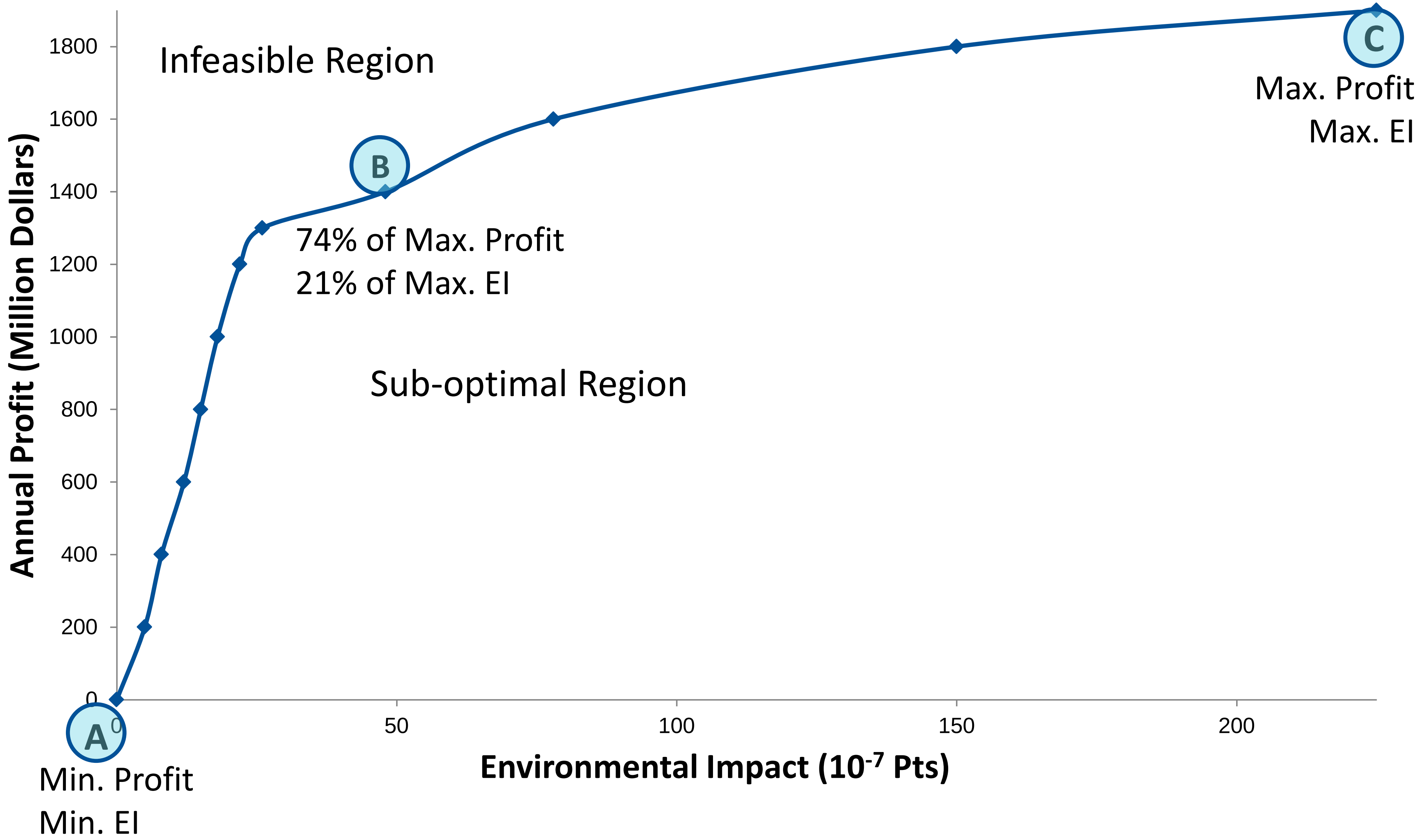
$$y^K \in Y = \{y^K \mid y^K \in \{0,1\}^m, E y^K \leq e\}$$

Mixed Integer Non-Linear Problem (MINLP)

Environmental Impact

SimaPro using a liquid fuels database.

Multi-Objective Optimisation



Chosen Pretreatments

Pretreatment:

Steam explosion (acid catalysed & uncatalysed)

Acid pretreatment

Delignification:

Using NaOH

Hydrolysis:

Acid

Enzymatic

Steam Explosion Model

Mass balance of pilot-scale pretreatment of sugarcane bagasse by steam explosion followed by alkaline delignification.

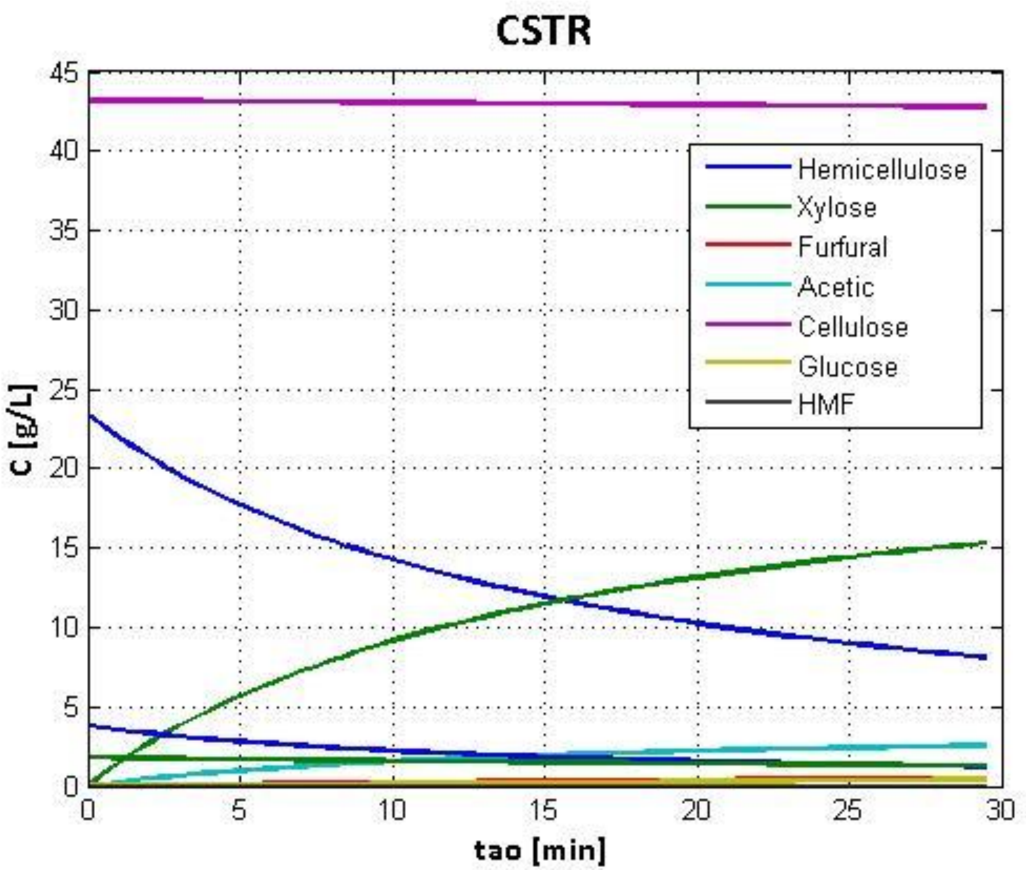
Rocha, G. J. M., Martín, C., Vinícius, F. N., Gómez, E. O., & Gonçalves, A. R.

- CTBE's Aspen simulation based on Rocha's paper.
  - Uncatalysed, 11 barg, 190°C
  - Acid catalysed, 5 barg, 150°C
- Conversions for individual reactions.
- Used in General Algebraic Modelling Software (GAMS).

Acid Pretreatment Model

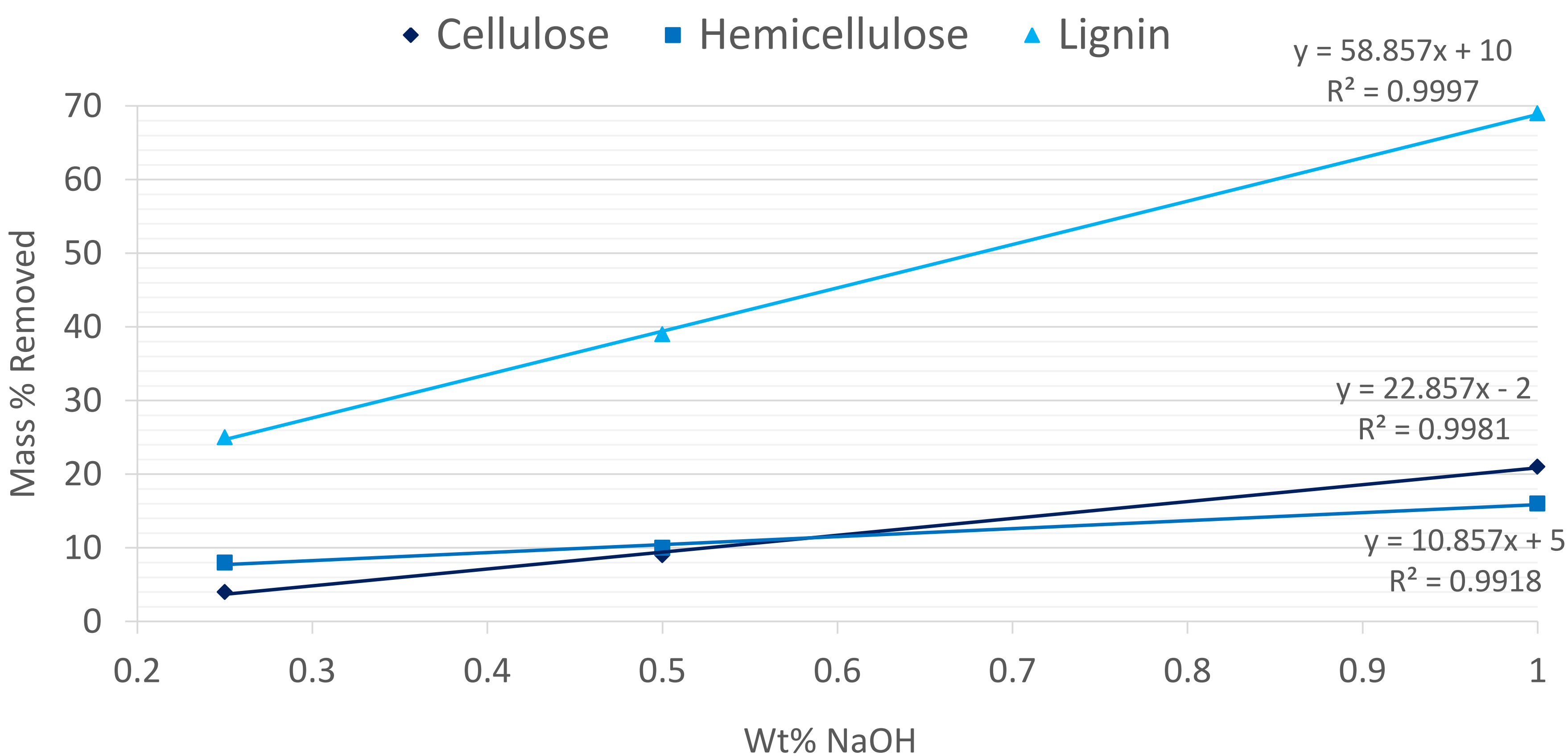
Kinetic study of the acid hydrolysis of sugar cane bagasse.

Aguilar, R., Ramırez, J., Garrote, G., & Vazquez, M.



Delignification Model

Chemical & morphological characterization of sugarcane bagasse submitted to a delignification process for enhanced enzymatic digestibility.



Acid Hydrolysis Model

Dilute acid hydrolysis of sugar cane bagasse at high temperatures: A kinetic study of cellulose saccharification and glucose decomposition. Part I: sulfuric acid as the catalyst.

Gurgel, L. & Marabezi, K.

- Kinetic equations for cellulose reactions with Arrhenius temperature relationship.
- Conversion factors for hemicellulose to xylose and xylose to furfural.
- GAMS model optimises T (between 180 & 230°C), tao, acid percentage (0.07, 0,14 or 0.28 wt%)

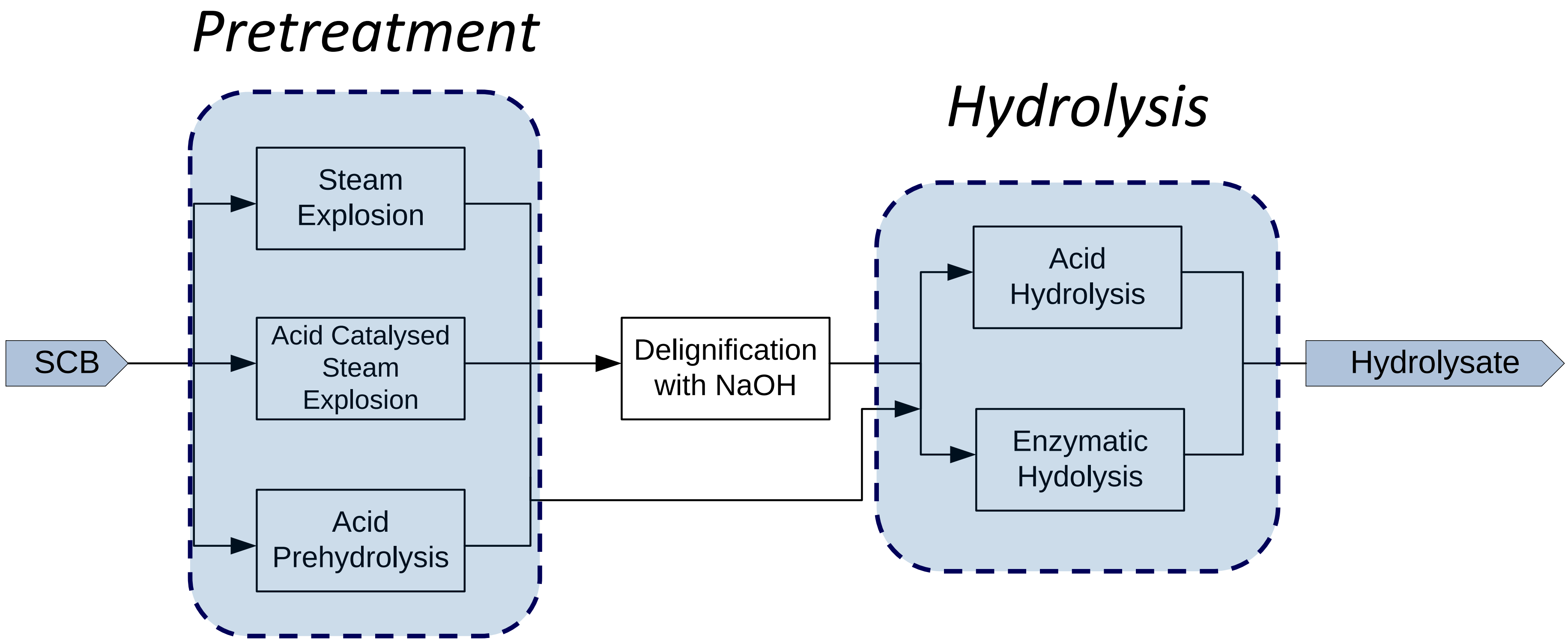
Enzymatic Hydrolysis Model

Technological Assessment Program (PAT). The Virtual Sugarcane Biorefinery (VSB).

Bonomi, A. et al.

- CTBE's Aspen simulation.
- Conversions for individual reactions.
- Fixed T, tao and enzyme loading.
- Least flexible model.

Superstructure



Challenges

- Creating a meaningful economic objective function
- Finding good data
  - Kinetic of acids is well researched
  - Steam explosion more black box approach
  - Trade secrets around enzyme mixtures
- Combining models
  - Acid prehydrolysis & acid hydrolysis
  - Effects of pretreatment on hydrolysis
  - Effects of delignification on hydrolysis

Limitations

- Hard to quantify physical effects
- Experiments have very specific conditions
  - Difficult to adjust experimental to new situations
  - Little flexibility in some models (eg. fixed residence time, water to solids ratio)
- Solvers very sensitive to initialisations (local optima)

Conclusion

- Multi-objective modelling
  - Economic and environmental objectives
- Pretreatment, delignification, hydrolysis
  - Kinetics and simulations
- Combining models and incorporating delignification

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Thank you.