Process Synthesis for Fuel Ethanol Production from Lignocellulosic Biomass Using an Optimization-Based Strategy

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Outline

1. Introduction
2. Case study
3. Summary

Motivation

- Fuel ethanol demand is on the increase, for reasons this audience is well aware of!
- Cost-effective process technologies with less expensive feedstocks, such as lignocellulosic biomass, are required.
- Evaluating alternative designs experimentally is difficult and expensive.
- Automated tools based on optimisation and simulation can help identify the most cost-effective process alternatives.

Lignocellulosic biomass

- An abundant and cheap feedstock suitable for energy production.
- Mainly agricultural and forestry residues and agro-industrial wastes.
- Can be converted to liquid biofuels such as ethanol which can be used directly or as an oxygenate for gasoline.
- The conversion of lignocellulosic biomass is a complex process:
    - Cellulose and hemicellulose must be transformed into fermentable sugars.
    - Post-fermentation steps include concentration and de-hydration.

Automated process design

Knowledge based

- Make use of heuristic rules.
- Are based on the experience of researchers and engineers.
- Provide qualitative ranking of design alternatives.

Optimisation based

- Based on a superstructure of design alternatives.
- Modelled using mixed integer nonlinear programming (MINLP).
- Provides quantitative ranking.

Jacaranda

- Object oriented framework for process design and optimisation [Fra06].
- Extensible and adaptable for a wide range of problems.
- Can simultaneously solve reaction and separation sections.
- Able to handle complex models (e.g. physical property estimation methods).
- Supports both deterministic and stochastic optimisation procedures.
- Supports multi-criteria optimisation.

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Objective

- Design and optimise process for the production of ethanol from lignocellulosic biomass.
- Consider alternative transformation routes.
- Analyse impact of these alternatives on the separation section.
- Rank alternatives based on economic criteria.

Alternative transformation routes

Cellulose hydrolysis (CH):

$$\begin{aligned}(\text{Cellulose})_n + \frac{n}{2}\ H_2O &\longrightarrow \frac{n}{2}\ \text{Cellobiose}\\ (\text{Cellulose})_n + n\ H_2O &\longrightarrow n\ \text{Glucose}\\ \text{Cellobiose} + 2\ H_2O &\longrightarrow 2\ \text{Glucose}\end{aligned}$$

Hexose fermentation (HF):

$$\begin{aligned}\text{Glucose} &\longrightarrow \boxed{C_2H_5OH} + 2\ CO_2\\ \text{Glucose} + 1.2\ NH_3 &\longrightarrow 6\ \text{S. cerevisiae} + 2.4\ H_2O + 0.3\ O_2\end{aligned}$$

Alternative transformation routes

Simultaneous saccharification and fermentation (SSF):

$$\begin{aligned}
(\text{Cellulose})_n + \frac{n}{2}\ H_2O &\rightarrow \frac{n}{2}\ \text{Cellobiose} \\
(\text{Cellulose})_n + n\ H_2O &\rightarrow n\ \text{Glucose} \\
\text{Cellobiose} + 2\ H_2O &\rightarrow 2\ \text{Glucose} \\
\text{Glucose} &\rightarrow \boxed{C_2H_5OH} + 2\ CO_2 \\
\text{Glucose} + 1.2\ NH_3 &\rightarrow 6\ \text{S. cerevisiae} + 2.4\ H_2O + 0.3\ O_2
\end{aligned}$$

Alternative transformation routes

Simultaneous saccharification and cofermentation (SSCF):

$$\begin{aligned}
(\text{Cellulose})_n + \frac{n}{2}\ H_2O &\rightarrow \frac{n}{2}\ \text{Cellobiose} \\
(\text{Cellulose})_n + n\ H_2O &\rightarrow n\ \text{Glucose} \\
\text{Cellobiose} + 2\ H_2O &\rightarrow 2\ \text{Glucose} \\
\text{Glucose} &\rightarrow \boxed{C_2H_5OH} + 2\ CO_2 \\
\text{Glucose} + 1.2\ NH_3 &\rightarrow 6\ \text{Z. mobilis} + 2.4\ H_2O + 0.3\ O_2 \\
3\ \text{Xylose} &\rightarrow 5\ \boxed{C_2H_5OH} + 5\ CO_2 \\
\text{Xylose} + NH_3 &\rightarrow 5\ \text{Z. mobilis} + 2\ H_2O + 0.25\ O_2
\end{aligned}$$

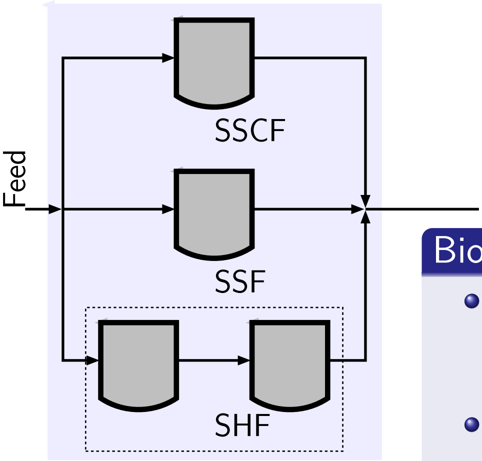
Process superstructure

Process superstructure

Biological transformations

- simultaneous saccharification and co-fermentation
- simultaneous saccharification and fermentation

Process superstructure



Biological transformations

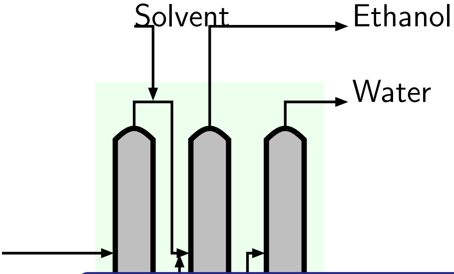
- simultaneous saccharification and co-fermentation
- simultaneous saccharification and fermentation

Process superstructure

Separation and purification

- Consider distillation alone but this could be relaxed.
- Must handle non-ideal mixture behaviour.

Process superstructure



Separation and purification

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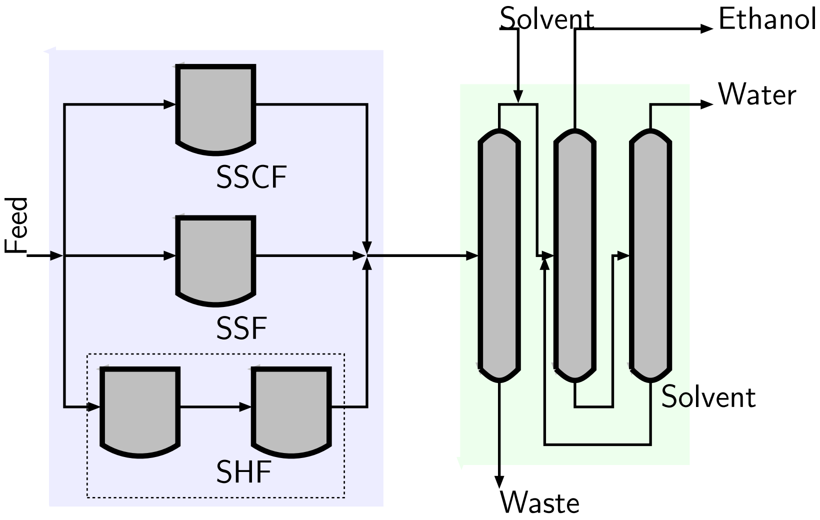
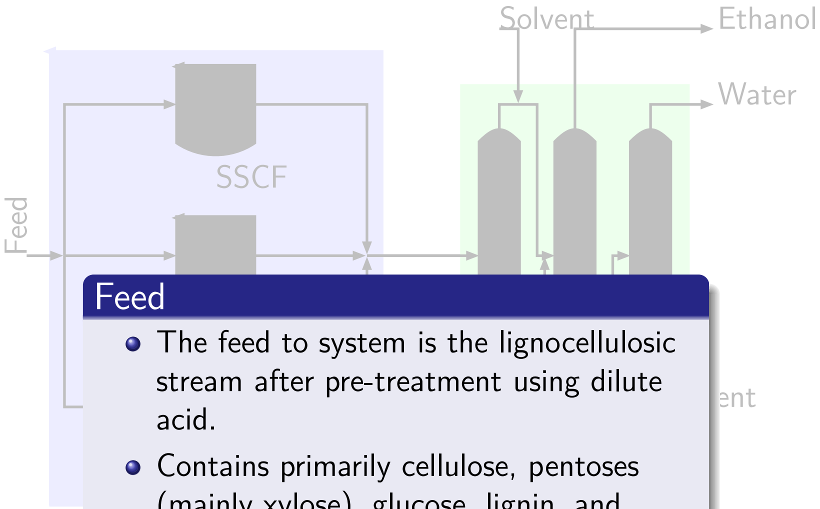


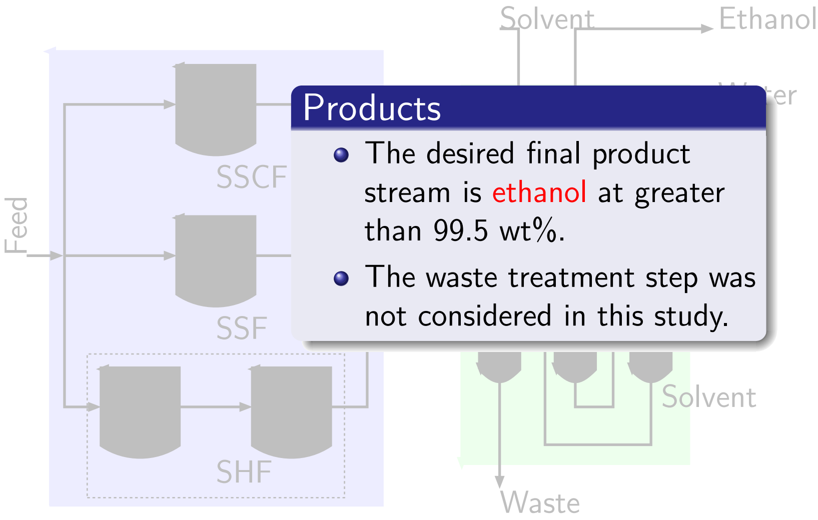
Models



Feed

- The feed to system is the lignocellulosic stream after pre-treatment using dilute acid.
- Contains primarily cellulose, pentoses (mainly xylose), glucose, lignin, and water.

Models



Products

- The desired final product stream is ethanol at greater than 99.5 wt%.
- The waste treatment step was not considered in this study.

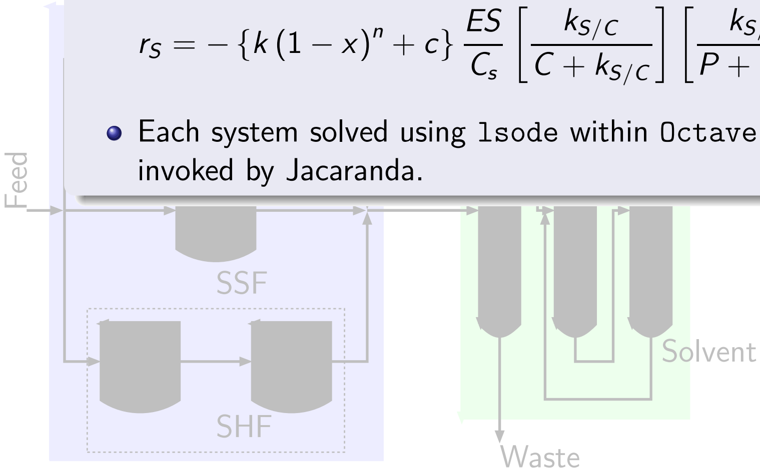
Mod

Reactor Models

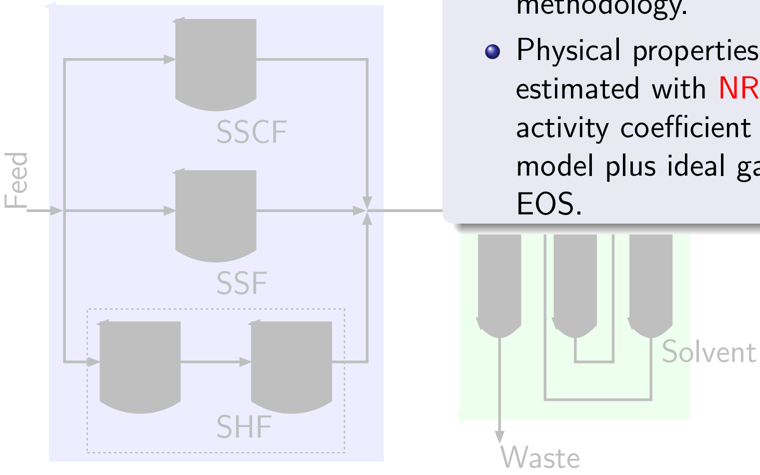
- Rate based for system of differential equations for each reactor, e.g. [SHL95]:

$$r_S = -\left\{k\left(1-x\right)^n + c\right\}\frac{ES}{C_s}\left[\frac{k_{S/C}}{C+k_{S/C}}\right]\left[\frac{k_{S/P}}{P+k_{S/P}}\right]$$

- Each system solved using `lsode` within `Octave` invoked by Jacaranda.



Models



Distillation Models

- Designs generated using Fenske, Underwood & Gilliland short-cut methodology.
- Physical properties estimated with NRTL activity coefficient model plus ideal gas EOS.

Computational aspects

- Design variables:
  - two binary variables for feed splitting,
  - residence time for each reactor, and
  - recovery of light and heavy keys for each column

  $\Rightarrow$ MINLP with total of 2 binary and $4 + 3 \times 2 = 10$ continuous real valued variables.
- The nonlinear problem is solved using a genetic algorithm (population replacement policy, elite size of 1, mutation rate of 10%, crossover rate of 70% and roulette wheel selection).
- Jacaranda will calculate the make-up of ethylene glycol required and the solvent recycle stream flow rate.

Results

SSCF configuration best performing

- Integration gives immediate consumption of glucose formed, avoiding inhibition of cellulose-degrading enzymes (cellulases).
- The utilization of xylose allows an increase in the content of fermentation sugars ⇒ increase in ethanol.
- Enhanced utilisation of the feed-stock is not a characteristic of the SSF process.
- The SHF requires two bioreactors, increasing capital cost in comparison.

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Summary

- Results demonstrate that the genetic algorithm used by Jacaranda handles the complexity of the problem design robustly.
- The solutions obtained show variability in the technological option. From 10 different runs:
  - three of the solutions corresponded to SSCF configurations (two of them with the best values of the objective function),
  - six solutions to the SSF process, and
  - one solution to the SHF configuration.
- Next steps are to use more rigorous models for distillation for non-ideal behaviour and to include yet more transformation steps.

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