

# Predictive Modeling Can De-Risk Biobased Production

James Gardner, Gilbert Yang, Phil Coffman, Akash Narani, and Deepti Tanjore  
Advanced Biofuels (and Bioproducts) Process Demonstration Unit (AB-PDU),  
Lawrence Berkeley National Laboratory, Emeryville, CA

## Introduction

Technologies developed to generate bio-based products are based on single feedstock types. While this approach is applicable for corn stover in the MidWest, for states such as California, with abundant but diverse feedstocks, technologies should be developed to accommodate multiple feedstock input to a single biorefinery. This project established the influence of mixing feedstocks on downstream sugar recovery and thereby fuel production for Imperial County as a case study. We relied on statistical approaches and developed a predictive model to identify optimal biomass concentrations and reaction types, temperatures, and times to maximize sugar yield and minimize furfural production.

## Predictive Model generated by SAS JMP®

Feedstocks with 1-100% of  
Corn Stover (CS)  
Loblolly Pine (LP)  
Energy Cane (EC)

Temperature – Scaled variable (1 – 100%)  
Acid (Ac) – 140 to 180°C  
Alkali (AL) – 55 to 120°C  
Hydrothermal (Hy) – 140 to 180°C

Pretreatments – Categorical variable  
Acid – 1% w/w H<sub>2</sub>SO<sub>4</sub>  
Alkali – 1% w/w NaOH  
Hydrothermal – Water only

Time – Scaled variable (1 – 100%)  
Acid – 5 to 50 minutes  
Alkali – 1 to 24 hours  
Hydrothermal – 5 to 50 minutes

Table1: Experimental Design generated by SAS JMP®

Whole plots	PT	Temp%	°C	Time %	Min	CS	LP	EC
1	Hy	1	140	39	26	0.0	1.0	0.0
1	Ac	1	140	100	60	0.3	0.4	0.3
1	Al	1	55	100	1440	0.0	0.0	1.0
1	Al	1	55	39	589	0.0	0.5	0.5
1	Al	1	55	100	1440	0.0	1.0	0.0
1	Hy	1	140	100	60	0.0	0.0	1.0
2	Ac	100	180	1	5	0.0	0.6	0.4
2	Ac	100	180	60	38	1.0	0.0	0.0
2	Al	100	120	1	60	0.0	1.0	0.0
2	Al	100	120	1	60	0.0	0.0	1.0
2	Hy	100	180	1	5	0.0	0.0	1.0
3	Hy	39	155	100	60	0.5	0.5	0.0
3	Ac	39	155	1	5	0.0	0.0	1.0
3	Hy	39	155	1	5	1.0	0.0	0.0
3	Al	39	80	1	60	0.3	0.4	0.3
3	Ac	39	155	1	5	0.4	0.6	0.0
3	Al	39	80	100	1440	1.0	0.0	0.0
4	Ac	80	172	80	49	0.0	1.0	0.0
4	Hy	80	172	80	49	1.0	0.0	0.0
4	Hy	80	172	80	48.8	0.0	1.0	0.0
4	Hy	80	172	1	5.0	0.5	0.0	0.5
4	Al	80	107	80	1159	0.2	0.4	0.4
4	Ac	80	172	80	48.8	0.0	0.0	1.0

## Methods and Materials

Compositional Analysis of Feedstocks  
Pretreatment Reactor  
Pretreatment Heating Medium

Enzyme Loading  
Enzymatic Hydrolysis Conditions

NREL Laboratory Analytical Protocols  
15 ml SS316 tube reactor  
SBL-2D Fluidized Sandbath (Technique)  
or MaxQ8000 Incubator (Thermo)  
CTec2 (40 mg/ g glucan)  
50°C and 24 hours

## Pretreatment and Enzymatic Hydrolysis of Mixed Feedstocks

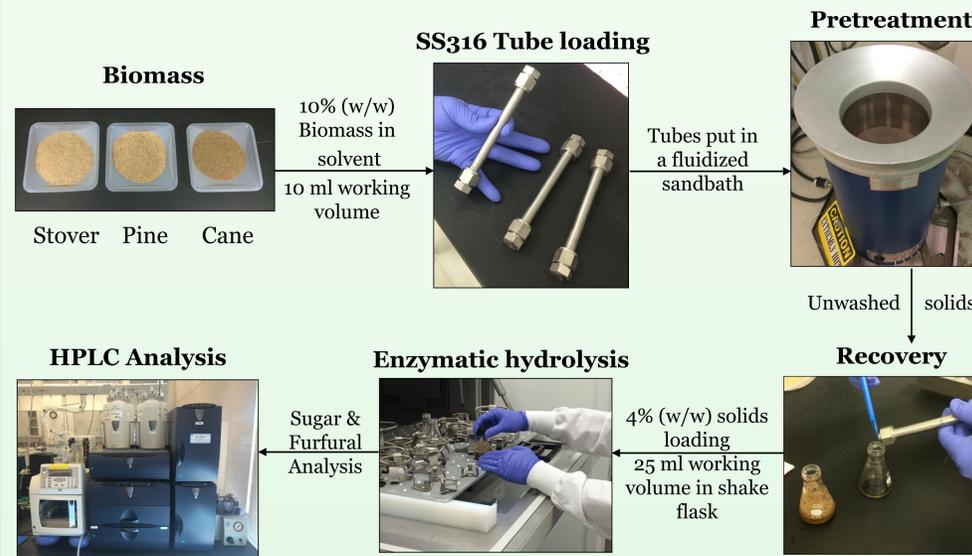


Figure 1. Pretreatment and Enzymatic Hydrolysis at Small scale for Mixed feedstocks

## The Model can generate Continuous Envelope of Feedstock Mixtures

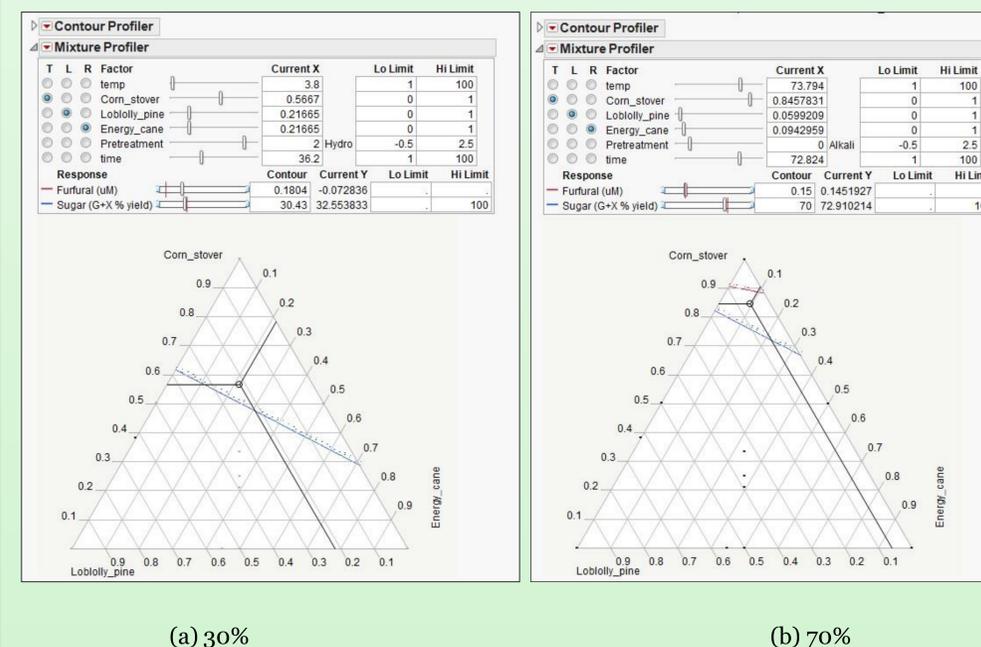


Figure 2. A Ternary Plot of Mixed Feedstock Composition for Predetermined Sugar Yields

## Alkali Pretreatment shows Highest Sugar Yields for Mixed Feedstocks

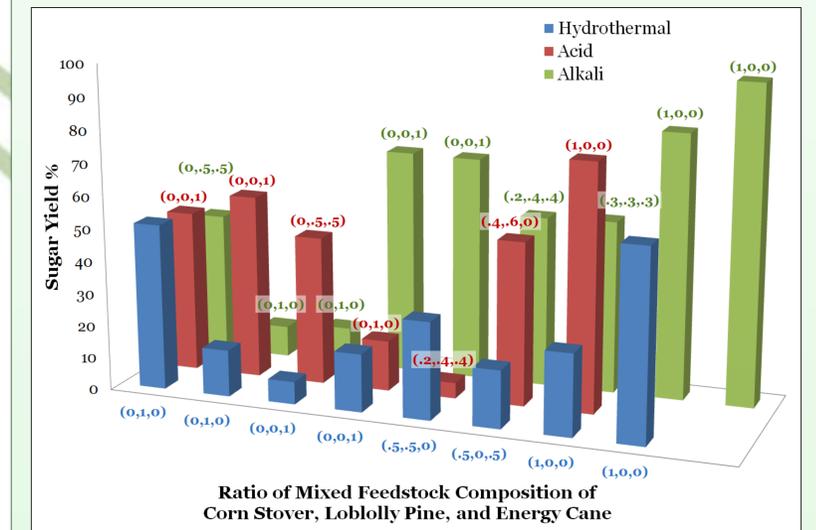


Figure 3. Sugar yields of mixed feedstocks with different pretreatments

## Summary/Conclusion

- Results from the treatments were fed into the predictive model to determine several combinations of feedstocks and pretreatments to achieve more than 70% theoretical sugar yield.
- Alkali treatment was most successful in deconstructing mixed feedstocks as it led to highest sugar yields in multiple treatment conditions when compared to Acid and Hydrothermal treatments.
- Predictions made from this study will reduce the risk in establishing a biorefinery in Imperial County by reducing its dependence on one feedstock and simultaneously maintaining overall product yields.
- Predictive modeling can be applied to convert mixed feedstocks in several geographic areas for the sustenance of bio-based economy. We will continue to perform several treatments in the future with varied feedstock compositions and pretreatments to build a robust global model.

## Acknowledgements

This work was funded by DOE – EERE Division, BioEnergy Technologies Office (BETO). We would like to thank our collaborators: Kevin Kenney, Vicki Thompson, and team from Idaho National Laboratory (INL) and Terrestrial Carbon Analytics (TCA).



## Contact Information

Akash Narani, M.S. Chemical Engineering  
Associate Process Engineer  
AB-PDU, LBNL  
Email: Anarani@lbl.gov  
Office :510-486-4528; Cell: 716-866-4967

