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DOE Bioenergy Technologies Office (BETO) 2015 Project Peer Review

Technical Market Analysis for Biochemical Conversion

March 23, 2015
Biochemical Conversion
Jim Collett and Mark Butcher
PNNL

Goal Statement

- **Challenge: Process and economic data on hydrocarbon production** via bioconversion that are freely available to industry are limited.
  - **Data at industrially-relevant scales** are limited because published research focuses mainly on compound discovery at lab-scale production levels (<5g/L).
  - **Data on the upgrading options for hydrocarbon fuel precursors** are limited because most bioconversion microbes do not directly produce market-ready diesel, jet, or other fuels.
- **Goal: Provide industry and BETO with rapid, preliminary assessments** of the potential of biochemical production of hydrocarbon fuels and products, and **tools to evaluate and track new approaches** in production technology, economics, and sustainability.

Quad Chart Overview

Timeline

- Project start date (2010)
- Project end date (2017)
- Percent complete (50)

Budget

	Total Costs FY 10 –FY 12	FY 13 Costs	FY 14 Costs	Total Planned Funding (FY 15-Project End Date
DOE Funded	$1.219 M	$210 K	$159 K	$469 K
Project Cost Share (Comp.)*				

Barriers

- At-A. Need for Comparable, Transparent, and Reproducible Analysis
- Bt-J. Catalyst Development
- Bt-K. Biochemical Conversion Process Integration

Partners and Advisors

- INL
- NREL
- University of Kansas, Berl Oakley (polyketide biosynthesis expert)

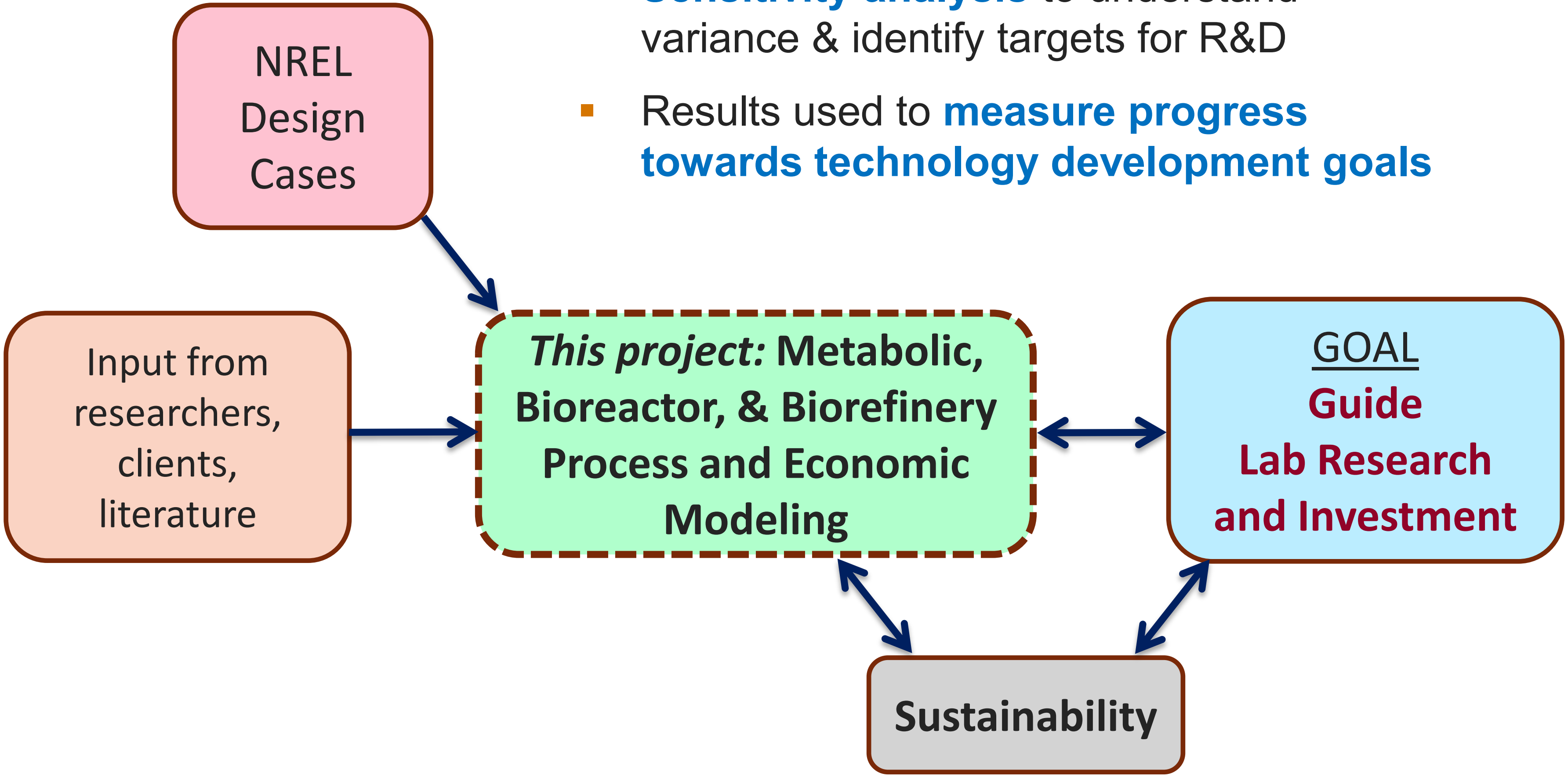
1 - Project Overview

- **History**
    - Bio-based products focus: **"Top 10 Products from Biomass"** (2003) and **"Products from Lignin"** (2007).
    - Techno-economic assessments (TEA) of **fungal ethanol production** (2008-11).
    - Survey and economic assessments of microbial production of **hydrocarbon fuels and co-products** (2010-12).
    - Preliminary **metabolic modeling and TEA of hydrocarbon production from oleaginous yeast** via bioconversion of pretreated corn stover (2013).
    - **Metabolic modeling of genetic engineering strategies** to improve hydrocarbon production from of oleaginous yeast (2014).
    - Evaluation of **options for maximizing feedstock lignin in the final fuel** (2014).
- **High Level Objective**
    - Use **flexible and rapid modeling** to establish preliminary cost and performance targets for **bioconversion** (titer, rate, yield) and **biorefinery unit operations**.

2 – Approach (Technical)

TECHNICAL APPROACH

- **Quick screening**, then detailed analysis
- **Sensitivity analysis** to understand variance & identify targets for R&D
- Results used to **measure progress towards technology development goals**



NREL Design Cases

Input from researchers, clients, literature

This project: **Metabolic, Bioreactor, & Biorefinery Process and Economic Modeling**

GOAL
Guide Lab Research and Investment

Sustainability

Approach (Management)

Structure

- **Project Management Plan** (PMP) describes scope, budget, schedule
- **Annual Operating Plan** (AOP) completed before each fiscal year
  - Specifies quarterly and annual **milestones** and **deliverables**
- **Quarterly reporting** to BETO (written reports plus regularly scheduled calls)

Challenges to project success

- The **potential titer, rate, and yield of candidate microbial catalysts** must be well understood.
- **Relevant experimental data are needed for** biorefinery process models.
- **Appropriate biorefinery unit operations** must be identified and their cost and performance accurately predicted.

Critical success factors

- Defining **real opportunities for profitable hydrocarbon production**
- **Making results public** (MYPP and published reports)

3 – Technical Accomplishments/ Progress/Results – FY 13

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Metabolic Network Reconstruction for the Oleaginous Yeast *Lipomyces starkeyi*

- A preliminary **genome-scale, stoichiometric model** of *L. starkeyi* metabolism based on the JGI's NRRL Y-11558 reference genome was constructed using the iMM904 model for *S. cerevisiae* as a template.
- At least one *L. starkeyi* enzyme could be mapped to more than 90% of the **1044 enzyme-catalyzed reactions** in the iMM904 model *(examples below)*

Rxn description	Formula	Gene-reaction association
phosphofructokinase	atp[c] + f6p[c] -> adp[c] + fdp[c] + h[c]	(Lsta_59861 and Lsta_59861)
glucose 6 phosphate isomerase	g6p[c] <=> f6p[c]	Lsta_1064
phosphoglycerate kinase	3pg[c] + atp[c] <=> 13dpg[c] + adp[c]	Lsta_75322
phosphoglycerate mutase	2pg[c] <=> 3pg[c]	(YKL152C or YDL021W or YOL056W)
pyruvate kinase	adp[c] + h[c] + pep[c] -> atp[c] + pyr[c]	(Lsta_215 or Lsta_215)

3 – Technical Accomplishments/ Progress/Results – FY 13

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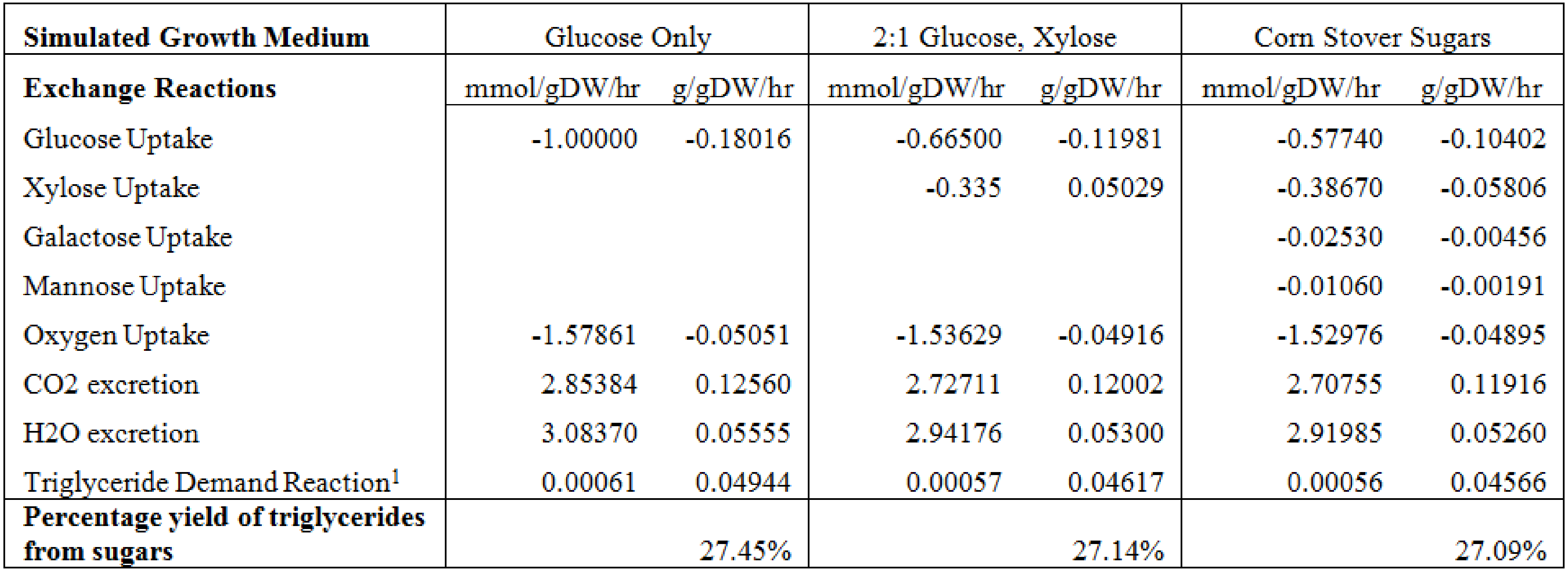
Metabolic Model Prediction of Maximum Biochemically Feasible Triglyceride Yield

Steady state mass fluxes for simulated growth of *L. starkeyi* on various sugar substrates as predicted by flux balance analysis with the objective function set to maximize triglyceride yield.



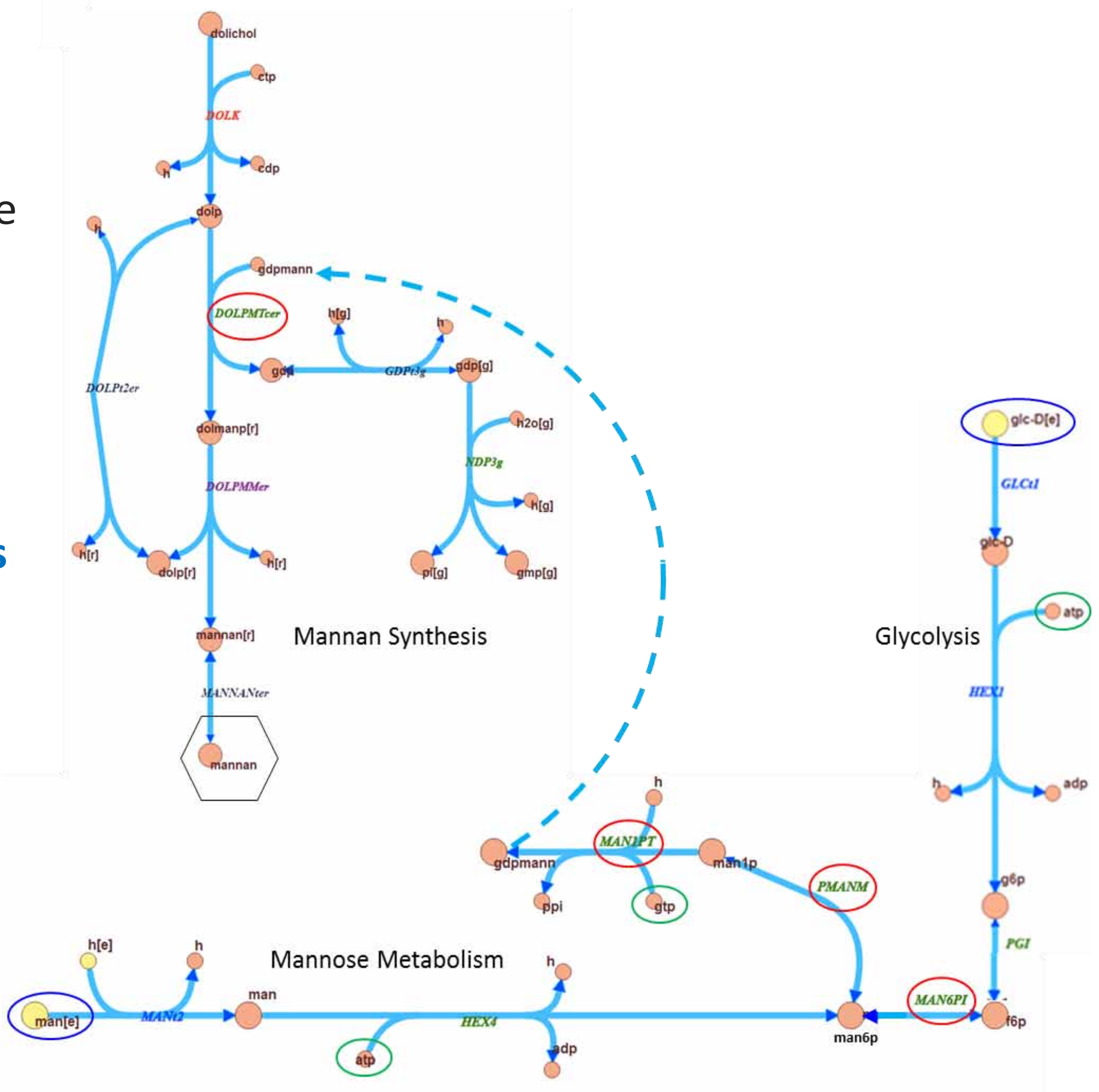
Simulated Growth Medium	Glucose Only		2:1 Glucose, Xylose		Corn Stover Sugars	
Exchange Reactions	mmol/gDW/hr	g/gDW/hr	mmol/gDW/hr	g/gDW/hr	mmol/gDW/hr	g/gDW/hr
Glucose Uptake	-1.00000	-0.18016	-0.66500	-0.11981	-0.57740	-0.10402
Xylose Uptake			-0.335	0.05029	-0.38670	-0.05806
Galactose Uptake					-0.02530	-0.00456
Mannose Uptake					-0.01060	-0.00191
Oxygen Uptake	-1.57861	-0.05051	-1.53629	-0.04916	-1.52976	-0.04895
CO2 excretion	2.85384	0.12560	2.72711	0.12002	2.70755	0.11916
H2O excretion	3.08370	0.05555	2.94176	0.05300	2.91985	0.05260
Triglyceride Demand Reaction[1]	0.00061	0.04944	0.00057	0.04617	0.00056	0.04566
Percentage yield of triglycerides from sugars		27.45%		27.14%		27.09%

[1] The mmol/gDW/hr values of the Triglyceride Demand Reaction are scaled 100-fold lower than the other mass fluxes in the table because MW of the generic triglyceride metabolite in the metabolic model is scaled 100-fold higher, with a chemical formula of C_{5160},H_{9566},O_{600}.

3 – Technical Accomplishments/ Progress/Results – FY 14

Excretion of galacto-mannan by wild type *L. starkeyi* was identified as a non-productive side reaction.

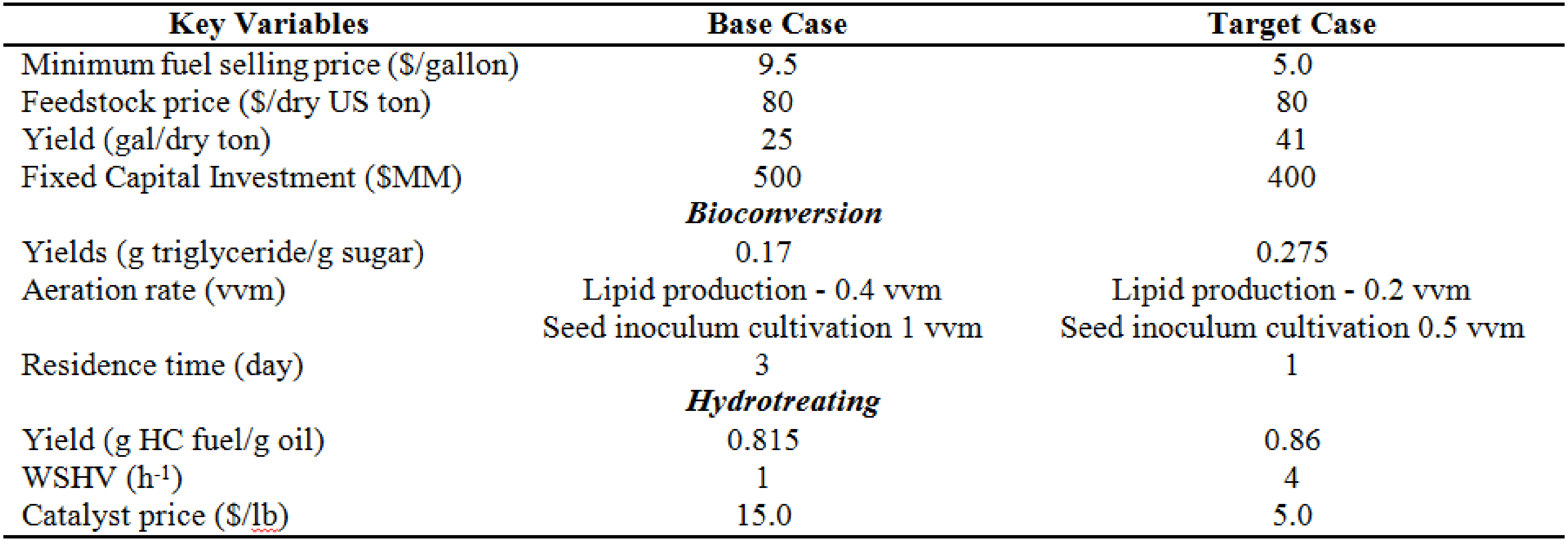
Using the **metabolic model**, four enzyme genes in the mannan synthesis pathway were identified as **candidates for suppression via genetic engineering**.



3 – Technical Accomplishments/ Progress/Results – FY 13

CHEMCAD preliminary process model for

- **bioconversion** of pretreated corn stover to lipids
- **solvent extraction** of lipids
- **hydrotreating** to upgrade the lipids to diesel and jet fuel.



Key Variables	Base Case	Target Case
Minimum fuel selling price (\$/gallon)	9.5	5.0
Feedstock price (\$/dry US ton)	80	80
Yield (gal/dry ton)	25	41
Fixed Capital Investment (\$MM)	500	400
	Bioconversion	
Yields (g triglyceride/g sugar)	0.17	0.275
Aeration rate (vvm)	Lipid production - 0.4 vvm Seed inoculum cultivation 1 vvm	Lipid production - 0.2 vvm Seed inoculum cultivation 0.5 vvm
Residence time (day)	3	1
	Hydrotreating	
Yield (g HC fuel/g oil)	0.815	0.86
WSHV (h^{-1})	1	4
Catalyst price (\$/lb)	15.0	5.0

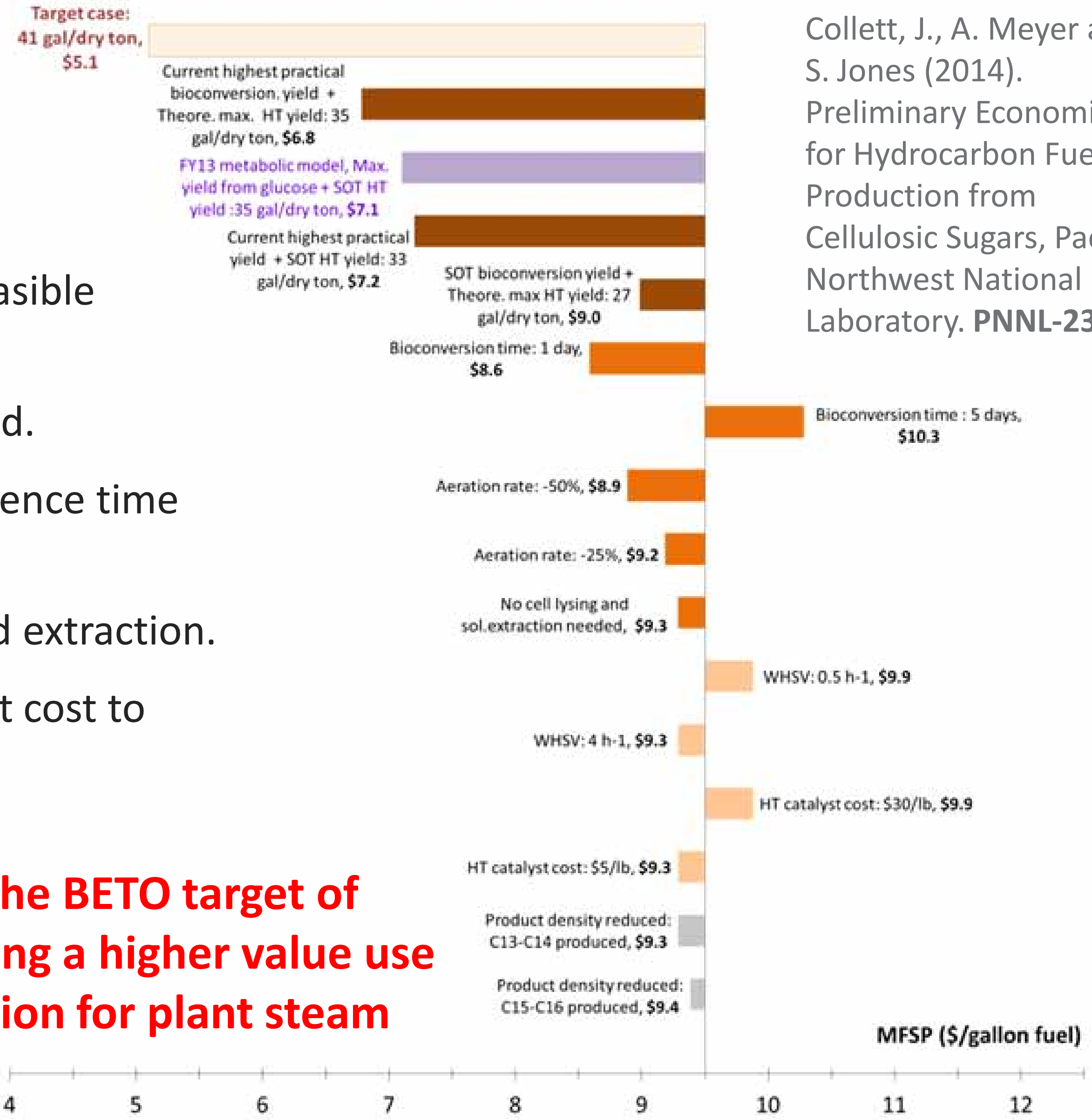
Collett, J., A. Meyer and S. Jones (2014). **Preliminary Economics for Hydrocarbon Fuel Production from Cellulosic Sugars**, Pacific Northwest National Laboratory. **PNNL-23374**.

3 – Technical Accomplishments/ Progress/Results – FY 13

Sensitivity Analysis

Targets for reducing the MFSP to $5/gal gge:

- Attain max biochemically feasible triglyceride yield (27.5%).
- Attain 85% hydrotreater yield.
- Reduce bioconversion residence time to 24 hours.
- Eliminate cell lysing and lipid extraction.
- Reduce hydrotreater catalyst cost to $5/lb. and WHSV to 4.

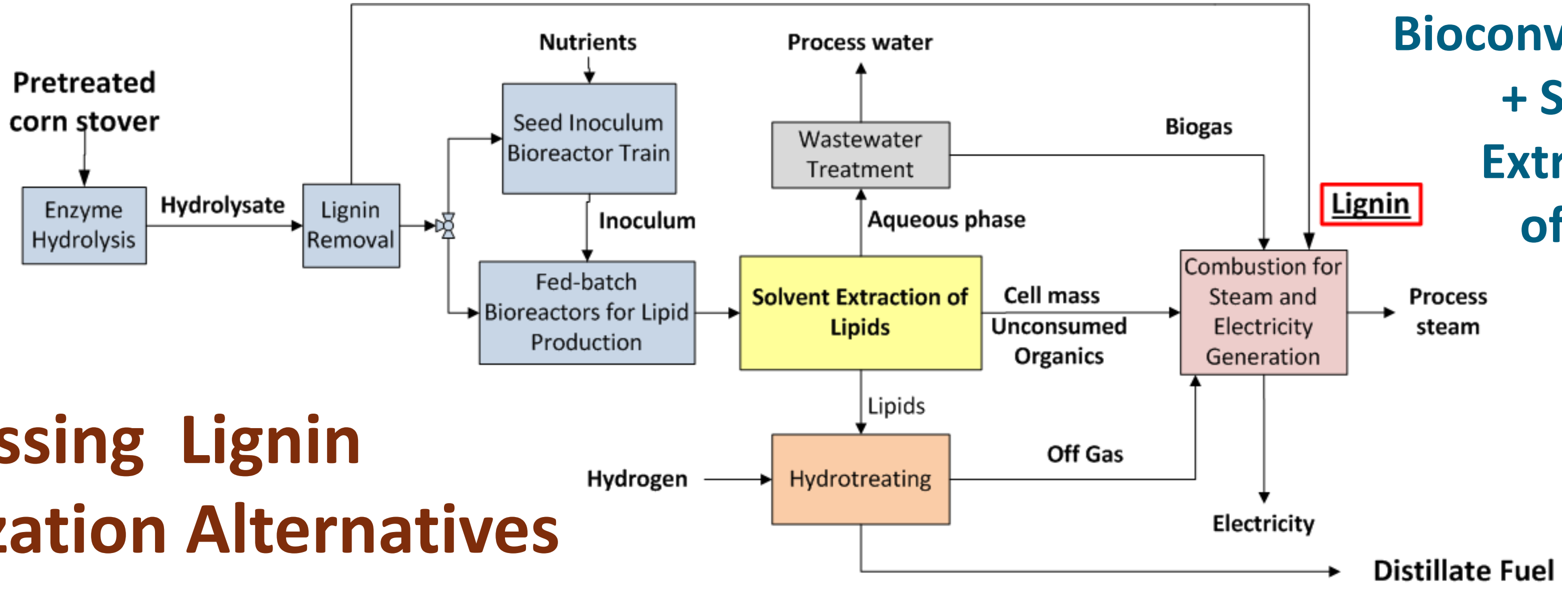


Collett, J., A. Meyer and S. Jones (2014). Preliminary Economics for Hydrocarbon Fuel Production from Cellulosic Sugars, Pacific Northwest National Laboratory. **PNNL-23374**.

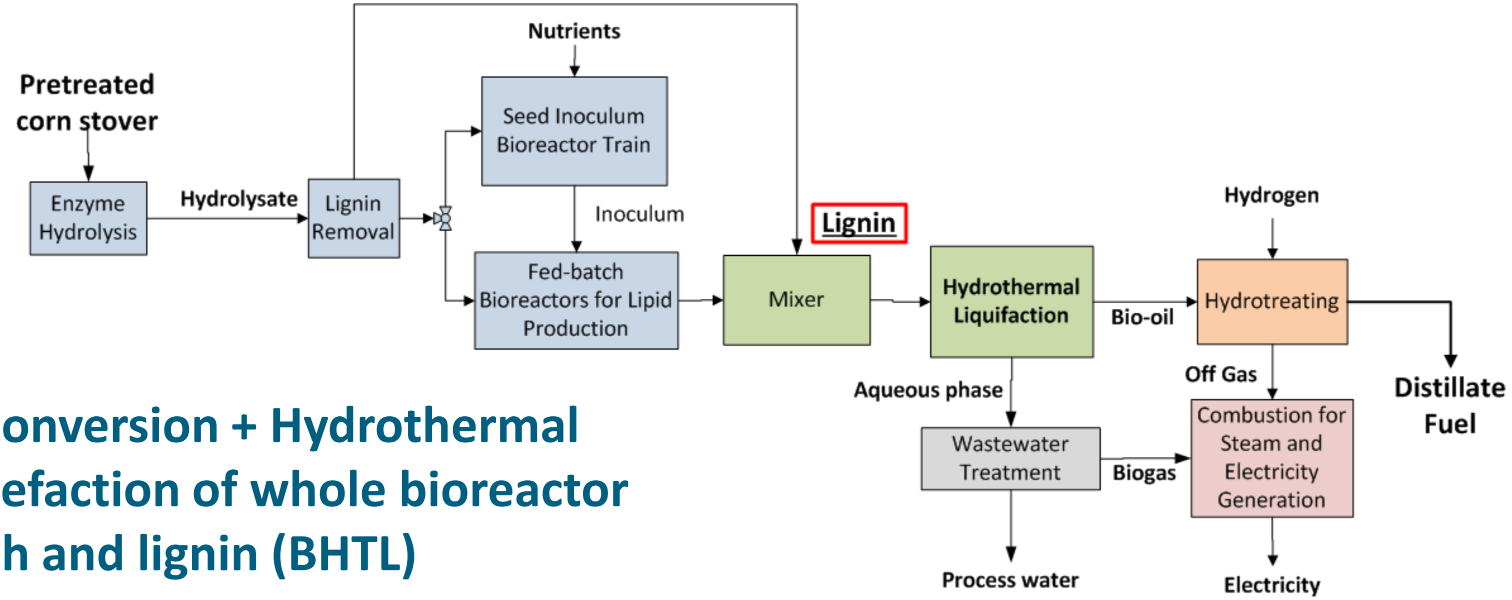
Reducing the MFSP to the BETO target of $3/gal will require finding a higher value use for lignin than combustion for plant steam

3 – Technical Accomplishments/ Progress/Results – FY 14

Bioconversion + Solvent Extraction of Lipids (BSLE)



Assessing Lignin Utilization Alternatives



Bioconversion + Hydrothermal Liquefaction of whole bioreactor broth and lignin (BHTL)

3 – Technical Accomplishments/ Progress/Results – FY 14

An **updated CHEMCAD process model** was used to compare the cost and performance of:

- bioconversion + **solvent extraction of lipids + lignin combustion** for steam (**BSLE Case**)
- bioconversion + **hydrothermal liquefaction of whole bioreactor broth and lignin** (**BHTL Case**)

Performance - BSLE vs. BHTL

Biorefinery Model Inputs and Outputs	Units	BSLE Case	BHTL Case
Corn Stover Feed (dry basis)	mtpd	2000.00	2000.00
Hydrotreater Hydrogen	lb H_2/lb HT feed	0.02	0.03
Triglyceride Lipid Yield (from bioconversion)	ton/dry ton feedstock	0.15	0.15
Bio-oil yield (includes bioconversion triglycerides)	ton/dry ton feedstock	n/a	0.25
Distillate Fuel Production Rate	mmgal/yr	28.40	41.10
Distillate Fuel Yield	gal/dry ton feedstock	39.00	57.00
Distillate Fuel Yield	ton/dry ton feedstock	0.13	0.20
Total Water Usage	gal/gal product	31.72	17.34
Electricity Consumption	MW	42.19	8.39
Electricity Sold to Grid	MW	8.18	0.00
Energy efficiency (fuel/feedstock + hydrogen)	%, HHV basis	0.32	0.48
Carbon Efficiency (C in fuel/C in feedstock)	%	23.86%	38.19%

Model assumptions based on NREL 2013 sugars-to-hydrocarbons design case, PNNL studies of hydrothermal liquefaction of algae and woody biomass, and PNNL bioreactor data. See additional slides for reference list.

3 – Technical Accomplishments/ Progress/Results – FY 14

Conclusion:

The BHTL case could **expand our options** for producing **superior fuels at a lower price** than the BSLE case.

Note: The base CHEMCAD model will be adapted for evaluating isoprenoid and polyketide production in FY15.

Costs (2011 US Dollar)	**BSLE Case**	**BHTL Case**
Installed Costs	$ M	$ M
Corn Stover Pretreatment and Conditioning	55.3	55.3
Enzyme Hydrolysis and Bioconversion	77.0	77.0
Cellulase Enzyme Production	12.7	12.7
Hydrothermal Liquefaction	Not used	98.9
Hydrotreating and Product Separation	22.9	34.6
Wastewater Treatment	40.1	43.3
Product and Feed Chemical Storage	3.2	3.6
Utilities	11.7	11.2
Additional Direct Cost	29.4	48.7
Total Installed Cost (TIC)	325.1	441.1
Fixed Capital Investment	520.0	705.8
Total Project Investment (TPI)	**547.8**	**742.9**
Operating Costs	$/gal product	$/gal product
Dry Biomass	2.04	1.41
Catalysts & Chemicals	0.73	0.56
Waste Disposal	0.04	0.03
Electricity and other utilities	-0.12	0.12
Fixed Costs	0.49	0.45
Capital Depreciation	0.61	0.57
Average Income Tax	0.34	0.32
Average Return on Investment	1.60	1.50
Minimum Fuel Selling Price, $/gallon	**5.73**	**4.97**
Minimum Fuel Selling Price, $/gge*	**5.45**	**4.54**
*gallon gasoline equivalent		

3 – Technical Accomplishments/ Progress/Results – FY 15

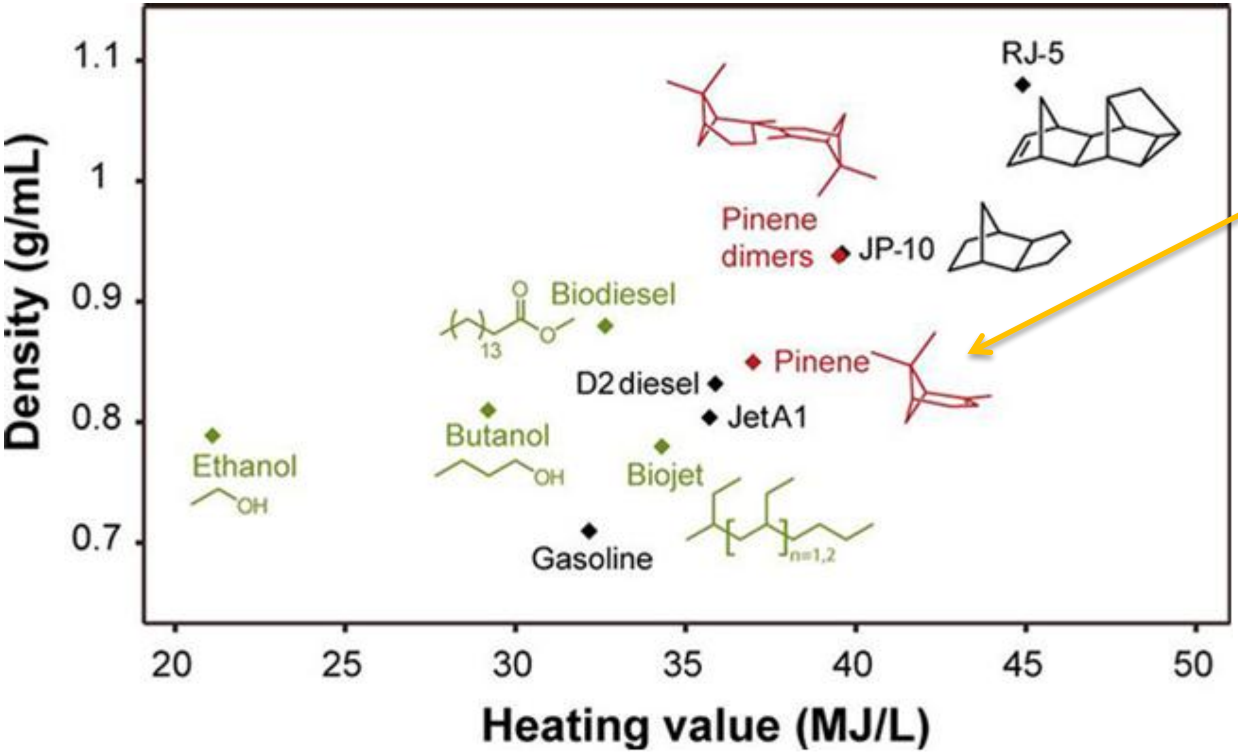
High-energy blendstocks for petroleum jet and diesel fuels

BiofuelsDigest

Making superfuels affordable, via biofuels: the JP-10 story

February 5, 2013 | Jim Lane

http://www.biofuelsdigest.com/bdigest/2013/02/05/making-superfuels-affordable-biofuels-and-jp-10/



JP-10 is a high-energy synthetic jet fuel that costs **$13-$25/gallon**.

High-density fuel candidates comparable to JP-10 have been synthesized from pinene, a woody **plant isoprenoid** (Harvey, et al., 2009)

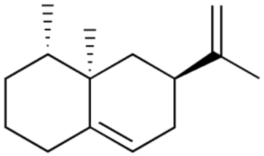
Fungi produce a wide variety of isoprenoids and polyketides that may be excellent blendstocks for improving petroleum jet fuel performance.

3 – Technical Accomplishments/ Progress/Results – FY 15

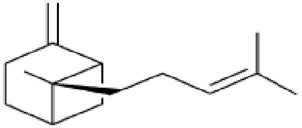
- FY15 Objective: **evaluate isoprenoid and polyketide compounds** to estimate baseline and targeted product titer, rate, and yield levels for a **hypothetical biorefinery using filamentous fungi for bioconversion**
    - **Literature search** for polyketide and isoprenoid compounds produced by filamentous fungi species
    - **Preliminary assessment** of isoprenoids and polyketides based on chemical structures and properties
    - **Compilation of a short list of candidate compounds** for use as hydrocarbon components of diesel and jet fuel (shown on next slide)
- Next step: **select one or more candidates** from short list to use in predicting production potential and for developing a **preliminary biorefinery process model**

3 – Technical Accomplishments/ Progress/Results – FY 15

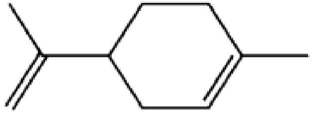
Isoprenoid and Polyketide Candidates				
Compound	**Type**	**Chemical conversion process**	**Final carbons**	**Hydrocarbon fuel**
Aristocholene	Bicyclic sesquiterpene	Very mild hydrogenation	C13	Jet
β-trans-bergamotene	Bicyclic sesquiterpene	Very mild hydrogenation	C15	Jet
(2Z,4Z)-4,6-Dimethylocta-2,4-dienoic	Polyketide	Carboxylic acid reduction	C10	Jet
4-hydroxy-3-methyl-6-(2-oxoundecyl)-2-pyrone	Polyketide	Decarbonylation	C20 or C21	Diesel
Limonene	Cyclic monoterpene	Mild hydrogenation	C10	Jet



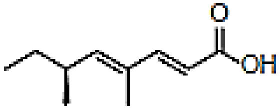
Aristolochene



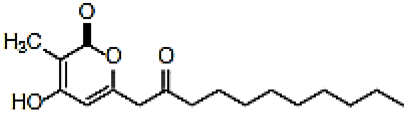
β-trans-bergamotene



Limonene



(2Z,4Z)-4,6-Dimethylocta-2,4-dienoic acid



4-hydroxy-3-methyl-6-(2-oxoundecyl)-2-pyrone

4 – Relevance

This project follows key recommendations made by **industry stakeholders** at the 2014 PRINCE workshop hosted by BETO:

- Addressing the **critical need for a greater variety of TEAs** for novel and unoptimized processes to evaluate the economics and feasibility of market entry for specific fuels and chemicals.
- Integration of **R&D data to understand specifications for biofuels and bio-based chemicals** and the specific impacts of their properties, such as compatibility with the existing petroleum infrastructure.
- Development of **modeling tools for metabolic pathways** of interest.
- Optimization focused on ***industrially relevant organisms.***

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Process Integration and Carbon Efficiency Workshop Summary Report

Summary Report from the June 11–12, 2014, Workshop in Lakewood, Colorado

December 2014

This project supports **BETO Analysis and Sustainability activities for Biochemical Conversion R&D** to understand the impact of biochemical and chemical conversion technologies with respect to environmental and economic metrics.

The **Technical and Market Analysis** produced by this project will improve the viability of biorefineries and support the growth of a nationwide bioeconomy that will reduce GHG emissions and our dependence on foreign oil.

5 – Future Work

- Proposed Work for FY16
  - Update the **CHEMCAD biorefinery process models for lipid, isoprenoid, and polyketide hydrocarbon production** with the latest data from the literature and ongoing experiments at PNNL.
  - Compile performance and physical specifications for **home heating oil, marine fuels, lubricants, and higher value jet fuels**.
  - **Characterize fungal metabolic processes** and **predict the maximum yields** for production of isoprenoid and polyketide compounds from biomass sugars.
  - Solicit expert opinion on the utility of fungal **isoprenoid and polyketide compounds as building blocks** for chemical synthesis of commodity chemicals.

Summary

- **Overview:** Primary objective is to **establish preliminary bioconversion titer, rate, and yield envelopes for hydrocarbon fuels** using techno-economic and market analysis to support BETO goals in transportation fuel development.

- **Approach:** Integrate data from literature, in-house R&D, and clients for **quick screening and follow-up analysis** of novel bioconversion processes and products.

- **Technical Accomplishments/Progress/Results:**
  - Preliminary **metabolic model for *Lipomyces starkeyi*** was validated with bioreactor data and used to estimate max biochemically feasible lipid yield.
  - **Prioritized process improvements** that may **reduce MFSP from $9 to $5.5/gge**.
  - Identified **lignin utilization alternative** that may further **reduce MFSP to $4.5/gge.**
  - Initiated evaluation of potential **polyketide and isoprenoid hydrocarbon fuel precursors** to prioritize candidates for R&D.

- **Relevance: Addresses a critical need for rapid integration of R&D data into TEAs** to evaluate the feasibility of market entry for novel fuels and chemicals.

- **Future work: 1) Estimate maximum yield** of promising polyketide and isoprenoid fuel precursors. **2) Update preliminary process models** for hydrocarbon fuels with experimental data. **3) Expand analysis** to other hydrocarbon fuels and chemicals.

Acknowledgements

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy BIOENERGY TECHNOLOGIES OFFICE

Pacific Northwest
NATIONAL LABORATORY

Biochemical Analysis: Jim Collett, Mark Butcher, Sue Jones, Aye Meyer, Yunhua Zhu,

Supporting Teams

Fungal Genomics: Jon Magnuson, Ken Bruno, Mark Butcher, Jim Collett, David Culley, Ziyu Dai, Shuang Deng, Beth Hofstad, Sue Karagiosis, Ellen Panisko

Advanced SCADA: Jim Collett, Erik Hawley, Richard Zheng, Richard Daniel

Additional Slides

Approach (Technical)

- Biocatalyst and chemical catalyst experts are engaged for:
  - Evaluation of **fuel precursor candidates**
  - Development of **hybrid processes** to leverage **the best** biochemical and chemical technologies

- **Inputs for process and metabolic models** come from published literature and from related AOP projects on fungal genomics and bioprocess development.

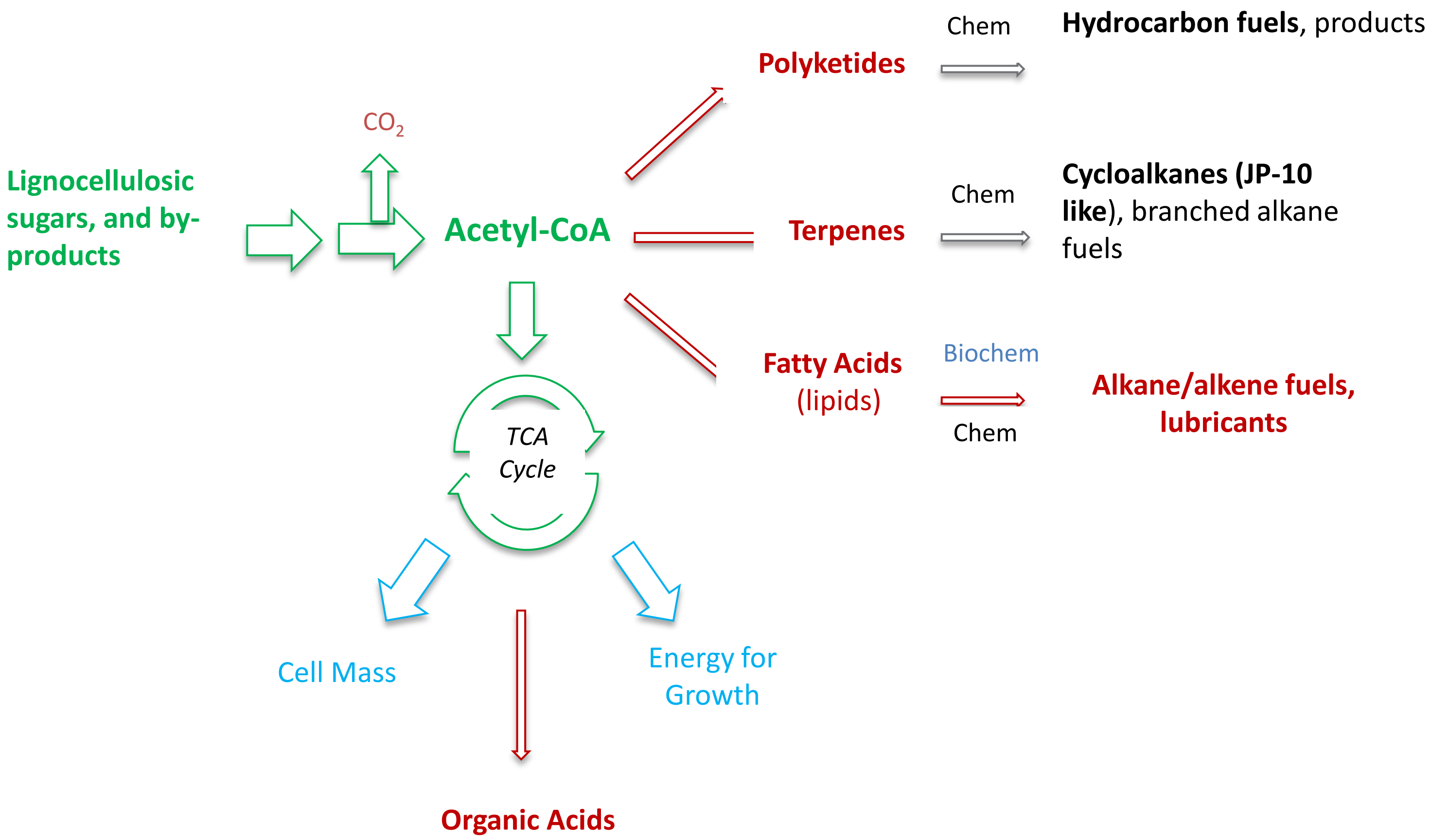
- Technical challenges for biochemical hydrocarbon fuel R&D:
  - **Microbial strains** with better pathway enzymes **for improved hydrocarbon production** must be developed.
  - Biochemical processes must be **optimized under industrially relevant conditions**
  - Process models must include validated experimental data that **scale up to commercial levels without losing performance**

Approach (Technical)

- **Pathways to Commercialization**
  - Producing **hydrocarbons as fuel precursors appears feasible.**
  - **Isoprenoids and polyketides** are promising blend components or precursors for **high value, high-density jet and missile fuels** such as RJ-4, RJ6 and JP-10.
  - Challenges
    - **Engineering production strains** that reach productivities required **to meet economic targets**
    - **Scaling processes** to commercial levels **without losing performance**
  - This project will help **quantify** these challenges

Approach (Technical)

- Isoprenoid (terpene) and polyketide pathways produce precursors to hydrocarbon fuels



Lignocellulosic sugars, and by-products

CO_2

Acetyl-CoA

Polyketides

Chem

Hydrocarbon fuels, products

Terpenes

Chem

Cycloalkanes (JP-10 like), branched alkane fuels

Fatty Acids (lipids)

Biochem

Chem

Alkane/alkene fuels, lubricants

TCA Cycle

Cell Mass

Energy for Growth

Organic Acids

- Increasing availability of genome sequences and use of bioinformatics are increasing potential for production improvements and new product discovery

3 – Technical Accomplishments/ Progress/Results

Key Milestones and Deliverables	Due Date	Completed
Use *Lipomyces starkeyi* metabolic model to identify at least one side reaction that does not contribute to fatty acid synthesis and/or inhibit overall biochemical conversion productivity and assess the benefits and risks of eliminating this side reaction	31-Dec-13	✓
Use *L. starkeyi* model to estimate the increases in growth rate and specific lipid yield that might be attained by the near complete suppression of mannan synthesis	31-Mar-14	✓
Update TEA assessment for bioconversion of lignocellulosic sugars to hydrocarbons by oleaginous yeast to include alternative processing schemes identified from the metabolic model	30-Jun-14	✓
Final report summarizing FY14 results from metabolic modeling and techno-economic analysis and the progress made on increasing carbon efficiency to facilitate advantageous economics	30-Sep-14	✓
Complete a broad inventory of polyketide and isoprenoid compounds reported to be produced by *Aspergillus* species	31-Dec-14	✓
Complete a preliminary, literature-based assessment of candidate Aspergillus polyketide or isoprenoid compounds for suitability for hydrocarbon components of diesel or jet fuel	31-Mar-15	✓
Calculate the predicted yield of most promising polyketide or isoprenoid fuel precursor compounds	30-Jun-15	On schedule
Assemble preliminary biorefinery process model for producing hydrocarbon fuel precursors using fungi	30-Sep-15	On schedule
Final report summarizing FY15 findings and preliminary process model	30-Sep-15	On schedule

3 – Technical Accomplishments/ Progress/Results – FY 13

Initial validation of the *L. starkeyi* metabolic model via comparison of Flux Balance Analysis (FBA) predictions of log phase cell growth with bioreactor data.

	Bioreactor Experiment		Metabolic Model*	
Metabolites	mmol/gDW/hr	g/gDW/hr	mmol/gDW/hr	g/g DW/hr
Glucose	-1.053	-0.190	-1.050	-0.189
O2	-2.862	-0.092	-2.737	-0.088
CO2	2.521	0.111	2.806	0.123
Ammonium	-0.332	-0.006	-0.544	-0.010
Cell mass growth		0.113		0.097

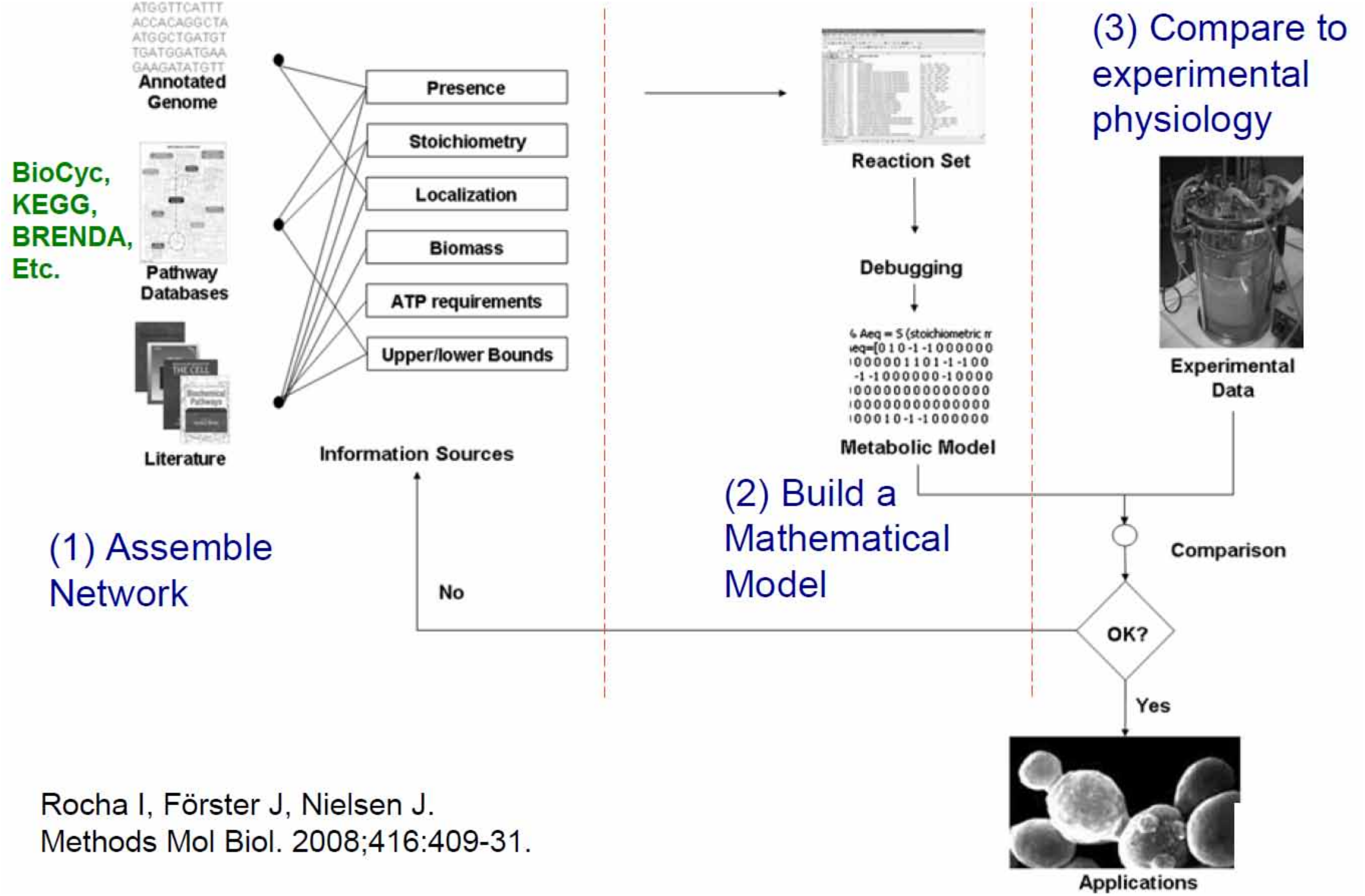
*Model glucose exchange flux was constrained to match bioreactor experiment; all other model fluxes were predicted by flux balance analysis.

mmol/gDW/hr = millimoles of metabolite produced or substrate consumed per gram of dry weight of cell mass per hour.

g/gDW/hr = grams of metabolite produced or substrate consumed per gram of dry weight of cell mass per hour.

Negative values indicate consumption; positive values indicate production

Metabolic Network Reconstruction



BioCyc,
KEGG,
BRENDA,
Etc.

(1) Assemble Network

(2) Build a Mathematical Model

(3) Compare to experimental physiology

Rocha I, Förster J, Nielsen J.
Methods Mol Biol. 2008;416:409-31.

FBA of COBRA Models

A COBRA model is composed of vectors and matrices that hold:

- the reaction network stoichiometry
- gene lists
- protein lists (enzymes)
- gene-protein-reaction associations

Typical procedure for simulating metabolism:

1. The matrix of stoichiometric coefficients is translated into a system of linear equations.
2. An objective function is selected (i.e. cell growth).
3. Exchange flux constraints are set.
4. FBA is used to find an optimal distribution of fluxes through the network that maximizes the objective function

$$
\begin{array}{c|cccccccc}
 & \text{GLCt1} & \text{HEX1} & \text{PGI} & \text{PFK} & \text{FBP} & \text{FBA} & \text{TPI} & \text{EX\_glc} \\
\hline
\text{glc-D[e]} & -1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\
\text{glc-D} & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
\text{atp} & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\
\text{H} & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
\text{adp} & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
\text{g6p} & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\
\text{f6p} & 0 & 0 & 1 & -1 & 1 & 0 & 0 & 0 \\
\text{fdp} & 0 & 0 & 0 & 1 & -1 & -1 & 0 & 0 \\
\text{pi} & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
\text{h2o} & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
\text{g3p} & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\
\text{dhap} & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0
\end{array}
$$

Stoichiometric Matrix for Glycolysis Pathway

- Schellenberger J, Que R, Fleming RM, Thiele I, Orth JD, Feist AM, Zielinski DC, Bordbar A, Lewis NE, Rahmanian S, Kang J, Hyduke DR, Palsson BØ. Nat Protoc. 2011
- http://opencobra.sourceforge.net/openCOBRA/Welcome.html

Feedstock and Financial Assumptions

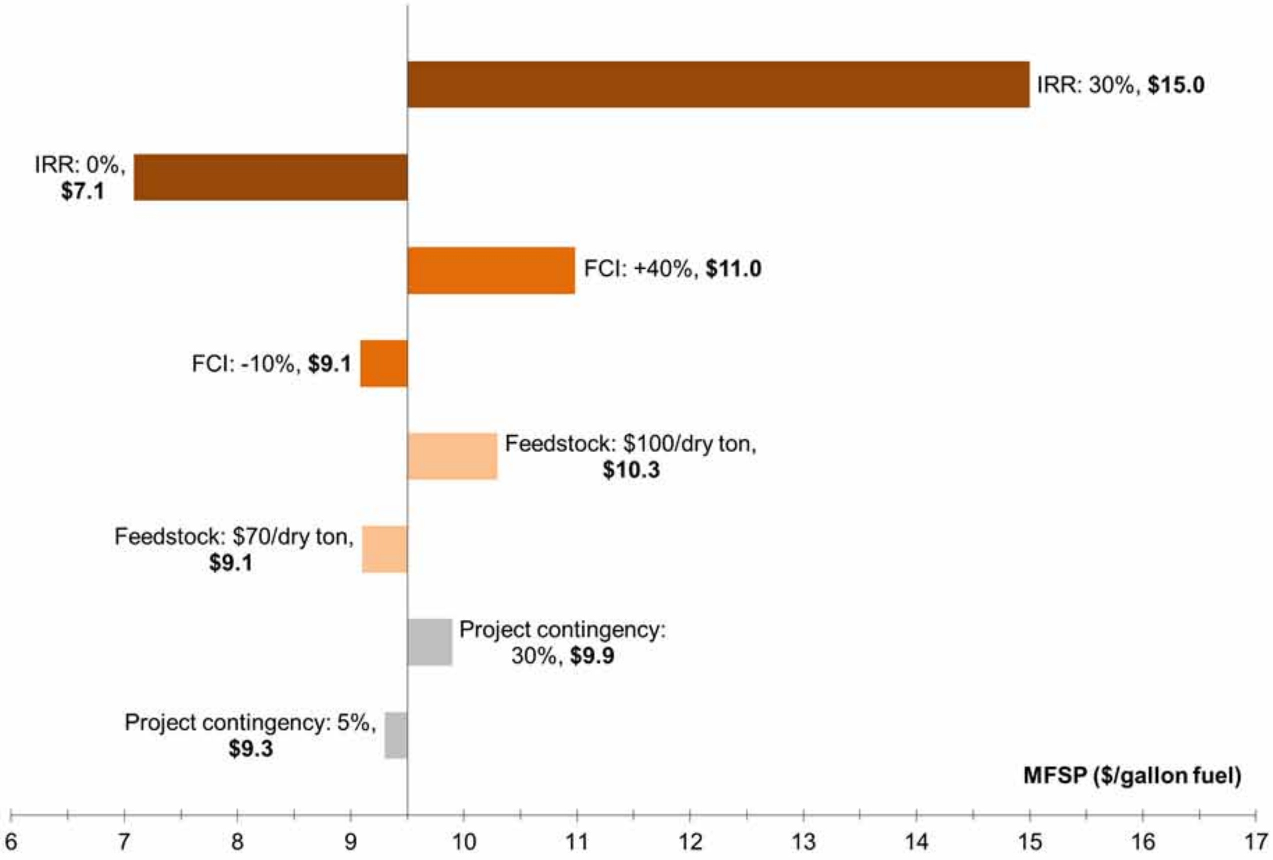


Figure 4. Fuel price sensitivities to feedstock costs and financial assumptions

Collett, J., A. Meyer and S. Jones (2014). Preliminary Economics for Hydrocarbon Fuel Production from Cellulosic Sugars, Pacific Northwest National Laboratory. **PNNL-23374**.

BSLE vs. BHTL Model Details

Biorefinery Performance Results

Bioconversion + Solvent Lipid Extraction (BSLE)
vs.
Bioconversion + Hydrothermal Liquifaction (BHTL)

	Unit	BSLE Case	BHTL Case
Feedstocks and Raw Materials			
Corn Stover, dry basis	mtpd	2,000	2,000
Corn Stover, wet basis, with 20% moisture	lb/h	229,647	229,647
Hydrotreater (HT) Hydrogen	lb H_2/lb HT feed	0.0166	0.0282
Intermediate Products			
Triglyceride lipid yield from fermentation	ton/dry ton feedstock	0.145	0.145
Bio-oil yield	ton/dry ton feedstock	n/a	0.248
Bio-oil total production	lb/h	n/a	42,921
Bio-oil percentage from lignin	w/w	n/a	16.6%
Bio-oil percentage from yeast	w/w	n/a	5.4%
Bio-oil percentage from triglyceride lipids	w/w	n/a	59.3%
Bio-oil percentage from unreacted sugars & other organics	w/w	n/a	18.7%
Final Products			
Distillate Fuel production rate	mmgal/yr	28.4	41.1
Distillate Fuel yield	gal/dry ton feedstock	39	57
Distillate Fuel yield	ton/dry ton feedstock	0.126	0.197
Water Usage			
Cooling Water Make-up	gal/gal product	30.6	17.34
Boiler Feedwater Make-up	gal/gal product	1.12	0*
Total Water Usage	gal/gal product	31.72	17.34
Electricity Usage			
Electricity consumption	MW	42.19	8.39
Electricity generation	MW	50.36	6.00
Electricity purchased from grid	MW	0	2.09
Electricity sold to grid	MW	8.18	0
Energy Efficiency			
Feedstock, higher heating value (HHV) basis	MMBtu/hr	1400.1	1400.1
Hydrogen HHV	MMBtu/hr	61.1	81.9
Distillate Fuel HHV	MMBtu/hr	472.1	709.1
Eefficiency, Distillate Fuel/feedstock + hydrogen	%, HHV basis	0.323122198	0.47845563
Carbon Efficiency, C in Distillate Fuel/C in feedstock	**%**	**23.86%**	**38.19%**

BSLE vs. BHTL Model Details

Biorefinery Performance Results

Bioconversion + Solvent Lipid Extraction (BSLE)
vs.
Bioconversion + Hydrothermal Liquifaction (BHTL)

	BSLE Case		BHTL Case	
Installed Cost (2011 US Dollar)	million $	% of total TIC	million $	% of total TIC
Corn Stover Pretreatment and Conditioning	55.3	17.0%	55.3	12.5%
Enzyme Hydrolysis and Bioconversion	77.0	23.7%	77.0	17.5%
Cellulase Enzyme Production	12.7	3.9%	12.7	2.9%
Hydrothermal Liquefaction	Not used		98.9	22.4%
Hydrotreating and Product Separation	22.9	7.0%	34.6	7.8%
Wastewater Treatment	40.1	12.3%	43.3	9.8%
Product and Feed Chemical Storage	3.2	1.0%	3.6	0.8%
Utilities	11.7	3.6%	11.2	2.5%
Additional Direct Cost	29.4	9.0%	48.7	11.0%
Total Installed Cost (TIC)	325.1	77.6%	441.1	87.3%
Fixed Capital Investment	520.0		705.8	
Total Project Investment (TPI)	547.8		742.9	
Operating Cost	$/gal product	% of total	$/gal product	% of total
Dry Biomass	2.04	35.6%	1.41	28.4%
Catalysts & Chemicals	0.73	12.7%	0.56	11.3%
Waste Disposal	0.04	0.7%	0.03	0.6%
Electricity and other utilities	-0.12	-2.1%	0.12	2.5%
Fixed Costs	0.49	8.6%	0.45	9.0%
Capital Depreciation	0.61	10.6%	0.57	11.5%
Average Income Tax	0.34	5.9%	0.32	6.4%
Average Return on Investment	1.60	27.9%	1.50	30.3%
Minimum Distillate Fuel Selling Price, $/gallon	**5.73**	100.0%	**4.97**	100%
Contributions		% of total		% of total
Feedstock cost	2.04	35.6%	1.41	28.4%
Biochemical conversion cost	1.83	32.0%	1.27	25.5%
Thermochemical and other conversion cost	1.86	32.4%	2.29	46.1%
Minimum Distillate Fuel Selling Price, $/gge*	**5.45**		**4.54**	

BSLE vs. BHTL Model References

- Collett, J., A. Meyer and S. Jones (2014). Preliminary Economics for Hydrocarbon Fuel Production from Cellulosic Sugars, Pacific Northwest National Laboratory. **PNNL-23374**.

- Davis, R., Biddy, M., Tan E, Tao, L., Jones, S. (2013). Biological Conversion of Sugars to Hydrocarbons Technology Pathway. NREL/TP-5100-58054; PNNL-22318. Denver, CO, National Renewable Energy Laboratory and Pacific Northwest National Laboratory.

- Elliott, D. C., T. R. Hart, A. J. Schmidt, G. G. Neuenschwander, L. J. Rotness, M. V. Olarte, A. H. Zacher, K. O. Albrecht, R. T. Hallen and J. E. Holladay (2013). "Process development for hydrothermal liquefaction of algae feedstocks in a continuous-flow reactor." Algal Research-Biomass Biofuels and Bioproducts **2**(4): 445-454.

- Zhu, Y. H., M. J. Biddy, S. B. Jones, D. C. Elliott and A. J. Schmidt (2014). "Techno-economic analysis of liquid fuel production from woody biomass via hydrothermal liquefaction (HTL) and upgrading." Applied Energy **129**: 384-394.

(Not a template slide – for information purposes only)

- *The following slides are to be included in your submission for Peer Evaluation purposes, but* ***will not*** ***be part of your oral presentation*** *–*
- *You may refer to them during the Q&A period if they are helpful to you in explaining certain points.*

Responses to Previous Reviewers' Comments

- Reviewer comment: It would appear that from an economical modeling standpoint there could be significant overlap between the work presented here and the work presented by NREL. A consolidated approach may be advantageous and should be considered; i.e., rather than two national laboratories developing economic models let one take the lead.

- PI Response: The two efforts compliment each other with NREL's main focus being on metabolic engineering in *Zymomonas* bacteria and PNNL's exclusively focused on fungi and yeast. Supporting more than one bioconversion approach for hydrocarbon fuel production may reduce risk for BETO, especially if engineered metabolic pathways can be made transferable across organisms to maximize bioconversion yield and efficiency.

Responses to Previous Reviewers' Comments

- Reviewer comment: Definitely needed work in order to understand the technical / economic issues of HC production prior than to start doing R&D. The initial conclusion though is that it doesn't appear possible to achieve $3/gal unless there is some co-product value of the lignin (or something else).
- PI Response: We agree that hydrocarbon production through biochemical processes will be challenging both technically and economically. Our analysis emphasized the importance of finding a higher valued use for lignin besides power generation to achieve the BETO goal of producing a hydrocarbon fuel with an MFSP of $3/gallon. We have proposed under a related project a hybrid process that would maximally incorporate lignin carbon into the final fuel product.

Publications, Patents, Presentations, Awards, and Commercialization

Publications:

- Jovanovic I, SB Jones, DM Santosa, Z Dai, KK Ramasamy, and Y Zhu. 2010. A survey of Opportunities for Microbial Conversion of Biomass to Hydrocarbon Compatible Fuels . PNNL-19704.
- Ryan Davis, Mary Biddy, Eric Tan, Ling Tao, and Sue Jones. Biological Conversion of Sugars to Hydrocarbons Technology Pathway. (2013) NREL/TP-5100-58054; PNNL-22318.
- Mary Biddy and Sue Jones. Catalytic Upgrading of Sugars to Hydrocarbons Technology Pathway (2013) NREL/TP-5100-58055; PNNL-22319.
- PA Meyer, IJ Tews, JK Magnuson, SA Karagiosis and SB Jones, “Techno-economic analysis of corn stover fungal fermentation to ethanol”. Applied Energy (2013) 111:657–668.
- Collett, J., A. Meyer and S. Jones (2014). Preliminary Economics for Hydrocarbon Fuel Production from Cellulosic Sugars, Pacific Northwest National Laboratory. PNNL-23374.

Presentations:

- Jovanovic I, and SB Jones. 2010. “Novel Microbial Conversion of Biomass to Hydrocarbon Compatible Fuels." Abstract submitted to 33ed Symposium on Biotechnology for Fuels and Chemicals, Seattle, WA. PNNL-SA-76722
- Tews IJ, SB Jones, and P Meyer. Technoeconomic Assessment of Cellulosic Bio-Conversion Processes; Near and Future Possibilities. (2011) Recent Advances in Fermentation Technology, Marcos Island, FL. PNNL-SA-82679.
- Meyer P, IJ Tews, SB Jones, and JK Magnuson. 2011. "A Techno-economic Analysis for Cellulosic Ethanol Production from by Fungal Fermentation." Abstract submitted to 243rd ACS (American Chemical Society) National Meeting & Exposition, San Diego, CA. PNNL-SA-83738.