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A process economic assessment of hydrocarbon biofuels production using chemoautotrophic organisms

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HIGHLIGHTS

- Process model presented for microbial hydrocarbon production from H_2, O_2 and CO_2.
- Economic analysis is used to obtain capital, operating cost and fuel cost estimate.
- Electricity cost is found to be >90% of fuel cost.
- Specific fuel productivity target $\geqslant 0.3$ g-fuel/gDW-h is needed for feasibility.
- Economic feasibility requires LCOE <2¢/kWh LCOE for target specific productivity.

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ABSTRACT

Economic analysis of an ARPA-e Electrofuels (http://arpa-e.energy.gov/?q=arpa-e-programs/electrofuels) process is presented, utilizing metabolically engineered *Rhodobacter capsulatus* or *Ralstonia eutropha* to produce the C_{30+} hydrocarbon fuel, botryococcene, from hydrogen, carbon dioxide, and oxygen. The analysis is based on an Aspen plus® bioreactor model taking into account experimentally determined *Rba. capsulatus* and *Rls. eutropha* growth and maintenance requirements, reactor residence time, correlations for gas–liquid mass-transfer coefficient, gas composition, and specific cellular fuel productivity. Based on reactor simulation results encompassing technically relevant parameter ranges, the capital and operating costs of the process were estimated for 5000 bbl-fuel/day plant and used to predict fuel cost. Under the assumptions used in this analysis and crude oil prices, the Levelized Cost of Electricity (LCOE) required for economic feasibility must be less than 2¢/kWh. While not feasible under current market prices and costs, this work identifies key variables impacting process cost and discusses potential alternative paths toward economic feasibility.

1. Introduction

Fossil fuels have provided a readily accessible and energy-dense fuel source to pave the way for science and technology advancements. However, fossil fuel reservoirs, which accumulated over millions of years, are a finite resource that must be replaced with more sustainable alternative liquid fuels. Corn ethanol, the most widely produced biofuel in the United States, made up less than 5% of transportation fuels in 2011 (www.eia.gov). Furthermore, there is ongoing controversy related to corn-ethanol contributing to higher food prices. Additional constraints on alternative fuel technologies include valuation of carbon credits and assurance of economic and political energy security. These competing issues demand the development of transformative technologies for producing renewable liquid fuels able to meet our society's growing energy needs.

The Electrofuels initiative, administered by the United States Department of Energy's Advanced Research Projects Agency – Energy (ARPA-E), aimed to develop liquid biofuels that avoid the issues encountered in the current generation of biofuels: (1) the reliance of biomass-derived technologies on the inefficient process of photosynthesis, (2) the relatively energy- and resource-intensive nature of agronomic processes, and (3) the occupation of large areas of arable land for feedstock production (http://arpa-e.energy.gov/?q=arpa-e-programs/electrofuels). To address these issues, the

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List of symbols and abbreviations

a, b, c, d	stoichiometric coefficients in cell growth equation
bbl	US fluid barrel
C_{fuel}	concentration of fuel in the bioreactor, mol L^{-1}
C_i	liquid phase concentration of i-th gas component, mol L^{-1}
D_i	diffusion coefficient of i-th gas component, $m^2\ s^{-1}$
$\frac{dc_i}{dt}$	rate of consumption of i-th gas component, mol $L^{-1}\ h^{-1}$
$\left[\frac{dc_i}{dt}\right]_{growth}$, $\left[\frac{dc_i}{dt}\right]_{fuel}$, $\left[\frac{dc_i}{dt}\right]_{maint}$, $\left[\frac{dc_i}{dt}\right]_{total}$	rate of substrate utilization for growth, fuel synthesis, maintenance requirements and total respectively, mol $L^{-1}\ h^{-1}$
EROI	Energy Return on Investment
F	rate of liquid feed into reactor, L h^{-1}
gDW	grams dry weight
GTR_i	gas transfer rate of i-th gas component, mol $L^{-1}\ h^{-1}$
H_i	Henry's law coefficient of i-th gas component, atm L mol^{-1}
IGCC	integrated gasification combined cycle
K_La_i	gas–liquid mass transfer coefficient of the i-th component, h^{-1}
LCOE	Levelized Cost of Electricity
m_{H_2}, m_{O_2}	maintenance coefficient of cells on H_2 and O_2 respectively mol $gDW^{-1}\ h^{-1}$
NGCC	natural gas combined cycle
PC	pulverized coal
$\bar{P}_f$	volumetric fuel productivity, g-fuel $L^{-1}\ h^{-1}$
P_{tot}	total pressure, atm
R_{fuel}	specific fuel productivity, g-fuel·$gDW^{-1}\ h^{-1}$
r_{growth}	rate of growth of cells, gDW $L^{-1}\ h^{-1}$
V	reactor volume, L
X	cell density, gDW L^{-1}
Y_{f/H_2}	yield of fuel on H_2, g-fuel·(mol-H_2)$^{-1}$
y_i	gas phase mole fraction of i-th component
$Y^T_{H_2}$	true growth yield of cells on H_2, gDW mol^{-1}
ε	cell recycle efficiency
μ, $\mu_{\max}$	specific growth rate and maximum specific growth rate of cells, h^{-1}
τ	residence time through reactor, V/F, h^{-1}

Electrofuels initiative funded research efforts that sought to develop biological processes that would convert distributed, off-grid, renewable electricity into alternative liquid fuels. The logic of this approach rests in its ability to provide a reliable energy source for the transportation sector by storing transiently-available electrical energy in a chemical bond (Fig. 1A). In addition, the Electrofuels approach is synergistic with advances in photovoltaic cells.

Under the Electrofuels initiative, a range of approaches to this challenge were funded (summary found in (Tuerk, 2011)). The concept for our approach is depicted schematically in Fig. 1A, and involves collecting and transporting electrons to a centralized bioreactor for biological capture of the reducing power in the chemical bonds of a hydrocarbon fuel. This proceeds by: (1) the capture of solar energy into electrical energy via photovoltaic cells (with demonstrated laboratory efficiencies upwards of 40%, a sevenfold improvement on photosynthesis), (2) the use of the generated electricity to split water into molecular hydrogen (H_2) and oxygen (O_2), and (3) feeding these gases, along with carbon dioxide (CO_2) emitted from point sources such as a biomass or coal-fired power plant, to a microbial bioprocessing platform. Our proposed microbial bioprocessing platform leverages a chemolithoautotrophic microorganism naturally able to utilize these gases as growth substrates, and genetically modified to produce a triterpene hydrocarbon fuel molecule native to the alga *Botryococcus braunii*. The details and rationale of these choices are discussed below.

This exercise of using process economic analyses to research priorities is an important aspect of the ARPA-E program. An initial analysis of the economic feasibility of the microbial process, based on microbial energetic theory, can be found in an extensive thesis (Tuerk, 2011). A preliminary process economic model can also be found in a co-author's honors thesis (Myers, 2013). In this work, we expand upon these previous analyses by constructing a more detailed bioreactor model in Aspen Plus® (described in Section 2.2). Furthermore, we examined specific scenarios based on reactor residence time (τ), specific fuel productivity (R_{fuel}) and gas–liquid mass transfer coefficient (k_La) to predict their effect on the overall process volumetric fuel productivity ($\bar{P}_f$) and fuel cost ($/bbl-fuel). The ultimate goal of this analysis was to identify limiting parameters for the process and ranges of these variables needed to achieve economic feasibility.

1.1. Rationale for selection of the microbial bioprocessing platform

Biological approaches for producing alternative fuels are benefitting from advances in molecular biology. These developments have increased the range of fuel molecule targets that can be synthesized by living organisms (Farmer and Liao, 2001; Kim et al., 2006), as well as expanded the selection of alternative hosts for production through the development of new genetic engineering tools (Steinbrenner and Sandmann, 2006). However, current works most frequently uses *Escherichia coli* or yeast as the microbial host with carbohydrate (i.e. fixed-carbon) based substrates. Our approach to the Electrofuels initiative leverages developments in alternative hosts capable of autotrophic growth on H_2 as well as developments in fuel targets.

1.1.1. Microbial host selection

For this economic analysis, we decided to include two different chemolithoautotrophs (microbes growing on H_2, O_2 and CO_2) based on specific differences in their physiology, metabolism and energetic yields. Initially motivated by the production of the industrially relevant biopolymer poly-hydroxy butyrate (PHB), the chemoautotrophic growth mode was developed as an alternative approach to bioprocessing using *Ralstonia eutropha* (Tanaka et al., 1995). High-density growth (40–90 gDW/L) of *Rls. eutropha* on gaseous substrates was achieved in high gas–liquid-mass-transfer bioreactors with controlled addition of inorganic nutrients, demonstrating the technical feasibility of such a process. We are also investigating the use of *Rhodobacter capsulatus*, a purple non-sulfur facultative phototroph, as a candidate because of its capability of diverse metabolic modes (including autotrophic), ability to utilize a range of growth substrates, and innate high level production of carotenoids (Hunter et al., 2009) indicating that pathways for isoprenoid biosynthesis are already present in this organism. We have recently achieved significant milestones, including production of >100 mg/L botryococcene, by genetically engineering *Rba. capsulatus* (Khan et al., 2013), validating its poten-