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# Life cycle optimization for sustainable design and operations of hydrocarbon biorefinery via fast pyrolysis, hydrotreating and hydrocracking

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#### ABSTRACT

This paper addresses the optimal design and operation of hydrocarbon biorefinery via fast pyrolysis, hydrotreating and hydrocracking of hybrid poplar feedstock under economic and environmental criteria. The hydrocarbon biorefinery encompasses fast pyrolysis for crude bio-oil production, upgrading of the bio-oil through hydrotreating, separation and hydrocracking of long chained hydrocarbons into gasoline and diesel range products, and steam reforming for hydrogen production. We propose a bi-criteria nonlinear programming (NLP) model that seeks to maximize the economic performance measured by the net present value (NPV) and to minimize the environmental impacts. The environmental objective is measured with the global warming potential (GWP) metric according to the life cycle assessment procedures, which covers gate-to-gate environmental impacts of the hydrocarbon biorefinery. The multiobjective NLP model simultaneously determines the production capacity, size of each process units, operational conditions, the flow rates of species and streams at each stage of the process, hydrocarbon biofuel yields, and consumption rate of feedstock, steam, electricity, and natural gas. The bi-criteria NLP model is solved with the  $\varepsilon$ -constraint method, and the resulting Pareto-optimal curve reveals the tradeoff between the economic and environmental dimensions of the sustainable hydrocarbon biorefinery. The optimization results reveal that the unit production cost of the hydrocarbon biofuels is \$2.31 per gallon of gasoline equivalent (GGE) for the maximum NPV solution and \$3.67/GGE for the minimum GWP design. The corresponding greenhouse emission is 8.07 kgCO<sub>2-eq</sub>/GGE.

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#### 1. Introduction

The global economy is heavily reliant on the supply of petroleum based fuels, which are limited resource, environmentally unfriendly, and potentially unstable leading to political vulnerability. In recent years, researchers have put much effort into the development of sustainable and environmentally benign biofuels. Hydrocarbon biorefinery technologies, which convert a wide variety of cellulosic materials to liquid transportation fuels, have been considered as promising approaches to overcome the market barrier resulting from the current vehicle technologies and fuel distribution infrastructure (National Advanced Biofuels Consortium, 2012; The National Academies, 2009). In this respect, the U.S. government proposed the Energy Independence and Security Act of 2007 (Public Law 110-140, 2007) that requires the total amount of biofuel production to increase from 4.7 billion gallons per year in 2007 to 36 billion gallons per year by 2022. Therefore, considering the short time to achieve the goal and the investment on new

infrastructures, it is appealing to investigate infrastructurecompatible fuels. Hydrocarbon biofuels provide vehicle performance similar to or better than their conventional counterparts (National Advanced Biofuels Consortium, 2012). Moreover, they can use the current fuel distribution and utilization infrastructure that includes pipelines, pumping stations, and vehicles without significant changes (National Advanced Biofuels Consortium, 2012; You & Wang, 2011). The main advantage of hydrocarbon biofuels is that they are more sustainable than their petroleum counterpart, because they produce less life cycle environmental impact and reduce the consumption of nonrenewable primary energy resources. Furthermore, hydrocarbon biorefinery via fast pyrolysis followed by hydrotreating and hydrocracking can potentially produce hydrocarbon biofuels at lower production cost, and environmental emissions compared to other biomass conversion pathways. Hence, the goal of this work is to design and optimize the hydrocarbon biorefinery via fast pyrolysis, hydrotreating and hydrocracking under economic and environmental criteria to ensure they are economically competitive and environmentally sustainable.

During the past decade, considerable efforts have been made to convert biomass to chemicals and liquid fuels. Experimental studies have been undertaken on biofuel productions (Maschio,

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#### Nomenclature

#### Sets/indices

set of emissions in the life cycle emission inventories

el set of elements in biomass

set of chemical species indexed by i set of equipment indexed by *l*  $L_{eq}$ st(i)set of species *j* in stream st set of biofuels product q

**Parameters** 

CEPCI chemical engineering plant cost index

 $ECC_{h}^{l}$ base case purchase cost of equipment *l* in \$MM

fsc unit price of biomass feedstock in \$/kg **INCP** percentage of investment incentive

**INCM** maximum allowable investment incentive in \$MM

cost of buildings factor including services  $K_{blg}$ 

 $K_{cns}$ cost of construction factor  $K_{ctg}$ project contingency factor  $K_{elc}$ electrical systems cost factor Keng engineering cost factor

equipment purchase installation factor  $K_{pei}$ 

 $\dot{K_{pp}}$ cost of piping factor

cost instrumentation and controls factor  $K_{icf}$ 

 $K_{lg}$ legal and contractors fee factor

 $K_{lnd}$ cost factor of land

 $K_{om}$ O&M cost as percentage of the total equipment pur-

chase cost

working capital cost factor  $K_{wcp}$ 

LCIE<sup>cat</sup> life cycle emissions inventory of chemical b per

functional unit associated with emissions source

category cat

 $Mw_{i/i}$ molar mass of species *j* or element *i* 

number of carbon atoms nC nΗ number of hydrogen atoms nOxnumber of oxygen atoms natural gas price in \$/kg ngc unit cost of power in \$/kWh рс

the market price of biofuels q in \$/gallon  $p_q$ 

 $Q_{stm}$ heat per kmol of steam

 $R_{tax}$ income tax

reactor product distribution of species R S split fraction of species and streams sf

sizing factor

conversion rate of species in water gas shift reaction

unit cost of steam in \$/kmol stmc

annual operating hours of the biorefinery h/year  $T_{op}$ lifespan of the hydrocarbon biorefinery in years  $t_{ls}$ the unit value of volumetric incentive in \$/gallon of  $v_{inc}$ 

biofuels produced

mole fraction

the damage factor that accounts for the GWP asso- $\Pi_{cat}$ 

ciated with chemical species b

#### Variables

annual gross profit in \$MM AGP **APAT** annual profit after tax in \$MM CtCh

annual catalyst and chemical cost in \$MM **ECCl** base case purchase cost of equipment *l* in \$MM

molar flow rate

**FIXC** fixed O&M cost in \$MM **FSC** feedstock cost in \$MM

FSCtrans feedstock cost transportation cost in \$MM

total molar flow rate

**GWP** global warming potential in ktonCO<sub>2-eq</sub>/year GWPcat global warming potential contribution of category

cat in ktonCO<sub>2-eq</sub>/year

**INCV** total volumetric incentive in \$MM INCC total investment incentive in \$MM

LCI<sub>b</sub>cat life cycle emissions inventory entry of chemical b

associated with

m mass flow rate  $\bar{m}$ total mass flow rate

NGC annual natural gas cost in \$MM NPV net present value in \$MM PC annual power cost in \$MM STMC annual steam cost in \$MM

TAC total annualized operating in \$MM cost **TPEC** total equipment purchase cost in \$MM **TPIC** total purchase investment cost in \$MM Vq annual gallons of biofuels q production

#### **Superscripts**

average avg condenser con cyc cvclone cmb combustor dem demister

distillation column/product splitter dis

dry dryer

hpf high pressure flash hts high temperature shift

hyc hydrocracker hydrotreater hvt kdr knock out drum lpf low pressure flash pyrolysis

pyr auench qnc rfm steam reformer

tot total

#### Subscripts

air air bms biomass

cat emission source categories

chr char

dbms dried biomass

elec electricity consuming units

exh exhaust stream dsl diesel fd feed stream fuel gas fg gasoline gasl

heatc heat consuming units

liq liquid natural gas ng pd product stm steam vap vapor

Koufopanos, & Lucchesi, 1992; Meesuk, Cao, Sato, Ogawa, & Takarada, 2011; Salema & Ani, 2011) and techno-economic analysis of hydrocarbon biorefineries based thermochemical conversion pathways was conducted (Jones et al., 2007; Swanson, Platon, Satrio, & Brown, 2010; Wright, Daugaard, Satrio, & Brown, 2010). These technologies are based on biomass gasification followed by Fisher–Tropsch (FT) or fast pyrolysis followed by hydroprocessing.

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