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Power and Chemical Production Analysis Based on Biomass Gasification Processes

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It is necessary to systematically evaluate site-wide energy efficiency and chemical production for biomass to transportation liquid (BTL) processes. BTL processes consist of biomass collection, biomass fast pyrolysis, bio-oil gasification, water gas shift, acid gas removal, CO_2 capture and storage (CCS), Fischer-Tropsch (FT) synthesis, and syncrude refining. Operating parameters determine the transportation liquid production, the exhaust tail gas, and process energy and power demands. For the tail gas treatment, it could burn in utility systems to generate steam and power and realize whole system power and energy self-sufficiency. The components H₂ and CO in the tail gas recovered and recycled to the FT synthesis for more oil production either. However, the tail gas recovery scenario pays for the cost of burning extra fuel in utility systems and more CO_2 emission to the environment.

In this paper, BTL process and utility systems are investigated and optimized simultaneously based on system simulation and mathematical programming method. The correlation among process key operating parameters, tail gas treating scenarios, product outputs, and utility system performance are addressed firstly based on the simulation, and then a MILP model is formulated to achieve an optimal BTL process design and utility system configuration. Barley straw to transport fuel production as well as utility systems are designed as the example to illustrate the optimization methodology.

1. Introduction

Biomass is considered as a promising clean-energy option of renewable resources with greenhouse gas emissions reduction. There are wide sources of biomass for chemical production (Eller Z et al. (2013)) such as banana waste (Souza et al. 2013) and barley straw. Biomass can be converted into bio-oil by biochemical or thermochemical method. The bio-oil is the feed for transportation fuel production (Kreutz et al., 2008).

The research on BTL has been developed mostly focused on experiment research (Jaimes Figueroa et al., 2013), production efficiency improvement (NG, 2010), and techno-economic performance estimation (Ng et al., 2011). Baliban et al. (2010, 2011) compared hybrid biomass, coal, and natural gas processes, and introduced a three-stage decomposition framework to determine the minimum utility requirement, the minimum number of heat exchanger matcher, and the minimum annualized cost of heat exchanges in a series of paper (Elia et al., 2010). Baliban et al. (2013) also analysed the conversion of hardwood biomass to liquid transportation fuels. Ljungstedt et al. (2013) quantified the opportunity for heat integrated FT crude production, co-located with a typical Scandinavian Kraft pulp and paper mill. Garcia et al. (2013) simulated different bioprocesses to evaluate bioproducts from pretreated lignocellulosic materials. Peduzzi et al. (2013) investigated process integration of lignocellulosic biomass into liquid fuels through thermo-chemical conversion to save energy based on energy and mass balances and pinch analysis of centralised and decentralised configurations.

The operating condition of BTL processes affect process heating, cooling, power, and electricity demands, which are the basis of utility system design. The process tail gas mainly contains CO, H_2 , and CH₄. It can

burn as utility fuel for heat and power generation in utility systems. The components H₂ and CO in the tail gas can be recycled to the FT production by auto thermal reforming (ATR) for more oil production.

In this work, BTL processes and utility systems are simulated simultaneously using Aspen Plus to address the effect of key operating parameters and tail gas treating on process products, process energy and power demands, utility fuel selection, and utility system performance. A MILP model is formulated for the total site optimization. Barley straw to the transport fuel production is designed as the example by the integration of production processes and utility systems to enhance the energy efficiency and material production of the whole system.

2. BTL processes and utility systems simulation

BTL processes include biomass pyrolysis to produce bio-oil, bio-oil gasification for syngas generation, water gas shift to adjust syngas H_2/CO molar ratio, syngas purification for acid gas removal, and liquid transportation oil production by Fischer-Tropsch (FT) synthesis and syncrude refining and tail gas treatment.

Biomass fast pyrolysis produces bio-oil with water, char and non-condensable gases. The char and non-condensable gases can combust for pyrolysis heating. Bio-oil is gasified for raw syngas production. Syngas mainly consists of CO, H_2 , CO₂ and H_2O . The H_2/CO mole ratio in the syngas is required to reach 2.06 - 2.20 by water gas shift operation. Syngas purification is carried out by Selexol unit to reduce CO₂ content less than 20 ppm. CO₂ is pressed to 80bar, and then restored in a deep geology.

The purified syngas converts to be alkanes, alkenes and oxygenated chemicals through FT synthesis using iron or cobalt catalysts. In this work, FT conversion to straight-chain paraffins (C1 to C60) follows the Anderson-Schulz-Flory distribution (NG, 2010). The conversion rate is mainly determined by FT operating temperature and H₂ and CO contents in the FT feed. The FT synthesis products are separated into syncrude and FT tail gas. The syncrude is refined by hydrocracking to obtain gasoline, kerosene, and diesel. Both FT tail gas and syncrude refining gas contribute to the process tail gas, which mainly contains light hydrocarbons and unreacted H₂ and CO. There are two scenarios of tail gas treatment. The first is tail gas combustion in utility systems to satisfy process energy and power demands. The second is H₂ and CO recovery from the tail gas by membrane separation, pressure swing adsorption (PSA), and auto thermal reforming (ATR) to increase product output with the cost of burning extra fuel in utility systems.

Utility system consists of boilers, gas turbines, heat recovery steam generator (HRSG), steam turbines, and other auxiliary components. The source of very high pressure (VHP) steam and power is fuel combustion in boilers and gas turbines with heat recovery steam generators (HRSG). Natural gas, coal and FT tail gas are fuel options.

2.1 System simulation

Both BTL processes and utility systems are simulated using Aspen Plus to determine quantitative relationships among process operating parameters, process products, tail gas treatment, process utility demands, and steam and power generation in utility systems. The simulation is wholly converged. Figure 1 illustrates the simulation of Selexol and CO₂ compression. Figure 2 shows the utility system simulation. The simulation of other units is not listed in this paper.

Besides process stream data, process energy and power demands are obtained from the simulation. They are the basis of utility system design.

However, process energy targets are less than process energy demand obtained from the simulation. In BTL process, the process heat recovery within individual unit would reduce the process heating and cooling demands. Process indirect heat recovery through utility steam mains would reduce utility VHP steam demand and save fuel burning in boilers. For example, the heat integration in Selexol can save cold utility demand. In the unit of gasification, VHP steam is generated from high temperature syngas which is exhausted from the gasifier. Shaft power and electricity are required by refrigerant production, compressors, pumps, etc.

2.2 Sensitivity analysis

Key operating parameters are identified based on sensitivity analysis. FT synthesis plays an important role in the product distribution, FT tail gas, and process utility demands. Key operating parameters are FT operating temperature and the molar ratio H_2/CO in the FT feed. The quantitative analysis of tail gas treatment and fuel selection in utility systems on product yields, system energy and power efficiency, and CO_2 emission are addressed as well.



Figure 1: Selexol and CO2 compression



Figure 2: Utility systems simulation

3. Integration optimization

Both the production process and the utility system are designed to maximize the profit by optimizing key process operating parameters, tail gas treatment, and utility system configuration simultaneously.

3.1 Optimization model

The optimization model is shown in Eq (1). The profit is products incomes C_{prod} minus the feed cost C_{feed} , system operating cost *COP*, and whole system equipment depreciation cost. F_{ann} is a depreciation factor. BTL process products of gasoline, kerosene, and diesel, contribute to product incomes C_{prod} .

$$Max Profit = C_{prod} - C_{feed} - COP - F_{ann}^* (CAP_{proc} + CAP_{util})$$
(1)

The feed cost contains the cost of biomass, steam and O_2 consumption as reactants in gasification, shift, and AFT units. System operating cost includes fuel consumption in utility systems, electricity import or export to the grid, and cooling water supplement in the utility system.

The process equipment cost is calculated based on Eq (2) (Kreutz et al., 2008). Eq (3) estimates the heatexchanger cost (Yee & Grossmann, 1990). Utility system capital cost including boilers, gas turbine, HRSGs, and steam turbines is determined by equipment type, size and operating load.

$C_{PRO} = C_0 * \left(\frac{S}{S_0}\right)^f$	(2)
$C_{HEX} = 1200 * (A^2)^{0.6}$	(3)

Decision variables in the optimization include process operating parameters and equipment selection (equipment type and size). Based on sensitivity analysis, FT feed H₂/CO molar ratio (x_1) and FT reaction temperature (x_2) are decision variables in the optimization. For the tail gas treatment, the syncrude refining exhaust is burned as utility fuel, and the FT tail gas has two treatment options: one burns as utility fuel, and the other is recycled for CO, H₂ recovery by ATR. The percent of FT tail gas for reforming is the third operating variable (x_3) in the optimization.

Utility system item size is expressed by the maximum steam load (MS) for boilers, steam turbines, and HRSGs, and the maximum power generation (WS) for gas turbines. Steam distribution load (M) at every steam head, and power generation (W) by gas turbines and steam turbines are continuous variables. Electricity import and export to grid are allowable in the design.

The utility system item selection is 0-1 variable (y) in the model.

3.2 Constraints

Mass and energy balance are equality constraints. Steam production constraint of the sum of steam production no less than process steam demands is an inequality constraint. Equipment models provide equipment operating performance, including boilers for steam generation, gas turbines for power generation, HRSGs for VHP steam generation, steam turbines for steam distribution and shaft power generation, and let down valves for steam pressure reduction. Eq (4) is the boiler performance model, which provides the relationship of fuel consumption and VHP steam production at full load and part load operation. Eq (5) shows boiler efficiency model (Aguilar, 2005).

$$[aM^{\max} + (1+b)M][(1+\varphi)C_p\Delta T^{SAT} + q] = q_{fuel}$$
(4)

$$\eta = \frac{M / M^{\max}}{(1+b)(M / M^{\max}) + a}$$
(5)

The operating variables vary in limited ranges due to the reaction restriction.

 $\begin{array}{l} x_1 \! \in \! [2.06, \, 2.20] \\ x_2 \! \in \! [220 \ ^\circ \! C, \ 240 \ ^\circ \! C] \\ x_3 \! \in \! [0, \, 1]. \end{array}$

3.3 Solution

The MILP model is solved using the DICOPT solver of GAMS 23.6 to obtain optimal operation parameters and utility system configuration.

4. Barley straw to transport fuel design

Barley straw to transport fuel production is designed by the integration and optimization of production processes and utility systems.

The barely straw feed rate is 100t/h. Annual operating time is 8300h. Equipment depreciation rate is 0.05. Table 2 shows material and power price data. Steam mains data are listed in Table 3. The whole system is designed using the proposed methodology.

The optimal operating variables are listed in Table 4. When FT synthesis feed H_2/CO molar ratio is 2.06, FT reaction temperature is 201.6°C, full FT synthesis tail gas is recycled by reforming, and natural gas combusts as fuel in the utility system, the whole site is economic.

Figure 2 is the optimized utility system configuration. 10.382t/h natural gas is consumed in a gas turbine for power and energy production.

Table 5 compares the process and system performance at the optimal design with that at condition 1. The condition 1 is non- optimal design with key operating parameters listed in Table 4. From the economic analysis, the total profit based on the optimal design increases 17.28% compared with that at condition 1. The products income increases 17.45%, and the utility system operating cost reduces 31.58%. From the product distribution in the optimal design, 5.46t/h gasoline, 6.394t/h kerosene, and 4.594t/h diesel are produced. More kerosene and diesel are produced with less gasoline output compared with that at condition 1.

5. Conclusions

Both of BTL production and utility systems are investigated based on the simulation of production processes and utility systems to assess process product outputs, process energy and power demands, and utility system performance. The site- wise system are optimized simultaneously to achieve the optimal system economic profit by taken into account of process operating parameters such as FT operating temperature and FT feed H_2/CO molar ratio, tail gas treatment scenarios, utility system configurations, and utility fuel selection. Barley straw to transport fuel production is designed based on the proposed methodology to determine key operating parameters, tail gas treatment, and utility configuration. The design achieves higher product outputs and higher energy and power efficiencies. However, the increased product yield through tail gas recovery costs extra natural gas combustion in the utility system and more CO_2 emission.

Table 2: Price data

Electricity	VHP steam	Natural gas	Fresh water	Cycle water	Gasoline	Kerosene	Diesel
\$/kW∙h	\$/t	\$/t	\$/t	\$/t	\$/t	\$/t	\$/t
0.104	17.183	220	0.538	0.0242	1572	1500	1420

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Figure 2: Optimal utility system configuration

Table 3: Steam mains data

Steam	T _{sat}	Tope	Pope
headers	°C	°C	bar
VHP	318	540	110
HP	257	430	45
MP	188	260	12
LP	144	180	4

Table 4:	Operating	parameters	determination
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_	Condition 1	Optimal design
H ₂ /CO	2.1	2.06
FT temperature, °C	240	201.6
Recycle tail gas percent	80%	100%

Table 5: The optimal design

	Condition 1	Optimal design
Annual gross profit/(10 ⁸ \$/a)	1.58	1.91
Products income/(10 ⁸ \$/a)	1.75	2.12
Feed cost/(10 ⁶ \$/a)	3.00	3.20
Capital cost (10 ⁷ \$)	62.657	62.618
Operating cost/(10 ⁷ \$/a)	-1.75	-1.33
Gasoline/(t/h)	7.594	5.460
Kerosene/(t/h)	4.036	6.394
Diesel/(t/h)	1.642	4.594
Natural gas/(t/h)	8.143	10.382
Electricity export /(kW·h)	37010	37110

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Nomenclature

 $\begin{array}{l} \mathsf{A}-\mathsf{heat}\ \mathsf{exchanger}\ \mathsf{area},\ \mathsf{m}^2\\ \mathsf{C}-\mathsf{Equipment}\ \mathsf{capital}\ \mathsf{cost},\ \$\\ \mathsf{C}_{\mathsf{HEX}}-\mathsf{Heat}\ \mathsf{exchanger}\ \mathsf{capital}\ \mathsf{cost},\ \$\\ \mathsf{CAP}\ -\ \mathsf{Capital}\ \mathsf{cost},\ \$/a\\ \mathsf{COP}\ -\ \mathsf{Operating}\ \mathsf{cost},\ \$/a\\ \mathsf{C}_o\ -\ \mathsf{Equipment}\ \mathsf{reference}\ \mathsf{cost},\ \$\\ \mathsf{C}_{\mathsf{prod}}\ -\ \mathsf{Products}\ \mathsf{income},\ \$/a\\ \mathsf{C}_{\mathsf{feed}}\ -\ \mathsf{Feed}\ \mathsf{cost},\ \$/a\\ \mathsf{f}\ -\ \mathsf{Equipment}\ \mathsf{size}\ \mathsf{index}\\ \mathsf{F}_{\mathsf{ann}}\ -\ \mathsf{Depreciation}\ \mathsf{factor}\\ \end{array}$

MS - Mass flowrate, t/h

- M Steam flowrate at different steam mains, kg/s
- S_o Equipment reference size
- W Power, MW
- WS Equipment size expressed by power output, MW
- a, b regression parameters of boiler hardware model
- φ boiler blowdown rate, kg/kg
- C_p specific heat capacity, KJ/(kg*K)
- q effective heat steam
- η boiler efficiency

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