CHEMICAL ENGINEERING TRANSACTIONS Volume 25, 2011
Editors Jiří Jaromír Klemeš, Petar Sabev Varbanov, Hon Loong Lam
Copyright © 2011, AIDIC Servizi S.r.l., ISBN 978-88-95608-16-7 ISSN 1974-9791
DOI: 10.3303/CET1125032

Automated Targeting for Synthesis of a Syngas-Based Integrated Biorefinery

Douglas H.S. Tay, Denny K.S. Ng*

Department of Chemical and Environmental Engineering, The University of Nottingham, Malaysia Campus, Broga Road, 43500 Semenyih, Selangor DE, Malaysia.
Denny.Ng@nottingham.edu.my

The increasing world energy consumption and public awareness towards environmental sustainability have motivated a shift to reduce fossil fuels dependence by increasing the production and usage of renewable energy. Liquid biofuels generated from biomasses are among the promising forms of renewable energy as they can be produced from a wide variety of renewable feedstocks. Integrated Biorefinery that utilises biomasses as feedstocks to produce multiple products via various biomass conversion technologies, analogous to petroleum refinery, is a newly-proposed concept. Gasification process is recognised as one of the promising options for initial conversion of biomass to intermediates. In this work, a multiple-cascade automated targeting approach is presented to locate the optimum performance targets of a syngas-based integrated biorefinery.

1. Introduction

There is an increased attention to the issues of energy security, resource diversification, and efficiency enhancement to further reduce fossil fuels dependence. Biofuels are among the promising forms of renewable energy produced via a biorefinery. To enhance the overall process and economic performances, the concept of integrated biorefinery which integrates multiple platforms as a whole is proposed (Fernando et al. 2006). Gasification process is an attractive technology for the initial processing of biomass as it is robust and can handle a wide range of feedstocks (Dermibas 2009). This process typically operates in a temperature range of 1,000° C – 1,400° C to convert biomass into syngas. As syngas is a multifunctional intermediate for the production of various value-added products as well as power and heat, syngas-based integrated biorefinery is proposed.

In order to optimise the production of syngas for production in an integrated biorefinery, a systematic synthesis technique is needed. In this work, a multiple-cascade automated targeting approach is presented to optimise the operating condition of a gasifier and optimum allocation of syngas for downstream processes. Based on the proposed approach, maximum economic potential of a syngas-based integrated biorefinery can be determined. In addition, minimum external heat input requirement to attain optimum gasification temperature is determined. Besides, optimum allocation of raw material to produce syngas that fulfil the requirement of downstream processes, based on the H_2/CO ratio of syngas, can also be determined, prior detail design.

Please cite this article as: Tay D.H.S. and Ng D.K.S., 2011, Automated targeting for synthesis of an syngas-based integrated biorefinery, Chemical Engineering Transactions, 25, 189-194
DOI: 10.3303/CET1125032

2. Multiple-cascade Automated Targeting

Recently, Ng (2010) extended the use of automated targeting for the synthesis of an integrated biorefinery. As reactions are involved in gasification process and with syngas specification measured in term of H_2/CO ratio, the previous work is not directly applicable in synthesis of a syngas-based integrated biorefinery. In order to overcome the limitations of previous work, a generic multiple-cascade approach is developed in this work. The problem of synthesizing syngas-based integrated biorefinery may be formally stated as follows. A set of biomass sources i, SRB_i can be converted to syngas p (INTER_p). Each source i has given a flowrate of $F_{\text{SRB}i}$ and is characterised based on the quality of the stream (e.g., specific heat content, oxygen content, etc.). A set of gasifier sinks SKG_j, which represents the different operating parameters of a gasifier, to convert sources i into syngas p is specified. Each sink is characterised by the predefined quality. The addition of reactants/oxidants r, SRR_r to facilitate the gasification process is also taken into consideration. Based on the gasification models (e.g., Mountouris et al., 2008; Tay et al. 2010, etc.), the syngas p composition produced from SKG_j can be determined.

To allow syngas p to be further processed into the final products p', a set of process sinks j', $\text{SK}_{j'}$ is specified. Each sink j' is characterised by the minimum requirement of H_2/CO ratio. To standardise the quality measurement of sink j' and syngas p, syngas p is also characterised based on H_2/CO ratio which can be computed based on its syngas composition. Meanwhile, the process conversion factors ($X_{j'p'}$) of syngas p to final product, $\text{PROD}p'$ via $\text{SK}_{j'}$ is also specified. Since $X_{j'p'}$ is always given in term of CO conversion, therefore, CO flowrate is used as the quality measurement of syngas p. Besides, external syngas source from steam methane reformer, SMR (F^{SMR}) can be supplied into integrated biorefinery to improve the quality of the syngas from biomass gasification. As abovementioned problem can be divided into two sub-problems, two sets of cascade will be utilised in this work.

The objective of this work is to locate the maximum economic potential (EP) of a syngas-based integrated biorefinery, which indirectly determines the minimum requirement of external heat input, H^{heat} and F^{SMR}, optimum gasification operation and syngas network that that fulfil the requirement of downstream processes.

To address the abovementioned problem the sources/sinks is first arranged in descending sequence, with the highest quality on top of the cascades (k = 1). In the first set of cascade, the specific heat content is used as the quality measurement, thus, the biomass sources (SRB_i), gasifier sinks (SKG_j), additional reactants r required for the gasification process (SRR_r) at various temperature are arranged in a descending order based on the specific heat content. The net material flow cascade from the earlier level k – 1 (δ^{I}_{k-1}) with the flow balance at level k forms the net material flowrate (δ^{I}_k) as followed:

$$\delta^{\text{I}}_k = \delta^{\text{I}}_{k-1} + (\Sigma_i F_{\text{SRB}i} + \Sigma_r F_{\text{SRR}r} - \Sigma_j F_{\text{SKG}j})_k \quad (1)$$

As there is no additional supply of resource (biomass) from the final level (k = n), a constraint (Equation 2) is added.

$$\delta^{\text{I}}_k = 0 \quad (2)$$

The corresponding heat load cascading is performed next to determine the minimum amount of external heat required to be supplied. Within each interval, the heat load is given by the product of the net material flow from level k (δ^{I}_{k}) and the difference between two adjacent levels ($H_k - H_{k+1}$). As in the material flow cascade, the residual heat load of each level k ($\varepsilon 1_k$) is cascaded down to the next level. Thus, the heat load balance at the k-th level can be determined by Equation 3.

$$\varepsilon^{I}_{k} = \varepsilon^{I}_{k-1} + \delta^{I}_{k}(H_k - H_{k+1}) \tag{3}$$

where ε^{I}_{k-1} is the residue heat load that is cascaded from level $k - 1$.

As external heat (H^{heat}) is allowed to be supplied into the gasifier attained the desired gasification temperature, the first level of the heat cascading at $k = 1$, ε^{I}_{1} is expressed as followed:

$$\varepsilon^{I}_{1} = H^{\text{heat}} \tag{4}$$

Note that residual heat load, ε must take a positive value, to ensure that a feasible source-sinks allocation solution (Ng, 2010). Thus, Equation 5 is included as a constraint in the formulation of the model.

$$\varepsilon^{I}_{1} \geq 0 \tag{5}$$

In case where the residual heat load is determined to be zero at level k ($\varepsilon^{I}_{k} = 0$), a pinch point occurs. Following the "golden rule" of pinch analysis, the targeted heat load is supplied to the sinks above the pinch point with the available sources (Ng, 2010). Therefore, if pinch point is located at the last level ($\varepsilon^{I}_{n} = 0$), all sinks are to be supplied with external heat sources.

In the second set of cascade for the conversion of syngas p to final products p', H_2/CO ratio and CO molar flow are used as quality and quantity measurements respectively. Note that the previous set of cascades is measured in mass flowrate, while, the intermediate cascade is measured in molar flowrate, Equation 6 is included in model to conversion mass flow to molar flow.

$$F_{\text{SRS}p} = \Sigma_j (F_{\text{SKG}j} X_{jp}) \qquad \forall p \tag{6}$$

where $F_{\text{SRS}p}$ is the corresponding syngas flowrate (in term of CO molar flowrate) produced from gasifier sink j and X_{jp} is the mass to molar conversion factor.

Following the same principle, the material cascade of syngas p is arranged in descending order based on the H_2/CO ratio. The CO flow cascade is performed based on equation below:

$$\delta^{II}_{k} = \delta^{II}_{k-1} + (\Sigma_i F_{\text{SRS}p} - \Sigma_j F_{\text{SKP}j'})_k \tag{7}$$

where $F_{\text{SKP}j'}$ are the flowrate of various process sinks that convert syngas into value added products p'.

In order to ensure the H_2/CO ratio of process sinks, j' is fulfilled, H_2 load cascading is performed next. Within each interval, the H_2 load is given by the product of the net CO flowrate from level k ($\varepsilon^{II}{}_k$) and the difference between the two adjacent levels (R_k and R_{k+1}).

$$\varepsilon^{II}{}_k = \varepsilon^{II}{}_{k-1} + \delta^{II}{}_k (R_k - R_{k+1}) \tag{8}$$

In addition, Equations 9 and 10 are also included to ensure no additional CO and H_2 are generated from the last level n.

$$\delta^{II}{}_n = 0 \tag{9}$$
$$\varepsilon^{II}{}_n = 0 \tag{10}$$

The syngas, $\text{SKP}_{j'}$ which meets the minimum syngas requirement of processes j' is to be further converted to value added products, PRODp'. Based on the given CO molar conversion factor ($X_{j'p'}$), $F_{\text{PROD}p'}$ is expressed as below:

$$F_{\text{PROD}p'} = \Sigma_{j'}(F_{\text{SKP}j'} \cdot X_{j'p'}) \quad \forall p \tag{11}$$

To target the maximum economic potential (EP) of a syngas-based integrated biorefinery, Equation 12 is maximised and set as the optimisation objective.

$$\text{EP} = \Sigma_p(\text{P}_p \cdot F_{\text{PROD}p'}) - [\Sigma_i(\text{C}_{\text{SRB}i} F_{\text{SRB}i}) + \Sigma_r(\text{C}_{\text{SRR}r} \cdot F_{\text{SRR}r}) + \text{C}^{\text{SRM}} F^{\text{SMR}} + \text{C}^{\text{heat}} H^{\text{heat}}] \tag{12}$$

where $\text{P}_{p'}$ is the selling price of product p'; $\text{C}_{\text{SRB}i}$, $\text{C}_{\text{SRR}r}$, C^{SMR} and C^{heat} are the cost of biomasses *i,* reactants *r*, syngas from SMR and external heat source respectively.

3. Case Study

Large quantity of oil palm waste, known as Empty Fruit Bunches (EFB) is produced in the palm oil industry. Thus, a syngas-based integrated biorefinery that utilise EFB as feedstock is proposed. Based on the model, the optimum gasification temperature, amount of external heat required, the minimum amount of syngas required from SMR and the optimum product portfolio can be determined. The syngas composition and its corresponding specific heat content from oxygen gasification of EFB are determined and tabulated in Tables 1 – 2 (Tay et al., 2010).

Table 1 Physical Properties of EFB (Tay et al. 2010)

Biomass	**C**	**H**	**O**	**Moisture Content (%wt)**	**Specific Heat Content** (MJ/kg)	**MW**	**SRB$_i$**	**Price** (US$/kg)
EFB	1	0.97	0.584	9.5%	-5.1615	24.834	SRB$_1$	0.004

Table 2 Composition of syngas produced from per kmol of EFB and its properties (Tay et al. 2010)

T (K)	SKG_j	H_2	CO	CO_2	H_2O	CH_4	H_2/CO ($R_{j'}$)	Specific Heat Content	CO (mol/kg biomass)	SKS_p
		(kmol / kmol EFB)						$\frac{MJ}{kg\ syngas}\ \frac{kg\ syngas}{kg\ biomass}$		
1500	SKG_1	0.623	0.999	0.000	0.001	0.001	0.624	-1.9758	0.04023	SRS_1
1400	SKG_2	0.622	0.998	0.001	0.001	0.001	0.623	-2.2126	0.04018	SRS_2
1300	SKG_3	0.618	0.995	0.003	0.004	0.002	0.621	-2.4743	0.04006	SRS_3
1200	SKG_4	0.608	0.985	0.012	0.010	0.004	0.617	-2.8384	0.03966	SRS_4

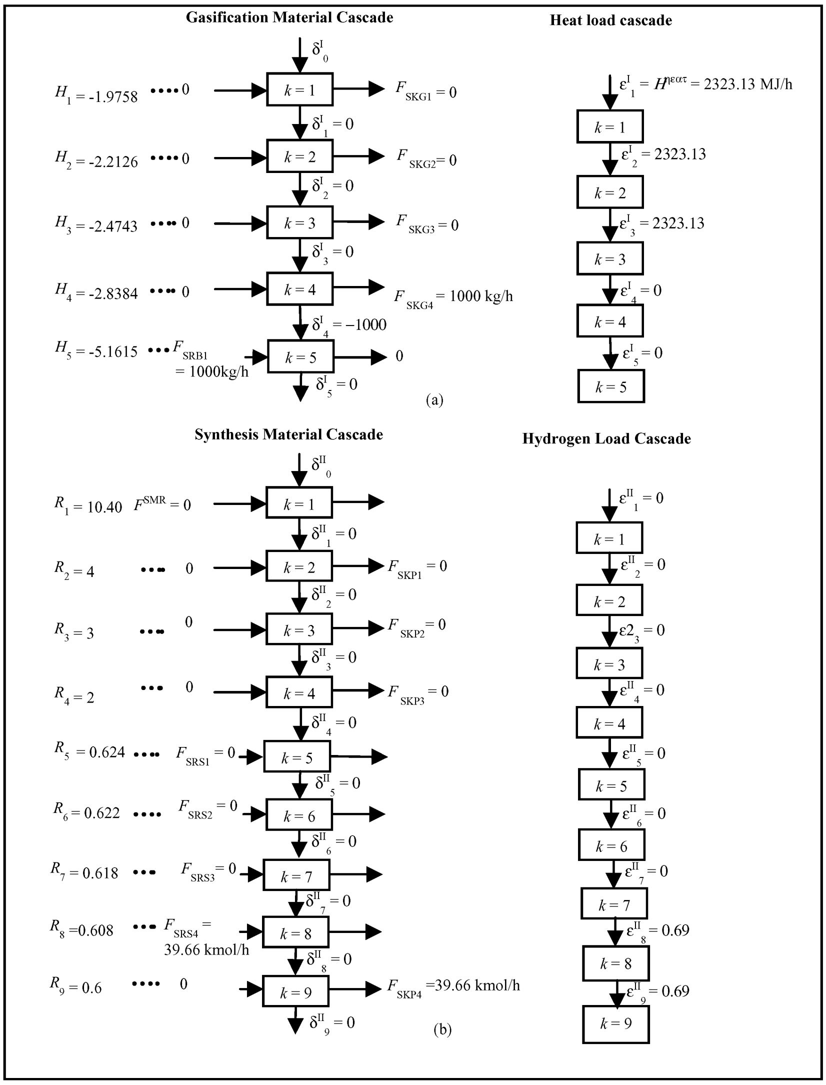

Figure 1 Generic BCD for (a) EFB Gasification (b) Syngas Synthesis

Table 3 Syngas requirement for synthesis processes and produce/utilities/raw materials specifications

Processes	**Process sinks** ($SKP_{j'}$)	**Min H_2/CO** ($R_{j'}$)	**CO molar Conversion**	**Product** ($PROD_{p'}$)	**Product Price** ($P_{p'}$, US$)
Mix-alcohol synthesis	SKP_1	4	0.30	$PROD_1$	0.62/kg
Methanol Synthesis	SKP_2	3	0.99	$PROD_2$	0.10/kg
Dimethyl-Ether synthesis	SKP_3	2	0.90	$PROD_3$	0.39/kg
Fischer Tropsch Synthesis	SKP_4	0.6	0.80	$PROD_4$	0.51/kg
Syngas from SMR	SRR_{ext}	10.40	-	-	102/kg
Electricity	H^{heat}	-	-	-	0.017/MJ

Solving the proposed the model (Equations 1-11) with the objective function to maximise Equation 12 yields the result in Figure 1. As shown in Figure 1, the minimum amount of heat required (H^{heat}) for the gasification process is located at 2323.13 MJ/h. Note that no syngas from SMR is required ($F^{SMR} = 0$). Based on the conversion factor in Table 3, the FT-crude is selected as the final product at a production rate of 448.70kg/h (assuming CO conversion of 0.80 and average C_7 FT-crude with MW of 99). Based on the optimised result, the maximum EP is targeted at US$ 185.46/h with EFB feed rate of 1000kg/h.

4. Conclusion

A multiple-cascade automated targeting approach is presented to locate the optimum economic performance of a syngas-based integrated biorefinery. In this work, the first set of cascade is used to target the optimum gasifier operating temperature to produce syngas intermediates from biomass; while, a second set of cascade is used to target the optimum allocation of syngas intermediates to various technologies to produce value added products.

References

Demirbas M.F., 2009, Biorefineries for biofuel upgrading: A critical review, Applied Energy, 86, S151-S161

El-Halwagi M.M. and Manousiothakis V., 1990, Automatic synthesis of mass-exchange networks with single component targets, Chem. Eng. Sci., 9, 2813-2831

Fernando S, Adhikari S, Chandrapal C and Murali N., 2006, Biorefineries: Current status, challenges, and future direction, Energy & Fuels, 20(1), 1727-1737

Mountouris A., Voutsas E. and Tassios D., 2008, Plasma gasification of sewage sludge: Process development and energy optimization, Energy Conversion and Management, 49(8), 2264-2271

Ng D.K.S., 2010, Automated targeting for the synthesis of an integrated biorefinery, Chem. Eng. J., 162(1), 67–74

Tay D.H.S., Kheireddine H., Ng D.K.S and El-Halwagi M.M., 2010, Synthesis of an integrated biorefinery via the biomass gasification thermodynamic equilibrium optimization model, 13th Asia Pacific Confederation of Chemical Engineering Congress - APCChE 2010, Taipei, Taiwan, Oral Session 6 [10216]