Process Simulation and Scheduling of Bio-succinic Acid Production from Palm Biomass

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Abstract This chapter describes process modelling of bio-succinic acid production from palm biomass. Batch scheduling is carried out to determine the time bottleneck of the process, i.e. equipment that limits the annual production due to its long cycle time. In this case, the fermenter is identified as the time bottleneck, as it has the longest cycle time. Therefore, debottlenecking strategy is applied where additional fermenters are added to reduce the cycle time. Doing so leads to increased batches and annual production of the bio-succinic acid. With deployment of five fermenters, an increase of 340% of bio-succinic acid was resulted, as compared to that of the base case process.

Keywords Process simulation · Process scheduling · Palm biomass · Succinic acid · SuperPro designer · Debottlenecking

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1 Introduction

With the increasing consciousness on environmental impact of the fossil-based petrochemical industries, research on biochemical production was emerging in recent years. The US Department of Energy (US DOE) listed 12 chemical building blocks which have the potential to be commercially produced through biological pathway (Werpy & Peterson, 2004). In this regard, succinic acid appeared to be among the top rank in the list. Succinic acid is also known as amber acid or butanedioic acid, which is a dicarboxylic acid with molecular formula of $C_4H_6O_4$. Such acid is an intermediate in the tricarboxylic acid cycle produced during aerobic metabolism, and an end product of anaerobic metabolism (Tan et al., 2014). This chemical can be produced via various strict and facultative anaerobic microorganisms and used as a precursor in many industries, such as pharmaceutical, food, agriculture, polymer, cosmetic and textile industries. In the pharmaceutical industries, for instance, succinic acid is used in the preparation of active calcium succinate, active pharmaceutical ingredients, vitamin A, anti-inflammatory-erthyrodiol derivates, sedative, antipasmer, etc. Succinic acid is utilized in a polyester synthesis and acts as an intermediate in the manufacturing of plasticizer, resins, biodegradable solvents, engineering plastics, surfactants, detergents, etc. The major market potential of succinic acid lies as a precursor for the production of other chemicals (Allied Market Research, 2020).

Compared to the fossil-based succinic acid production, bio-succinic acid production is a benign environmental route (Xu et al., 2021). The usability of renewable raw materials and its carbon dioxide (CO_2) fixation are the major advantages of bio-succinic acid production. Apart from being carbon neutral, it requires 30–40% lower energy consumption as compared to conventional fossil-based succinic acid. These factors have led to the commercialization of bio-based succinic acid in recent years (Kuenz et al., 2020). In fact, production of bio-succinic acid could serve as a downstream process for CO_2-producing biofuel industries such as bio-methane, bio-ethanol and bio-hydrogen plants as it could absorb CO_2 in the process, reducing CO_2 concentration while purifying the biogas in the process. (Tan et al., 2018).

In this chapter, a commercial process simulation tool, i.e. SuperPro Designer (SPD) v12 (www.intelligen.com) is used to model a newly developed bio-succinic acid production process from palm biomass, i.e. oil palm frond (OPF) that is collected from the oil palm plantation. The process was developed based on laboratory-scale experimental work (Luthfi et al., 2016).

2 Process Simulation

Figure 1 shows the simulation flowsheet developed in SPD for a bio-succinic acid production process. The process is operated in batch mode, with an annual operating time of 7920 h. The feed stream of the process consisted of 1000 kg of OPF. Note that OPF is a lignocellulose material, and is modelled as a stock mixture in SPD.

The properties of OPF are given in Table 1, obtained from OPF sample taken from the oil palm estate of Universiti Kebangsaan Malaysia, located at Bangi, Selangor, Malaysia (Tan et al., 2017).

As shown in Fig. 1, the OPF is sent to the ball mill where its juice is pressed from the fresh OPF, before being sent for centrifugation. Apart from juice removal, the ball mill also serves as physical treatment that enlarges the surface area of the bagasse, so to allow more effective pretreatment at later stage. The OPF juice from the centrifuge is transferred to the fermenter, while the separated bagasse from ball mill and centrifuge are sent to the Pretreatment Section. This follows the same process as reported by Luthfi et al. (2017).

In the Pretreatment Section, the OPF bagasse is first treated with sodium hydroxide (NaOH) of 4 wt%; the latter disrupts the crystalline structure of the lignocellulosic bagasse, so to recover its fermentable sugars. The liquid effluent from the pretreatment unit is then cooled to 40 °C before it is sent to a rotary siever. The latter removes the black liquor, which consists of hydrolyzed xylan and lignin. Effluent from the rotary siever is transferred into the enzymatic reactor. In the enzymatic reactor, hydrochloric acid (HCl) is first used to neutralize the NaOH content, while enzyme (consisting of cellulase and xylanase) is later used to break down the structural carbohydrate of pretreated bagasse into fermentable sugars (Luthfi et al., 2019). The hydrolysate from the enzymatic reactor is then sent for membrane filtration to remove all suspended solids. The filtrate (OPF sugar) is sent to the fermenter.

In the fermenter, OPF juice (extracted in ball mill) and OPF sugar (from pretreatment section) are first transferred in from their operations. Mineral mixture (consisting 50 wt% of potassium dihydrogen phosphate (KH_2PO_4) and sodium chloride) are next added into the fermenter (Tan et al., 2016), which is then followed by sterilization-in-place (SIP). The SIP ensures no other microbe presence in the fermenter prior to the charging of the necessary microbes, i.e. *Actinobacillus succinogenes*. Fermentation process is next initiated upon the charging of inoculum *Acinobacillus succinonogenes*. Throughout the fermentation process which takes a total duration of 24 h, CO_2 is charged to fermenter, while its temperature is maintained at 37 °C (Luthfi et al., 2018). Upon the completion of fermentation process, product from the fermenter is sent to the Downstream Processing Section.

In the Downstream Processing Section, several processing units are used for the purification of bio-succinic acid. Two units of membrane filtration are used to remove the suspended solids and liquid content from the fermentation broth. The suspended solid are mainly due to microbe and other traces of impurities resulted from enzymatic hydrolysis and OPF juice. Filtrate from the membrane unit is sent to a flash evaporator, where the product is further concentrated in the medium to allow a more efficient crystallization process (Luthfi et al., 2020). Effluent from the evaporator is then mixed with concentrated HCl in order to reduce its pH value, before being sent to the crystallization, where succinic acid solids are formed. Concentrated HCl is used to lower the pH for the optimum succinic acid crystallization. Products from the crystalizer are dried in a drum dryer. The latter removes remaining moisture of the crystals. Dried crystals from the drum dryer are ready for sale. Detailed setting for all units are shown in Table 2.

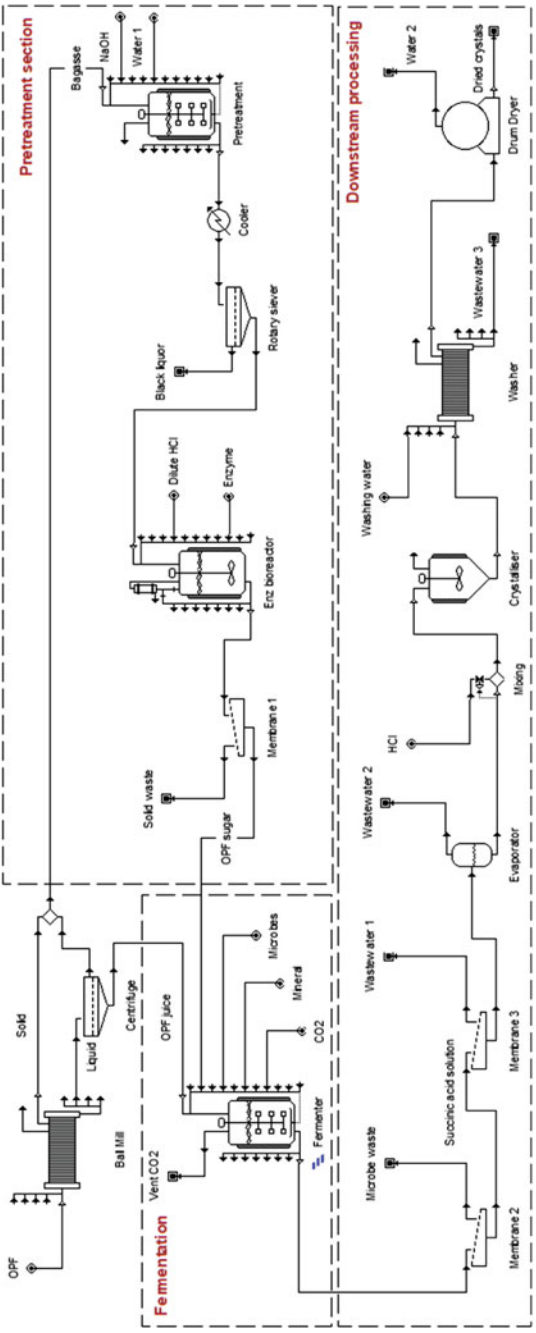

Fig. 1 Simulation flowsheet for bio-succinic acid production in SuperPro Designer (SPD) v12

Table 1 Properties for OPF feed stream

Properties	Value
Pressure	1 bar
Temperature	25 °C
Mass flow	1000 kg
Composition (wt%)	
Ash	2.21
Fructose	0.02
Glucan	29.31
Glucose	1.25
Lignin	15.43
Sucrose	0.09
Water	41.67
Xylan	10.02

3 Process Scheduling

Details of scheduling for each process units, such as duration and start time are given in the last two column of Table 2 (all units are assume to have zero set-up time). The operation Gantt chart of the process is shown in Fig. 2. SPD determines that the overall process has a batch time of 62 h, while its minimum cycle time is identified as 40 h. With the annual operation time of 7920 h, the minimum cycle time determines that the process has a yearly production of 197 batches, which is equivalent to an annual production of 6878 kg of bio-succinic acid products.

4 Options for Debottlenecking

SPD next identifies that the fermenter is the *time bottleneck* of this process (see Fig. 2 for its longest cycle time among all units, i.e. 40 h). To improve the overall annual productivity, the minimum cycle time is to be reduced. One potential solution is to make use of multiple units of fermenter. This may be done using the staggered mode function of SPD. Results of the latter are shown in Table 3. As shown, with five fermenters, the annual production is increased to 30,303 kg/y, i.e. 340% of the base case process. Note however that the use of multiple fermenters will increase the capital expenditure of the process. However, during the course of this process simulation work, economic feasibility study was not carried out due to the lack of process economic data.

Table 2 Important setting and scheduling data for all units (set-up time is assumed as zero)

Processes	Important setting	Duration	Start time
Ball mill	Removal of ash, glucan, lignin, water and xylan (99% removal for all)	4 h	Beginning of the batch
Centrifuge	Removal of ash, glucan, lignin and xylan (100% removal for all)	30 min	After completion of ball mill procedure
Pretreatment	Transfer in bagasse	15 min	After completion of ball mill procedure
	Charge-in NaOH (28.1 kg)	15 min	After completion of previous operation
	Charge-in water (607.7 kg)	1 h	After completion of previous operation
	Agitation	1 h	After completion of previous operation
	Heating (to 98 °C)	1 h	Start with agitation operation
	Transfer-out bagasse	30 min	After completion of previous operation
Cooler	Exit temperature: 40 °C	30 min	Start with transfer-out of Pretreatment procedure
Rotary siever	Split %: ash (30.18), glucan (4.27), NaOH (79.5), water (79.5), xylan (73.3)	1	After completion of cooler procedure
Enzymatic bioreactor	Transfer-in	30 min	After completion of rotary siever procedure
	Charge HCl (3539.3 kg, with 0.0364% HCl and 99.9636% water)	10 min	After completion of previous operation
	Reaction 1 (neutralization), with mass stoichiometry: 36.46 HCl + 40 NaOH → 58.44 NaCl + 18.02 H_20 (100% conversion) Final temperature: 40 °C	20 min	Start with charging of HCl
	Agitation	20 min	Start with Reaction 1
	Charge enzyme (0.18 kg)	5 min	After completion of previous operation
	Heating (final temperature: 40 °C)	6 h	Start with charging of enzyme

(continued)

Table 2 (continued)

Processes	Important setting	Duration	Start time
	Reaction 2 (glucan conversion), with mass stoichiometry: 180.16 glucan → 180.16 glucose (88.4% conversion) Final temperature: 40 °C	6 h	Start with Heating
	Reaction 3 (xylan conversion), with mass stoichiometry: 150.13 xylan → 150.13 xylose (89.93% conversion) Final temperature: 40 °C	6 h	Start with Reaction 2
	Transfer-out	20 min	After completion of previous operation
Membrane 1	Removal of enzyme (99%)	1 h	Start with transfer-out of Enzymatic bioreactor procedure
Fermenter	Transfer-in OPF juice	30 min	After completion of centrifuge procedure
	Transfer-in OPF sugar	1 h	Start with Membrane 1 operation
	Charge mineral (6.27 kg for both KH_2PO_4 and sodium chloride)	10 min	After completion of previous operation
	SIP (100 kg/h m^3)	30 min	After completion of previous operation
	Charge CO_2 (10.87 kg)	24 h	After completion of previous operation
	Charge microbe (0.519 kg)	15 min	Start with charging of CO_2
	Agitate	24 h	Start with charging of microbe
	Reaction (fermentation)	24 h	Start with agitation
	Transfer-out	30 min	After completion of previous operation
Membrane 2	Removal of microbe (99%)	1 h	After fermentation procedure completed
Membrane 3	Removal of NaCl (100%), NaOH (100%) and water (32.26%)	1 h	After Membrane 2 procedure completed
Evaporator	Removal of water (80%), and acetic acid (70%) Temperature: 70 °C	1 h	After Membrane 3 procedure completed
Mixer	Mixing of HCl (input mass ratio of 0.01)	10 min	After completion of Evaporation procedure

(continued)

Table 2 (continued)

Processes	Important setting	Duration	Start time
Crystallizer	Evap. Data: Water in vapor phase (82.18%) Crystal. Data: succinic acid	6 h	Start with Mixing procedure
Washer	Filtration: removal of succinic acid solid (100%) and glucose (0.1%) Loss on drying (LOD): 10%	2 h	After completion of Cyrtalization procedure
	Cake wash	30 min	After completion of previous operation
Drum dryer	Filtration: removal of water (calculated based on final LOD) Final LOD: 1%	6 h	After completion of Washer procedure

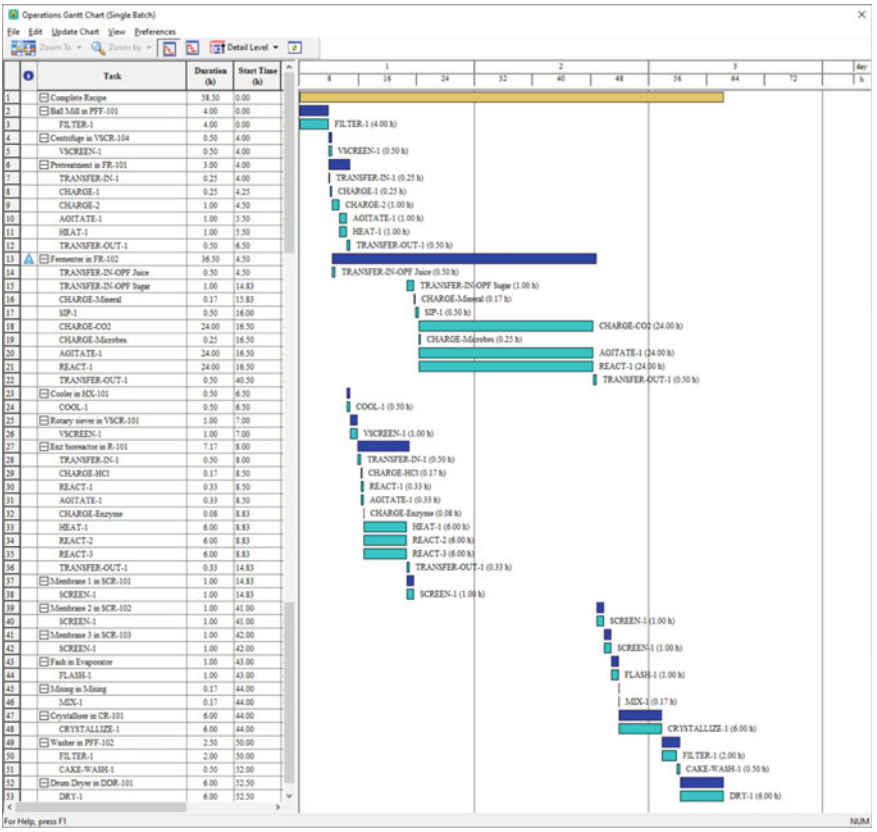

Fig. 2 Operational Gantt chart for bio-succinic acid production

Table 3 Summary of production with different units of fermenters

Numbers of fermenter	Number of annual batches	Annual production (kg/y)
1	97	6878
2	393	13,722
3	590	20,600
4	786	27,444
5	1097	30,303

5 Conclusion

In this chapter, a production process of bio-succinic acid crystal is modelled using SuperPro Designer v12. Scheduling is also performed to identify the time bottleneck of the process, which limits the annual production. The fermenter which has 40 h cycle time is determined as the time bottleneck. More fermenters are hence added to reduce the cycle time, and hence increase the number of batches and annual production of the bio-succinic acid product. Doing this leads to 340% increase of production, as compared to that of the base case process. Detailed economic evaluation should be carried out next in order to identify economic hotspots of the process.

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