Supplementary Information

Biochemical to enable Biorefinery: A case study of polyphenols extraction from Bio-oil for Utilization as Biodiesel Antioxidants

Xiaopeng Shi[a], Haotong Lin[a], Qi Ouyang[a], Guanqun Luo[b], Xianghong Lu[c], jianbing Ji[c] and Kaige Wang[1,*]

[a] State Key Laboratory of Clean Energy Utilization, Zhejiang University, Hangzhou 310027, China

[b] Cryogenic Center, Hangzhou City University, Hangzhou 310015, China

[c] College of Chemical Engineering, Zhejiang University of Technology, Hangzhou 310014, China.

* Corresponding author. Email address: kaigewang@zju.edu.cn

1. Theoretical induction time calculation method

The calculation formula is as follows:

$$IP_n = \frac{C_r \cdot C_a}{C_m} \cdot IP_m \tag{1}$$

$$IP_t = \sum_{i=1}^{n} IP_n \tag{2}$$

In the formula, IP_n represents the theoretical induction time of the *n-th* phenolic compound in the fraction; C_r denotes the relative content of the *n-th* phenolic compound in the fraction; C_a is the addition concentration of the fraction; C_m refers to the addition concentration of the corresponding model compound of the *n-th* phenolic compound, which is 0.1 wt.% in this study; IP_m is the induction time of the *n-th* phenolic model compound; and IP_t represents the total theoretical induction time of the phenolic compounds in the fraction. Here, n=1,2,3.

In addition, based on the addition concentrations of model compounds other than phenolic compounds and their corresponding average reduction in induction time for biodiesel, a functional relationship between the concentration of other compounds in the fraction and the percentage reduction in the fraction's induction time was established. The correlation coefficient was found to be 0.9989. The fitted formula is as follows:

$$y(x) = \frac{\sum_{i=0}^{k} IP_k / IP_0}{k} \cdot 100\% \tag{3}$$

$$Y = a \cdot (X - b)^c \tag{4}$$

In the formula, x represents the addition concentration, which in this study was 0.1 wt.%, 0.2 wt.%, and 0.5 wt.%; y is the percentage reduction in average induction time caused by the other model compounds at the concentration x; IP_k is the induction time of the *k-th* model compound; IP_0 is the induction time of pure biodiesel; k=1，2，3，…; Y is the theoretical percentage reduction in induction time caused by other compounds; X represents the total concentration of other compounds; and a, b, and c are the fitting parameters. a =0.24547 ± 0.0334，b= − 0.0419 ± 0.02473，c= − 0.44249 ± 0.11945.

To comprehensively consider the impact of phenolic compounds and other compounds on the antioxidant properties of the distillate, the total theoretical induction time of the distillate can be calculated using the following equation(IP_T) ：

$$IP_T = IP_t \cdot Y \tag{5}$$

2. Process flow for graded utilization of bio-oil

The bio-oil is transferred from biorefinery to the distillation tower (D1), with no chemical reactions involved in the process. Under atmospheric pressure, the bio-oil is heated from room temperature to 110 °C in D1 for dehydration. The water vapor is cooled and transferred to the wastewater treatment unit (W1), while the remaining distillation fractions are cooled and transferred to the next-stage distillation tower (D2). The dehydrated bio-oil is distilled under a pressure of approximately 1 kPa to separate the 110 ~ 250 °C (after reaction, the biodiesel precursor) and 250 ~ 300 °C fractions, while the heavy fraction above 300 °C is designated as the bio-bitumen additive. All products are cooled by the cooling system (C1 ~ 5), with the biodiesel precursor and bio-bitumen additive sent to the storage system. At room temperature, the 250 ~ 300 °C fraction is sequentially extracted with 15 wt.% NaOH solution, 15 wt.% hydrochloric acid solution, and dichloromethane solvent in a mass ratio of 1:2. The extracted components are transferred to the solvent distillation recovery system (D4), while the remaining extraction components are sent to the acid-base solution recovery system (ARS). The sodium hydroxide and hydrochloric acid in the extraction process neutralize to produce sodium chloride, which is recovered through an electrolytic process for reuse of sodium hydroxide and hydrochloric acid. The wastewater generated during the process is transferred to WT. The extraction components are then separated from the dichloromethane solvent by vacuum distillation at 40°C to obtain bio-antioxygen, which is used as a biodiesel antioxidant, and is sent to the storage system. The dichloromethane solvent is recovered and reused. Wastewater generated from distillation, extraction, acid-base/solvent recovery, and other processes is treated biologically and recycled.

The specific technical parameters of this project were as follows: dehydration rate was 10%, dichloromethane recovery rate was 99.8%, sodium hydroxide recovery rate was 90%, hydrochloric acid recovery rate was 90%, wastewater recovery rate was 95%, extraction efficiency was 95%, biodiesel yield was 30%, bio-antioxygen yield was 19%, and bio-bitumen additive yield was 32%.

Tab. S1. Oxidation induction period of other model compounds

Chemical	Addition concentration		
	0.1 wt.%	0.2 wt.%	0.5 wt.%
Acetic acid	0.03	0.02	0.01
2- Acetylfuran	0.68	/	/
Cyclopentanone	0.43	0.43	0.23
5- Hydroxy -2- pentanone	0.62	/	/
Furfural	0.38	0.30	0.28
Furfuryl alcohol	0.62	/	/
Methyl-phenoxide	0.57	0.45	0.25

Tab. S2. Technical indictors

Technical indictors	Parameters
Dehydration rate	10%
Dichloromethane recovery rate	99.8% [1]
Sodium hydroxide recovery rate	90%
Hydrochloric acid recovery rate	90%
Wastewater recovery rate	95% [2]
Extraction efficiency	95%
Biodiesel precursor yield	30%
Bio-antioxygen yield	19%
Bio-bitumen additive yield	32%

Tab. S3. The equipment acquisition costs (base year: 2019)

Equipment	Converted costs ($)
Distillation unit [3]	798159.34
Cooling unit [4]	729972.53
Extraction unit [1]	664601.65
Solvent distillation recovery unit [1]	135741.76
Acid-base recovery unit [5]	1252005.49
Wastewater treatment unit [6]	1112239.01
Storage unit [7]	13131.87
Total	4705837.91

Tab. S4. The project investment cost calculation factors and results

	Calculation factors	Cost ($)
Total installation and equipment purchase cost. (TIEC)	**302% TPEC**	14211634.62
Total Purchased Equipment Cost (TPEC)	**100% TPEC**	4705837.91
Equipment installation	39% TPEC	1835274.73
Instruments and Control	26% TPEC	471002.75
Piping	10% TPEC	1223516.48
Electronic Systems	31% TPEC	1458804.95
Warehouse	29% TPEC	1364697.80
Site Development	12% TPEC	564697.80
Service Facilities	55% TPEC	2588214.29
Total Indirect Costs (TIC)	**89% TPEC**	4188200.55
Engineering	32% TPEC	1505865.38
Construction	34% TPEC	1599986.26
Legal and Contractor Costs	23% TPEC	1082348.90
Total Direct and Indirect Costs (TDIC)	**TIEC+TIC**	18399835.16
Contingency	20% TDIC	3679972.53
Fixed Capital Investment (FCI)	**TIEC+TIC+Contingency**	22079793.96
Working Capital (WC)	15% FCI	3311964.29
Land Use (LU)	6% TPEC	282348.90
Total Project Investment (TPI)	**FCI+WC+LU**	25674107.14

The equipment installation required a significant amount of materials and labor, including concrete and steel for support structures, electrical wiring, cables, pipelines, and valves. These factors contributed to the equipment installation costs, which could be estimated by applying a certain proportion factor (i.e., installation factor) to the equipment purchase cost. This led to the calculation of direct costs, which was the sum of the equipment purchase cost and the equipment installation cost. Indirect costs were expenses related to the construction of facilities, which were not characterized by equipment or materials. These included project costs, construction costs, legal and contractor fees. Construction costs represented labor-related benefits, such as retirement

benefits, workers' compensation, unemployment insurance, machinery rental, and cleanup costs after project completion. Contingency costs were additional expenses caused by project delays due to weather, construction errors, or inaccurate cost estimates. Working capital (WC) and land acquisition costs (LU) represented the project's operational cash flow and the cost of land acquisition for building facilities, respectively. Both were non-depreciable costs and did not lose value with usage. Working capital ensured the normal operation of the project, covering prepayments for raw material purchases, utility costs, labor wages, and supplies for ongoing operations. Working capital remained tied up throughout the project's lifespan and was recovered in monetary form after the project was completed.

Tab. S5. Project Operating Cost Calculation Basis and Results

	Calculation Basis	Cost ($ per year)
Equipment Capacity Factor f_0	96%	
Raw Material Cost		2449725.27
Bio-oil	54.95 $/t	2310439.56
99% Sodium Hydroxide	412.09 $/t	99766.48
36% Hydrochloric Acid	41.21 $/t	25041.21
Dichloromethane	453.30 $/t	14491.76
Water	0.70 $/t	58914.84
Electricity	0.0834 $/kWh	1754203.30
Operational Labor	Estimated based on scale [7]	296703.30
Managerial Labor	20% Operational labor	89010.99
Maintenance and Repair	5% FCI	1103983.52
Operational Loss	15% Maintenance and repair costs	165604.40
Research Cost	15% Labor costs	57857.14
Variable Costs (VC)		5976002.75
Employee Benefits, Social Security Tax, Unemployment Insurance, etc.	65% Labor and maintenance costs	968310.44
Local Taxes	1.5% FCI	331195.05
Insurance	1% FCI	220796.70
Fixed Costs (FC)		1520329.67
Project Loan	Self-financed	
Annual Total Operating Cost	**DC+FC+CC**	7496304.95

Operating costs were calculated based on Fixed Capital Investment (FCI). Variable Costs (VC) included raw material costs, labor costs, water and electricity costs, and maintenance and repair costs. The unit prices for raw materials were referenced from various sales websites, and water and electricity prices were based on the relevant department's charging standards. Labor costs were estimated based on the actual scale of operations, with 30 operational workers, each

earning $824.18 per month, and 20% of the operational workforce (6 people) assigned to management, earning $1,236.26 per month. Fixed Costs (FC) consisted of employee benefits, local taxes, insurance, and other related expenses.

Tab.S6. Discounted Cash Flow Analysis Factors

Factors	Set Value
Factory lifetime	20 years
Annual operating time	8410 hours
Equity financing	100% (Self-financed)
Construction period	3 years
Year 1: Project preparation	8% FCI
Year 2: Engineering construction, etc.	60% FCI
Year 3: Process equipment installation, etc.	32% FCI
Start-up period	6 months
Revenue	50%
Variable operating costs	75%
Fixed operating costs	100%
Depreciation rate	Double Declining Balance Method (200%DB)
Depreciation period	7 years
Benchmark discount rate i_0	10%
Income tax rate	25%
Biodiesel price	54.95 $/t
Bio-bitumen price	412.09 $/t

The double declining balance method was used to calculate the depreciation of fixed assets, with a depreciation period (payback period) of 7 years. This method provided the shortest payback period and the maximum tax deduction [7]。The calculation formula was as follows:

$$Annual\ depreciation\ rate = \frac{2}{Depreciation\ period} \times 100\% \quad (6)$$

$$\begin{cases} Depreciation\ expense\ for\ the\ current\ year \\ = Depreciation\ balance\ from\ the\ previous\ year \times Annual\ depreciation\ rate \\ Depreciation\ balance\ for\ the\ current\ year \\ = Depreciation\ balance\ from\ the\ previous\ year - Depreciation\ expense\ for\ the\ current\ year \end{cases} \quad (8)$$

The net present value (NPV) was the difference between the future cash flows generated by the project investment, discounted at the benchmark discount rate, and the investment costs：

$$NPV = \sum_{t=0}^{n} (CI_t - CO_t)\,(1 + i_0)^{-t} = \sum_{t=0}^{n} CF_t\,(1 + i_0)^{-t} \quad (9)$$

In the equation, CI_t represented the cash inflow in year t; CO_t represented the cash outflow in year t; i_0 was the benchmark discount rate; CF_t was the net cash flow in year t; and n denoted the project lifespan in years.

Tab.S7. Discounted Cash Flow Analysis ($)

Years	-2	-1	0	1	2	3
Fixed Assets	1766383.53	13247876.48	7065534.12			
Land Acquisition	282350.31					
Working Capital			3311969.12			
Total Investment Cost	2048733.84	13247876.48	10377503.24			
Main Product Sales Revenue						
By-product Sales Revenue				4678640.11	6238186.81	6238186.81
Total Sales Revenue				11108044.04	14810725.38	14810725.38
Variable Operating Costs				5229006.84	5976007.81	5976007.81
Fixed Operating Costs				1520302.45	1520302.45	1520302.45
Total Operating Costs				6749309.28	7496310.26	7496310.26
Depreciation Expense				6308512.61	4506080.43	3218628.88
Depreciation Balance				15771281.52	11265201.09	8046572.20
Net Income [a]	-2048733.84	-13247876.48	-10377503.24	-1949777.85	2808334.69	4095786.24
Preliminary Losses	0.00	2048733.84	15296610.32	25674113.56	27623891.41	24815556.72
Taxable Income	-2048733.84	-15296610.32	-25674113.56	-27623891.41	-24815556.72	-20719770.48
Tax Payable						
Annual Cash Inflow [b]	-2048733.84	-13247876.48	-10377503.24	4358734.75	7314415.12	7314415.12
Discount Factor [c]	1.21	1.10	1.00	0.91	0.83	0.75
Annual Net Present Value [d]	-2478967.95	-14572664.13	-10377503.24	3962486.14	6044971.18	5495428.34

Tab.S7. Discounted Cash Flow Analysis ($)

Years	4	5	6	7	8	9
Fixed Assets						
Land Acquisition						
Working Capital						
Total Investment Cost						
Main Product Sales Revenue	8572538.57	8572538.57	8572538.57	8572538.57	8572538.57	8572538.57
By-product Sales Revenue	6238186.81	6238186.81	6238186.81	6238186.81	6238186.81	6238186.81
Total Sales Revenue	14810725.38	14810725.38	14810725.38	14810725.38	14810725.38	14810725.38
Variable Operating Costs	5976007.81	5976007.81	5976007.81	5976007.81	5976007.81	5976007.81
Fixed Operating Costs	1520302.45	1520302.45	1520302.45	1520302.45	1520302.45	1520302.45
Total Operating Costs	7496310.26	7496310.26	7496310.26	7496310.26	7496310.26	7496310.26
Depreciation Expense	2299020.63	1642157.59	1172969.71	837835.51		
Depreciation Balance	5747551.57	4105393.98	2932424.27	2094588.77		
Net Income [a]	5015394.49	5672257.53	6141445.41	6476579.62	7314415.12	7314415.12
Preliminary Losses	20719770.48	15704375.99	10032118.46	3890673.04		
Taxable Income	-15704375.98	-10032118.45	-3890673.04	2585906.57	7314415.12	7314415.12
Tax Payable				646476.64	1828603.78	1828603.78
Annual Cash Inflow [b]	7314415.12	7314415.12	7314415.12	6667938.48	5485811.34	5485811.34
Discount Factor [c]	0.68	0.62	0.56	0.51	0.47	0.42
Annual Net Present Value [d]	4995843.95	4541676.32	4128796.65	3421706.76	2559171.48	2326519.52

Tab.S7. Discounted Cash Flow Analysis ($)

Years	10	11	12	13	14	15
Fixed Assets						
Land Acquisition						
Working Capital						
Total Investment Cost						
Main Product Sales Revenue	8572538.57	8572538.57	8572538.57	8572538.57	8572538.57	8572538.57
By-product Sales Revenue	6238186.81	6238186.81	6238186.81	6238186.81	6238186.81	6238186.81
Total Sales Revenue	14810725.38	14810725.38	14810725.38	14810725.38	14810725.38	14810725.38
Variable Operating Costs	5976007.81	5976007.81	5976007.81	5976007.81	5976007.81	5976007.81
Fixed Operating Costs	1520302.45	1520302.45	1520302.45	1520302.45	1520302.45	1520302.45
Total Operating Costs	7496310.26	7496310.26	7496310.26	7496310.26	7496310.26	7496310.26
Depreciation Expense						
Depreciation Balance						
Net Income [a]	7314415.12	7314415.12	7314415.12	7314415.12	7314415.12	7314415.12
Preliminary Losses						
Taxable Income	7314415.12	7314415.12	7314415.12	7314415.12	7314415.12	7314415.12
Tax Payable	1828603.78	1828603.78	1828603.78	1828603.78	1828603.78	1828603.78
Annual Cash Inflow [b]	5485811.34	5485811.34	5485811.34	5485811.34	5485811.34	5485811.34
Discount Factor [c]	0.39	0.35	0.32	0.29	0.26	0.24
Annual Net Present Value [d]	2115017.75	1922743.41	1747948.55	1589044.14	1444585.58	1313259.62

Tab.S7. Discounted Cash Flow Analysis ($)

Years	16	17	18	19	20
Fixed Assets					
Land Acquisition					-282350.31
Working Capital					-3311969.12
Total Investment Cost					-3594319.43
Main Product Sales Revenue	8572538.57	8572538.57	8572538.57	8572538.57	8572538.57
By-product Sales Revenue	6238186.81	6238186.81	6238186.81	6238186.81	6238186.81
Total Sales Revenue	14810725.38	14810725.38	14810725.38	14810725.38	14810725.38
Variable Operating Costs	5976007.81	5976007.81	5976007.81	5976007.81	5976007.81
Fixed Operating Costs	1520302.45	1520302.45	1520302.45	1520302.45	1520302.45
Total Operating Costs	7496310.26	7496310.26	7496310.26	7496310.26	7496310.26
Depreciation Expense					
Depreciation Balance					
Net Income [a]	7314415.12	7314415.12	7314415.12	7314415.12	10908734.55
Preliminary Losses					
Taxable Income	7314415.12	7314415.12	7314415.12	7314415.12	10908734.55
Tax Payable	1828603.78	1828603.78	1828603.78	1828603.78	2727183.64
Annual Cash Inflow [b]	5485811.34	5485811.34	5485811.34	5485811.34	8181550.91
Discount Factor [c]	0.22	0.20	0.18	0.16	0.15
Annual Net Present Value [d]	1193872.38	1085338.53	986671.39	896973.99	1216135.41

[a]：Net Income = Total Sales − Total Costs − Depreciation；

[b]：Annual Cash Inflow = Total Sales − Total Costs − Tax Amount；

[c]：*Discount Factor*$=（1+i_0）^{-t}$，i_0 is the base discount rate, t is the year；

[d]：Annual Net Present Value = Annual Cash Inflow × Discount Factor

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