

ICE Corporation
Business Development

TO: Y. Roman and T. Kinney
FROM: Akorfa Dagadu, Eliana Shin, Lucy Kanas
SUBJECT: Preliminary Design for Terephthalic Acid Process

This report presents the preliminary process design, safety evaluation and economic assessment for the proposed PET recycling glycolysis process for BHET production. We evaluate the technical feasibility, safety, environmental impact, and economic viability for integrating this recycling process into ICE Corporation's operations.

With Aspen Plus simulation, the process demonstrates a stable operation that achieves the target BHET yield of 60,000 tonnes with a high purity of 99.6%. Effective phase separation, controlled recycling of ethylene glycol (EG) and temperature-pressure control strategies support these operations. By incorporating closed-loop EG recovery, fresh solvent demand and wastewater generation significantly decrease. The report systematically identifies key safety risks associated with reactor overheating, pressure relief, dust and purging through a preliminary hazard analysis (PHA) which outlines appropriate safeguards and recommendations for a safe startup and operation.

From an economic standpoint, the process demonstrates strong performance, with a net present value of \$106 million and an internal rate return of 49%, exceeding the minimum required investment return of 12.5%. With an initial capital investment of \$105.5 million and annual operating and material costs of \$85.7 million in subsequent years, producing 60,000 tonnes of BHET annually yields a gross profit per year of \$33.3 million and a weighted average cost of capital of \$25.7 million. Additionally, the safety profile includes resolvable data gaps, reduced environmental impact with recycling of solvent.

Given the quality of product and favorable economic and safety indicators, we recommend proceeding with the construction of this design of PET depolymerization plant that produces 60,000 tonnes of BHET per year and expect to achieve a 49% IRR on the investments.

Process Flow Diagram and M&EB

Table 1 and Figure 1 summarise the complete mass and energy balances for all major process streams across the system. The PET feed enters the CSTR at elevated temperature and pressure, where it reacts with excess ethylene glycol in the presence of zinc acetate forming BHET. Downstream flash separation, filtration and condensation steps aim to remove vapour phase EG as well as solid impurities, purifying the BHET product stream and recovering EG for recycle stream. The table also reports operating pressures, temperatures, phases and specific enthalpies for each stream, these form the basis for energy balance and utility calculations.

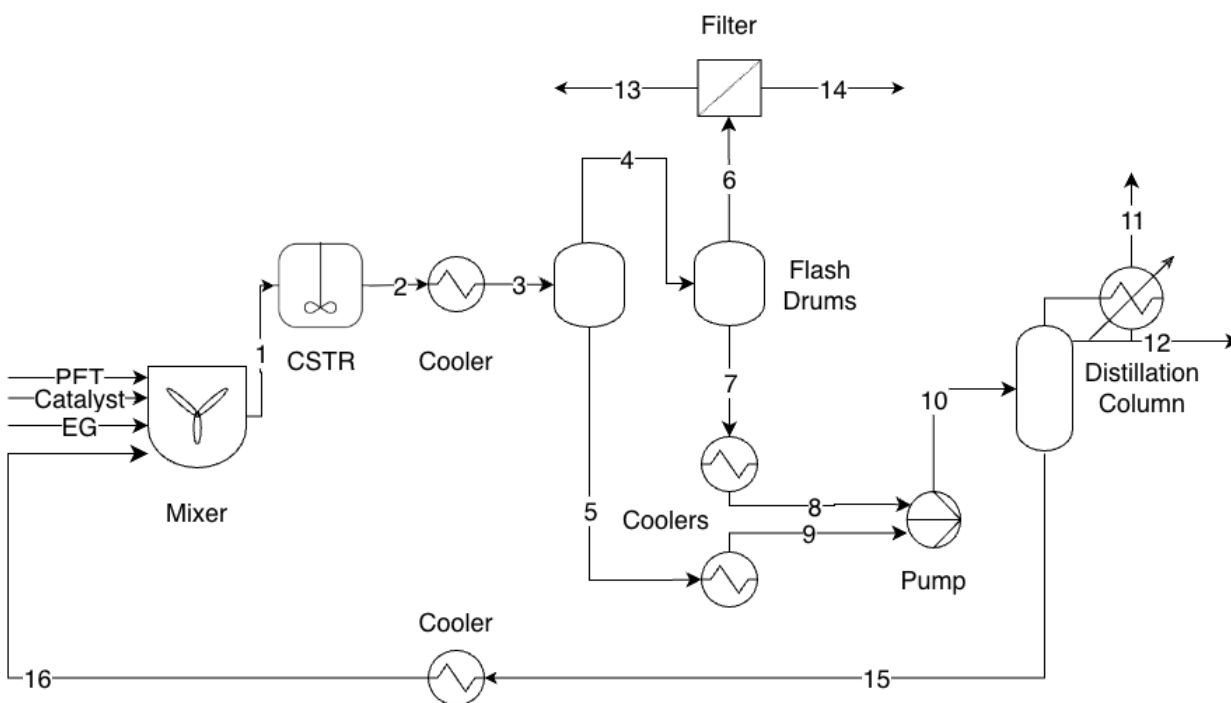


Figure 1. Process Flow Diagram for PET recycling via glycolysis including an EG recycling loop for waste minimisation and a filter for high purity BHET product. For clarification, see appendix **Table A1** for the diagram key.

Flows in kg/hr, pressures nominal

Stream no.	1	2	3	4	5	6	7	8	9
Stream Components	CSTR Inlet	CSTR Outlet	Cooler 1 Outlet	Flash 1 Slurry	Flash 1 EG Vapor	Unfiltered BHET product	Flash 2 EG Vapor	Cooler 3 Outlet	Cooler 2 Outlet
PET	5650	244	244	12.3	232	9.91	2.41	2.41	232
EG	44600	42800	42800	63.5	42700	7.69	55.8	55.8	42700
Zinc Catalyst	352	352	352	352	-	352	-	-	-
BHET	107	7260	7260	7150	104	7150	2.87	2.87	104
Solid impurities	143	143	143	TRACE	143	TRACE	-	-	143
Water	143	143	143	0.0102	143	TRACE	0.0102	0.0102	143
Total	50995	50942	50942	7578	43322	7520	61.1	61.1	43322
Pressure (Bar)	1.5	2.6	1	0.01	0.01	0.0025	0.0025	0.05	0.05
Temperature (c)	115	240	60	160	160	180	180	15	15
Specific enthalpy (kJ/kg)	-6550	-6350	-6860	-4250	-6100	-4190	-5820	-5820	-7400
Phase	liquid	liquid	liquid	liquid	vapour	liquid	vapor	liquid	liquid

Line no.	10	11	12	13	14	15	16
Stream Components	Column Feed	Condenser Outlet	Waste Stream	BHET Product	Purge Stream	Column EG Outlet	Cooler 4 Outlet/ Recycle
PET	234	TRACE	0.531	8.92	0.991	234	234
EG	42800	1.03	21000	0.769	6.92	21800	21800
Zinc Catalyst	0	-	-	17.6	334	-	-
BHET	107	TRACE	TRACE	7150	3.58	107	107
Solid Impurities	143	97.5	45.4	-	-	TRACE	TRACE
Water	143	0.496	142	TRACE	-	TRACE	TRACE
Total	43427	99.0	21188	7177	345	22141	22141
Pressure (Bar)	1	1	1	0.0025	0.0025	1	1.5
Temperature (c)	15.1	74.4	74.4	180	180	197	25
Specific enthalpy (kJ/kg)	-7400	1800	-7320	-4380	-277	-6860	-7340
Phase	liquid	vapour	liquid	solid	liquid	liquid	liquid

Table 1. Mass and energy balance tables.

Piping and Instrument Diagram

In this proposed PET depolymerization system, PET enters the mixer in a 20%wt slurry in ethylene glycol, alongside 0.065%wt catalyst zinc acetate. The mixture then enters a CSTR, where the temperature and pressure are monitored with indicator-controllers to prevent thermal runaway and ensure adequate conversion. Additionally, a liquid level indicator manipulates a valve at the outlet of the reactor to maintain uniform residence time and ensure consistent flow rate. The reacted mixture passes through a cooler with a simple temperature controller before entering a series of two flash separators. A liquid level controller in between the separators controls a valve that prevents vapor from entering the liquid line. The hot BHET slurry then enters a filter where the BHET solid cake can be separated from the remaining mother liquor and dissolved catalyst. As for the vaporized EG from both flash separators, the two streams pass through coolers to convert back to liquid phase, are merged, and are pumped into the distillation column. Within the column, a number of controllers including pressure and liquid level control the reflux ratio and ensure an efficient and safe process. The recycled EG is then cooled and funneled into the mixer with a valve controlled by a flow indicator to make sure the recycle stream does not overload the system and cause instability and downstream issues.

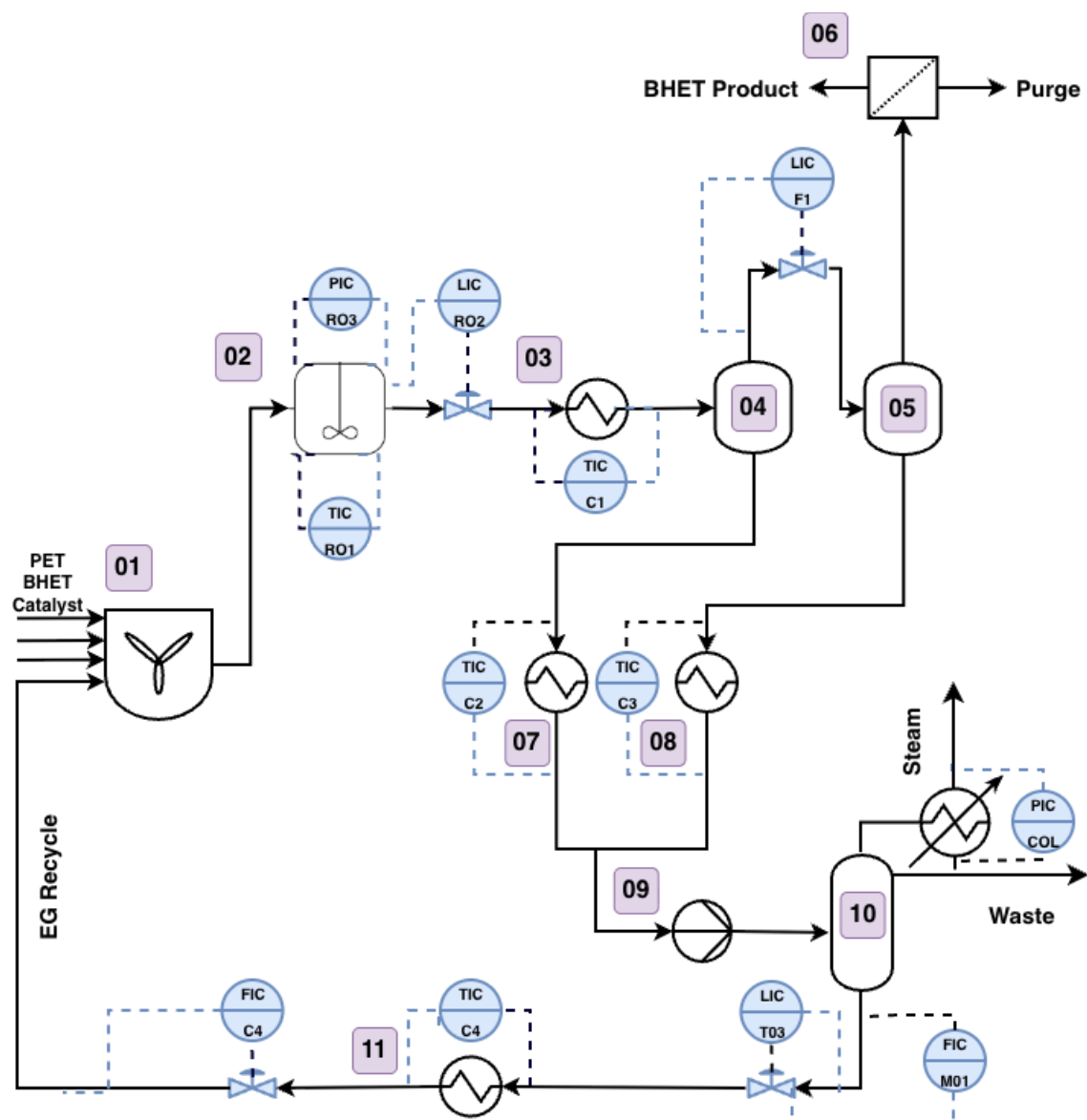


Figure 2. Process and Instrumentation Diagram for PET recycling process. Key controls are identified on the diagram however see following Process Control section for a detailed explanation on the purpose for each controller.

Process Control

The control strategy for the PET depolymerization process is designed to

- (1) maintain stable reactor operating conditions,
- (2) ensure consistent phase separation in the flash drums,
- (3) deliver a conditioned and steady feed to the EG purification column, and
- (4) achieve the required EG purity in the distillate while protecting equipment in the column.

The plant operates near steady state, and control loops are implemented to reject disturbances, maintain production and purity levels, regulate temperatures, and ensure safe operation. Although we did not run Aspen Dynamics, the control structure is based on standard industrial practice and Aspen plus design and stream results. A simple P&ID (PFD + valves + controller tags) accompanies this description.

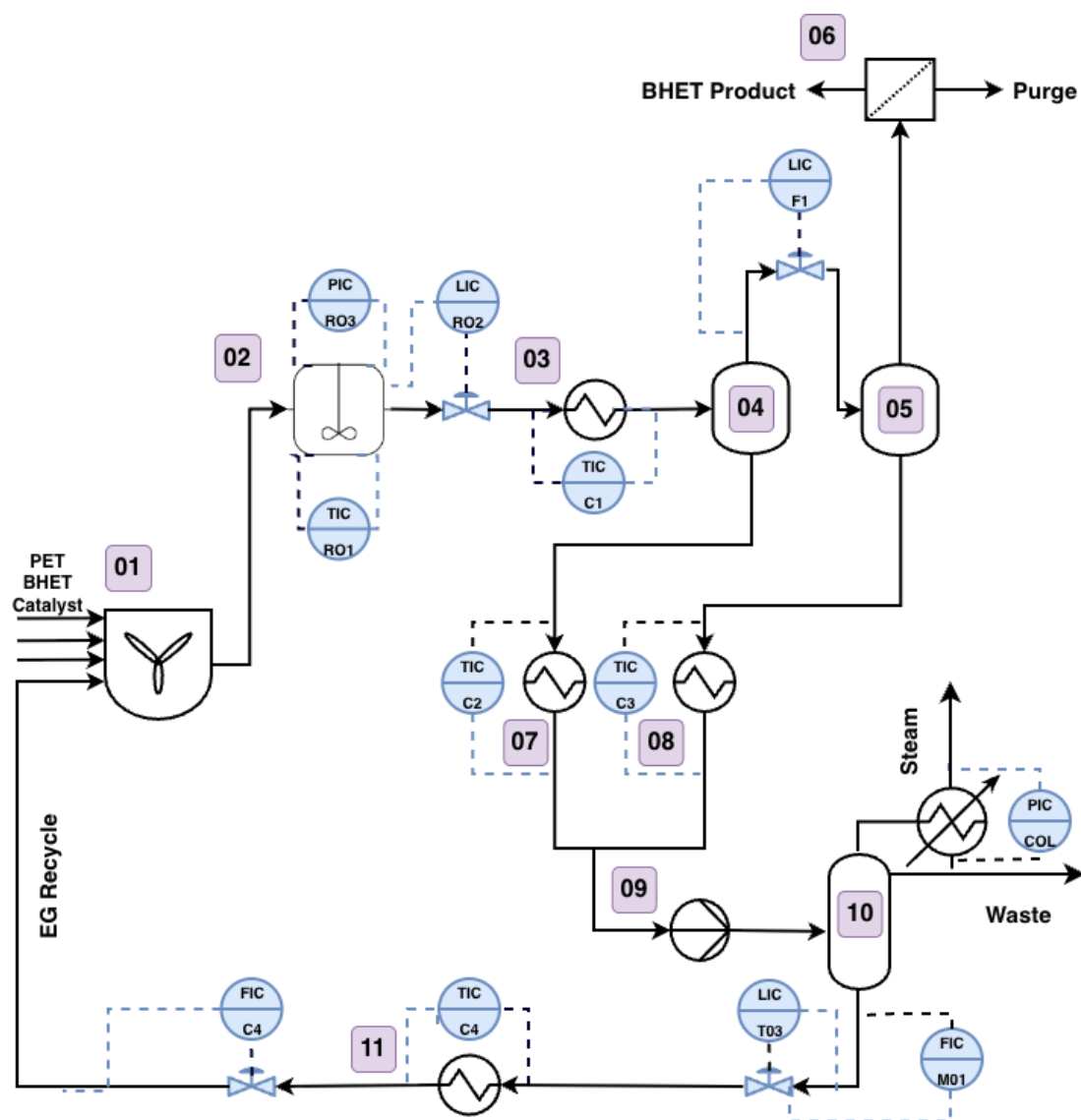


Figure 2. Same as above.

Tag	Controlled Variable (CV)	Manipulated Variable (MV)	Purpose
TIC-R01	Reactor temperature	Hot-oil valve to jacket	Manipulates heat input to control temperature and reaction kinetics to maintain BHET yield.
PIC-R02	Reactor pressure	Vent valve	Protects equipment and maintains liquid phase.
LIC-R03	Reactor liquid level	Reactor outlet stream valve	Maintains residence time in reactor, Maintains reaction inventory and dampens flow surges to downstream separation units.
TIC-E01	Cooler 1 outlet temperature	Cooling water valve	Ensures feed is sub-cooled to minimize vapor load on the flash vessel.
LIC-F01	Flash 1 liquid level	Flash 1 bottoms valve	Ensures stable phase split and prevents entrainment.
TIC-E02	Cooler 2 outlet temperature	CW valve	Conditions EG for downstream cooling/pumping.
TIC-E03	Cooler 3 outlet temperature	CW valve	Ensures proper temperature for EG conditioning.
PIC-T01	Column overhead pressure	Condenser CW valve	Fixes boiling point profile and prevents flooding.
FIC-T02	Bottoms flow	Reflux control valve internal to column	Controls column separation efficiency and distillate purity.
LIC-T03	Bottoms level	Bottoms product valve	Prevents reboiler dry-out; maintains column material balance.
TIC-E04	Cooler 4 outlet temperature	CW valve	Ensure proper temperature for recycled EG.
FIC-M01	Recycle EG flow	Recycle valve	Maintain recycle stream to the system, preventing over or underload that would cause the process to become unsteady.

Table 2. Controlled variables and manipulated variables of each controller. The primary objective of the control system is to maintain high-yield production of BHET while ensuring safe operation and environmental compliance. We employed a control strategy where unit operations, including the reactor, flash, and column, have local regulation to isolate disturbances before they propagate downstream.

I. Reactor and Reaction Section

The kinetics of the glycolysis reaction is highly dependent on temperature. Therefore, **TIC-R01** is the primary quality controller. It manipulates the hot oil jacket valve to maintain the setpoint operating temperature which directly influences BHET yield. To ensure safety and proper phase equilibrium,

PIC-R02 controls the reactor pressure by manipulating the vent valve. This loop is critical for preventing over-pressure scenarios and protecting the vessel integrity. Simultaneously, **LIC-R03** regulates the reactor liquid level by manipulating the outlet valve. This level control is essential for maintaining a constant residence time for the reaction. It also serves as the first line of defense against feed surges by smoothing the flow to downstream units.

II. Separation and Conditioning

Downstream of the reactor, the process focuses on conditioning the stream for separation. We use **TIC-E01** on the reactor effluent cooler to regulate the stream temperature, with similar temperature controllers on the other coolers in the system. This ensures the feed enters the flash tank at the precise condition required for a consistent vapor-liquid split. The flash liquid level is governed by **LIC-F01** to prevent vapor blow-through into the liquid line.

A key design feature is the flow control strategy entering the distillation column. We merged the streams from coolers C2 and C3 prior to the feed pump and installed **FIC-P01** on this combined line. Distillation columns are sensitive to feed rate fluctuations which can cause weeping or flooding on the trays. We used a flow controller here to hard-set the feed rate to the column. This forces upstream disturbances to be absorbed as level changes in the flash tank or reactor rather than upsetting the column profile.

III. Distillation and Recycle

For the distillation column, **PIC-T01** stabilizes the vapor density and boiling point profile by adjusting condenser duty. To ensure product quality, we utilize a flow controller on the reflux line, **FIC-T02**. This loop maintains the specific liquid-to-vapor ratio required for separation efficiency and fixes the distillate purity via reflux ratio. At the bottom of the column, **LIC-T03** actively regulates the sump level by manipulating the bottoms product valve. This control loop serves to automatically close the column's overall material balance. It ensures that the rate of product removal exactly matches the liquid that flows down the trays. By keeping the sump inventory within a fixed range, **LIC-T03** keeps the reboiler heating elements submerged to prevent dryout and accommodates dynamic changes in feed rate without needing manual operator intervention. Finally, **FIC-M01** on the recycle stream manipulates a valve leading to the mixer in order to ensure a constant flow rate and prevent over or underload that would affect the reaction stoichiometry and load on downstream unit operations.

IV. Safety and Response to Upsets

The process is designed with significant hydraulic capacitance (liquid holdup) in the reactor and flash vessels. These vessels act as temporary storage in the event of a downstream blockage or valve failure. For example, if the column feed pump trips, **LIC-F01** will close the flash outlet. The liquid level in the flash will rise until it triggers an alarm. This alarm is interlocked to cut the fresh feed to the reactor. This approach ensures that a single equipment failure results in a safe process shutdown rather than a material spill or pressure release.

Economic Estimates

Initial investment for equipment and installation totaled to \$19.8M. The equipment sizing and estimated costs were calculated using methods and parameters given in Towler & Sinnott: Section 7.5.2, Table 7.2, Table 15.1; Perry's Chemical Engineers' Handbook: Section 11-58, Section 10-27, Section 14; McCabe, Smith, and Harriott's *Unit Operations of ChemE*.

I. Equipment Sizing

#	Equipment	Method	Sizing
01	mixer	volume = residence time $\times$ vol. flow rate	volume = 5,541 m ³
02	reactor CSTR, carbon steel with hot oil jacket	volume = residence time $\times$ vol. flow rate	volume = 382.61 m ³ length = 10.31 m diameter = 6.87 m
03	heat exchanger 1	area = heat duty / (U $\times$ ΔT_{lm})	area = 1521.12 m ²
04	flash separator 1	Souders–Brown equation @ 80% flood, 5 minute holdup, +20% surge, L/D = 3	volume = 16.677 m ³
05	flash separator 2	Souders–Brown equation @ 80% flood, 5 minute holdup, +20% surge, L/D = 3	volume = 15.907 m ³
06	filter	area = flow rate / filtration rate	area = 120 m ²
07	heat exchanger 2	area = heat duty / (U $\times$ ΔT_{lm})	area = 42.46 m ²
08	heat exchanger 3	area = heat duty / (U $\times$ ΔT_{lm})	area = 0.40 m ²
09	pump	electrical power = density $\times$ gravity $\times$ vol. flow rate $\times$ pump head / (pump efficiency $\times$ motor efficiency)	power = 1.778 kW
	tower	column diameter = sqrt(4 $\times$ vapor vol. flow / pi flooding vapor velocity) $\rightarrow$ volume = $\pi \times r^2 \times h$	volume = 7.05 m ³ diameter = 1.44 m
10	reboiler	area = heat duty / (U $\times$ ΔT_{lm})	area = 158.95 m ²
	condenser	area = heat duty / (U $\times$ ΔT_{lm})	area = 94.02 m ²
	accumulator	volume = $\frac{1}{2} \times$ residence time $\times$ vol. flow rate	volume = 5.80 m ³
11	heat exchanger 4	area = heat duty / (U $\times$ ΔT_{lm})	area = 7.80 m ²

Table 3. Equipment sizing calculations using standard chemical engineering equations.

II. Estimated Costs

#	Equipment	Type	S		a	b	n	Cost
01	mixer	static mixer	99.52	L/s	570	1170	0.4	\$7,938.01
02	reactor	CSTR	382.61	m ³	61,500	32,500	0.8	\$3,846,696.37
03	heat exchanger	shell & tube	1521.12	m ²	28,000	54	1.2	\$383,623.07
06	filter	vacuum drum	120	m ²	-73,000	93,000	0.3	\$318,054.53
07	heat exchanger	shell & tube	42.46	m ²	28,000	54	1.2	\$32,852.55
08	heat exchanger	shell & tube	0.40	m ²	28,000	54	1.2	\$28,017.98

09	pump	explosion proof motor	1.778	kW	-1100	2100	0.6	\$1866.05
	reboiler	thermosiphon	148.95	m ²	30,400	122	1.1	\$60,371.22
10	condenser	shell & tube	94.02	m ²	28,000	54	1.2	\$40,596.74
	accumulator	cone roof tank	5.80	m ³	5800	1600	0.7	\$11,276.71
11	heat exchanger	shell & tube	7.80	m ²	28,000	54	1.2	\$28,635.20
				C_{ref}			n	
04	flash separator		16.677 m ³		50,000	\$/m ³	0.6	\$270,545.78
05	flash separator		15.907 m ³		50,000	\$/m ³	0.6	\$262,980.15
10	tower		7.05 m ³		53,500	\$/m ³	0.6	\$172,690.03
Raw Total								\$5,466,144.36
Lang Factor (for mixed fluids-solids processing plants)								3.63
Total Capital Cost (factored for equipment + installation)								\$19,842,104.03

Table 4. Total capital cost estimations using Towler reference parameters and associated equations.

After estimating a raw total for equipment costs of approximately \$5.47M, the Lang factor for mixed fluids-solids processing was implemented to calculate the total cost of equipment and installation.

Additionally, the initial investments will include the first year of plant operation. Raw materials and utilities were estimated using market research, standard utility pricing, and Aspen simulation software. Calculations were made under the assumption of a 350-day operating year, with Towler & Sinnott parameters for operators, positions, and shifts from Section 8.5.

Raw Materials	Price	System Usage	Annual Cost
PET flake	\$1323 / metric ton ¹	5415 kg / hr	\$60,177,978
ethylene glycol	\$705 / metric ton ²	22799.1 kg / hr	\$1,851,651.71
zinc acetate	\$2500 / metric ton ³	351.975 kg / hr	\$84,474
Utilities			
cooling water	\$2e-05 / kg	15,108,788 kg / hr	\$2,538,276.34
hot oil	\$3.54 / hr (Aspen)	-	\$297,761.52
electricity	\$0.0775 \$ / kWhr	14756.37 kW	\$9,606,399.57
wastewater treatment	\$1.10 / m ³	19.82 m ³ / hr	\$183,130.33
solid waste to landfill	\$40 / Mg	380.3 kg / hr	\$127,779.48

¹ Argus Media. *Argus Recycled Polymers — Report Sample*. March 7, 2025.

² Lang, W. T., et al. (2023). Chemical recycling of polyethylene terephthalate, an industrial and sustainable opportunity for Northwest of England. *Journal of Environmental Chemical Engineering*, 11(5), 110585. <https://doi.org/10.1016/j.jece.2023.110585>

³ MarketResearchReportStore. (n.d.). *Anhydrous Zinc Acetate Report*.

<https://www.marketresearchreportstore.com/reports/2030004/anhydrous-zinc-acetate?utm>

Labor	
operating labor	\$5,760,000
supervision	\$1,440,000
overhead	\$3,600,000
Total Annual Operating Cost	
	\$86,667,450.95

Table 5. Operating costs including labour and utilities.

The total initial investment, consisting of capital, installation, and operating cost for one year, totals to approximately \$105.5M. With a 50/50 split between debt and equity, a loan of \$52.8 will be paid off over 10 years with interest at a debt rate of 5%, yielding an annual payment of \$6.8M.

The product BHET has an average selling price of \$1,980 per metric ton. Given the Aspen process simulation results, the total annual revenue is estimated to be \$118.9M. In addition to the loan/debt service, the plant operates with additional economic parameters: a corporate tax rate of 10%, location factor (United States) of 1.04, and an investor return of 12.5%.

Year	Revenue	Costs	Gross Profit	Debt Service	Profit after debt service	Tax (w/o Depreciation)	Depreciation	Book Profit	Deprec. Benefit	WACC
0		\$105.5M								-\$52.8M
1	\$118.9M	\$85.7M	\$33.3M	\$6.8M	\$26.4M	\$2.6M	\$21.1M	\$5.3M	\$2.1M	\$25.9M
2	\$118.9M	\$85.7M	\$33.3M	\$6.8M	\$26.4M	\$2.6M	\$21.1M	\$5.3M	\$2.1M	\$25.9M
3	\$118.9M	\$85.7M	\$33.3M	\$6.8M	\$26.4M	\$2.6M	\$21.1M	\$5.3M	\$2.1M	\$25.9M
4	\$118.9M	\$85.7M	\$33.3M	\$6.8M	\$26.4M	\$2.6M	\$21.1M	\$5.3M	\$2.1M	\$25.9M
5	\$118.9M	\$85.7M	\$33.3M	\$6.8M	\$26.4M	\$2.6M	\$21.1M	\$5.3M	\$2.1M	\$25.9M
6	\$118.9M	\$85.7M	\$33.3M	\$6.8M	\$26.4M	\$2.6M		\$26.4M		\$23.8M
7	\$118.9M	\$85.7M	\$33.3M	\$6.8M	\$26.4M	\$2.6M		\$26.4M		\$23.8M
8	\$118.9M	\$85.7M	\$33.3M	\$6.8M	\$26.4M	\$2.6M		\$26.4M		\$23.8M
9	\$118.9M	\$85.7M	\$33.3M	\$6.8M	\$26.4M	\$2.6M		\$26.4M		\$23.8M
10	\$118.9M	\$85.7M	\$33.3M	\$6.8M	\$26.4M	\$2.6M		\$26.4M		\$23.8M
11	\$118.9M	\$85.7M	\$33.3M		\$33.3M	\$3.3M		\$33.3M		\$29.9M
12	\$118.9M	\$85.7M	\$33.3M		\$33.3M	\$3.3M		\$33.3M		\$29.9M
13	\$118.9M	\$85.7M	\$33.3M		\$33.3M	\$3.3M		\$33.3M		\$29.9M
14	\$118.9M	\$85.7M	\$33.3M		\$33.3M	\$3.3M		\$33.3M		\$29.9M
15	\$118.9M	\$85.7M	\$33.3M		\$33.3M	\$3.3M		\$33.3M		\$29.9M
NPV										\$106.0M
IRR										49%

Table 6. Net Present Value and Internal Rate of Returns Calculations.

Given these parameters, the net present value (NPV) is \$106M and the internal rate of return (IRR) is 49%. The process is expected to generate \$106M more than the minimum return required by investors, compensating for its capital and operating expenses over its lifetime and creating substantial economic value. The IRR of 49% also demonstrates strong project profitability relative to the target investor return of 12.5%. The proposed BHET process exceeds the minimum required performance and offers a favorable margin for economic viability under the assumed market and operating conditions.

Safety and Environmental Summary

A detailed Failure Mode and Effects Analysis (FMEA) was conducted on the revised process design (Reactor → Vacuum Flash → Distillation). No show-stoppers were identified that would require abandoning the design. However, the shift to a vacuum-driven separation process introduces high-severity risks that require specific engineering safeguards in the detailed design phase.

Key Hazards and Critical Safeguards

A total of 36 failure modes were scored using a severity × occurrence × detection method on a scale from 1–10. The highest values correspond to the Hazards listed below.

Hazard / Failure Mode	Consequences	Existing Safeguards	Recommended Actions
Reactor overheating (loss of cooling or agitator trip)	Rapid pressure rise; potential vessel rupture; release of hot glycol vapor.	Jacket temperature control, Pressure Safety Valve on reactor.	Add a spare cooling pump with automatic changeover if the main one fails. Install Independent High-Temperature Trip (SIS) to cut heat source and inject quench; size PSV for two-phase flow.
Vacuum System Air Ingress (Flash Drums)	Oxygen enters hot vessel (160°C); potential internal fire/explosion atmosphere.	Vacuum-rated vessel design; Nitrogen blanketing on seals.	Install Oxygen Analyzers on vacuum exhaust lines interlocked to N ₂ purge; implement strict leak-testing protocols.
Blocked vent / undersized relief	PSV opens releasing hot EG vapor.	Pressure Safety Valve, Heat Tracing.	Add a rupture disk upstream. Set up a regular testing plan for relief devices.
BHET dust generation	Combustible dust risk, respiratory risk.	Local collection, PPE.	Carry out a Dust Hazard Analysis; use N ₂ purge where feasible to reduce ignition risk
Nitrogen purging / confined space	Asphyxiation hazard to personnel.	Permits, Adequate Ventilation.	Install fixed O ₂ monitors near purge points; reinforce training and rescue plans

Outstanding Data Gaps

- Vacuum Integrity: Verification of gasket materials and flange ratings to prevent oxygen ingress at 0.01 bar operation.
- Relief System Protection: Validation of PSV sizing for two-phase flow during a runaway reaction scenario.
- Pump Cavitation: NPSH calculations for the transfer pump (Stream 9) moving boiling liquid from vacuum to pressure.
- Dust Ignition Risk
- Oxygen Deficiency Protection

Environmental Summary

The process generates distinct waste streams that define the scope for the utility and treatment facilities. While the benefit of the recycling plant outweighs these impacts, the following streams define the magnitude of the waste treatment task:

- Liquid Effluent (Wastewater): The primary liquid waste (Stream 12) contains approximately 21,000 kg/hr of water mixed with ethylene glycol and dissolved organics. This stream requires a dedicated glycol recovery unit or specialized wastewater treatment (pH control and solids removal) before discharge.
- Solid/Sludge Waste (Spent Catalyst): Stream 14 removes the bulk of the spent Zinc Acetate catalyst (334 kg/hr) along with minor BHET residues. This material must be handled as hazardous chemical waste due to heavy metal content and requires controlled off-site disposal to minimize landfill impacts.
- Vapor Emissions: Minor losses from nitrogen purging and vacuum exhaust (Stream 11) will contain volatile organics and require scrubbing or flaring to minimize atmospheric release.

A closed-loop recycling stream returns unreacted ethylene glycol and dissolved organics back to the reactor, minimising fresh solvent demand and wastewater generation. While efforts are made to reduce environmental impact, the benefit of the recycling plant should outweigh the impacts posed by the process design. With the addition of the recycling stream, operating and environmental costs are minimised.

Aspen Plus Model

The PET glycolysis process simulation was developed in Aspen Plus to understand mass and energy streams and verify the feasibility of the proposed recycling process. The property method selected for the simulation is the NTRL method, which is compatible with our system involving polymers and organic solvents. The NTRL method accounts for the nonideal interactions between the EG solvent and the aromatic BHET monomer, which is critical in predicting phase behavior in the flash separators. Also, without this method, the model would not be able to predict the correct VLE required in the EG recycle loop.

The reaction in the CSTR was modeled with a 2nd-order reaction in PET and EG, using Power Law kinetics in Aspen Plus. The pressure in the reactor was also set to ensure liquid phase through the reaction. These simplifications allowed for convergence of the reactor heat duty and effluent composition.

Another notable simplification in the Aspen model involves BHET purification. In the actual process, solid cake and mother liquor can be separated via crystallization, or solubility differences. In Aspen Plus, all components are listed in liquid form rather than solids, so the flash separator and filter serve as the purification unit operations. The solid impurities entering with PET feed are modeled as inert ash to track accumulation without interfering with reaction stoichiometry and kinetics.

The process also features a closed-loop recycle of EG solvent. To ensure convergence, the tear stream was initialized with estimates from manual mass balances. We also assumed that trace accumulation of water and impurities in the recycle loop reaches a steady state that does not significantly impact solvent quality.

Sources

1. Argus Media. *Argus Recycled Polymers — Report Sample*. 7 Mar. 2025.
2. Chu, Mingyu, Weilin Tu, Qiao Zhang, Wenyu Huang, Jinxing Chen, and Ding Ma. “Co-recycling of plastics and other waste materials.” *Nature Reviews Clean Technology*, vol. 1, 2025, pp. 320–332. <https://doi.org/10.1038/s44359-025-00055-z>.
3. Green, Don W., and Marylee Z. Southard, editors. *Perry's Chemical Engineers' Handbook*. 9th ed., McGraw-Hill, 2018.
4. Lang, W. T., et al. “Chemical recycling of polyethylene terephthalate, an industrial and sustainable opportunity for Northwest of England.” *Journal of Environmental Chemical Engineering*, vol. 11, no. 5, 2023, p. 110585. <https://doi.org/10.1016/j.jece.2023.110585>.
5. MarketResearchReportStore. *Anhydrous Zinc Acetate Report*. n.d. <https://www.marketresearchreportstore.com/reports/2030004/anhydrous-zinc-acetate>.
6. McCabe, Warren L., Julian C. Smith, and Peter Harriott. *Unit Operations of Chemical Engineering*. 7th ed., McGraw-Hill, 2004.
7. Towler, Gavin, and Ray Sinnott. *Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design*. 3rd ed., Butterworth-Heinemann, Sept. 2021.

Appendix**Table A1.** Process Flow Diagram Key

Process Flow Diagram Key	
	Mixer
	CSTR
	Heat Exchanger
	Flash Drum
	Centrifugal Pump
	Distillation Column
	Condenser
	Filter