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Process Simulation of Dimethyl Terephthalate from Polyethylene Terephthalic Bottle Waste

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ABSTRACT: To safeguard the petroleum feedstock and lessen the special problems that polyethylene terephthalate (PET) bottle litter poses for the environment. PET was converted using chemical recycling technology into useful things with a significant and prosperous industrial application. This work employed ASPEN PLUS V10 to simulate the chemical methanolysis depolymerization process of PET plastic wastes using a continuous stir tank reactor for the manufacture of pure dimethyl terephthalate (DMT) and EG, with methanol recovered for industrial usage. Excess methanol (CH₃OH) was used to break down PET trash. The reaction's ideal operating conditions were a mean PET particle size of 127.5 m, 1000 kg/h of PET depolymerized at a CH₃OH:PET (w/w) ratio of 6:1, 571.15 K temperature, 80.92 bar pressure, and 1.8667 h residence time. It is a first-order reaction in terms of PET. The process produced 1003.9357 kg/h of DMT, 320.9803 kg/h of EG, and 99.35% of the PET was depolymerized. Selectivity values for DMT and EG were 0.7578 and 0.2422, respectively. Techniques such as filtration, distillation, and crystallization were utilized to separate the component mixtures. It was possible to obtain heat from the transportation, reaction, and separation operations. Through this endeavour, the production of DMT and EG was improved while using less processing heat. In the future, commercial processes can be scaled up using the procedures and their operating conditions.

KEY WORDS: Continuous stir tank reactor, Crystallizer, Distillation column, Dimethyl terephthalate, Ethylene glycol, Filter, Methanol, Polyethylene terephthalate, Terephthalic acid.

I. INTRODUCTION

PET plastic is a cost-effective and long-lasting polymer that is used in a variety of products, including packaging, bottles, straws, bags, and much more, which keeps the plastic production and disposal cycle going nonstop. Due to increased urbanization, there is an increase in global population demand for extra PET bottle plastic use. PET bottles for soft drinks and water have a very short shelf life. They lack enough worth to be kept since they are so cheap and because their disposal is done improperly. They end up in landfills instead. It builds up over time and becomes a significant environmental issue globally (Dussud et al., 2018). It has as well become a liability or problem for the industries to solve (Chen et al., 2021).

A significant amount of garbage is produced with limited PET recycling capabilities as a result of the expanding population, together with advancements in technology and PET bottle delivery services. Previous studies indicate that plastic bottles disintegrate between 70 and 450 years old, demonstrating that plastics do not quickly biodegrade (Delaney, 2013; Chan, 2016). Another goal is to find a way to modernize, enhance, and develop PET bottle trash disposal techniques. This is necessary to meet the vision and insight that these practices must be environmentally sound and sustainable.

According to Geyer et al. (2017), just 9% of the 6,300 metric tons of plastic waste produced in 2015 PET plastic is a cost-effective and long-lasting polymer that is used in a variety of products, including packaging, bottles, straws, bags, and much more, which keeps the plastic production and disposal cycle going nonstop. Also, the production of PET packaging bottles has increased as a result of these products' attributes, which include good mechanical properties, ease of manipulation to fabricate any shape or product of interest, breadth of their products, and future promise in research for more products, combined with daily new innovation (Sarioğlu and Kaynak, 2017). PET bottle trash is readily thrown out and is allowed to clog gutters and drains and leave behind litter everywhere. Due to its non-biodegradability and the potential for very slow disintegration caused by photochemical reactions, electrolyte corrosion,



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hydrolysis, microbes, and other factors. It builds up over time and becomes a significant environmental issue globally (Dussud et al., 2018).

Recycling is the most recent technique for handling PET bottle waste. If the appropriate sub-method is not used and is not handled appropriately, the method itself has various problems (Raheem et al., 2019). The primary problem with recycling is that it can only return one kind of pure, unadulterated plastic waste to the way it was when it was produced. Thus, the problem of plastic waste at the disposal site is not addressed (Soong et al., 2022). For secondary (mechanical) recycling, only monolayer plastics are permitted, which adversely impacts the environment and causes physical damage to objects. A study on the creation of PET flakes and the mechanical recycling process was also conducted by (Zhang et al., 2020). Gas and liquid fuel are the only by-products of pyrolysis and gasification (tertiary recycling) that have been studied in depth. The pyrolysis of PET bottle waste was made possible by the use of LCA (Davidson et al., 2021). PET bottle waste can only be partially decomposed by the time-consuming process of enzymelysis (tertiary recycling by biodegradation). Solvolysis, or tertiary recycling through chemical depolymerization, is pricy, harmful for the environment, and demanding to separate the finished product from the process. Recycling from the Quaternary recovers energy along with CO_2 emissions and other priceless materials and recovering PET monomers is not covered by it (Samak et al., 2020).

For chemical recovery, there are numerous different types of hydrolysis, such as neutral, acid, and alkaline hydrolysis (Čolnik et al., 2021); alcoholysis (Jiang et al., 2022); aminolysis (Jiang et al., 2022); glycolysis (Raheem and Uyigue, 2010; Yun et al., 2022); and ammonolysis (Benyathiar et al., 2022). The only process that may convert PET bottle waste into DMT is alcoholysis (methanolysis).

PET bottle waste was solvolyzed (chemically recycled) in this work to identify methods for making PET bottle waste digestion into DMT novel and industrially viable at a reasonable low cost of production. The design, modelling, and simulation of the process led to the development of a simple and efficient separation technique. It was established to be used later to create a life cycle inventory for recycling PET bottle waste into DMT. Hope can be found in future studies on the effects on the environment and the economy provided by measurements of materials and energy. A straightforward and effective separation technique was developed through planning, modelling, and process simulation. It was made with the intention of being used later to compile a life cycle inventory of the PET bottle debris that was recycled and turned into DMT. The quantification of materials and energy can be used to further research the consequences for the environment and the economy. The planning, modelling, and simulation of the process led to the development of an easy-to-use separation technique. It was established to be used later to create a life cycle inventory for recycling PET bottle waste into DMT. Hope can be found in future studies on the effects on the environment and the economy. The planning, modelling, and simulation of the process led to the development of an easy-to-use separation technique. It was established to be used later to create a life cycle inventory for recycling PET bottle waste into DMT. Hope can be found in future studies on the effects on the environment and the economy provided by measurements of materials and energy can be used to further research the consequences on the environment and energy. The quantification of materials and energy can be used to further research the consequences on the environment and the economy.

II. PET BOTTLE WASTE-METHANOLYSIS METHOD OF DIGESTION TO DMT DESIGN, MODELING, AND SIMULATION (DMS) USING ASPEN PLUS WITH THE ASPEN POLYMER FEATURE

PET (the reactant) and CH₃OH (the reactant and solvent) flow into the reactor while the product(s) of the reaction simultaneously exit the vessel in a reaction vessel created and simulated using CSTR. It becomes a useful instrument for continuous chemical processing by allowing input and output streams to flow constantly. It is designed to handle a very viscous PET substance and has a tank reactor, feed and exit pipelines, and an embedded impeller. A vortex should be able to form in order to ensure that the reactants are evenly mixed. PET was chosen due to its wellknown potential for scaling up and superiority in sturdy, solid handling since it is a solid substance. Because CSTR cascades have better heat transmission capabilities, their pseudo-plug flow characteristics improve residence time distribution control. It is a potential solution for ultra-high-temperature processes like PET and superheated methanol. They also exhibit increased resilience to more potent reactions and reagent concentrations. They are perfect for reactions with fast kinetics because they can run for long periods of time and create large amounts of product per unit of time. They operate continuously and have fewer running costs. The feed adopts a homogeneous composition throughout the reactor and operates in a steady state with a constant flow of reactants and products. The material in the tank and the exit stream share the same chemical make-up. CSTRs, which have greater heat transfer properties than batch reactors, may be used to remove heat from the reaction mixture more quickly and effectively. This can shorten response times and lower the risk of overheating. The most common applications for continuous stirred-tank reactors in industrial processing where continuous agitation is necessary include the polymer (PET) sector and homogenous liquid-phase



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flow processes. They may be used singly, successively, or as a part of a battery. The temperature of the reacting mixture, T, should stay constant at the proper value as the CSTR control target. The temperature of the coolant is the sole variable that may be changed. Both the CSTR method and the temperature control system are original and well-designed. Due to their rapid control speed, high control precision, high heat exchange efficiency, and low heat-carrying agent consumption, they are advantageous for energy savings and consumption reduction. They are quite simple to use and put into action. To ensure the correct mixing of materials that are continuously introduced into the reactor and to create mixes with similar chemical compositions at the input and output.

A DMS of PET Bottle Waste Methanolysis Method of Digestion to DMT Process

Information from the experimental study on the methanolysis digestion of PET bottle trash into DMT was used in the DMS processing. All of the reaction modelling equations for the Aspen Plus with Polymer feature's CSTR were already present in the program. The tolerance for the component attributes is 0.001 due to the software's efficacy. Data from the PET bottle waste methanolysis technique of digesting for the DMT experiment and CSTR are shown in Table 1.

Operating conditions	Values	Units	Operating conditions	Values	Units
CH ₃ OH : PET	6:1		Total reactor actual volume,	90.1646	m ³
			Va		
Temperature	571.15	K	Order of reaction	1st	Based on
				order	PET
Pressure	80.92	bar	Reaction rate constant, k	6.1676	s^{-1} (or sec ⁻¹)
Residence time	1.8667	h	Activation energy (E _a)	96.5628	kJ/mole
Total reactor volume, V _t	81.9678	m ³			

Table 1.	PET b	ottle waste	e methano	lvsis m	ethod of	digestion	to DMT	reaction of	operating	conditions

The simulation was done based on the computational flow diagram (CFD) shown in Figures 1(a and b) below:



Figure 1a: Process flow diagram of methanolysis method of polyethylene terephthalate bottles waste chemical recycling into dimethyl terephthalate



Figure 1b: Process flow diagram methanolysis method of polyethylene terephthalate bottles waste chemical recycling into dimethyl terephthalate



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B PET Bottle Waste Methanolysis Method of Digestion Chemical Reaction Model

The PET neutral hydrolysis chemical recycling into TPA was simulated using a kinetic Segment-based power law reaction model, which is consistent with work by (Saidi and Kadkhodayan, 2020), who used Aspen Plus to simulate and measure the recovery efficiency of copper in the leaching process of copper oxide in H_2SO_4 solution. A power law representation of the molarity concentration basis (C_i) was used, as shown in the following equation (1).

$$r = kT^n e^{-Ea/_{RT}} \Pi(C_i)^{\alpha_1} \tag{1}$$

If the reference temperature T_0 is not stated, the above equation (1) is appropriate. Otherwise, if a reference temperature T_0 is supplied, the equation (2) below is appropriate.

$$r = k \left(\frac{T}{T_o} \right)^n e^{\left(\left(-Ea/R \right) \left[\frac{1}{T} - \frac{1}{T_o} \right] \right)} \Pi(C_i)^{\alpha_1}$$

$$\tag{2}$$

Where T is temperature in degrees K, To is reference temperature in degrees K, r is reaction rate, and n is the exponential factor, Ea stands for activation energy, R for the universal gas law constant, C for molarity (kg mol/m³), i for component index, and Π for the product operator. Relevant and suitable models can also be developed for the work, as was done by Castillo Gonzalez et al. (2020), who developed mathematical models for continuous biodiesel reactors that can be used for economic analysis of supply changes in continuous processes of biodiesel.

It should be noted that the depolymerisation of PET using CH_3OH to produce DMT is the first-order reaction involving the methanolysis digestion of PET. Selectivity was 0.7578, PET conversion was 99.35%, and DMT (monomer) yield was 99.35%. The EG yield and selectivity were, respectively, 99.35% and 0.2422. The reaction route is shown in Eq. (3).

 $1 \text{ mole of } \begin{array}{c} C_{10}H_8O_4 + 2 \text{ moles of } \begin{array}{c} CH_3OH \\ Methanol \end{array} \rightarrow 1 \text{ mole of } \begin{array}{c} CH_3OH \\ Methanol \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } \begin{array}{c} C_6H_4(COOCH_3)_2 \\ Dimethyl \text{ terephthalate } \end{array} + 1 \text{ mole of } Dimethyl \end{array} + 1 \text{ mole of } Dimethyl Dimethyl$

II. Chemical Recycling of PET Bottles Waste Using Methanolysis Method: Process Design, Modelling, and Simulation Procedure

Experimental data from Liu et al. (2015) were used to mimic the chemical methanolysis technique of depolymerizing PET into DMT. The method used was neutral hydrolysis digestion of PET bottle waste. For CSTR with agitation, the Aspen Plus v10 with polymer function was used. The data used is shown in Table 1 above.

A Methanolysis Method of PET Bottle Waste Digestion to DMT Process Description

The basis of this concept is a 1000 kg/h PET garbage bottle. Figures 1(a) and (b) were used for simulation and modelling. In Feed 1, PET powder and methanol were combined in a 1:1 mass ratio at operating temperatures of 298.15 K and 1.01325 bar. The transport medium for PET was methanol. Feed 2 was 5000 kg/h of methanol that was moved into reactor 1 by pump 2 running at 82.00 bars and heated by heater 2 (pre-heating) to a temperature of 571.15 K. Heaters 1 and 2 provided input and output for the pumps 1 and 2, which raised the pressure to 82.00 bar and moved streams 1 and 2 of materials into the reactor. At the entrance of reactor 1, pre-heaters 1 and 2 heated the output streams of pumps 1 and 2 to a temperature of 571.15 K, as well as their respective input and output results. We needed these pre-heaters to help us heat the reactants to reactor 1's desired supercritical operating temperature. Achieving the desired conversion by beginning the reaction right away in the reactor was crucial for steady-state performance. By reducing the amount of energy used to heat the reactor rather than heating it completely, it aids in system optimization. This decreased the amount of heater needed to heat the heat transfer medium, which in turn reduced the size of the heating exchanger required for reactor 1, always optimized energy, and increased the process economics (Luyben, 2012). In reactor 1, the mass ratio of ethanol to PET was 6:1. To encourage PET's full conversion to DMT and the better selectivity of the DMT product over EG, there was an excess of methanol.

A mixture of 6000 kg/h of methanol and 1000 kg/h of PET was used in Reactor 1 (the CSTR reactor). It had a volume of 90.1646 m3 and ran at a temperature of 571.15 K and an operating pressure of 80.92 bar. According to the



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information in Table 1 above, Reactor 1 was used to depolymerize PET into DMT. It is evident that yields of DMT and EG with corresponding selectivity of 99.35% were obtained, which is similar to the value reported in the literature. At the identical optimal working conditions of 571.15 K temperature, 80.92 bar pressure, and 1.8667 h of residence time, there are hardly any changes between them. Additionally, the process's selectivity of 0.7578 for DMT and 0.2422 for EG demonstrated its viability and demonstrated that it is more likely to produce DMT than EG.

Additionally, by contrasting those with the authors' earlier efforts, which are described below, the data and findings of this study were confirmed. The work of Liu et al. (2015) gets the closest (99.35% DMT) despite the variations in operating conditions for converting PET bottle waste into DMT. The results of DMT production show a declining trend, with values of 93.10 percent by Pham and Cho (2021), 91.0 percent by Tang et al. (2022), and 89.10 percent by Jiang et al. (2022). Ma et al. (2022) and Tollini et al. (2022) both produced the poorest results, with 78.40% and 71.00%, respectively.

Filter 1 received the reactor 1 product mixture at a higher pressure of 80.92 bar. A 0.0009 mass fraction (6.4864 kg/h) of solid, unreacted PET was filtered out by filter 1 at 1.01325 bar and 571.50 K, while pump 3 at 2.0265 bar sent it to the next stage of treatment. Pump 4 running at 2.0265 bar transferred the remaining 0.9991 total mass fractions of DMT (0.1436), methanol (0.8106), and EG (0.0459) to liquid mixture separation (distillation). Pump 4 working at 2.0265 bar through cooler 1 pumped Filter 1's liquid filtrate stream into Radfrac distillation column 1, which contained 0.0459 (320.89 kg/h) mass fractions of EG, 0.8106 (5668.69 kg/h) mass fractions of Methanol, and 0.1435 (1003.94 kg/h) mass fractions of DMT. The temperature was 571.15 k, and the pressure was 1.01325 bar. Before entering distillation column 1, it was cooled down to 337.85 K in cooler 1 at a pressure of 2.0265 bar, which is the boiling point of methanol, the stream's most volatile component. The pressure in Radfrac Distillation Column 1 was 1.01325 bar. Methanol was collected as an overhead product and moved by pump 5 through the commercial or re-use area of refrigerator 1.

Pump 6 operated at 2.0265 bar, and cooler 2 cooled the bottom products stream of distillation column 1, which contained a mixture of 0.2420 (320.63 kg/h) mass fractions of EG, 0.7578 (1003.94 kg/h) mass fractions of DMT, and a trace amount of 0.0002 (0.2581 kg/h) mass fractions of methanol at 490.59 K and 1.01325 bar pressure. With this cooling, the stream temperature was intended to be brought within 10 degrees of the crystallizer's operational range. A crystallizer cooler, chiller, or refrigerator works best when the operating temperatures of the input stream and crystallizer are no more than 10 degrees apart. Crystallizer 1 uses a refrigerator to cool the stream of its contents to 298.15 K at 1.0133 bar pressure. The following requirements (rules) should be followed while selecting a temperature: (1) Unless it is a trace component that may or may not be soluble in other components with higher freezing points, its operating temperature must be higher than the freezing points of all other components in the crystallizing stream, excluding the crystallizing component. (2) The operating temperature of the crystallizing stream must be lower than the boiling point of all its constituents. The freezing points for EG in this situation are 260.15 K, DMT is 413.80 K, and trace methanol is 175.47 K. The freezing point of DMT is much lower than 298.15 K, which is higher than that of EG and methanol. Methanol's (in trace) boiling points are 337.85 K, EG's are 470.45 K, and their respective values are 559.20 K. The requirements were satisfied, which gave us the chance to recover a very high DMT. In crystallizer 1, at its operating settings and with the solvents available, DMT had a solubility of 0.122. It equated to 1.3574 g of DMT/L of solvent mixture, or 0.122 g of DMT per 100 g of the solvent combination. The product stream contained a 0.7575 (1003.55 kg/h) mass fraction of DMT crystal, a 0.0003 (0.38 kg/h) mass fraction of DMT, a 0.242 (321.63 kg/h) mass fraction of EG, and a 0.0002 (0.26 kg/h) mass fraction of methanol at a temperature and pressure of 298.15 K and 1.0133 Bar, respectively. Pump 7 pushed the product stream from crystallizer 1 into filter 2 at a pressure of 2.0265 bar. Filter 2 specifies phase separation of percentage of liquid to fraction of solid to fraction of solid to fraction of solid at 1.0133 bar pressure. Heater 3 was used to extract DMT for packaging for sale or further processing.

The mass fraction mixture that went through filter 2 for filtration was 0.9980 (320.63 kg/h) of EG, 0.0008 (0.26 kg/h) of methanol, and 0.0012 (0.38 kg/h) of DMT waste (designated as E-M-D-W-1) that was transported into the EG recovery section or waste pond by pump 8 running at 2.0265 bar pressure.

IV. Results and Discussion for the Methanolysis Method of PET Digestion into DMT

Using intermediate products and recovered materials, the overall material and energy balances for the chemical recycling of a 1000 kg/h flow rate of PET bottle waste into DMT using the methanolysis process were determined. The



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in-line processing scope of this effort, as shown below, included the reaction and separation of the recovered and produced components.

The stoichiometry equation for the reaction is shown in equation 3 above. The reaction rate constant, k, for reactor 1 is 6.1676, and the activation energy, Ea, is 96.5628 kJ/mol. According to equation (3), one mole of PET reacts with two moles of CH₃OH to produce one mole of DMT, one mole of EG, and one mole of CH₃OH. This work was built on the depolymerisation of PET bottle waste at a rate of 1000 kg/h utilizing the methanolysis method, and the anticipated results were based on the reaction equation (3). Table 2 presents the findings from both this study and Liu et al. (2015). It is clear that the 99.35% yields for DMT and EG and the accompanying selectivity were consistent with Liu et al. (2015) findings. They hardly differ from one another at the same optimal operating conditions of 571.15 K, 80.92 bar pressure, and 1.8667 h residence time. Additionally, the process' selectivity for DMT, which was 0.7578, and EG, which was 0.2422, both showed that it was viable and that it preferred the production of DMT over EG.

Table 2: Validation of this work of methanolysis method of depolymerisation of PET bottle waste into DMT (reactor 1 products) with that of Liu et al. (2015)

Reactor 1 output						
Component	Quantity (kg)	%	Mass	Mole	% yield	selectivity
			fractio	fraction		
PET conversion	993.5136	99.35				
Unreacted PET	6.4864	0.65	0.0009	0.0002		
Methanol	331.3123	5.52				
conversion						
Unreacted +	5668.6877	94.48	0.8098	0.9446		
excess						
Expected DMT	1010.4865					
Produced DMT	1003.9357		0.1435	0.0276	99.35	0.7578
Expected EG	322.9841					
Produced EG	320.9803		0.0458	0.0276	99.35	0.2422
Produced EG Property	320.9803	This wor	0.0458 k	0.0276 (Liu et al.,	99.35 2015)	0.2422 Difference
Produced EG Property	320.9803	This wor Value	0.0458 k Unit	0.0276 (Liu et al., Value	99.35 2015) Unit	0.2422 Difference Value
Produced EG Property Temperature	320.9803	This worValue571.1	0.0458 k Unit K	0.0276 (Liu et al., Value 571.15	99.35 2015) Unit K	0.2422 Difference Value
Produced EG Property Temperature Pressure	320.9803	This wor Value 571.1 80.92	0.0458 k Unit K bar	0.0276 (Liu et al., Value 571.15 80.92	99.35 2015) Unit K bar	0.2422 Difference Value
Produced EG Property Temperature Pressure Residence time	320.9803	This wor Value 571.1 80.92 1.866	0.0458 k Unit K bar h	0.0276 (Liu et al., Value 571.15 80.92 1.8667	99.35 2015) Unit K bar h	0.2422 Difference Value
Produced EG Property Temperature Pressure Residence time (Mass ratio) CH ₃ OH	320.9803	This wor Value 571.1 80.92 1.866 6:1	0.0458 k Unit K bar h	0.0276 (Liu et al., Value 571.15 80.92 1.8667 6:1	99.35 2015) Unit K bar h	0.2422 Difference Value
Produced EG Property Temperature Pressure Residence time (Mass ratio) CH ₃ OF	1:PET	This wor Value 571.1 80.92 1.866 6:1 Value	0.0458 k Unit K bar h Unit	0.0276 (Liu et al., Value 571.15 80.92 1.8667 6:1 Value	99.35 2015) Unit K bar h Unit	0.2422 Difference Value Value Value
Produced EG Property Temperature Pressure Residence time (Mass ratio) CH ₃ OH yield of DMT	320.9803	This wor Value 571.1 80.92 1.866 6:1 Value 99.35	0.0458 k Unit K bar h Unit %	0.0276 (Liu et al., Value 571.15 80.92 1.8667 6:1 Value 99.79	99.35 2015) Unit K bar h Unit %	0.2422 Difference Value Value Value 0.44 (%)
Produced EG Property Temperature Pressure Residence time (Mass ratio) CH ₃ OH yield of DMT yield of EG	320.9803	This wor Value 571.1 80.92 1.866 6:1 Value 99.35 99.35	0.0458 k Unit k bar h Unit % %	0.0276 (Liu et al., Value 571.15 80.92 1.8667 6:1 Value 99.79 99.79	99.35 2015) Unit K bar h Unit % %	0.2422 Difference Value Value Value 0.44 (%) 0.44 (%)
Produced EG Property Temperature Pressure Residence time (Mass ratio) CH ₃ OH yield of DMT yield of EG Selectivity of DMT	1:PET	This wor Value 571.1 80.92 1.866 6:1 Value 99.35 99.35 0.757	0.0458 k Unit bar h Unit % %	0.0276 (Liu et al., Value 571.15 80.92 1.8667 6:1 Value 99.79 99.79 0.7577	99.35 2015) Unit K bar h Unit % %	0.2422 Difference Value Value Value 0.44 (%) 0.44 (%) 0.0001

By comparing the data and findings of this study to earlier research by the authors named below, the data and findings were further confirmed. The work of Liu et al. (2015) gets the closest (99.35% DMT) despite the variations in operating conditions for converting PET bottle waste into DMT. The results of DMT production show a declining trend, with values of 93.10 percent by Pham and Cho. (2021), 91.0 percent by Tang et al. (2022), and 89.10 percent by Jiang et al. (2022). Ma et al. (2022) and Tollini et al. (2022) both produced the poorest results, with 78.40% and 71.00%, respectively.

Table 3: Summary of the overall material balance of the waste system boundary of the neutral hydrolysis method of chemical recycling of PET bottles in terms of feeds, wastes generated, and products (recovered materials and purified products).



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Operation (Component	PET	CH ₃ OH		Operation / Componen	PET	CH ₃ OH	DM	EG
Gomponent				Componen			1	
Feed 1	1000.00	1000.00		Product 1 (PET-R-	6.49			
Feed 2		5000.00		Product 2 (MEOH-		5668.43	0.00	0.26
				R-1)			(trac	
Total (kg/h)	1000.00	6000.00		Product 3 (Heater 3-			1003	
				PDT)			.55	
Feeds grand total	7000.00			Products Total	6.49	5668.43	1003	0.26
(kg/h)				(kg/h)			.55	
Operation /	EG	CH ₃ OH	DMT	Products grand	6678			
/ Component				total (kg/h)	.73			
Waste 1 (E-M-D-W-	320.63	0.26	0.38					
1)								
Wastes total (kg/h)	320.63	0.26	0.38					
Wastes grand total (kg/h)	321.27							

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Energy balances are: cooling is 17375482.49 kJ/h with 831163.95 kg/h of cooling water; refrigeration using propane is 907687.08 kJ/h and 226921.47 kg/h; heating is 6623.4349 kJ/h using 3.2570 kg/h of medium pressure steam (MPS); 10596299.0937 kJ/h using 6212.5791 kg/h of high pressure steam (HPS); and 13853629.7594 kJ/h using 23089.3523 kg/h of fired heat steam (FHS). Total steam energy consumed for this came to 24456552.288 kJ/h, with 29305.1884 kg/h of burned heat steam in addition to medium and high pressure steam. Additionally, 69.01 kWh of power are needed for pumping.

VI. CONCLUSION AND FUTURE WORK

The methanolysis digestion method approach to chemical recycling was used to carry out the experimental PET digestion into DMT. To solve the problems with product mix separation, particularly PET bottle garbage, CSTR used the data for design, modelling, and simulation in the Aspen Plus V10 simulator. Another objective is the commercial production of DMT from PET bottle waste. DMT and EG yields grow with increasing residence time and the CH₃OH:PET reactant ratio until reaction equilibrium is attained. DMT and EG yields of 99.35 percent each were attained, with selectivity of 0.7578 for DMT and 0.2422 for EG. The best operating parameters for this technique were a 1.8667-hour residence period, 571.15 K, autogenous pressure, and a CH₃0H:PET weight ratio of 6. Aspen Plus V10 software was used to mimic eight pumps: a reflux pump, a reboiler, a condenser, two filters, a distillation column, a crystallizer, three heaters, two coolers, and a refrigerator in order to separate the combination of products. The reactor's outputs were CH₃OH (5668.69 kg/h), EG (320.89 kg/h), unreacted PET (6.49 kg/h), and DMT (1003.93 kg/h). Unreacted PET was fully removed by Filter 1. In a distillation column, methanol that was 100 percent pure was recovered. Filter 2 divided the filtrate into 100% pure DMT and 99.80% pure EG after EG crystallized into DMT. The total amount of feed materials used per hour was 7000 kg, which matched the amount of products and waste intended for recovery. The system generated 17375482.49 kJ/h of cooling energy using a total of 831163.95 kg/h of cooling water. Using 226921.47 kg/h of propane, the energy needed for refrigeration was 907687.08 kJ/h. The system's 24456552.288 kJ/h total heating energy need was met by running 3.2570 kg/h of medium-pressure steam, 6212.5791 kg/h of high-pressure steam, and 23089.3523 kg/h of fired heat steam. Pumping used 69.01 kWh in total of electricity. The system generated 17375482.49 kJ/h of cooling energy using a total of 831163.95 kg/h of cooling water. Using 226921.47 kg/h of propane, the energy needed for refrigeration was 907687.08 kJ/h. The system's 24456552.288 kJ/h total heating energy need was met by running 3.2570 kg/h of medium-pressure steam, 6212.5791 kg/h of high-pressure steam, and 23089.3523 kg/h of fired heat steam. Pumping used 69.01 kWh of electricity in total.

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