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Sustainable Polyurethane Technology

PEP Report 10E

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Glossary

AlkPO	Alkoxylated polyol
barg	Bar gauge
BFD	Block flow diagram
BFW	Boiler feedwater
bhp	Brake horsepower
BL	Battery limit
BLI	Battery limits investment
°C	Degrees Celsius
CAGR	Compound annual growth rate
capex	Capital expenditure
CC	Cyclic carbonate
¢/gal	Cents per gallon
CHW	Chilled water
¢/kWh	Cents per kilowatt-hour
¢/lb	Cents per pound
¢/Mgal	Cents per thousand gallons
cP	Centipoise
CSBO	Carbonated soybean oil
CSTR	Continuous stirred tank reactor
¢/TR-h	Cents per refrigeration ton-hour
CW	Cooling water
CWR	Cooling water return
CWS	Cooling water supply
DABCO	1,4-diazabicyclo-[2,2,2]-octane (33%) in dipropylene glycol (67%)
DEG	Diethylene glycol
DI	Deionized
$/h	Dollars per hour
$/kg	Dollars per kilogram
DM	Demineralized
DMC	Double metal cyanide
$/Mlb	Dollars per thousand pounds
$/Mscf	Dollars per thousand standard cubic feet
$/t	Dollars per metric ton
EO	Ethylene oxide
EOL	End-of-life
EPC	Engineering procurement and construction
ESBO	Epoxidized soybean oil
ETP	Effluent treatment plant
°F	Degrees Fahrenheit
FOB	Free/freight on board
ft	Feet
ft dia	Feet diameter
G&A	General and administrative
gal	Gallons
GHG	Greenhouse gas
gpm	Gallons per minute
HO	Hot oil
HVAC	Heating, ventilation and air conditioning
kg	Kilograms
$kgCO_2eq$	Kilograms of CO_2 equivalent
kg/h	Kilograms per hour
kg/m^3	Kilograms per cubic meter
kg/min	Kilograms per minute
kg/y	Kilograms per year
kJ/h	Kilojoules per hour

kW	Kilowatts
kWh	Kilowatt-hour
kWh/lb	Kilowatt-hour per pound
lb	Pounds
lb/h	Pounds per hour
lb/lb	Pounds per pound
LP	Low-pressure
LPC	Low-pressure condensate
LPS	Low-pressure steam
m^3	Cubic meters
mb	Millibar
MDI	Methylene diphenyl diisocyanate
mg KOH/g	Milligrams of KOH per gram
min	Minutes
Mlb/h	Thousand pounds per hour
mm	Millimeters
MMBtu	Million British thermal units
MMBtu/h	Million British thermal units per hour
MMBtu/lb	Million British thermal units per pound
m/min	Meters per minute
MMlb/y	Million pounds per year
MMt/y	Million metric tons per year
MOC	Material of construction
Mol. wt.	Molecular weight
MPag	Megapascals gauge
Mscfh	Thousand standard cubic feet per hour
Niax	Bis (2-dimethylaminoethyl) ether (70%) in dipropylene glycol (30%)
NIPU	Non-isocyanate polyurethane
PEP	Process Economics Program
PFD	Process flow diagram
PHU	Polyhydroxyurethane
PO	Propylene oxide
ppm	Parts per million
ppmw	Parts per million by weight
psig	Pounds per square inch gauge
PU	Polyurethane
PVC	Polyvinyl chloride
R&D	Research and development
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RePO	Recycled polyol
ROI	Return on investment
scf	Standard cubic feet
sq ft	Square feet
SS	Stainless steel
TBAB	Tetrabutylammonium bromide
TDI	Toluene diisocyanate
TDS	Total dissolved solids
TFC	Total fixed capital
TFE	Thin-film evaporator
TR	Refrigeration ton
TR-h	Refrigeration ton-hour
TRL	Technology readiness level
t/t	Metric tons per metric ton
t/y	Metric tons per year
USGC	US Gulf Coast
UV	Ultraviolet
VDR	Vacuum distillation reactor

wt%	Weight percent
w/w	Weight by weight
y	Years

Abstract

Polyurethanes (PUs) are ranked among the sixth most manufactured polymers worldwide and are widely used in a variety of applications because of the diverse properties they offer. Nevertheless, PUs are raising questions around their environmental, legislative, health, and recycling concerns. Currently, the PU industries are heavily dependent on petroleum; the two major feedstocks — polyols and isocyanates — are largely petroleum-derived. Because of the depletion of fossil fuels, environmental concerns of greenhouse gas (GHG) emissions in the PU synthesis process, and the dramatically increased costs of petroleum feedstocks, many researchers are focusing on finding renewable resources to reduce the use of fossil fuels, with the anticipation of increased adaptation in the coming years. Moreover, sustainable feedstocks stand out as a viable option to synthesize greener PU. Bio-based polyfunctional short alcohol and isocyanate compounds have emerged to design fully bio-based PU materials with targeted chemical and mechanical properties.

In this report, we review the current industrial status of large-scale PU production via sustainable routes. A brief technology overview of various processes to produce PUs from renewable resources is presented, covering aspects such as process design, catalyst performance, process efficiency, and the overall technology readiness. A more in-depth analysis, including technoeconomic evaluations, is presented for the following three processes:

- Bio-based polyols: This technology utilizes bio-based feedstocks such as castor oil to produce polyols, which are essential for PU production. These bio-based polyols are then polymerized with isocyanates to form PU products, resulting in a reduced carbon footprint and a more sustainable alternative to traditional fossil-derived polyols.
- Non-isocyanate polyurethane (NIPU) route: NIPU represents an innovative method of synthesizing PU without the use of toxic isocyanates. This process involves the reaction of cyclic carbonates with amines. Cycloaddition of CO_2 to epoxidized soybean oil generates cyclic carbonates, which then react with diamines to form NIPUs. This approach not only eliminates the reliance on fossil fuels but also utilizes CO_2 as a raw material, helping to mitigate GHG emissions.
- Recycling of PU waste: This method emphasizes the chemical recycling of PU waste materials. Through glycolysis, discarded PU products are broken down into their original polyols, which can then react with isocyanates to produce new PUs. This process diverts waste from landfills and reduces the demand for virgin materials, promoting a circular economy in the PU industry.

The production economics assessment in this report is based on a US Gulf Coast location. An iPEP Navigator tool is also attached to the electronic version of this report. The interactive iPEP Navigator module provides an economic snapshot for each of the abovementioned processes, with options to choose from different units as well as regions of interest. Apart from the technical and economic analyses, we have also included material balance tables, a sized equipment list, and process flow diagrams for each of these technologies.

The technological and economic assessment of the process is the Process Economics Program's independent interpretation of a potential commercial process. Each of these is based on the information presented in the open literature, such as patents or technical articles, and may not reflect in whole or in part the actual plant configuration. We do believe that these sources are sufficient to represent the process and process economics within the range of accuracy necessary for the economic evaluations of the conceptual process designs.

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