IHS CHEMICAL

Upgradation of Pygas C\textsubscript{5} Cut to Produce Isoprene and Other Products

PEP Review 2016-06

April 2016

Rajesh Kumar Verma
Principal Analyst
Upgradation of Pygas C$_5$ Cut to Produce Isoprene and Other By-products

Rajesh Kumar Verma, Principal Analyst

Abstract
Pyrolysis gasoline, or Pygas, is a by-product of high-temperature naphtha cracking during ethylene and propylene production. Pygas is a naphtha-range product containing C$_5$- to C$_{12}$-range aromatics, di-olefins, olefins, and paraffins. Pygas has a high octane value, and thus is potentially a good blending material for motor gasoline after some treatment. It can also be further fractionated in various cuts, which can be used as feedstock to produce high-value products.

The focus of this review is to evaluate the value of upgradation routes for the Pygas C$_5$ cut. In this study, we have done a technoeconomic evaluation of the most recent GTC Technology process to produce polymer-grade isoprene, piperylene, and dicyclopentadiene (DCPD). The main product of the process is isoprene, while piperylene and dicyclopentadiene are by-products. We also assess and describe the differences between the older GTC process and the newer (current) version of the technology. (It should be noted that the older version was never offered by GTC for license.)

This review also presents technical and economic evaluation of a process for production of polymer-grade DCPD. In addition, a CDEtherol® process for production of TAME (tertiary amyl methyl ether) based on an isoamylene-rich stream as feedstock is presented.

The process economics include estimated capital costs and production costs; variable cost, plant cash cost, and plant gate cost are also presented separately as part of net production costs. A brief market overview summarizes the global supply and demand end-use market and demand drivers.

This review is based on data drawn from public information sources (mainly patents) with guidance from GTC Technology. Aspen Simulation Workbook™ models are developed for both the cases to evaluate the process economics (CAPEX and OPEX) with the help of the proprietary IHS PEP Cost index. Some of the technical and economic information used in the design was based on the author’s own engineering judgment.

The production economics presented in this review are based on a US Gulf Coast location and are in English units. However, we also attach an iPEP Navigator module with the PDF file of this review to allow a quick conversion of the process economics in other major regions (i.e., China, Germany, Japan, the Middle East, and Canada). With the selection of each competing process, the module also allows production economics to be reported in each region in either English or metric units.
# Contents

1 Summary
   Differences between the IHS results and licensor-offered recoveries 5

2 Introduction
   Overview 9
   Industrial application of isoprene and other by-products
      Isoprene 11
      DCPD (dicyclopentadiene) 12
      Piperylene 12
      TAME (tertiary amyl methyl ether) 12

3 Isoprene separation from Pygas C₅ cut
   Solvents and chemical treatments 14
   Industrial status
      Isoprene 15
      Piperylene 16
      Dicyclopentadiene 17
   Literature survey/patents summary 19
   Process description
      Isoprene concentration section GT-C₅<sup>SM</sup> 24
      Isoprene purification section GT-Isoprene™ 25
   Design basis 27
   Material balance 28
   Economics 30
   Environmental concerns 37

4 Etherol process for TAME production
   CDTech Etherol process 38
   Chemistry 38
   Catalyst 40
   Industry outlook 41
   Literature survey/patents summary 42
   Process description 44
   Design basis 47
   Material balance 47
   Economics 49

5 Ultrapure DCPD production
   Literature survey/patents summary 54
   Process description 55
   Material balance 57
   Economics 58
Tables

Table 1  Summary of isoprene production economics 7
Table 2  Typical composition for Pygas C₅ cut (naphtha cracker) with components MW and TBP 10
Table 3  DCPD consumption in each sector 17
Table 4  Companies producing isoprene worldwide—Capacity and processes being used 18
Table 5  Design basis for isoprene process 27
Table 6  Component balance for C₅ and isoprene section 28
Table 7  Isoprene separation from Pygas C₅ cut by solvent extraction—Major equipment 31
Table 8  Isoprene separation from Pygas C₅ cut by solvent extraction—Total capital investment 34
Table 9  Isoprene separation from Pygas C₅ cut by solvent extraction—Production costs 35
Table 10  Companies producing TAME with capacities 41
Table 11  Design basis for etherol process 47
Table 12  Component balance for TAME plant 47
Table 13  TAME production on product basis—Major equipment 49
Table 14  TAME production on product basis—Total capital investment 50
Table 15  TAME production on product basis—Production costs 51
Table 16  Component balance for ultrapure DCPD plant 57
Table 17  DCPD production cost on product basis—Major equipment 58
Table 18  DCPD production cost on product basis—Total capital investment 59
Table 19  DCPD production cost on product basis—Production costs 60

Figures

Figure 1  Block diagram for naphtha cracker to Pygas C₅ cut 9
Figure 2  Industrial applications of isoprene 11
Figure 3  Isoprene production (based on processes used) and major isoprene consumers—2015 16
Figure 4  Consumption of piperylene in each sector 17
Figure 5  Two-stage solvent extraction process 21
Figure 6  Single-stage solvent extraction process 23
Figure 7  Effect of plant design capacity on CAPEX 36
Figure 8  Effect of plant operating capacity on product value 36
Figure 9  Effect of by-product prices (piperylene) on product value 37
Figure 10  Effect of temperature on ether yield 39
Figure 11  Interbed cooling arrangements 43
Figure 12  Helices packing 44
Figure 13  Effect of plant design capacity on CAPEX 52
Figure 14  Effect of unit operating level on product value 52
Figure 15  Effect of TAME feed price on product value 53
Figure 16  Effect of unit operating level on product value 61
Figure 17  Effect of unit plant design capacity on product value 61
Figure 18  Process schematic for GTC (C₅ + DCPD) section—GT-C₅<sup>SM</sup> 67
Figure 19  Process schematic for GTC isoprene section—GT-ISOPRENE<sup>SM</sup> 68
Figure 20  Process schematic for ultrapure DCPD production 69
Figure 21  Process schematic for TAME production—CDEtherol® process 70