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PETROCHEMICALS 101

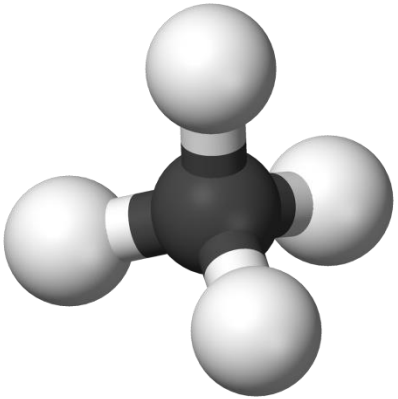
By Ben Gonzalez

OUTLINE

- Petrochemicals
- Hydrocarbon Chemistry
- Value Chain
- Economics
- Olefins
- Aromatics
- Polymers
- Outlook
- Appendix

WHAT ARE PETROCHEMCALS?

- Chemical products derived from petroleum, natural gas, and coal
- The two most common classes are olefins and aromatics
- Used as building blocks to producing plastics, solvents, foams fabrics, fibers, nylons and rubbers.
- Some aromatics can also be used as gasoline blending feedstock.
- Growth in production located where cheap feedstock



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HYDROCARBON CHEMISTRY

CLASSIFICATIONS

- Organic Chemistry – study of the structure of properties, composition, reactions, and preparation of carbon-containing compounds, including hydrocarbons.
- Hydrocarbons, compounds that contain only carbon and hydrogen, are the principal constituents of petroleum and natural gas, and can be classified into three categories
  - Aliphatics – alkanes (paraffins), alkenes (olefins), and alkynes.
  - Cycloaliphatics (cycloalkanes or naphthenes)
  - Aromatics

1. https://www.britannica.com/science/hydrocarbon

ALKANES

Paraffins - Straight Chain Compounds, saturated hydrocarbons, having formula C_nH_{2n+2}.

Formula	Name	Formula	Name
CH_4	Methane	C_6H_{14}	Hexane
C_2H_6	Ethane	C_7H_{16}	Heptane
C_3H_8	Propane	C_8H_{18}	Octane
C_4H_{10}	Butane	C_9H_{20}	Nonane
C_5H_{12}	Pentane	$C_{10}H_{22}$	Decane

Ethane, Propane, Butane, Naphtha, and Gas Oil are used as feed in steam crackers to produce ethylene, propylene, butadiene, benzene, toluene, and xylene.

1. Leffler, William (2000). Petroleum Refining in Nontechnical Language

2. https://www.britannica.com/science/hydrocarbon

ALKENES

- Olefins – Unsaturated hydrocarbons, containing a carbon-carbon double bond
- Main Olefins: Ethylene, Propylene, Butylene
- Key characteristic is absence of two hydrocarbons, formula C_nH_{2n}
- Chemically unstable, can be reacted with some other compound with ease

1. Leffler, William (2000). Petroleum Refining in Nontechnical Language

2. https://www.britannica.com/science/hydrocarbon

CYCLOALKANES

- Also known as naphthenes
- Class of hydrocarbons bent into ring or cyclic shape with formula C_nH_{2n}
- Examples: cyclopropane, cyclobutane, cyclopentane, cyclohexane, etc.

1. Leffler, William (2000). Petroleum Refining in Nontechnical Language

2. https://www.britannica.com/science/hydrocarbon

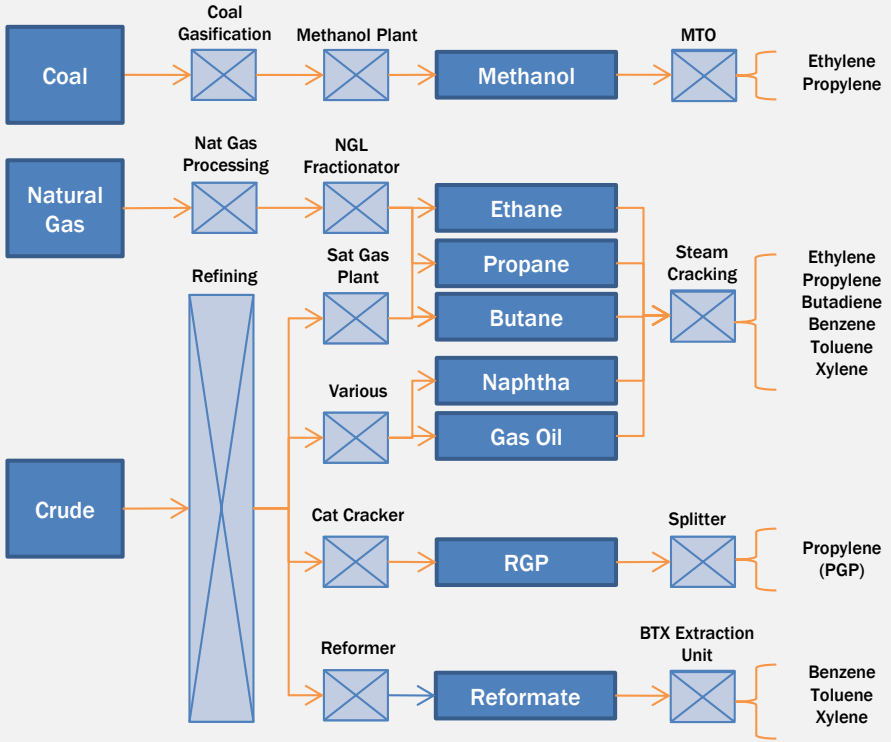
AROMATICS

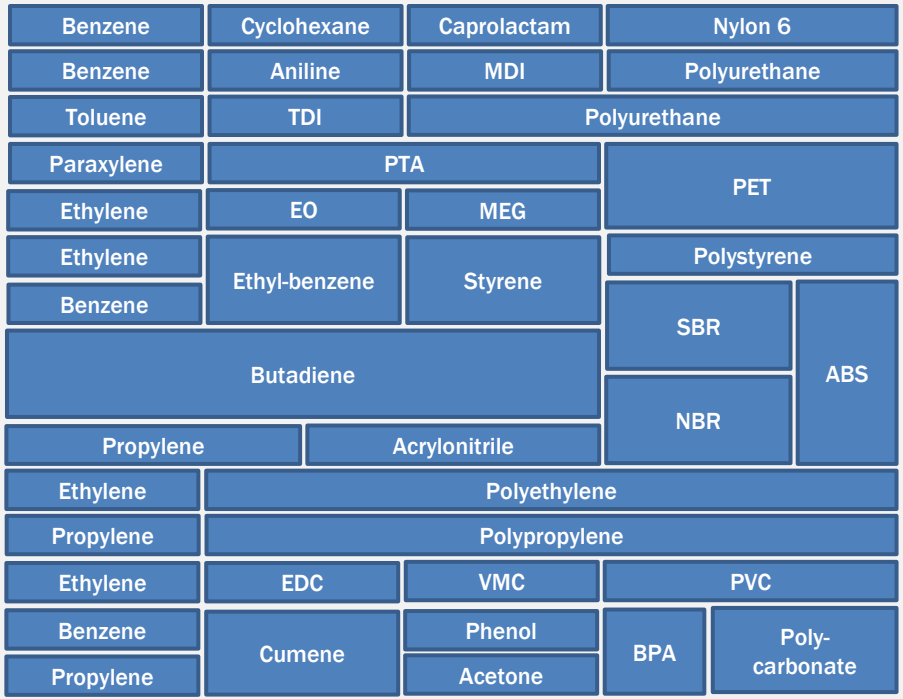
- Based on the benzene ring
  - A cyclohexane ring with a hydrogen atom removed from each carbon, and satisfying valence rules by putting double bonds between carbons.
- Referred to BTXs: Benzene, Toluene, and Xylenes
- Double bonds make the benzene ring unstable, used as building block in chemical industry
- Name aromatics came by characteristic smell of BTXs

1. Leffler, William (2000). Petroleum Refining in Nontechnical Language

2. https://www.britannica.com/science/hydrocarbon

PETROCHEMICAL VALUE CHAIN





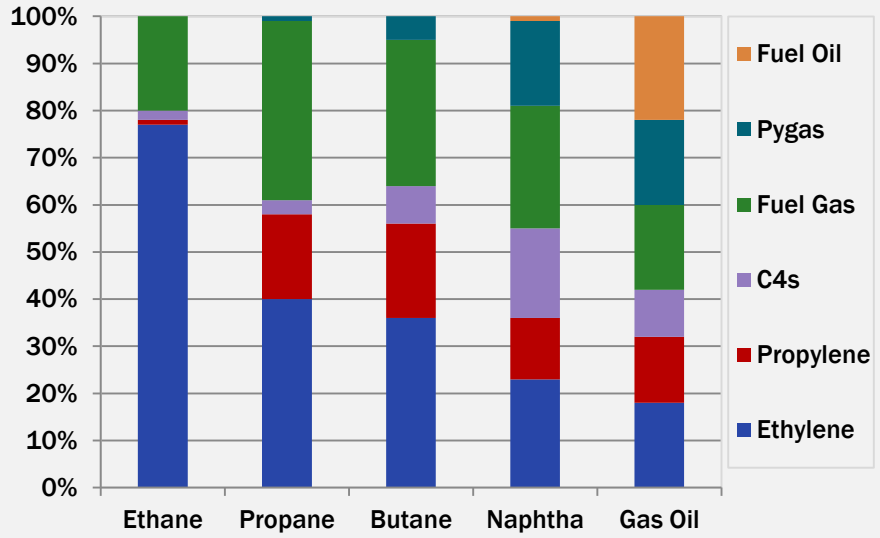
The process above goes from left to right, ending at the polymer. The blocks are not proportional to volume needed to produce the next product.

STEAM CRACKING

- Produces ethylene, the most fundamental petrochemical
- Uses ethane, propane, butane, naphtha or gas oil.
- Heavier feedstocks produce more co-products, Crude C4s and Aromatics
- Ethane yields the most ethylene, therefore requires less feed
- Ethane crackers typically have the lowest production costs
- Production costs for heavier feeds drop when prices for co-products rise
- Ethane is the preferred feedstock in regions where natural gas is abundant
- Where natural gas isn't abundant, naphtha is preferred

STEAM CRACKING YIELDS

Percentage of Product per Unit of Feed					
	Ethane	Propane	Butane	Naphtha	Gas Oil
	1	1	1	1	1
Ethylene	0.77	0.4	0.36	0.23	0.18
Propylene	0.01	0.18	0.2	0.13	0.14
C4s	0.02	0.03	0.08	0.19	0.1
Fuel Gas	0.2	0.38	0.31	0.26	0.18
Pygas		0.01	0.05	0.18	0.18
Fuel Oil				0.01	0.22



As previously mentioned, Ethane, Propane, Butane, Naphtha, and Gas Oil are used as feed in steam crackers. Ethane yields the most ethylene, and yields the least by-products. Heavier feedstock yields less ethylene, but yields more by-products. The feed slate can be mixed in more complex facilities.

1. Leffler, William (2000). Petroleum Refining in Nontechnical Language

STEAM CRACKER ECONOMICS

- Revenue – Costs = Margin
- Revenue – (Variable Costs + Fixed Costs) = Margin
- Revenue = Ethylene Price
- Variable Costs = Raw Materials – Co-Product Prices + Utilities
- Raw Materials = Feedstock + Catalysts
- Fixed Costs = Labor + Overhead + Maintenance + Taxes
- Ethylene – {[(Feedstock + Catalysts) – Co-Product Prices + Utilities] + [Labor + Overhead + Maintenance + Taxes]} = Margin

PRODUCTION MODEL (EXAMPLE)

Capacity	**1,000,000**	**mt/year**			
ISBL	1,680,001,633				
OSBL	672,000,653				
Other	588,000,572				
Total Capital Investment	**2,940,002,858**				
Variable Costs	**Per ton of ethylene**	**Unit**	**Market Price**	**Unit**	**Cost $/mt**
Raw Materials					
Feedstock					
Naphtha	3	mt	500	$/mt	1,500
Catalysts	*assumed value - 1 mt of ethylene at $5/mt*				5.00
Utilities					
Power	200	kwh	0.1	$/kwh	20
Fuel	8.15	MMBtu	6	$/MMBtu	48.90
Cooling Water	1	Mgal/mt	0.6	$/Mgal	0.6
Total Variable Costs					**1,574.50**
Co-Products/By-Products					**Co-Product Revenue $/mt**
Propylene	0.5	mt	800	$/mt	400
Crude C4s	0.3	mt	800	$/mt	240
Pygas	0.58	mt	800	$/mt	464
Fuel Oil	0.06	mt	300	$/mt	18
Hydrogen	0.56	mt	100	$/mt	56
Total Co-Product Credits					**1,178**
Fixed Costs					**Cost $/mt**
Labor	0.22	25/shift/mt	20	$/hr	4.38
Overhead	*75% of Labor Cost*				3.29
Maintenance	*3% of ISBL*				50.40
Taxes	*1.5% of Total Capital Investment*				44.10
Total Fixed Costs					**102.17**
Product					**Revenue $/mt**
Ethylene	1	mt	1,000	$/mt	**1,000**
Production Cash Cost					**498.67**
Margin					**501.33**

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OLEFINS

ETHYLENE

- Ethylene or ethene with formula C2H4 is the simplest member of the alkene (olefins) class of hydrocarbons.
- Ethylene is produced by steam cracking.
- Most of ethylene production goes into producing polyethylene, and is the most widely used petrochemical.
- Ethylene is also an important natural plant hormone, and is used in the agriculture industry to promote ripening.

OTHER ETHYLENE PROCESSES

- CTO – coal is gasified to produce a syngas which is then converted to methanol; methanol is then converted to ethylene and propylene.
- MTO – methanol is converted to olefins;
- Ethanol to Ethylene – dehydration of ethanol from sugar cane (brazil) or corn (US).

ETHYLENE DERIVATIVES

- Polyethylene – the largest demand for ethylene making up more than half of ethylene consumption globally; includes low density polyethylene (LDPE), linear low density polyethylene (LLDPE), and high density polyethylene (HDPE). Major applications include packaging.
- Ethylbenzene – used to produce styrene which is used to produce polystyrene plastics, ABS/SAN plastics, SBR rubber, and unsaturated polyesters.
- Ethylene Dichloride – used to make vinyl chloride monomer to make polyvinyl chloride (PVC, vinyl)
- Ethylene Oxide – used to make ethylene glycol which makes solvents, and PET plastic/polyester when combined with paraxylene.
- Vinyl Acetate - used to produce a wide range of adhesives and paints.
- Ethyl alcohol (ethanol) – used in pharmaceuticals, cosmetics, detergents, printing inks, and more.

PROPYLENE

- Propylene or propene with formula C3H6 is the second simplest member of the alkene (olefins) class of hydrocarbons.
- Propylene is produced at the petroleum refinery in the fluid catalytic cracking unit (FCC) and steam cracker, both as by-products.
- Propylene is sold in the merchant market as refinery, chemical, or polymer grade propylene based on its purity.
  - Refinery-grade propylene (RGP) is made up of 65-75% propylene while the rest is mostly propane.
  - Chemical-grade propylene (CGP) is made up of 92% or more propylene.
  - Polymer-grade propylene (PGP) is 99.5 wt% minimum propylene.

PROPYLENE BY SOURCE

- Propylene is produced mostly as by-products from steam cracking and refining in the FCC process; also produced from on-purpose technologies such as propane dehydrogenation (PDH), olefin metathesis, coal-to-olefins (CTO), methanol-to-olefins (MTO), and coal to propylene (CTP).
- In the US, propylene is mostly sourced from the FCC process, then sent to splitters, due to more cracking of ethane derived from shale gas
- Globally, the majority of propylene is sourced from the steam cracking process.

REFINERY GRADE PROPYLENE (RGP)

- In a petroleum refinery, propylene is a by product of fluid catalytic cracking (FCC).
- The propylene/propane (PP) stream, also known as RGP, is feedstock to the alkylation unit for the production of alkylate to be used in gasoline blending as an octane enhancer.
- RGP is sold in the merchant market to midstream or chemical companies with splitters to separate the propane from the propylene.
-
- When RGP spot prices increase, the splitter operator will increase PGP prices to maintain a margin over the feedstock price.

ON PURPOSE PROPYLENE

- PDH – propane is selectively dehydrogenated to propylene; in spite of simple chemistry, industrial implementation is complicated.
- CTO – coal is gasified to produce a syngas which is then converted to methanol; methanol is then converted to ethylene and propylene.
- MTO/MTP – methanol is converted to olefins; the MTP process produces more propylene than ethylene
- Metathesis – also known as olefins conversion technology (OCT); reaction, promoted by catalyst, between ethylene and butene to form propylene.

PROPYLENE DERIVATIVES

- Polypropylene – produced by process of polymerization where short chains (propylene) are joined to make long chains (polypropylene).
- Propylene Oxide – used to make intermediaries that in turn make solvents and polyurethanes.
- Acrylonitrile – used to make rubber, ABS and SAN plastic, and acrylic fiber
- Cumene – used to make intermediaries that in turn make polycarbonate, epoxy and phenolic resins, PMMA, and solvents.
- Acrylic Acid – used to make super-absorbants
- Butyraldehyde – used to make intermediaries to make plasticisers, solvents, and acrylic esters
- Isopropanol – used to make intermediaries to make PMMA and solvents.

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AROMATICS

AROMATICS

- Benzene with formula C_6H_6 is composed of 6 carbon atoms formed in a ring with 1 hydrogen atom attached to each.
- Toluene (Methylbenzene) with formula C_7H_8 is mostly used as a solvent and used for enhancing octane in the gasoline blend pool.
- Xylene (Dimethylbenzene) with formula C_8H_{10} exists in three isomeric forms, used as solvents, gasoline blending, and feed for the production of dyes, fibers, and films.
  - Metaxylene (1,2-Dimethylbenzene) or m-xylene
  - Orthoxylene (1,3-Dimethylbenzene) or o-xylene
  - Paraxylene (1,4-Dimethylbenzene) or p-xylene

AROMATIC PRODUCTION

- Mostly Produced at the petroleum refinery and steam cracker.
  - In a refinery, benzene, toluene, and xylene are produced in an aromatics extraction unit using reformate as feed
  - Produced in steam crackers that use heavier feedstock like butane, naphtha, and gas oil; pygas is sent to an aromatics extraction unit to produce benzene, toluene, and xylene.
- Metallurgical coke production – bituminous coal is fed into ovens and heated at high temperatures. Coke oven gas is recovered, and cooled. Light oil is removed from the gas and fractionated to recover benzene, toluene and xylene.
- On purpose benzene production
  - Toluene Disproportionation (TDP) – Toluene and hydrogen are converted in a reactor with a catalyst to produce benzene and methane.
  - Hydrodealkylation (HDA) – less valuable toluene feed is converted to higher valued benzene and paraxylene, mixed with hydrogen and passed over a catalyst.

BENZENE DERIVATIVES

- Alkylbenzene used to make surfactants, which are used to produce detergents
- Cyclohexane – used to produce caprolactam, which is used to produce nylon
- Cumene – used to produce phenol and acetone, which are used to produce BPA for the production of polycarbonate and epoxy resins, phenolic resins, PMMA, and solvents
- Ethylbenzene - used to produce styrene which is used to produce polystyrene plastics, ABS/SAN plastics, SBR rubber, and unsaturated polyesters
- Aniline – used to produce diphenylmethane diisocyanate (MDI), which is used to produce polyurethane

TOLUENE AND XYLENE DERIVATIVES

- Toluene Diisocyanate – Used to produce polyurethane for foams, insulation, and coatings for furniture
- Trinitrotoluene (TNT) – prepared by the nitration of toluene with a mixture of nitric acid and sulfuric acid for the production of explosives. Not produced commercially.
- Solvents – used for solvents in adhesives, paints, and industrial cleaners.
- Orthoxylene – used for the production of plasticisers
- Paraxylene – used to produce PET/polyester

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POLYMERS

POLYMERS

- Polyethylene Teraphthalate (PET)/Polyester – Type 1 plastic produced from MEG and PTA from Paraxylene. Used mostly for disposable soft drinks and bottled water as well as fabric referred to as polyester.
- High Density Polyethylene (HDPE) – Type 2 plastic produced from ethylene. Used mostly for milk jugs, detergent bottles, juice bottles, toiletry bottles, toys….
- Polyvinyl Chloride (PVC)/Vinyl – Type 3 plastic produced from ethylene and chlorine. Used for cooking oil bottles, plumbing pipes, toys….
- Low Density Polyethylene (LDPE) – Type 4 plastic produced from ethylene. Used to produce grocery bags, food wraps, bread bags….
- Polypropylene (PP) – Type 5 plastic produced from propylene. Used to produce medicine bottles, electrical cable insulation, carpeting, mats, rope, Tupperware, plastic bottles, textiles, chairs, auto components…
- Polystyrene (PS) – Type 6 plastic produced from ethylene and benzene (ethylbenzene). Used for production of polystryene foam, disposable coffee cups, plastic food boxes, packing foam, insulation….

http://learn.eartheasy.com/2012/05/plastics-by-the-numbers/

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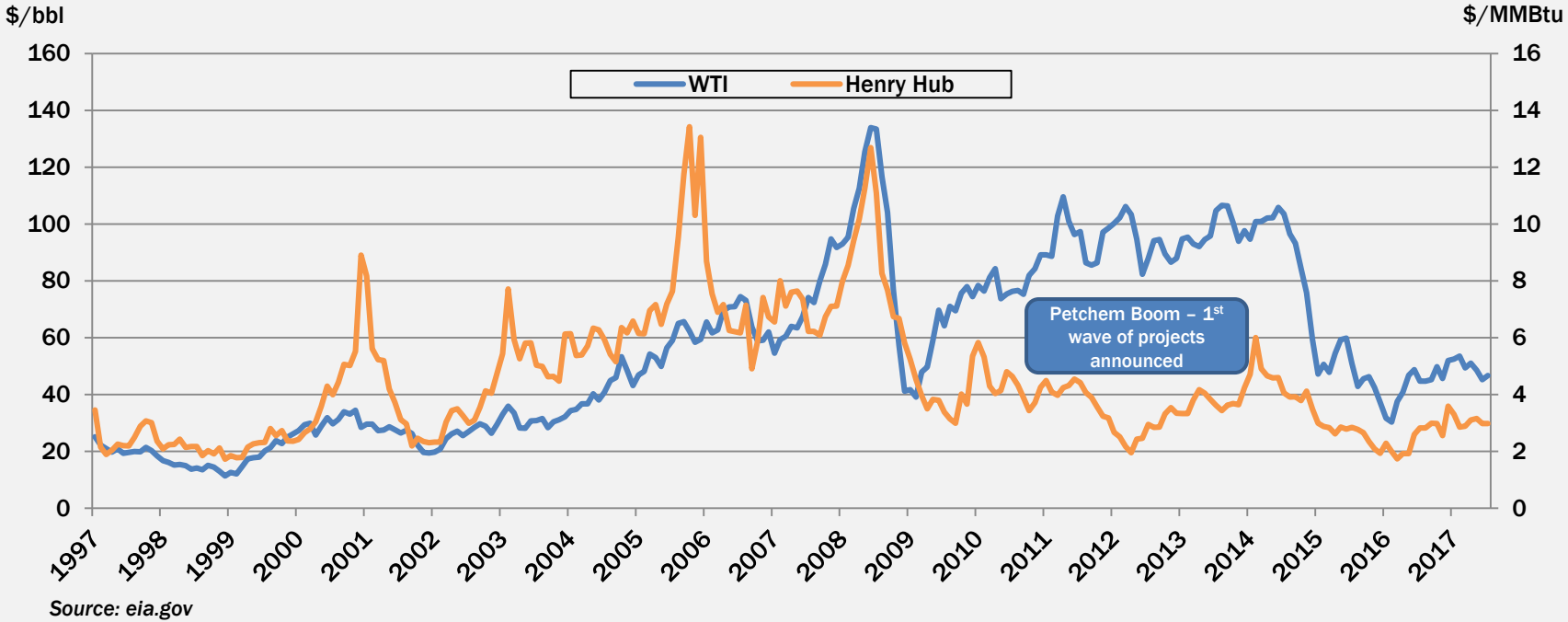
US PETROCHEMICALS

TOP 10 US PETROCHEMICAL COMPANIES IN 2016

Rank	COMPANY	CHEMICAL SALES ($ MILLIONS)	SECTOR	HEADQUARTERS
1	Dow Chemical	$48,158	Diversified	Midland, Mich.
2	ExxonMobil	26,058	Petrochemicals	Irving, Texas
3	DuPont	19,679	Diversified	Wilmington, Del.
4	PPG Industries	14,270	Paints, inorganics	Pittsburgh
5	Praxair	10,534	Industrial gases	Danbury, Conn.
6	Huntsman Corp.	9,657	Diversified	The Woodlands, Texas
7	Eastman Chemical	9,008	Diversified	Kingsport, Tenn.
8	Air Products	8,554	Industrial gases	Allentown, Pa.
9	Chevron Phillips	8,455	Petrochemicals	The Woodlands, Texas
10	Ecolab	7,653	Process services	St. Paul

Source: http://cen.acs.org/content/cen/articles/95/i19/Top-50-US-chemical-producers.html

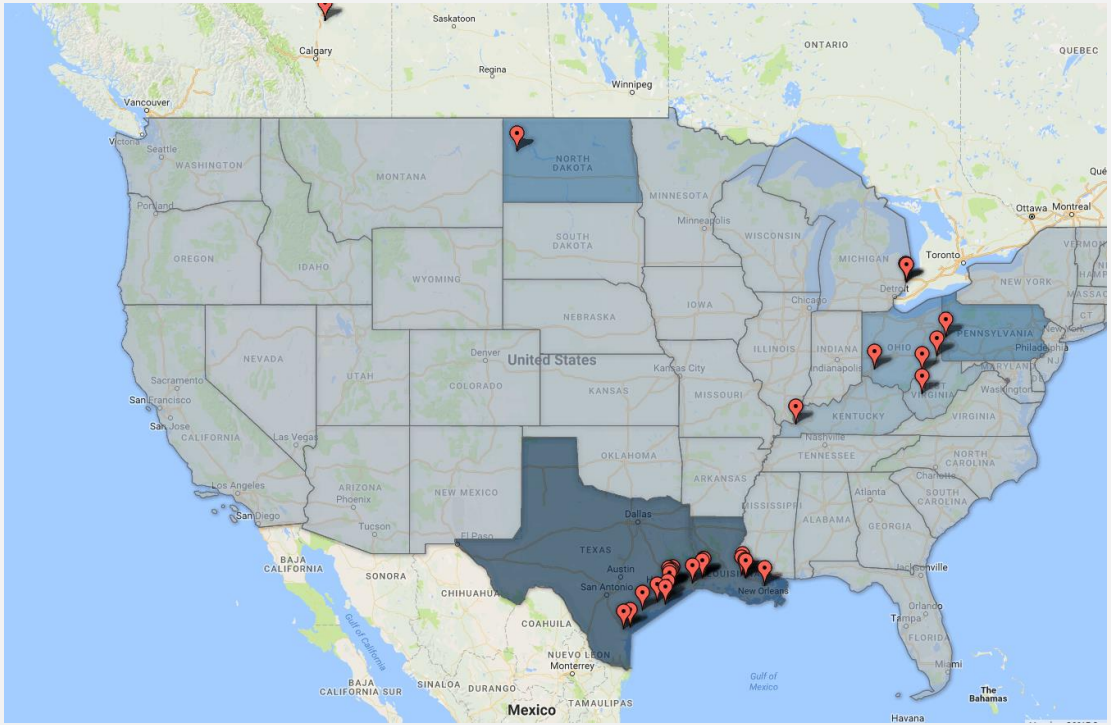
THE SHALE BOOM



Source: eia.gov

The spread between natural gas and crude prices at the end of 2009 through the end of 2014 incentivizes new ethylene projects.

PROPOSED ETHYLENE PROJECTS DURING THE US SHALE BOOM



- The US shale boom is responsible for a renaissance in the petrochemical industry.
  - New Steam Crackers
  - Capacity Expansions
  - Terminals
  - Vessels
  - Pipelines
  - Storage tanks and caverns
- All the proposed ethylene projects, greenfield and brownfield, are located near the shale plays.
- Of the proposed projects outside the USGC region, only the Shell project in Pennsylvania has been sanctioned. The PTTGC cracker in Ohio is expected to be sanctioned soon.

Source: http://analysis.petchem-update.com/engineering-and-construction/multimedia-mapping-us-ethane-cracker-construction-projects

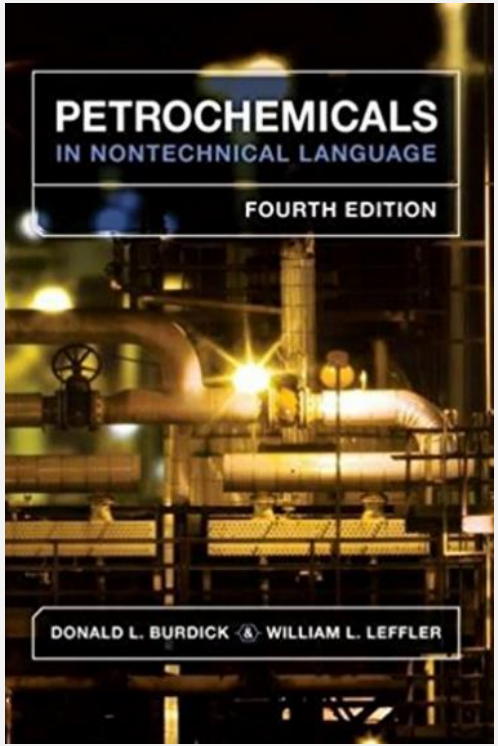
MARKET ANALYSIS

- Price Forecast
  - Long Term: Mostly tied to the energy value, feedstock price, or margin.
  - Short Term: Varies with supply, demand, and inventory fluctuations

- Supply Demand Forecast
  - Long Term: Demand is strongly tied to GDP. Supply forecast is based on how much product is needed to meet the demand. Facilities in forecast should be located in places with feedstock advantage.
  - Short Term: Monitor upcoming projects and maintenance schedule for all facilities on supply and demand side.

- Outlook
  - Global petrochemicals demand is expected to increase faster than refined products. Demand for refined products is expected to peak soon in the US, and within a decade or two globally according to multiple industry reports. Global petrochemical demand is expected to grow between 1-1.5 times faster than global GDP.

LITERATURE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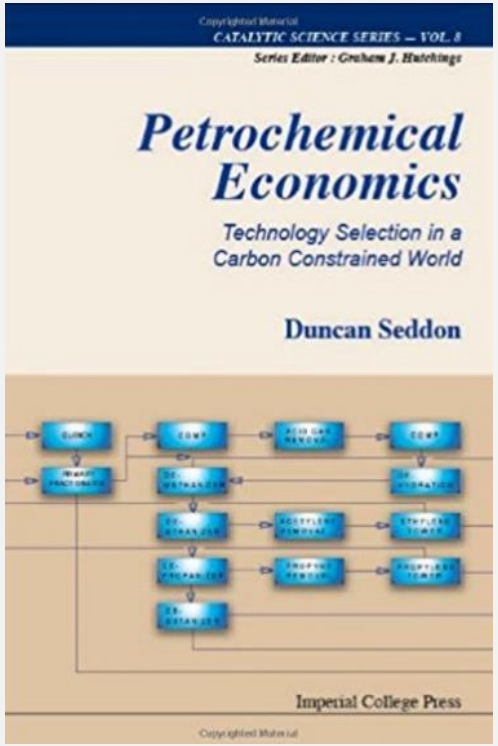
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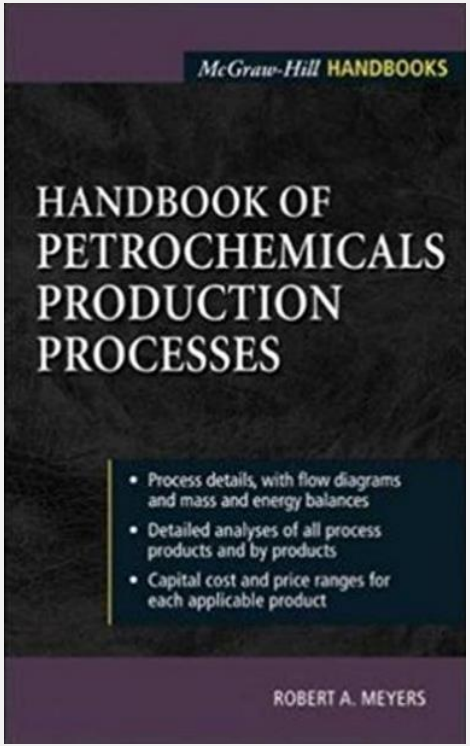
McGraw-Hill HANDBOOKS
HANDBOOK OF PETROCHEMICALS PRODUCTION PROCESSES
• Process details, with flow diagrams and mass and energy balances
• Detailed analyses of all process products and by products
• Capital cost and price ranges for each applicable product
ROBERT A. MEYERS

Q&A

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