Supplementary Information for Chemical Networks: a methodology to rapidly assess the environmental impact of chemical processes

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Introduction to graph theory

A brief introduction of terms is presented here (1).

In graph theory, a graph is defined as a structure to model relations between objects (hereby referred to as nodes), with nodes (or vertices or points) linked by edges (Figure S1a). These edges may have direction (leading to a directed graph, Figure S1b); multiple directed edges may link nodes (leading to a multidirected graph, Figure S1c) and weights may then be assigned to edges (leading to a multidirected weighted graph, Figure S1d).

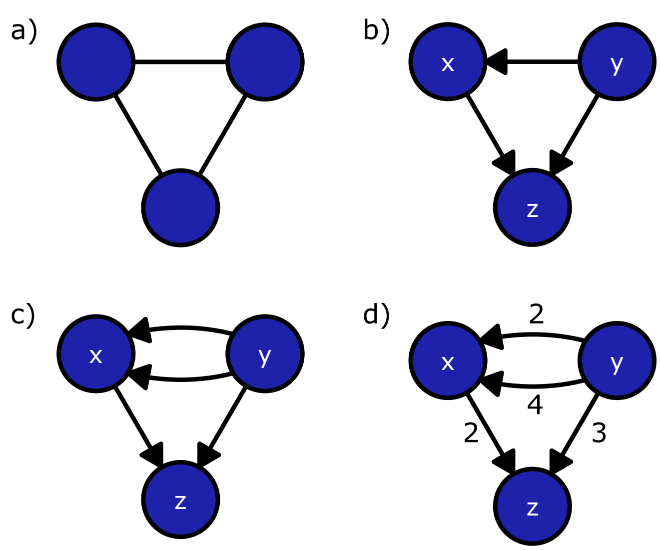

Figure S1: Examples of a) a graph with three nodes and three edges; b) a labelled directed graph; c) a labelled multidirected graph; d) a labelled, weighted multidirected graph.

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The degree of a node is the number of edges that are incident to it. So, in Figure S1c, *y* and *x* have a degree of 3, whereas *z* has a degree of 2. Indegree and outdegree are measures for nodes in directed graphs, where indegree is the number of head ends adjacent to a node, and outdegree the number of tail ends. So, in Figure S1c, *y* has an indegree of 0 and an outdegree of 3, whereas *x* has an indegree of 2 and an outdegree of 1. A node with an indegree of 0 (*y*) is named a source, and a node with an outdegree of 0 (*z*) is named a sink.

Graphs can contain subgraphs called paths. These are linear graphs with terminal nodes (two nodes with a degree of 1) which may be connected by other nodes (with a degree of 2).

Figure S2 demonstrates different possible paths from x and y to z.

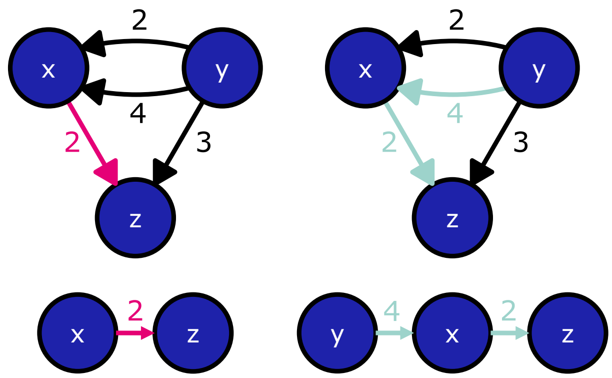

Figure S2: Examples of weighted subgraph paths from x to z and y to z via x.

Graph theory allows for the calculation of the shortest path from a source node to a sink (or target) node. This may be assigned from the number of edges, or steps, required (in this case the shortest path from *x* to *z* is equal to the shortest path from *y* to *z*, which is equal to 1), or if the graph is weighted, from the lowest weight path.

This is calculated from the sum of the weights of the edges of a path. The shortest path from *y* to *z* in Figure S2 is equal to 3. The longest path is equal to 6. There are several algorithms (Dijkstra's, Bellman-Ford, A*) for efficiently calculating the shortest path from source to target node (2).

It is possible for graphs to contain loops, (for instance if there existed a path from *x* back to *y*, or a path from *y* to *y*) but this is not relevant to this methodology.

Defining other variables

Feedstock consumption

Feedstock consumption is simply defined as the mass of primary feedstock consumed per mass of target product.

E-factor

The environmental factor, or E-factor, of a process is a metric of green chemistry, considering the mass of waste produced. It is primarily used in the fine chemicals industry, and was defined by Roger A. Sheldon (3) as:

$$\text{E-factor} = \frac{m_{\text{waste}}}{m_{\text{useful products}}} \qquad S1$$

The mass of all useful products is calculated from the sum of the masses of useful products. As $m_{\text{useful product}} < 0$, it is trivial to calculate this sum by summing all negative masses and multiplying by -1.

$$\frac{m_{\text{useful products}}}{m_{\text{target product}}} = -\sum \frac{m_{\text{useful product}}}{m_{\text{target product}}} \qquad S2$$

$$\text{where } m_{\text{target product}} > 0,\ m_{\text{useful product}} < 0$$

This value may also be used to convert net CO_2e per metric ton of target product to per metric ton of all useful products, via modification of equation S2.

The mass of total waste is calculated from the sum of the mass of all the feedstock minus the mass of all the useful products. As the consumption of useful products is negative, summing up all consumptions gives the total mass of waste.

$$\frac{m_{\text{waste}}}{m_{\text{target product}}} = \sum \frac{m_{\text{component}}}{m_{\text{target product}}} \qquad S3$$

$$\text{where } m_{\text{target product}} > 0,$$
$$\text{if component = feedstock, } m_{\text{feedstock}} > 0,$$
$$\text{if component = useful product, } m_{\text{useful product}} < 0$$

Energy consumption

Energy consumption is calculated in a similar way to equivalent CO_2 and divided into the same three variables.

Direct process energy consumption is calculated in much the same way as equivalent CO_2 but the enthalpy of combustion, ΔH_c, is used as the variable instead. This variable is defined per mass, rather than per mole, so if the units are given per mole than a conversion must be applied.

$$\frac{H_{\text{direct process}}}{m_{\text{target product}}} = \sum \frac{H_{\text{component}} \times m_{\text{component}}}{m_{\text{target product}}} \qquad S4$$

$$\text{where } m_{\text{target product}} > 0,$$
$$\text{if component = feedstock, } m_{\text{feedstock}} > 0,$$
$$\text{if component = useful product, } m_{\text{useful product}} < 0$$

Experimental data is required for accurate energy values. If no experimental data is available, energy E may be estimated from ΔH_f.

$$\frac{H_{\text{direct utilities}}}{m_{\text{target product}}} = \frac{H_{\text{natural gas}} + (L_{\text{steam}}(T, P) \times m_{\text{steam}})}{m_{\text{target product}}} \quad S5$$
$$\text{where } m_{\text{target product}} > 0$$

$$\frac{E_{\text{indirect utilities}}}{m_{\text{target product}}} = \frac{E_{\text{electricity}} + E_{\text{refrigeration}}}{m_{\text{target product}}} \quad S6$$
$$\text{where } m_{\text{target product}} > 0$$

Water consumption

Water consumption is calculated from the process water consumption plus the cooling water usage, at a set percentage bleed. Thus far, this percentage bleed has been set to 5%, but this could be varied for different regions, depending on ambient temperature etc.

$$\frac{\text{Net water consumption}}{m_{\text{target product}}} = \frac{\text{Process water consumption} + (\text{Cooling water bleed})}{m_{\text{target product}}} \quad S7$$
$$\text{where } m_{\text{target product}} > 0$$

Suggested improvements

The highest degree of uncertainty for the energy consumption is in direct process energy, due to the assignment of enthalpy values to the chemical feedstocks. Agreed upon values for the energies of ill-defined feedstocks, and potentially a move away from combustion enthalpy, may help rectify this.

The cooling water usage bleed should also be variable. This could be regional, with regions with a higher ambient temperature having a higher bleed, or process specific, based on temperatures etc. However, this level of detail may detract from the speed of data input, so an acceptable balance between accuracy and speed should be found.

More variables could be added to the processes, for example information on the safety of a process (toxicity, flammability etc.).

Building the network

The chemical pathways are built from pairs of nodes, with a weighted edge between them. Example data is presented in Table S1, and the graph illustrated in Figure S3.

Table S1: Example data for a multidirected, weighted chemical network.

Feedstock	Product	Weight
y	*x*	2
y	*x*	4
y	*z*	3
x	*z*	2

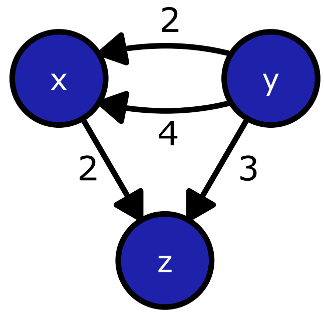

Figure S3: An example of a multidirected, weighted graph.

The consumption of each feedstock in a chemical pathway must be factored into the sustainability calculations. A solution presented is to treat feedstock consumption as another edge weight, and to create parallel network graphs with the two edge weightings. Each possible path can then be solved, and the weight, for example CO_2e, multiplied by the consumption weight, which has in turn been multiplied by the next consumption in the path. This requires the pathways to first be solved 'backwards', from target product to raw material.

Paths' weights may only be summed, not multiplied, so $\log 10^{\text{feedstock consumption}}$ is used as the edge weight. Table S2 shows a representative dataset, continuing the data from Figure S3, with feedstock consumption included.

Table S2: An example data set for processes from raw material y to target product z.

Target product	Feedstock	Product	Specific process	Feedstock consumption per metric ton product (t/t)	Net equivalent CO_2 per metric ton product (tCO_2e/t)
z	*y*	*x*	i	3	2
z	*y*	*x*	ii	4	4
z	*y*	*z*	iii	5	3
z	*x*	*z*	iv	3	2

To illustrate calculation of the net equivalent CO_2 per metric ton of *z* for each possible pathway, parallel network graphs weighted by $\log 10^{\text{feedstock consumption}}$ and CO_2e are drawn. These are first solved 'backwards', with *z* acting as the source, before the paths are flipped. This allows the accumulative consumption value to be calculated for each step, which can then be multiplied by the CO_2e value for that step in order to give the corrected CO_2e value.

In reality, the nodes for these graphs are the specific processes, other than the source/sink node of the target product *z*, but using the feedstocks and products as nodes is often more easy to visualise.

Figure S4 visualises the required graphs and calculations required to generate the data shown in Table S3.

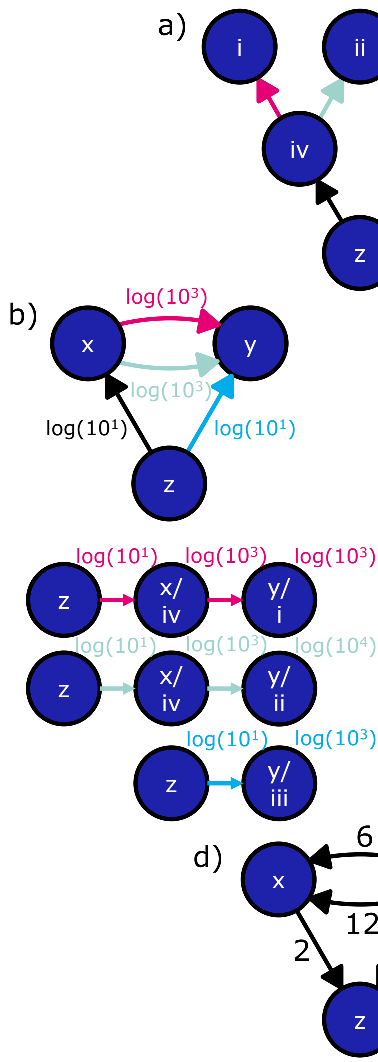

Figure S4: Graphs showing: a) a network directed from z to y, with the 'Specific process' acting as nodes; b) the possible paths from z to y, with edges weighted by $\log 10^{\text{feedstock consumption}}$; c) the possible paths from z to y, with edges weighted by the net equivalent CO_2 per metric ton of previous product; d) a network directed from y to z, with each edge weighted by the corrected net equivalent CO_2 per metric ton of z.

These data are presented in Table S3:

Table S3: Calculated data for the possible paths from y to z from the data given in Table S2. Numbers in brackets represent the consumption of y, which is irrelevant to the carbon calculations.

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Path steps	Individual consumption at each step (t/$t_{next\ product}$)	Accumulative consumption at each step (t/t_z)	Individual equivalent CO_2 at each step ($tCO_2e/t_{next\ product}$)	Corrected equivalent CO_2 at each step (tCO_2e/t_z)	Net equivalent CO_2 per metric ton *z* (tCO_2e/t_z)	Consumption of *y* per metric ton *z* (t/t)
i→iv→*z*	(3), 3, 1	(9), 3, 1	2, 2	6, 2	8	9
ii→iv→*z*	(4), 3, 1	(12), 3, 1	4, 2	12, 2	14	12
iii→*z*	(3), 1	(3), 1	3	3	3	3

In a practical implementation, all these data and more can be stored and filtered by the feedstocks or process steps used.

Water consumption network

An illustration of the chemical network is provided in Figure S5.

In this graph, each node is a chemical feedstock or product, and the edges between each node are weighted by the water consumption of the lowest water consuming route from that feedstock to one metric ton of the next product. The final products selected are the polymers LDPE, LLDPE, Bimodal HDPE, PP, PET, PVC, PBT and PAA.

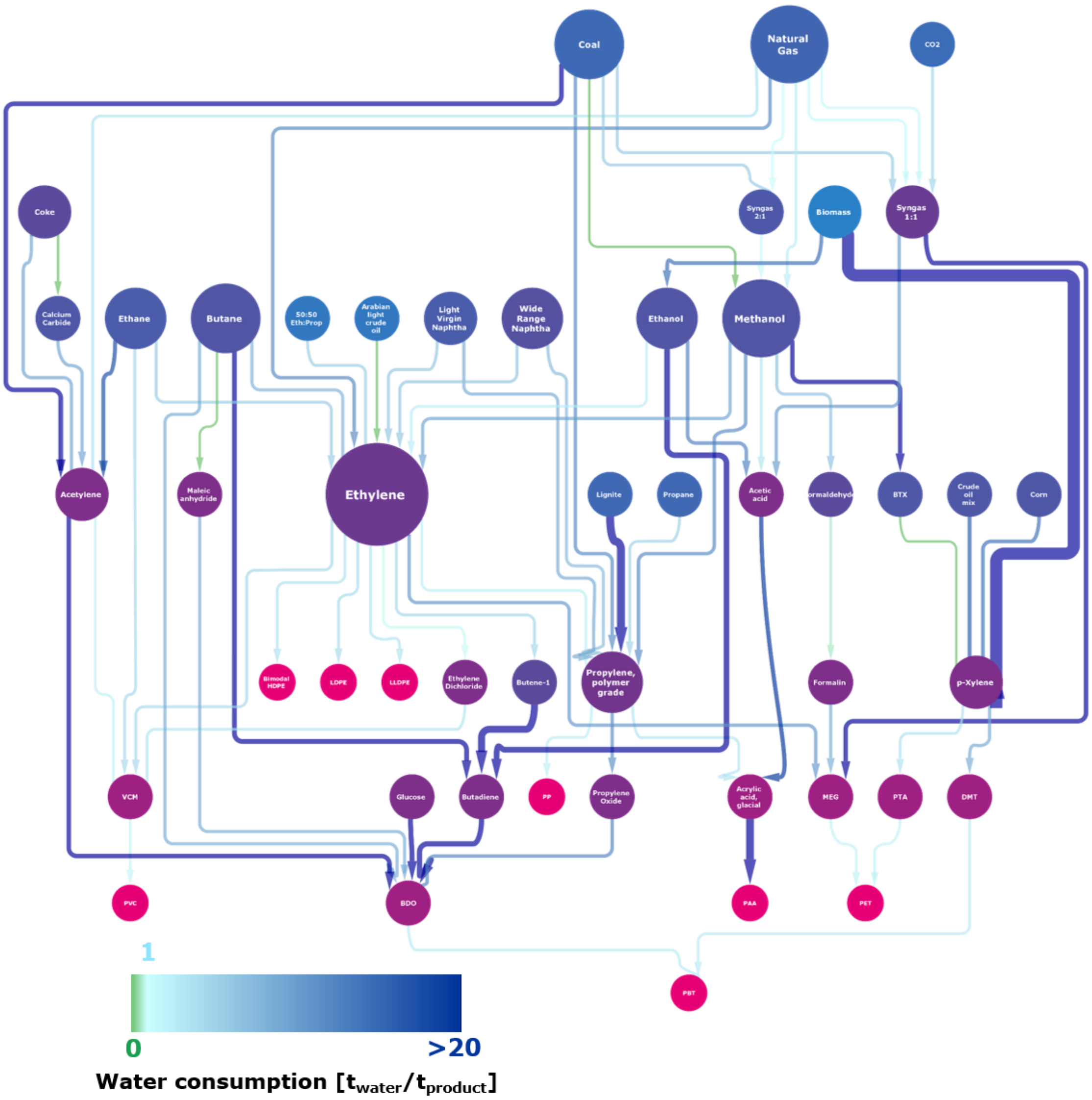

Figure S5: A representative chemical network for the plastics industry, with the targeted polymers LDPE, LLDPE, Bimodal HDPE, PP, PET, PVC, PBT and PAA. Each node represents a chemical feedstock or product, with the edges between each node weighted by the water consumption of the lowest water consuming route from that feedstock to one metric ton of the next product, according to the methodology described. The colour and thickness of the edges represent the edge weighting, the colour and size of each node represent the average shortest path length and the out degree of the nodes respectively. The process data are sourced from literature articles, internal analysis and IHS Markit PEP reports. Some process data includes integrated steps, leading to intermediate nodes being excluded, for example lignite to propylene. Analysis by the authors using the Python library NetworkX (4). The graph is plotted using Cytoscape (5, 6), and arranged using the yFiles hierarchic layout.

Table of process citations

Table S4: All industrial chemical processes cited from external sources, with the associated feedstock, product and reference (7).

Feedstock	Product	Reference	Process	Specific Process
50:50 Eth:Prop	Ethylene	IHS Markit: Ethylene via Ethane Steam Cracking PEP Report - 29H	Steam Cracking	Ethane:Propane 50:50 Steam Cracking
Acetic acid	Acrylic acid, glacial	External data	Formaldehyde route to acrylic acid	Acrylic acid via formaldehyde route
Acetylene	BDO	IHS Markit: Polybutylene Terephthalate (PBT) and Butanediol PEP Report - 96B	BDO Production	BDO from acetylene and formaldehyde
Acetylene	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Hydrochlorination	VCM from acetylene by hydrochlorination
Acrylic acid, glacial	PAA	IHS Markit: Superabsorbent Polymers PEP Report - 194A	Superabsorbent polymer production	Improved aqueous polymerization process to make SAP
Acrylic acid, glacial	PAA	IHS Markit: Superabsorbent Polymers PEP Report - 194A	Superabsorbent polymer production	Continuous reactor process to make SAP
Arabian light crude oil	Ethylene	IHS Markit: Crude Oil to Chemicals and Oxidative Coupling of Methane: Potential for Synergy? PEP Review - 2018-06	Oxidative Coupling	Chemicals from crude oil (Siluria OCM case)
Arabian light crude oil	Ethylene	IHS Markit: Crude Oil to Chemicals and Oxidative Coupling of Methane: Potential for Synergy? PEP Review - 2018-06	Steam Cracking	Chemicals from crude oil base case (ethane/propane recycled to steam cracking furnaces)
Arabian light crude oil	Ethylene	IHS Markit: Crude Oil to Chemicals and Oxidative Coupling of Methane: Potential for Synergy? PEP Review - 2018-07	Oxidative Coupling	Chemicals from crude oil (Siluria OCM case)
Arabian light crude oil	Ethylene	IHS Markit: Oxidative Coupling of Methane to Ethylene by Siluria Process PEP Review - 2014-07	Oxidative Coupling	Chemicals from crude oil (Siluria OCM case)
BDO	PBT	IHS Markit: Polybutylene Terephthalate (PBT) and Butanediol PEP Report - 96B	PBT Production	PBT from DMT
Biomass	Ethanol	IHS Markit: Cellulosic Bioethanol PEP Report - 263A	Cellulosic Bioethanol	Beta Renewables cellulosic ethanol plant
Biomass	Ethanol	IHS Markit: Cellulosic Bioethanol PEP Report - 263A	Cellulosic Bioethanol	POET-DSM cellulosic ethanol plant
Biomass	Ethanol	IHS Markit: Cellulosic Bioethanol PEP Report - 263A	Cellulosic Bioethanol	DuPont cellulosic ethanol plant
Biomass	p-Xylene	IHS Markit: Bio-Based Aromatics PEP Report - 287	Bio-based aromatics	para-Xylene from biomass via Anellotech process
BTX	p-Xylene	IHS Markit: Xylenes Separation PEP Report - 25C	Adsorption/isomerization	p-Xylene by Parex adsorption process
Butadiene	BDO	IHS Markit: 1,4-Butanediol and Tetrahydrofuran from Butadiene PEP Review - 82-2-2	BDO Production	BDO from BD

Butane	Ethylene	IHS Markit: Ethylene via Ethane Steam Cracking PEP Report - 29H	Steam Cracking	Butane Steam Cracking
Butane	BDO	IHS Markit: Polybutylene Terephthalate (PBT) and Butanediol PEP Report - 96B	BDO Production	BDO from Butane via MA
Butane	Butadiene	IHS Markit: On-Purpose Butadiene Production PEP Report - 35E	Butane dehydrogenation	1,3-Butadiene by butane dehydrogenation process
Butane	Maleic anhydride	IHS Markit: Maleic Anhydride from n-Butane by Scientific Design Co. Process PEP Review - 2020-14	Butane oxidation	Maleic anhydride from n-butane by Scientific Design Co. Process
Butane	Maleic anhydride	IHS Markit: Maleic Anhydride by Huntsman Technology PEP Review - 2020-08	Butane oxidation	Maleic anhydride by Huntsman Technology
Butene-1	Butadiene	IHS Markit: On-Purpose Butadiene Production PEP Report - 35E	Oxidative dehydrogenation	1,3-Butadiene by oxidative dehydrogenation
Calcium Carbide	Acetylene	IHS Markit: Acetylene PEP Report - 16A	Acetylene from calcium carbide	Acetylene from calcium carbide
Carbon dioxide (from air)	Methanol	IHS Markit: Green Methanol Production Process PEP Review - 2020-07	Methanol production	Green Methanol Production
Carbon dioxide (from air)	Syngas 1:1	IHS Markit: Carbon Dioxide Utilization Technologies PEP Report - 285A	CO2 to Syngas	Conversion of steam and CO2 to syngas for a F-T plant by co-electrolysis process
Coal	Syngas 2:1	IHS Markit: Syngas Production Economics of Chinese Coal Gasifiers PEP Report - 148D	Gassification	Syngas from bituminous coal by the ECUST gasifier
Coal	Syngas 2:1	IHS Markit: Syngas Production Economics of Chinese Coal Gasifiers PEP Report - 148D	Gassification	Syngas from bituminous coal by the HT-L gasifier
Coal	Methanol	IHS Markit: Methanol from Coal PEP Report - 43E	Methanol production	Methanol from coal
Coal	Propylene, polymer grade	IHS Markit: Propylene Process Summary PEP Review - 2016-11	Gassification	Siemens gasifier process
Coal	Acetylene	IHS Markit: Acetylene PEP Report - 16A	Arc process	Acetylene from coal by arc process using water quenching
Coal	Acetylene	IHS Markit: Acetylene PEP Report - 16A	Arc process	Acetylene from coal by arc process using hydrocarbon quenching
Coal	Syngas 1:1	IHS Markit: Syngas Production Economics of Chinese Coal Gasifiers PEP Report - 148D	Gassification	Syngas from bituminous coal by the ECUST gasifier
Coal	Syngas 1:1	IHS Markit: Syngas Production Economics of Chinese Coal Gasifiers PEP Report - 148D	Gassification	Syngas from bituminous coal by the HT-L gasifier
Coke	Acetylene	IHS Markit: Acetylene PEP Report - 16A	Acetylene from calcium carbide	Acetylene via calcium carbide integrated production
Coke	Calcium Carbide	IHS Markit: Acetylene PEP Report - 16A	Electrothermal process	Calcium carbide by electrothermal process
Coke	Calcium Carbide	IHS Markit: Acetylene PEP Report - 16A	Oxythermal process	Calcium carbide by oxythermal process
Coke	Calcium Carbide	IHS Markit: Acetylene PEP Report - 16A	Thermal process	Calcium carbide by thermal process using CO as heating medium
Corn	p-Xylene	IHS Markit: Bio-Based Aromatics PEP Report - 287	Bio-based aromatics	para-Xylene from corn via the Gevo process

Corn	p-Xylene	IHS Markit: Bio-Based Aromatics PEP Report - 287	Bio-based aromatics	para-Xylene from corn via the updated Gevo process
Corn	p-Xylene	IHS Markit: Bio-Based Aromatics PEP Report - 287	Bio-based aromatics	para-Xylene from corn via the Virent process
Crude oil mix	p-Xylene	IHS Markit: Crude Oil to P-Xylene – Zhejiang Refinery-PX Complex PEP Report - 303A	Crude oil to p-xylene	Zhejiang crude to p-xylene complex production
Crude oil mix	p-Xylene	IHS Markit: Crude Oil to p-Xylene Hengli Refinery-PX Complex PEP Report - 303	Crude oil to p-xylene	p-Xylene from crude oil via Hengli process
DMT	PBT	IHS Markit: Polybutylene Terephthalate (PBT) and Butanediol PEP Report - 96B	PBT Production	PBT from DMT
Ethane	Ethylene	IHS Markit: Ethylene from Ethane, by Oxidative Dehydrogenation PEP Review - 85-2-2	Oxidative dehydrogenation	Oxydehydrogenation of ethane Union Carbide technology
Ethane	Ethylene	IHS Markit: Ethylene by Non-Conventional Processes PEP Report 29F	Oxidative dehydrogenation	Ethylene from ethane by oxidative dehydrogenation
Ethane	Ethylene	IHS Markit: Ethylene via Ethane Steam Cracking PEP Report - 29H	Steam Cracking	Ethane (100%) Steam Cracking
Ethane	Acetylene	IHS Markit: Acetylene PEP Report - 16A	Acetylene from ethane	Acetylene from ethane by the Wulff process
Ethane	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Deoxydehydrochlorination	VCM by Dow ethane oxydehydrochloination process
Ethane	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Deoxydehydrochlorination	VCM from ethane by the Inovyl process
Ethanol	Ethylene	IHS Markit: Chemicals from Ethanol PEP Report - 235	Dehydration	Ethylene from ethanol by adiabatic fixed-bed catalytic dehydration
Ethanol	Ethylene	IHS Markit: Ethylene from Ethanol PEP Review - 79-3-4	Dehydration	Ethanol dehydrogenation (Fixed Bed)
Ethanol	Ethylene	IHS Markit: Ethylene from Ethanol PEP Review - 79-3-4	Dehydration	Ethanol dehydrogenation (Fluidised Bed)
Ethanol	Acetic acid	IHS Markit: Chemicals from Ethanol PEP Report - 235	Ethanol to acetic acid	Acetic acid from ethanol via acetaldehyde
Ethanol	Butadiene	IHS Markit: On-Purpose Butadiene Production PEP Report - 35E	Ethanol to butadiene	Ethanol to 1,3-butadiene by two-stage American process
Ethylene	Bimodal HDPE	IHS Markit: Bimodal HDPE PEP Report - 19G	Bimodal HDPE Production	LyondellBasell Hostalen ACP
Ethylene	Bimodal HDPE	IHS Markit: Bimodal HDPE PEP Report - 19G	Bimodal HDPE Production	Mitsui CX
Ethylene	Bimodal HDPE	IHS Markit: Bimodal HDPE PEP Report - 19G	Bimodal HDPE Production	INEOS Innovene S process
Ethylene	Bimodal HDPE	IHS Markit: Bimodal HDPE PEP Report - 19G	Bimodal HDPE Production	Univation UNIPOL PE process using PRODIGY Bimodal Catalyst
Ethylene	Bimodal HDPE	IHS Markit: Bimodal HDPE PEP Report - 19G	Bimodal HDPE Production	Univation UNIPOL PE process using PRODIGY Bimodal Catalyst for 400 ktpy plant capacity
Ethylene	Bimodal HDPE	IHS Markit: Bimodal HDPE production by a gas-phase process similar to LyondellBasell's Hyperzone Process PEP Review - 2017-05	Bimodal HDPE Production	Process similar to LyondellBasell Hyperzone PE process

Ethylene	LDPE	IHS Markit: LDPE Process Summary PEP Review - 2013-10	LDPE Production	ExxonMobil tubular
Ethylene	LDPE	IHS Markit: LDPE Process Summary PEP Review - 2013-10	LDPE Production	High-pressure autoclave process
Ethylene	LDPE	IHS Markit: LDPE Process Summary PEP Review - 2013-10	LDPE Production	SABTEC CTR tubular
Ethylene	LLDPE	IHS Markit: LLDPE Process Summary PEP Review - 2015-15	LLDPE Production	LLD production by a gas-phase process similar to the Innovene G process
Ethylene	LLDPE	IHS Markit: LLDPE Process Summary PEP Review - 2015-15	LLDPE Production	LLD production by a gas-phase process similar to the SPHERILENE S process
Ethylene	LLDPE	IHS Markit: LLDPE Process Summary PEP Review - 2015-15	LLDPE Production	LLD production by a slurry process similar to Chevron Phillips MarTECH slurry loop process
Ethylene	LLDPE	IHS Markit: LLDPE Process Summary PEP Review - 2015-15	LLDPE Production	LLD production by a solution process similar to Dow DOWLEX loop process (Ziegler)
Ethylene	LLDPE	IHS Markit: LLDPE Process Summary PEP Review - 2015-15	LLDPE Production	LLD production by a solution process similar to Dow DOWLEX loop process (metallocene)
Ethylene	LLDPE	IHS Markit: LLDPE Process Summary PEP Review - 2015-15	LLDPE Production	LLD production by a solution process similar to the SCLAIRTECH process
Ethylene	LLDPE	IHS Markit: LLDPE Process Summary PEP Review - 2015-15	LLDPE Production	LLD production by a solution process similar to the Advanced SCLAIRTECH process
Ethylene	LLDPE	IHS Markit: LLDPE Process Summary PEP Review - 2015-15	LLDPE Production	LLD, bimodal grade, production by a gas-phase process similar to the SPHERILENE C process
Ethylene	LLDPE	IHS Markit: LLDPE Process Summary PEP Review - 2015-15	LLDPE Production	LLD, bimodal grade, production by a hybrid process similar to the Borstar process
Ethylene	Propylene, polymer grade	IHS Markit: Propylene Process Summary PEP Review - 2016-11	Olefin conversion	Dimerization and OCT
Ethylene	Butene-1	IHS Markit: Dimerization of Ethylene to Butene-1 PEP Review - 84-3-3	Dimerization of ethylene	Dimerization of ethylene to butene-1
Ethylene	MEG	IHS Markit: Monoethylene Glycol (MEG) Process Summary PEP Review - 2014-11	EO hydration	Conventional EO hydration
Ethylene	MEG	IHS Markit: Monoethylene Glycol (MEG) Process Summary PEP Review - 2014-11	EO hydration	Selective EO hydration
Ethylene	MEG	IHS Markit: Monoethylene Glycol (MEG) Process Summary PEP Review - 2014-11	EO hydration	Shell OMEGA technology
Ethylene	MEG	IHS Markit: Monoethylene Glycol (MEG) Process Summary PEP Review - 2014-11	EO hydration	Dow METEOR technology

Ethylene	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Balanced process	VCM by a balanced process (Oxy Vinyls)
Ethylene	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Balanced process	VCM by a balanced process with heat and HCl recovery (Oxy Vinyls)
Ethylene	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Balanced process	VCM by a balanced process (Inovyl)
Ethylene	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Balanced process	VCM by a balanced process with heat and HCl recovery (Inovyl)
Ethylene	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Balanced process	VCM by a balanced process (Mitsui)
Ethylene	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Balanced process	VCM by a balanced process with heat and HCl recovery (Mitsui)
Ethylene	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Balanced process	VCM by a balanced process (Vinnolit)
Ethylene	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Balanced process	VCM by a balanced process with heat and HCl recovery (Vinnolit)
Ethylene	Ethylene Dichloride	IHS Markit: Vinyl Chloride PEP Report - 5D	Direct chlorination of Ethylene	Liquid-phase HTC process (Oxy Vinyls)
Ethylene	Ethylene Dichloride	IHS Markit: Vinyl Chloride PEP Report - 5D	Direct chlorination of Ethylene	Liquid-phase HTC process (Inovyl)
Ethylene	Ethylene Dichloride	IHS Markit: Vinyl Chloride PEP Report - 5D	Direct chlorination of Ethylene	Liquid-phase HTC process (Mitsui)
Ethylene	Ethylene Dichloride	IHS Markit: Vinyl Chloride PEP Report - 5D	Direct chlorination of Ethylene	Liquid-phase LTC process (Vinnolit)
Ethylene	Ethylene Dichloride	IHS Markit: Vinyl Chloride PEP Report - 5D	Direct chlorination of Ethylene	Gas-phase process (ICI)
Ethylene	Ethylene Dichloride	IHS Markit: Vinyl Chloride PEP Report - 5D	Oxychlorination	Fluidised-bed reactor, oxygen-based (Oxy Vinyls)
Ethylene	Ethylene Dichloride	IHS Markit: Vinyl Chloride PEP Report - 5D	Oxychlorination	Fluidised-bed reactor, air-based (Oxy Vinyls)
Ethylene	Ethylene Dichloride	IHS Markit: Vinyl Chloride PEP Report - 5D	Oxychlorination	Fixed-bed reactor, oxygen-based (Inovyl)
Ethylene	Ethylene Dichloride	IHS Markit: Vinyl Chloride PEP Report - 5D	Oxychlorination	Fixed-bed reactor, air-based (Inovyl)
Ethylene	Ethylene Dichloride	IHS Markit: Vinyl Chloride PEP Report - 5D	Oxychlorination	Fluidised-bed reactor, oxygen-based (Mitsui)
Ethylene Dichloride	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Pyrolysis	VCM from ethylene dichloride by pyrolysis (Generic)
Ethylene Dichloride	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Pyrolysis	VCM from ethylene dichloride by pyrolysis (Inovyl)
Ethylene Dichloride	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Pyrolysis	VCM from ethylene dichloride by pyrolysis (Mitsui)
Ethylene Dichloride	VCM	IHS Markit: Vinyl Chloride PEP Report - 5D	Pyrolysis	VCM from ethylene dichloride by pyrolysis (Vinnolit)
Formaldehyde	Formalin		Formaldehyde dilution to Formalin	Formaldehyde dilution to Formalin
Formalin	MEG	IHS Markit: MEG Process via Formaldehyde PEP Review - 2019-08	Formaldehyde to MEG	MEG process via Formaldehyde

Glucose	BDO	IHS Markit: Bio-Based 1,4-Butanediol PEP Report - 283	Bio-based BDO	1,4-Butanediol from glucose (direct route)
Glucose	BDO	IHS Markit: Bio-Based 1,4-Butanediol PEP Report - 283	Bio-based BDO	Bio-based 1,4-butanediol via succinic acid route (indirect route)
Light Virgin Naphtha	Ethylene	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Light Virgin Naphtha Maximum Ethylene Case Front-End Demethanizer
Light Virgin Naphtha	Ethylene	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Light Virgin Naphtha Maximum Ethylene Case Front-End Depropanizer
Light Virgin Naphtha	Ethylene	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Light Virgin Naphtha Maximum Ethylene Case Front-End Depropanizer with Gas Turbine Driver
Light Virgin Naphtha	Propylene, polymer grade	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Light Virgin Naphtha Maximum Propylene Case Front-End Demethanizer
Light Virgin Naphtha	Propylene, polymer grade	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Light Virgin Naphtha Maximum Propylene Case Front-End Depropanizer
Light Virgin Naphtha	Propylene, polymer grade	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Light Virgin Naphtha Maximum Propylene Case Front-End Depropanizer with Gas Turbine Driver
Light Virgin Naphtha	Propylene, polymer grade	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Superflex process
Light Virgin Naphtha	Propylene, polymer grade	IHS Markit: Propylene Process Summary PEP Review - 2016-16	Steam Cracking	Superflex process
Lignite	Propylene, polymer grade	IHS Markit: Propylene Process Summary PEP Review - 2016-11	Gassification	Shell gasifier process
Maleic anhydride	BDO	IHS Markit: Polybutylene Terephthalate (PBT) and Butanediol PEP Report - 96B	BDO Production	BDO from MA via DMM
MEG	PET	IHS Markit: Polyethylene Terephthalate PEP Report - 18D	PET Production	PET by a process similar to INVISTA CP process and Polymetrix EcoSphere SSP process (IV 0.82 dL/g)
MEG	PET	IHS Markit: Polyethylene Terephthalate PEP Report - 18D	PET Production	PET by a process similar to Uhde Inventa-Fischer Melt-to-Resin process (IV 0.82 dL/g)
Methanol	Ethylene	IHS Markit: Methanol to Olefins/Propylene Technologies in China PEP Report - 261A	Methanol-to-olefins	Methanol to olefins by the DMTO process
Methanol	Ethylene	IHS Markit: Methanol to Olefins Production in China II PEP Report - 261B	Methanol-to-olefins	Methanol to olefins by UOP Advanced MTO process
Methanol	Ethylene	IHS Markit: Methanol to Olefins Production in China II PEP Report - 261B	Methanol-to-olefins	Methanol to olefins by the DMTO-II process
Methanol	Ethylene	IHS Markit: Ethylene by Non-Conventional Processes PEP Report 29F	Methanol-to-olefins	UPO/Hydro MTO

Methanol	Ethylene	IHS Markit: Ethylene by Non-Conventional Processes PEP Report 29F	Methanol-to-olefins	Mobil MTE
Methanol	Propylene, polymer grade	IHS Markit: Propylene Process Summary PEP Review - 2016-11	Methanol-to-olefin	Lurgi MTP process
Methanol	Propylene, polymer grade	IHS Markit: Propylene Process Summary PEP Review - 2016-11	Methanol-to-olefin	JGC/MCC DTP process
Methanol	Acetic acid	IHS Markit: Acetic Acid, Update of the Celanese AO Plus Process PEP Review - 2013-01	Methanol carbonylation	Acetic acid via the Celanese AO Plus process
Methanol	Acetic acid	IHS Markit: Acetic Acid, Update of the BP Cativa Process PEP Review - 2013-07	Methanol carbonylation	Acetic acid via the BP Cativa process
Methanol	Acetic acid	IHS Markit: Acetic Acid by Chiyoda CT-ACETICA™ Process PEP Review - 2018-01	Methanol carbonylation	Acetic acid by the CT-ACETICA process
Methanol	BTX	IHS Markit: Unconventional Aromatics Processes PEP Report - 300	Methanol to aromatics	BTX aromatics production from methanol via Tsinghua process
Methanol	Formaldehyde	IHS Markit: Formaldehyde PEP Report - 23B	Formaldehyde production	Formaldehyde production by BASF silver catalyst process
Methanol	Formaldehyde	IHS Markit: Formaldehyde PEP Report - 23B	Formaldehyde production	Formaldehyde production by Dynea silver catalyst process
Methanol	Formaldehyde	IHS Markit: Formaldehyde PEP Report - 23B	Formaldehyde production	Formaldehyde production by D. B Western ferric-molybdate catalyst process
Methanol	Formaldehyde	IHS Markit: Formaldehyde PEP Report - 23B	Formaldehyde production	Formaldehyde production by Johnson Matthey ferric-molybdate catalyst process
Natural Gas	Syngas 2:1	IHS Markit: Synthesis Gas Production from Natural Gas Reforming PEP Report - 148B	Combined reforming	Syngas production for methanol by Lurgi two-stage process
Natural Gas	Syngas 2:1	IHS Markit: Synthesis Gas Production from Natural Gas Reforming PEP Report - 148B	Combined reforming	Syngas production for methanol by Haldor-Topsoe two-stage process
Natural Gas	Syngas 2:1	IHS Markit: Synthesis Gas Production from Natural Gas Reforming PEP Report - 148B	Combined reforming	Syngas production for methanol by Johnson Matthey/Davy two-stage process
Natural Gas	Syngas 2:1	IHS Markit: Syngas via MIDREX SynRG Reformer PEP Review - 2014-01	Steam methane reforming	Syngas via MIDREX SynRG reformer
Natural Gas	Methanol	IHS Markit: Liquid Phase Methanol PEP Review - 2009-15	Methanol production	Integrated ICI two-stage reforming and liquid phase methanol process
Natural Gas	Methanol	IHS Markit: Methanol PEP Report - 43F	Methanol production	Haldor Tosoe autothermal reforming-based process
Natural Gas	Methanol	IHS Markit: Methanol PEP Report - 43F	Methanol production	Casale combined reforming-based process
Natural Gas	Methanol	IHS Markit: Methanol PEP Report - 43F	Methanol production	Lurgi combined reforming-based process
Natural Gas	Methanol	IHS Markit: Methanol PEP Report - 43F	Methanol production	Johnson Matthey/Davy Two-stage reforming based process
Natural Gas	Ethylene	IHS Markit: Ethylene by Non-Conventional Processes PEP Report 29F	Ethylene from methanol	UPO/Hydro GTO

Natural Gas	Ethylene	IHS Markit: Ethylene by Non-Conventional Processes PEP Report 29F	Ethylene from methanol	Mobil MTE and ICI Methanol
Natural Gas	Ethylene	IHS Markit: Ethylene by Non-Conventional Processes PEP Report 29F	Oxidative Coupling	Ethylene from methane by oxidative coupling (The Arco Process)
Natural Gas	Ethylene	IHS Markit: Oxidative Coupling of Methane to Ethylene by Siluria Process PEP Review - 2014-07	Oxidative Coupling	Oxidative Coupling of Methane by Siluria Process
Natural Gas	Syngas 1:1	IHS Markit: Synthesis Gas Production from Natural Gas Reforming PEP Report - 148B	Autothermal reforming	Syngas production for F-T products by Topsoe autothermal process
Natural Gas	Syngas 1:1	IHS Markit: Synthesis Gas Production from Natural Gas Reforming PEP Report - 148B	Partial oxidation	Syngas production for F-T products by Shell partial oxidation process
Natural Gas	Ethylene	IHS Markit: Crude Oil to Chemicals and Oxidative Coupling of Methane: Potential for Synergy? PEP Review - 2018-07	Oxidative Coupling	Oxidative Coupling of Methane by Siluria Process
Natural Gas	Syngas 1:1	IHS Markit: Acetic Acid from Syngas via the BP SaaBre Process PEP Review - 2014-10	Syngas (SR~1) from natural gas	Syngas (SR 1) from Natgas via POX with H2 Skimming
Natural Gas	Acetylene	IHS Markit: Acetylene PEP Report - 16A	Arc process	Acetylene from natural gas by arc process
Natural Gas	Acetylene	IHS Markit: Acetylene PEP Report - 16A	Natural gas oxidation	Acetylene by partial oxidation of natural gas (with heat recovery)
Propane	Propylene, polymer grade	IHS Markit: Propane Dehydrogenation Process Technologies PEP Report - 267A	Dehydrogentation	CATOFIN process
Propane	Propylene, polymer grade	IHS Markit: Propane Dehydrogenation Process Technologies PEP Report - 267A	Dehydrogentation	Oleflex process
Propane	Propylene, polymer grade	IHS Markit: Propane Dehydrogenation Process Technologies PEP Report - 267A	Dehydrogentation	Uhde STAR process
Propylene Oxide	BDO	IHS Markit: Polybutylene Terephthalate (PBT) and Butanediol PEP Report - 96B	BDO Production	BDO from PO
Propylene, polymer grade	Acrylic acid, glacial	IHS Markit: Acrylic Acid Process Summary PEP Review - 2016-10	Acrylic acid from propylene	Glacial-grade acrylic acid by the Lurgi/Nippon Kayaku process
Propylene, polymer grade	Acrylic acid, glacial	IHS Markit: Acrylic Acid Process Summary PEP Review - 2016-10	Acrylic acid from propylene	Glacial-grade acrylic acid by the Mitsubishi process
Propylene, polymer grade	Acrylic acid, glacial	IHS Markit: Acrylic Acid Process Summary PEP Review - 2016-10	Acrylic acid from propylene	Glacial-grade acrylic acid by the updated Nippon Shokubai process
Propylene, polymer grade	Acrylic acid, glacial	IHS Markit: Acrylic Acid Process Summary PEP Review - 2016-10	Acrylic acid from propylene	Glacial-grade acrylic acid by the Nippon Shokubai process
Propylene, polymer grade	Acrylic acid, glacial	IHS Markit: Acrylic Acid Process Summary PEP Review - 2016-10	Acrylic acid from propylene	Glacial-grade acrylic acid by the BASF process
Propylene, polymer grade	Propylene Oxide	IHS Markit: Propylene Oxide by the BASF-Dow HPPO Process PEP Review - 2009-4	Oxidation of propylene	Propylene oxide by the BASF-Dow HPPO Process
Propylene, polymer grade	Propylene Oxide	IHS Markt: Propylene Oxide PEP Report - 2H	Oxidation of propylene	PO/TBA by the Lyondell process using TBHP
Propylene, polymer grade	Propylene Oxide	IHS Markt: Propylene Oxide PEP Report - 2H	Oxidation of propylene	PO/TBA by the Huntsman process using TBHP

Propylene, polymer grade	Propylene Oxide	IHS Markt: Propylene Oxide PEP Report - 2H	Oxidation of propylene	PO/SM by the Shell process using EBHP
Propylene, polymer grade	Propylene Oxide	IHS Markt: Propylene Oxide PEP Report - 2H	Oxidation of propylene	PO by the Sumitomo process using CHP
Propylene, polymer grade	Propylene Oxide	IHS Markt: Propylene Oxide PEP Report - 2H	Oxidation of propylene	PO by the BASF process using HP
Propylene, polymer grade	Propylene Oxide	IHS Markt: Propylene Oxide PEP Report - 2H	Oxidation of propylene	PO by the Degussa process using HP
Propylene, polymer grade	Propylene Oxide	IHS Markt: Propylene Oxide PEP Report - 2H	Oxidation of propylene	PO by the direct epoxidation of Aist-Nippon Shokubai
Propylene, polymer grade	Propylene Oxide	IHS Markt: Propylene Oxide PEP Report - 2H	Oxidation of propylene	PO by the Chlorohydrin process using lime
Propylene, polymer grade	Propylene Oxide	IHS Markt: Propylene Oxide PEP Report - 2H	Oxidation of propylene	PO by the Chlorohydrin process using cell liquor
Propylene, polymer grade	PP	IHS Markit: Polypropylene Process Summary PEP Review - 2014-03	PP Production	Bulk process similar to the Spheripol process
Propylene, polymer grade	PP	IHS Markit: Polypropylene Process Summary PEP Review - 2014-03	PP Production	Fluidised bed gas-phase process similar to Unipol process
Propylene, polymer grade	PP	IHS Markit: Polypropylene Process Summary PEP Review - 2014-03	PP Production	Vertical stirred-bed gas-phase process similar to Novolen PP process
Propylene, polymer grade	PP	IHS Markit: Polypropylene Process Summary PEP Review - 2014-03	PP Production	Horizontal stirred-bed gas-phase process similar to Innovene PP process
Propylene, polymer grade	PP	IHS Markit: Polypropylene Process Summary PEP Review - 2014-03	PP Production	Gas-phase process similar to Spherizone PP process
Propylene, polymer grade	PP	IHS Markit: Polypropylene PEP Report - 128E	PP Production	Gas-phase process similar to Unipol PP process
Propylene, polymer grade	PP	IHS Markit: Polypropylene PEP Report - 128E	PP Production	Gas-phase process similar to Novolen PP process
Propylene, polymer grade	PP	IHS Markit: Polypropylene PEP Report - 128E	PP Production	Gas-phase process similar to Spherizone PP process
PTA	PET	IHS Markit: Polyethylene Terephthalate PEP Report - 18D	PET Production	PET by a process similar to INVISTA CP process and Polymetrix EcoSphere SSP process (IV 0.82 dL/g)
PTA	PET	IHS Markit: Polyethylene Terephthalate PEP Report - 18D	PET Production	PET by a process similar to Uhde Inventa-Fischer Melt-to-Resin process (IV 0.82 dL/g)
p-Xylene	DMT	IHS Markit: Terephthalic Acid and Dimethyl Terephthalate PEP Report - 9E	DMT Production	Dimethyl terephthalate from p-xylene by succesive oxidations and esterifications
p-Xylene	PTA	IHS Markit: Purified Terephthalic Acid (PTA) PEP Report - 9H	Oxidation of p-xylene	PTA production from p-xylene by INVISTA process
p-Xylene	PTA	IHS Markit: Purified Terephthalic Acid (PTA) PEP Report - 9H	Oxidation of p-xylene	PTA production from p-xylene by Mitsubishi process

p-Xylene	PTA	IHS Markit: Purified Terephthalic Acid (PTA) PEP Report - 9H	Oxidation of p-xylene	PTA production from p-xylene by Dow-Davy COMPRESS process
Residual Oil	Acetylene	IHS Markit: Acetylene PEP Report - 16A	Acetylene from residual oil	Acetylene from residual oil by submerged flame process
Syngas 1:1	Acetic acid	IHS Markit: Acetic Acid from Syngas via the BP SaaBre Process PEP Review - 2014-10	Integrated syngas to acetic acid	Acetic Acid via the BP SaaBre Process
Syngas 1:1	MEG	IHS Markit: Monoethylene Glycol (MEG) Process Summary PEP Review - 2014-11	Coal-based syngas to MEG	Coal-based syngas process by Fujian
Syngas 1:1	MEG	IHS Markit: Monoethylene Glycol (MEG) Process Summary PEP Review - 2014-11	Coal-based syngas to MEG	Coal-based syngas process by Ube
Syngas 1:1	MEG	IHS Markit: Monoethylene Glycol (MEG) Process Summary PEP Review - 2014-11	Coal-based syngas to MEG	Coal-based syngas process by Sinopec
Syngas 2:1	Methanol	IHS Markit: Synthesis Gas Production from Natural Gas Reforming PEP Report - 148B, IHS Markit: Methanol PEP Report - 43F	Methanol production	Estimated Johnson Matthey/Davy methanol from syngas
VCM	PVC	IHS Markit: Vinyl Polymers PEP Report - 253	PVC Production	PVC by suspension polymerisation process
VCM	PVC	IHS Markit: Vinyl Polymers PEP Report - 253	PVC Production	PVC by bulk polymerisation process
VCM	PVC	IHS Markit: Vinyl Polymers PEP Report - 253	PVC Production	PVC by emulsion polymerisation process
VCM	PVC	IHS Markit: Vinyl Polymers PEP Report - 253	PVC Production	PVC by JNC polymerisation process
Wide Range Naphtha	Ethylene	IHS Markit: Naphtha Catalytic Cracking PEP Report - 29K	Catalytic Cracking	Wide Range Naphtha to Ethylene via ACO process
Wide Range Naphtha	Ethylene	IHS Markit: Naphtha Catalytic Cracking PEP Report - 29K	Catalytic Cracking	Wide Range Naphtha to Ethylene via downflow FCC process
Wide Range Naphtha	Ethylene	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Wide Range Naphtha Maximum Ethylene Case Front-End Demethanizer
Wide Range Naphtha	Ethylene	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Wide Range Naphtha Maximum Ethylene Case Front-End Depropanizer
Wide Range Naphtha	Ethylene	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Wide Range Naphtha Maximum Ethylene Case Front-End Depropanizer with Gas Turbine Driver
Wide Range Naphtha	Propylene, polymer grade	IHS Markit: Naphtha Catalytic Cracking PEP Report - 29K	Catalytic Cracking	Wide Range Naphtha to Propylene via ACO process
Wide Range Naphtha	Propylene, polymer grade	IHS Markit: Naphtha Catalytic Cracking PEP Report - 29K	Catalytic Cracking	Wide Range Naphtha to Propylene via downflow FCC process
Wide Range Naphtha	Propylene, polymer grade	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Wide Range Naphtha Maximum Propylene Case Front-End Demethanizer
Wide Range Naphtha	Propylene, polymer grade	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Wide Range Naphtha Maximum Propylene Case Front-End Depropanizer with Gas Turbine Driver

Wide Range Naphtha	Propylene, polymer grade	IHS Markit: Ethylene from Naphtha PEP Report - 29I	Steam Cracking	Wide Range Naphtha Maximum Propylene Case Front-End Depropanizer
Wide Range Naphtha	Acetylene	IHS Markit: Acetylene PEP Report - 16A	Naphha oxidation	Acetylene by partial oxidation of naphtha

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