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# **Example petrochemicals production system**

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This document defines the “processes” and “objects” which constitute the example model of petrochemical production processes and flows, to illustrate the use of the `flowprog` framework.

This is a simplified, illustrative version of a complete model developed as part of the C-THRU project.



## PRIMARY CHEMICALS

These processes produce primary chemicals such as ethylene and BTX.

### 1.1 Primary chemicals

These are the main primary chemicals modelled:

**i** *Object: Ethylene*

**i** *Object: Propylene*

**i** *Object: Benzene*

**i** *Object: Toluene*

**i** *Object: Xylenes*

**i** *Object: Butylenes*

**i** *Object: Butadiene*

A few additional “objects” need to be defined here.

## 1.2 Fossil feedstocks

**i** *Object: Butane*

**i** *Object: Ethane*

**i** *Object: Propane*

**i** *Object: Naphtha*

Steam cracking produces olefins (ethylene, propylene) from a range of fossil feedstocks. Two feedstocks are modelled, ethane and naphtha.

**i** *Process: SteamCrackingOfNaphtha*

Consumes:

Object	Amount
<i>sys:Naphtha</i>	2.6 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:Ethylene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Propylene</i>	0.5 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Butylenes</i>	0.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:PyrolysisGasoline</i>	0.4 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:MiscRefineryProducts</i>	0.5 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

This recipe represents a generic steam cracking process from naphtha.

**i** *Process: SteamCrackingOfEthane*

Consumes:

Object	Amount
<i>sys:Ethane</i>	1.3 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:Ethylene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Propylene</i>	0.1 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Butadiene</i>	0.1 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:MiscRefineryProducts</i>	0.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

This recipe represents a generic steam cracking process from ethane.

**i Process: CatalyticReformingOfNaphthaForToluene**

Consumes:

Object	Amount
<i>sys:Naphtha</i>	5.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:Toluene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Benzene</i>	0.3 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:OtherIndustrialGases</i>	0.3 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:MiscRefineryProducts</i>	2.9 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:WasteOtherChemicals</i>	0.5 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

This recipe represents generic catalytic reforming of naphtha for toluene.

**i Process: CatalyticReformingOfNaphthaForXylenes**

Consumes:

Object	Amount
<i>sys:Naphtha</i>	1.6 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:Xylenes</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Benzene</i>	0.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:OtherIndustrialGases</i>	0.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:WasteOtherChemicals</i>	0.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

## Example petrochemicals production system

This recipe represents generic catalytic reforming of naphtha for p-xylene.

To balance remaining demand not supplied by co-production of other processes, “on-purpose” production from propane and butane can be used.

### **i** Process: DehydrogenationOfPropane

Consumes:

Object	Amount
<i>sys:Propane</i>	1.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:Propylene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:MiscRefineryProducts</i>	0.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

This recipe represents generic dehydrogenation of propane for propylene.

### **i** Process: DehydrogenationOfButaneForButadiene

Consumes:

Object	Amount
<i>sys:Butane</i>	1.7 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:Butadiene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:MiscRefineryProducts</i>	0.7 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

This recipe represents generic dehydrogenation of butane for butadiene.

## 1.3 From ethyl alcohol

Ethyl alcohol (ethanol) is assumed to be produced from biomass, but with limited capacity.

**Object: EthylAlcohol / Ethyl alcohol**

Ethyl alcohol can be used to produce ethylene:

**Process: DehydrationOfEthylAlcohol**

Consumes:

Object	Amount	
<i>sys:EthylAlcohol</i>	1.6	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount	
<i>sys:Ethylene</i>	1.0	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:WasteOtherChemicals</i>	0.6	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

This recipe represents ethylene production from ethyl alcohol by dehydration.

## 1.4 Conversion processes

Many primary chemicals are produced as co-products, so to reach the required mix it is necessary to further convert unwanted co-products into demanded chemicals.

**Process: DistillationOfButylenesForButadiene**

Consumes:

Object	Amount	
<i>sys:Butylenes</i>	2.3	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount	
<i>sys:Butadiene</i>	1.0	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:WasteOtherChemicals</i>	1.3	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

This recipe represents distillation of butylenes for butadiene.

## Example petrochemicals production system

Pyrolysis gasoline, a co-product of steam cracking of heavier feeds, can be distilled to produce BTX:

### **i** *Object: PyrolysisGasoline*

PyrolysisGasoline is produced from steam cracking of naphtha, ethane, or crude oil, which is then distilled to produce BTX

### **i** *Process: DistillationOfPyrolysisGasolineForBTX*

Consumes:

Object	Amount
<i>sys:PyrolysisGasoline</i>	2.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:Benzene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Toluene</i>	0.5 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Xylenes</i>	0.3 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:WasteOtherChemicals</i>	0.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

This recipe represents distillation of pyrolysis gasoline for BTX.

Much of the toluene that is produced is converted to benzene and xylenes:

### **i** *Process: DisproportionationOfTolueneForXylenes*

Consumes:

Object	Amount
<i>sys:Toluene</i>	2.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:Xylenes</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Benzene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:MiscRefineryProducts</i>	0.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

This recipe represents disproportionation of toluene for p-xylene and benzene.

**i Process: DealkylationOfTolueneForBenzene**

Consumes:

Object	Amount
<i>sys:Toluene</i>	1.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:Benzene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:MiscRefineryProducts</i>	0.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

This recipe represents dealkylation of toluene for benzene.



## ORGANIC CHEMICALS

These processes synthesise downstream organic chemicals.

### **i** Process: StyreneSynthesis

Consumes:

Object	Amount
<i>sys:Ethylene</i>	0.3 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Benzene</i>	0.8 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:Styrene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:WasteOtherChemicals</i>	0.1 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

### **i** Process: EthyleneGlycolSynthesis

Consumes:

Object	Amount
<i>sys:Ethylene</i>	0.6 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:PureOxygen</i>	0.3 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Water</i>	0.4 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:EthyleneGlycol</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:WasteOtherChemicals</i>	0.4 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

### **i** Process: TerephthalicAcidSynthesis

Consumes:

Object	Amount	
<i>sys:Xylenes</i>	0.7	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:PureOxygen</i>	0.6	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount	
<i>sys:TerephthalicAcid</i>	1.0	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:WasteOtherChemicals</i>	0.3	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

### **i** Object: Styrene

### **i** Object: EthyleneGlycol / Ethylene glycol

### **i** Object: TerephthalicAcid / Terephthalic acid

## POLYMERS

These are the polymer objects modelled here:

**i Object: Polymers**

Children: *sys:PEPolyethylene sys:PPPolypropylene sys:PETPolyethyleneTerephthalate sys:SyntheticRubbers sys:OtherPolymers*

**i Object: PEPolyethylene / PE, Polyethylene**

Parents: *sys:Polymers*

**i Object: PPPolypropylene / PP, Polypropylene**

Parents: *sys:Polymers*

**i Object: PETPolyethyleneTerephthalate / PET, Polyethylene terephthalate**

Parents: *sys:Polymers*

**i Object: SyntheticRubbers / Synthetic rubbers**

Parents: *sys:Polymers*

**i Object: OtherPolymers / Other polymers**

Parents: *sys:Polymers*

Ending sub objects of “Polymers”

These are the polymerisation processes that produce them:

**i Process: ProductionOfPolymers**

Children: *sys:PolymerisationOfPE* *sys:PolymerisationOfPP* *sys:PolymerisationOfPET*  
*sys:PolymerisationOfStyreneButadiene* *sys:PolymerisationOfOtherPolymers*

**i Process: PolymerisationOfPE**

Consumes:

Object	Amount
<i>sys:Ethylene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:PEPolyethylene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:WasteOtherChemicals</i>	0.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:ProductionOfPolymers*

Assume a 97% process yield.

**i Process: PolymerisationOfPP**

Consumes:

Object	Amount
<i>sys:Propylene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:PPPolypropylene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:WasteOtherChemicals</i>	0.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:ProductionOfPolymers*

Assume a 97% process yield.

**i Process: PolymerisationOfPET**

Consumes:

Object	Amount
<i>sys:EthyleneGlycol</i>	0.3 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:TerephthalicAcid</i>	0.9 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:PETPolyethyleneTerephthalate</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Water</i>	0.2 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:ProductionOfPolymers*

**i Process: PolymerisationOfStyreneButadiene**

Consumes:

Object	Amount
<i>sys:Butadiene</i>	0.8 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Styrene</i>	0.3 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:SyntheticRubbers</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:WasteOtherChemicals</i>	0.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:ProductionOfPolymers*

Assume 25% styrene, 75% butadiene, with 2% polymerisation loss.

Similarly for polymerisation of “other polymers”:

**i Process: PolymerisationOfOtherPolymers**

Consumes:

Object	Amount
<i>sys:Butadiene</i>	0.3 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Styrene</i>	0.7 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:OtherPolymers</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:ProductionOfPolymers*

Similar to ABS, but for simplicity, removed Acrylonitrile from the demonstration model.

Ending sub processes of "ProductionOfPolymers"

## PRODUCTS

These are the product types that we are modelling (based on sectors) – just two for the purposes of this simplified model:

**i Object: Products**

Children: *sys:PackagingProducts sys:TransportationProducts*

**i Object: PackagingProducts**

Parents: *sys:Products*

**i Object: TransportationProducts**

Parents: *sys:Products*

Ending sub objects of “Products”

And end-of-life versions:

**i Object: EOLProducts**

Children: *sys:EOLPackagingProducts sys:EOLTransportationProducts*

**i Object: EOLPackagingProducts**

Parents: *sys:EOLProducts*

**i Object: EOLTransportationProducts**

Parents: *sys:EOLProducts*

Ending sub objects of “EOLProducts”

These are the processes that produce and use them:

**Process: ProductionOfProducts**

Children: *sys:ProductionOfPackagingProducts* *sys:ProductionOfTransportationProducts*  
*sys:EOLProcessingPackagingProducts* *sys:EOLProcessingTransportationProducts*

**Process: ProductionOfPackagingProducts**

Consumes:

Object	Amount	
<i>sys:PEPolyethylene</i>	0.5	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:PPPolypropylene</i>	0.2	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:PETPolyethyleneTerephthalate</i>	0.2	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:OtherPolymers</i>	0.1	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount	
<i>sys:PackagingProducts</i>	1.0	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:ProductionOfProducts*

**Process: ProductionOfTransportationProducts**

Consumes:

Object	Amount	
<i>sys:PEPolyethylene</i>	0.1	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:PPPolypropylene</i>	0.3	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:SyntheticRubbers</i>	0.3	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:OtherPolymers</i>	0.3	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount	
<i>sys:TransportationProducts</i>	1.0	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:ProductionOfProducts*

**Process: EOLProcessingPackagingProducts**

Consumes:

Object	Amount	
<i>sys:EOLPackagingProducts</i>	1.0	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount	
<i>sys:PEPolyethyleneAtEOL</i>	0.5	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:PPPolypropyleneAtEOL</i>	0.2	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:PETPolyethyleneTerephthalateAtEOL</i>	0.2	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:OtherPolymersAtEOL</i>	0.1	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:ProductionOfProducts*

**i Process: EOLProcessingTransportationProducts**

Consumes:

Object	Amount	
<i>sys:EOLTransportationProducts</i>	1.0	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount	
<i>sys:PEPolyethyleneAtEOL</i>	0.1	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:PPPolypropyleneAtEOL</i>	0.3	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:SyntheticRubbersAtEOL</i>	0.3	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:OtherPolymersAtEOL</i>	0.3	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:ProductionOfProducts*

Ending sub processes of “ProductionOfProducts”

**i Process: UseOfProducts**

Children: *sys:UseOfPackagingProducts* *sys:UseOfTransportationProducts*

**i Process: UseOfPackagingProducts**

Consumes:

Object	Amount	
<i>sys:PackagingProducts</i>	1.0	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

## Example petrochemicals production system

---

Produces:

Object	Amount
<i>sys:EOLPackagingProducts</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:UseOfProducts*

### **Process: UseOfTransportationProducts**

Consumes:

Object	Amount
<i>sys:TransportationProducts</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:EOLTransportationProducts</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:UseOfProducts*

Ending sub processes of “UseOfProducts”

## END-OF-LIFE PROCESSES

At the end-of-life of the end-use sector products, some of the polymers can be recovered. The processes that split end-of-life products into end-of-life polymers are generated from the product model, and generated recipes are included in *Products*.

### 5.1 End-of-life polymer streams

The following objects are defined to represent polymer streams recovered from end-of-life processes:

**i** **Object: PolymersAtEOL**

Children: *sys:PEPolyethyleneAtEOL* *sys:PPPolypropyleneAtEOL* *sys:PETPolyethyleneTerephthalateAtEOL*  
*sys:SyntheticRubbersAtEOL* *sys:OtherPolymersAtEOL*

**i** **Object: PEPolyethyleneAtEOL**

Parents: *sys:PolymersAtEOL*

PEPolyethylene recovered at the end-of-life products.

**i** **Object: PPPolypropyleneAtEOL**

Parents: *sys:PolymersAtEOL*

PPPolypropylene recovered at the end-of-life products.

**i** **Object: PETPolyethyleneTerephthalateAtEOL**

Parents: *sys:PolymersAtEOL*

PETPolyethyleneTerephthalate recovered at the end-of-life products.

**i** **Object: SyntheticRubbersAtEOL**

Parents: *sys:PolymersAtEOL*

## Example petrochemicals production system

SyntheticRubbers recovered at the end-of-life products.

### **i** *Object: OtherPolymersAtEOL*

Parents: *sys:PolymersAtEOL*

OtherPolymers recovered at the end-of-life products.

Ending sub objects of “PolymersAtEOL”

## 5.2 Mixed polymer streams

Polymers-at-end-of-life can end up mixed together, that can subsequently go to chemical recycling or their final treatment. Below are the representation of these mixing processes:

### **i** *Process: MixingWastePolymerStreams*

Children: *sys:MixingPEPolyethyleneAtEOL sys:MixingPPPolypropyleneAtEOL sys:MixingPETPolyethyleneTerephthalateAtEOL sys:MixingSyntheticRubbersAtEOL sys:MixingOtherPolymersAtEOL*

### **i** *Process: MixingPEPolyethyleneAtEOL*

Consumes:

Object	Amount
<i>sys:PEPolyethyleneAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:MixedPolymersAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:MixingWastePolymerStreams*

### **i** *Process: MixingPPPolypropyleneAtEOL*

Consumes:

Object	Amount
<i>sys:PPPolypropyleneAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:MixedPolymersAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:MixingWastePolymerStreams*

**i Process: MixingPETPolyethyleneTerephthalateAtEOL**

Consumes:

Object	Amount
<i>sys:PETPolyethyleneTerephthalateAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:MixedPolymersAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:MixingWastePolymerStreams*

**i Process: MixingSyntheticRubbersAtEOL**

Consumes:

Object	Amount
<i>sys:SyntheticRubbersAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:MixedPolymersAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:MixingWastePolymerStreams*

**i Process: MixingOtherPolymersAtEOL**

Consumes:

Object	Amount
<i>sys:OtherPolymersAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

## Example petrochemicals production system

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Produces:

Object	Amount
<i>sys:MixedPolymersAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:MixingWastePolymerStreams*

Ending sub processes of “MixingWastePolymerStreams”

The following objects are defined to represent polymer streams recovered from end-of-life processes:

**i** **Object: MixedPolymersAtEOL**

MixedPolymersAtEOL goes to chemical recycling or final treatment.

**i** **Object: Waste**

## RECYCLING PROCESSES

The polymers from end of life processes can be recycled. The thermoplastics polymers can be mechanically recycled; chemical recycling is not considered for this simplified model.

### 6.1 Mechanical recycling

#### **i** Process: MechanicalRecycling

Children: *sys:MechanicalRecyclingOfPEPolyethyleneAtEOL* *sys:MechanicalRecyclingOfPPPolypropyleneAtEOL*  
*sys:MechanicalRecyclingOfPETPolyethyleneTerephthalateAtEOL*

#### **i** Process: MechanicalRecyclingOfPEPolyethyleneAtEOL

Consumes:

Object	Amount
<i>sys:PEPolyethyleneAtEOL</i>	1.6 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
<i>sys:PEPolyethylene</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Waste</i>	0.6 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:MechanicalRecycling*

A yield of approximately 60% is assumed.

#### **i** Process: MechanicalRecyclingOfPPPolypropyleneAtEOL

Consumes:

Object	Amount
<i>sys:PPPolypropyleneAtEOL</i>	1.6 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

## Example petrochemicals production system

Produces:

Object	Amount	
<i>sys:PPPolypropylene</i>	1.0	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Waste</i>	0.6	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:MechanicalRecycling*

A yield of approximately 60% is assumed.

### **i** Process: MechanicalRecyclingOfPETPolyethyleneTerephthalateAtEOL

Consumes:

Object	Amount	
<i>sys:PETPolyethyleneTerephthalateAtEOL</i>	1.6	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount	
<i>sys:PETPolyethyleneTerephthalate</i>	1.0	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>
<i>sys:Waste</i>	0.6	<a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Parents: *sys:MechanicalRecycling*

A yield of approximately 60% is assumed.

Ending sub processes of “MechanicalRecycling”

## FINAL TREATMENT PROCESSES

Polymers at end-of-life that do not get recycled can to any of these:

**i** **Process: FinalTreatment**

Children: *sys:Landfilling sys:Incineration sys:Mismanagement*

**i** **Process: Landfilling**

Consumes:

Object	Amount
<i>sys:MixedPolymersAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
--------	--------

Parents: *sys:FinalTreatment*

**i** **Process: Incineration**

Consumes:

Object	Amount
<i>sys:MixedPolymersAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
--------	--------

Parents: *sys:FinalTreatment*

### **i** *Process: Mismanagement*

Consumes:

Object	Amount
<i>sys:MixedPolymersAtEOL</i>	1.0 <a href="http://qudt.org/vocab/quantitykind/Mass">http://qudt.org/vocab/quantitykind/Mass</a>

Produces:

Object	Amount
--------	--------

Parents: *sys:FinalTreatment*

Ending sub processes of "FinalTreatment"

## OTHER CHEMICAL SYNTHESIS

### 8.1 Wastes and other misc objects

**i** *Object: WasteOtherChemicals*

**i** *Object: OtherIndustrialGases*

**i** *Object: Water*

**i** *Object: PureOxygen*

**i** *Object: MiscRefineryProducts*



## PROCESS INDEX

### C

CatalyticReformingOfNaphthaForToluene  
(*primary-chemicals*), ??  
CatalyticReformingOfNaphthaForXylenes  
(*primary-chemicals*), ??

### D

DehydrogenationOfPropane (*primary-chemicals*),  
??  
DehydrogenationOfButaneForButadiene  
(*primary-chemicals*), ??  
DehydrationOfEthylAlcohol (*primary-chemicals*), ??  
DistillationOfButylenesForButadiene  
(*primary-chemicals*), ??  
DistillationOfPyrolysisGasolineForBTX  
(*primary-chemicals*), ??  
DisproportionationOfTolueneForXylenes  
(*primary-chemicals*), ??  
DealkylationOfTolueneForBenzene (*primary-chemicals*), ??

### E

EOLProcessingPackagingProducts (*products*),  
??  
EOLProcessingTransportationProducts  
(*products*), ??  
EthyleneGlycolSynthesis (*organic-chemicals*),  
??

### F

FinalTreatment (*final-treatment-processes*), ??

### I

Incineration (*final-treatment-processes*), ??

### L

Landfilling (*final-treatment-processes*), ??

### M

MixingWastePolymerStreams (*end-of-life-processes*), ??

MixingPEPolyethyleneAtEOL (*end-of-life-processes*), ??

MixingPPPolypropyleneAtEOL (*end-of-life-processes*), ??

MixingPETPolyethyleneTerephthalateAtEOL  
(*end-of-life-processes*), ??

MixingSyntheticRubbersAtEOL (*end-of-life-processes*), ??

MixingOtherPolymersAtEOL (*end-of-life-processes*), ??

Mismanagement (*final-treatment-processes*), ??

MechanicalRecycling (*recycling-processes*), ??

MechanicalRecyclingOfPEPolyethyleneAtEOL  
(*recycling-processes*), ??

MechanicalRecyclingOfPPPolypropyleneAtEOL  
(*recycling-processes*), ??

MechanicalRecyclingOfPETPolyethyleneTerephthalateAtEOL  
(*recycling-processes*), ??

### P

ProductionOfPolymers (*polymers*), ??

PolymerisationOfPE (*polymers*), ??

PolymerisationOfPP (*polymers*), ??

PolymerisationOfPET (*polymers*), ??

PolymerisationOfStyreneButadiene (*polymers*), ??

PolymerisationOfOtherPolymers (*polymers*),  
??

ProductionOfProducts (*products*), ??

ProductionOfPackagingProducts (*products*), ??

ProductionOfTransportationProducts  
(*products*), ??

### S

SteamCrackingOfNaphtha (*primary-chemicals*), ??

SteamCrackingOfEthane (*primary-chemicals*), ??

StyreneSynthesis (*organic-chemicals*), ??

### T

TerephthalicAcidSynthesis (*organic-chemicals*), ??

**U**

UseOfProducts (*products*), ??

UseOfPackagingProducts (*products*), ??

UseOfTransportationProducts (*products*), ??

## OBJECT INDEX

### B

Benzene (*primary-chemicals*), ??  
StyreneSynthesis (*consumes*), ??  
CatalyticReformingOfNaphthaForToluene (*produces*), ??  
CatalyticReformingOfNaphthaForXylenes (*produces*), ??  
DistillationOfPyrolysisGasolineForBTX (*produces*), ??  
DisproportionationOfTolueneForXylenes (*produces*), ??  
DealkylationOfTolueneForBenzene (*produces*), ??  
Butylenes (*primary-chemicals*), ??  
SteamCrackingOfNaphtha (*produces*), ??  
DistillationOfButylenesForButadiene (*consumes*), ??  
Butadiene (*primary-chemicals*), ??  
PolymerisationOfStyreneButadiene (*consumes*), ??  
PolymerisationOfOtherPolymers (*consumes*), ??  
SteamCrackingOfEthane (*produces*), ??  
DehydrogenationOfButaneForButadiene (*produces*), ??  
DistillationOfButylenesForButadiene (*produces*), ??  
Butane (*primary-chemicals*), ??  
DehydrogenationOfButaneForButadiene (*consumes*), ??

### E

Ethylene (*primary-chemicals*), ??  
StyreneSynthesis (*consumes*), ??  
EthyleneGlycolSynthesis (*consumes*), ??  
PolymerisationOfPE (*consumes*), ??  
SteamCrackingOfNaphtha (*produces*), ??  
SteamCrackingOfEthane (*produces*), ??  
DehydrationOfEthylAlcohol (*produces*), ??  
Ethane (*primary-chemicals*), ??  
SteamCrackingOfEthane (*consumes*), ??  
Ethyl alcohol (*primary-chemicals*), ??

DehydrationOfEthylAlcohol (*consumes*), ??  
EOLProducts (*products*), ??  
EOLPackagingProducts (*products*), ??  
EOLProcessingPackagingProducts (*consumes*), ??  
UseOfPackagingProducts (*produces*), ??  
EOLTransportationProducts (*products*), ??  
EOLProcessingTransportationProducts (*consumes*), ??  
UseOfTransportationProducts (*produces*), ??  
Ethylene glycol (*organic-chemicals*), ??  
EthyleneGlycolSynthesis (*produces*), ??  
PolymerisationOfPET (*consumes*), ??

### M

MixedPolymersAtEOL (*end-of-life-processes*), ??  
MixingPEPolyethyleneAtEOL (*produces*), ??  
MixingPPPPolypropyleneAtEOL (*produces*), ??  
MixingPETPolyethyleneTerephthalateAtEOL (*produces*), ??  
MixingSyntheticRubbersAtEOL (*produces*), ??  
MixingOtherPolymersAtEOL (*produces*), ??  
Landfilling (*consumes*), ??  
Incineration (*consumes*), ??  
Mismanagement (*consumes*), ??  
MiscRefineryProducts (*misc-processes*), ??  
SteamCrackingOfNaphtha (*produces*), ??  
SteamCrackingOfEthane (*produces*), ??  
CatalyticReformingOfNaphthaForToluene (*produces*), ??  
DehydrogenationOfPropane (*produces*), ??  
DehydrogenationOfButaneForButadiene (*produces*), ??  
DisproportionationOfTolueneForXylenes (*produces*), ??  
DealkylationOfTolueneForBenzene (*produces*), ??  
Naphtha (*primary-chemicals*), ??  
SteamCrackingOfNaphtha (*consumes*), ??

### N

Naphtha (*primary-chemicals*), ??  
SteamCrackingOfNaphtha (*consumes*), ??

CatalyticReformingOfNaphthaForToluene  
(consumes), ??

CatalyticReformingOfNaphthaForXylenes  
(consumes), ??

## O

OtherPolymersAtEOL (end-of-life-processes), ??

MixingOtherPolymersAtEOL (consumes), ??

EOLProcessingPackagingProducts (produces),  
??

EOLProcessingTransportationProducts  
(produces), ??

OtherIndustrialGases (misc-processes), ??

CatalyticReformingOfNaphthaForToluene  
(produces), ??

CatalyticReformingOfNaphthaForXylenes  
(produces), ??

Other polymers (polymers), ??

PolymerisationOfOtherPolymers (produces),  
??

ProductionOfPackagingProducts (consumes),  
??

ProductionOfTransportationProducts (con-  
sumes), ??

## P

PolymersAtEOL (end-of-life-processes), ??

PEPolyethyleneAtEOL (end-of-life-processes), ??

MixingPEPolyethyleneAtEOL (consumes), ??

EOLProcessingPackagingProducts (produces),  
??

EOLProcessingTransportationProducts  
(produces), ??

MechanicalRecyclingOfPEPolyethyleneAtEOL  
(consumes), ??

PPPolypropyleneAtEOL (end-of-life-processes), ??

MixingPPPolypropyleneAtEOL (consumes), ??

EOLProcessingPackagingProducts (produces),  
??

EOLProcessingTransportationProducts  
(produces), ??

MechanicalRecyclingOfPPPolypropyleneAtEOL  
(consumes), ??

PETPolyethyleneTerephthalateAtEOL (end-  
of-life-processes), ??

MixingPETPolyethyleneTerephthalateAtEOL  
(consumes), ??

EOLProcessingPackagingProducts (produces),  
??

MechanicalRecyclingOfPETPolyethyleneTerephthalateAtEOL  
(consumes), ??

PureOxygen (misc-processes), ??

EthyleneGlycolSynthesis (consumes), ??

TerephthalicAcidSynthesis (consumes), ??

Polymers (polymers), ??

PE, Polyethylene (polymers), ??

PolymerisationOfPE (produces), ??

ProductionOfPackagingProducts (consumes),  
??

ProductionOfTransportationProducts (con-  
sumes), ??

MechanicalRecyclingOfPEPolyethyleneAtEOL  
(produces), ??

PP, Polypropylene (polymers), ??

PolymerisationOfPP (produces), ??

ProductionOfPackagingProducts (consumes),  
??

ProductionOfTransportationProducts (con-  
sumes), ??

MechanicalRecyclingOfPPPolypropyleneAtEOL  
(produces), ??

PET, Polyethylene terephthalate (polymers),  
??

PolymerisationOfPET (produces), ??

ProductionOfPackagingProducts (consumes),  
??

MechanicalRecyclingOfPETPolyethyleneTerephthalateAtEOL  
(produces), ??

Propylene (primary-chemicals), ??

PolymerisationOfPP (consumes), ??

SteamCrackingOfNaphtha (produces), ??

SteamCrackingOfEthane (produces), ??

DehydrogenationOfPropane (produces), ??

Propane (primary-chemicals), ??

DehydrogenationOfPropane (consumes), ??

PyrolysisGasoline (primary-chemicals), ??

SteamCrackingOfNaphtha (produces), ??

DistillationOfPyrolysisGasolineForBTX  
(consumes), ??

Products (products), ??

PackagingProducts (products), ??

ProductionOfPackagingProducts (produces),  
??

UseOfPackagingProducts (consumes), ??

## S

SyntheticRubbersAtEOL (end-of-life-processes), ??

MixingSyntheticRubbersAtEOL (consumes), ??

EOLProcessingTransportationProducts  
(produces), ??

Synthetic rubbers (polymers), ??

PolymerisationOfStyreneButadiene (pro-  
duces), ??

ProductionOfTransportationProducts (con-  
sumes), ??

Styrene (organic-chemicals), ??

StyreneSynthesis (produces), ??

PolymerisationOfStyreneButadiene (*consumes*), ??

PolymerisationOfOtherPolymers (*consumes*), ??

## T

Toluene (*primary-chemicals*), ??

CatalyticReformingOfNaphthaForToluene (*produces*), ??

DistillationOfPyrolysisGasolineForBTX (*produces*), ??

DisproportionationOfTolueneForXylenes (*consumes*), ??

DealkylationOfTolueneForBenzene (*consumes*), ??

TransportationProducts (*products*), ??

ProductionOfTransportationProducts (*produces*), ??

UseOfTransportationProducts (*consumes*), ??

Terephthalic acid (*organic-chemicals*), ??

TerephthalicAcidSynthesis (*produces*), ??

PolymerisationOfPET (*consumes*), ??

## W

Waste (*end-of-life-processes*), ??

MechanicalRecyclingOfPEPolyethyleneAtEOL (*produces*), ??

MechanicalRecyclingOfPPPolypropyleneAtEOL (*produces*), ??

MechanicalRecyclingOfPETPolyethyleneTerephthalateAtEOL (*produces*), ??

WasteOtherChemicals (*misc-processes*), ??

StyreneSynthesis (*produces*), ??

EthyleneGlycolSynthesis (*produces*), ??

TerephthalicAcidSynthesis (*produces*), ??

PolymerisationOfPE (*produces*), ??

PolymerisationOfPP (*produces*), ??

PolymerisationOfStyreneButadiene (*produces*), ??

CatalyticReformingOfNaphthaForToluene (*produces*), ??

CatalyticReformingOfNaphthaForXylenes (*produces*), ??

DehydrationOfEthylAlcohol (*produces*), ??

DistillationOfButylenesForButadiene (*produces*), ??

DistillationOfPyrolysisGasolineForBTX (*produces*), ??

Water (*misc-processes*), ??

EthyleneGlycolSynthesis (*consumes*), ??

PolymerisationOfPET (*produces*), ??

## X

Xylenes (*primary-chemicals*), ??

TerephthalicAcidSynthesis (*consumes*), ??

CatalyticReformingOfNaphthaForXylenes (*produces*), ??

DistillationOfPyrolysisGasolineForBTX (*produces*), ??

DisproportionationOfTolueneForXylenes (*produces*), ??