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BASE IMPACTS® DATA DOCUMENTATION

CATEGORY: CHEMICALS, FINISHING PRODUCTS

3 levels of documentation are available for the datasets in Base Impacts®:

- A **general documentation** explaining general information on the datasets and data general requirements
- A **sectorial documentation**: one document per sector describing the available datasets and their characteristics (technological representativeness, geographical representativeness), and providing the information on the datasets in a common layout. Information comes from the consultation specifications, the dataset commissioner technical proposal and the metadata
- The **datasets metadata** can be viewed directly in the datasets sheets. They include more detailed information (flow diagrams, Etc.)

This document is the category documentation for chemicals, finishing products.

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A. PRESENTATION OF THE CHEMISTRY DATASETS

1. List of available datasets

The following datasets are available:

Technological representativity	Geographical representativity	Dataset type	Scope
Adhesive			
PVC adhesive	World	LCI results	Adhesive production
Hot-melt based on EVA	World	LCI results	Adhesive production
Phenolic resin adhesive modified with nitrile rubber	World	LCI results	Adhesive production
Crystallising Polyurethane adhesive	World	LCI results	Adhesive production
2-component PUR adhesive based on polyether and castor oil	World	LCI results	Adhesive production
Epoxy Adhesive Mix	World	LCI results	Adhesive production
Simple 2-component epoxy adhesive	World	LCI results	Adhesive production
Solvent-based polychloroprene adhesive of good heat resistance	World	LCI results	Adhesive production
Pressure sensitive adhesive based on natural rubber	World	LCI results	Adhesive production
Leather adhesive based on nitrile rubber	World	LCI results	Adhesive production
Water-based acrylic adhesive for PVC flooring	World	LCI results	Adhesive production
Polyester hot-melt for the textile industry	World	LCI results	Adhesive production
PVAc adhesive	World	LCI results	Adhesive production
UV-curing laminating adhesives	World	LCI results	Adhesive production
PUR dispersion adhesive	World	LCI results	Adhesive production

Technological representativity	Geographical representativity	Dataset type	Scope
Solvent-based polyurethane adhesive for the shoe industry	World	LCI results	Adhesive production
Finishing products			
PU lacquer black	World	LCI results	Lacquer production
Acrylic varnish	World	LCI results	Varnish production
PU varnish	World	LCI results	Varnish production
Polyester finish	World	LCI results	Finish production
Acrylic finish	World	LCI results	Finish production
PU finish	World	LCI results	Finish production
Mix varnish/lacquer maximum	World	LCI results	Mix production
Mix adhesive maximum	World	LCI results	Mix production
Mix adhesive PU maximum	World	LCI results	Mix production
Finish maximum	World	LCI results	Mix production

Table 1 : Available datasets

2. Structure of available datasets

Datasets must be distinguished between “partly terminated systems” and “LCI results”.

All Chemistry datasets are LCI results.

The following diagram is used to present the structure of the datasets:

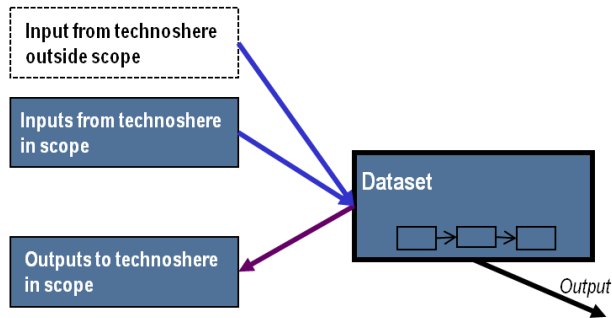


Figure 1 : Structure of the datasets

- The “LCI result” datasets represent a whole production process.

They represent inventories where the material and the process have already been aggregated. For example, “PP pipe, extruded” results from the aggregation of PP granulate dataset and extrusion process dataset.

The LCI results datasets include the following elements:

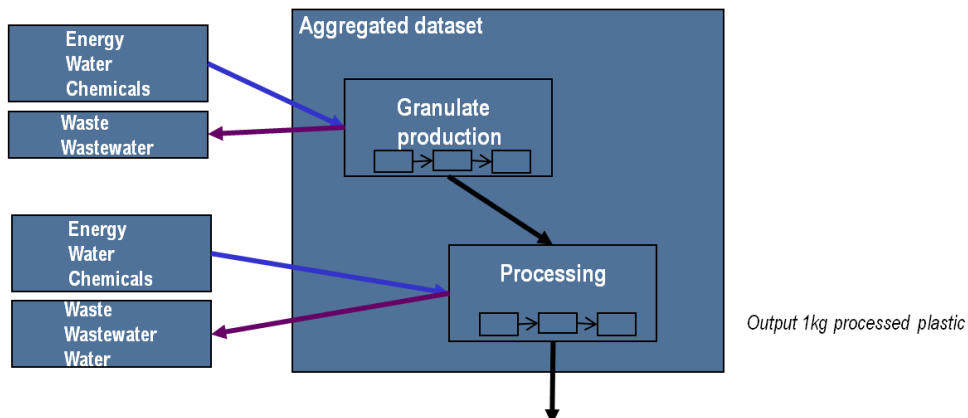


Figure 2 : Structure of the datasets – “LCI results”

B. SCOPE OF THE DATASETS

1. Reference flow, functional unit

The processes are provided for 1 kg of output.

2. System boundaries

2.1. General foreground system boundaries

No general rules are defined.

2.2. Dataset-specific foreground system boundaries

2.2.1. Adhesive

All adhesive datasets provided follow the same cut-off criteria and have the same data sources.

Data cut-off and completeness principles:

Coverage of at least 95% of mass and energy of the input and output flows, and 98% of their environmental relevance (according to expert judgment).

Data sources:

Müller and Rath (2010)

ULLMANN'S Encyclopedia of Industrial Chemistry

Individual industry data

2.2.1.1. PVC adhesive

A commercial PVC polymer is dissolved in suitable solvents, such as a ketone or tetrahydrofuran (THF); in this case specifically a mixture of butanone and cyclohexanone. The rheology (viscosity) is adjusted with additives such as pyrogenic silica. The solids content is approx 25%. The properties of the adhesive after curing are identical to PVC.

PVC adhesive is ideal for bonding PC. PVC adhesives are used in the construction industry to join PVC pipes and to bond PVC sheeting for garden ponds.

2.2.1.2. Hot-melt based on EVA

This dataset represents a general-purpose hot-melt based on Ethylene Vinyl Acetate (EVA) copolymer. EVA based adhesives are low-cost bulk adhesives that adhere well to all kind of substances and satisfy applications without specifically high requirements of heat resistance or adhesion. They are mainly used in packaging, book-binding, shoe-making or for the Do-It-Yourself (DIY) market.

EVA polymers are made by free-radical polymerization of ethylene and vinyl acetate. The hot-melt can be manufactured by simply stirring the components at elevated temperatures under exclusion of air. Resins are added typical at quantities of 30-40% in order to improve adhesion and tack, especially when molten in the precise moment when the substrates (i.e. components to be glued) are mated. Wax is typically added at around 30%, mainly to reduce cost and viscosity.

Quantities of one-third of polymer, one-third resin and one-third wax are typical of EVA hot-melt formulations.

This dataset represents a general-purpose hot-melt based on Ethylene Vinyl Acetate (EVA) copolymer. EVA based adhesives are low-cost bulk adhesives that adhere well to all kind of substances and satisfy applications without specifically high requirements of heat resistance or adhesion. They are mainly used in packaging, book-binding, shoe-making or for the Do-It-Yourself (DIY) market.

2.2.1.3. Phenolic resin adhesive modified with nitrile rubber

The adhesion is provided via reactive phenolic resin (in this case a novolak/urotropine-mixture) that enters into a polycondensation reaction to yield a highly cross-linked thermoset. Nitrile rubber is added to provide toughening by reducing the otherwise high brittleness. Acetone is used as solvent.

There is many applications. Adhesive exhibit high mechanical strength, excellent adhesion to many substrates, as well as excellent thermal and hydrolytic stability.

2.2.1.4. Crystallising Polyurethane adhesive

This is a guide formulation for making a crystalline polyurethane adhesive, including synthesis of the polymer. The polyester is a crystalline type with a molecular weight of approx 3500g/mol, while butanediol serves as a chain extender. The chain extender and polyester are used in roughly the same molar quantities, with 4,4'-MDI being the preferred isocyanate. The total hydroxyl content and the isocyanate are used stoichiometrically, i.e. $\text{NCO/OH} = 1$ and the solids content is 17%.

Solvent-based polyurethane adhesives show good adhesion to a variety of plastic substrates, e.g. soft PVC shoe soles.

2.2.1.5. 2-component PUR adhesive based on polyether and castor oil

2-component PUR adhesive usually cure by means of a polyaddition between an isocyanate and a polyol component.

The A-component (polyol) consists of the polyol and the necessary chain extenders, fillers, stabilisers, plasticisers, catalysts etc. Different mixtures of polyols are often used.

Castor oil yields polymer of high cohesive strength but significant brittleness; very inexpensive polyol; limestone flour is an inexpensive filler; pyrogenic silica is added for viscosity adjustment and to avoid settling of fillers; silicate in castor oil is used as molecular sieve (dessicant) for in-situ drying.

The B-component (hardener, isocyanate) consists of monomeric isocyanates or mixtures of prepolymers terminated with oligomeric isocyanate.

Typical applications are sandwich elements for caravans; flooring adhesive for parquet or metal floors; automotive industry to fasten plastic components to metal or to fasten different

plastic components together; headlamps to fasten glass or polycarbonate lens to plastic body. Energy consumption and material loss during adhesive application is not included.

2.2.1.6. Epoxy Adhesive Mix

The adhesive modeled based on epoxy, electricity and handling of manufacturing waste.

Simple 1-component epoxy adhesive are widely used in the automotive industry for gluing components at the body-in-white (BIW) level and for gluing headlamp lenses to the body. It is also used for bonding ceramic tiles in the construction industry.

2.2.1.7. Simple 2-component epoxy adhesive

The A-component is a combination of a liquid standard epoxy resin, a polyether-based flexibilised resin and an aluminium oxide filler (to reduce shrinking and lower price). The two resins are modeled via identical resin datasets as specific data is not available.

The B-component is pure triethylene tetraamine which is modeled as hexamethylene tetraamine due to lack of specific data.

Simple 2-component epoxy adhesive are widely used in the automotive industry for glueing components at the body-in-white (BIW) level and for glueing headlamp lenses to the body. It is also used for bonding ceramic tiles in the construction industry.

2.2.1.8. Solvent-based polychloroprene adhesive of good heat resistance

Fast crystallising polychloroprene at approx 20% make is suitable for contact adhesive that develop bond strength very fast. Adding reactive alkylphenolic resins in combination with magnesium oxide boosts heat resistance by forming chelates, and both magnesium oxide and tin oxide neutralise traces of released hydrogen chloride that can cause corrosion.

Solvents are petroleum ether/cycloaliphatic/ketone/ester blends.

With fast crystallising polychloroprene resin used as general-purpose contact adhesive.

2.2.1.9. Pressure sensitive adhesive based on natural rubber

Natural rubber latex is collected from rubber trees, coagulated, squeezed for water, and dried. As tackiness of natural rubber is low, resin is added as well as plasticising oil. Furthermore, polymeric trimethyldihydroquinoline is added as a stabilising agent.

Pressure sensitive adhesives based on natural rubber adhere well to non-polar substrates.

2.2.1.10. Leather adhesive based on nitrile rubber

Nitrile rubber is manufactured by free-radical-initiated hot-emulsion polymerisation of butadiene and acrylonitrile to yield a random copolymer. The nitrile rubber is masticated and dissolved along with a PVC copolymer with a total solids content of approx. 20%. Typical solvents are ketones (e.g. acetone or butanone), esters (ethyl and butyl acetate) and aromatic hydrocarbons. Fillers can be various oxides and silicates.

This adhesive is formulated to adhere to leather. Nitrile rubber in general adhere well to substrates as glass, metals, and wood, and to plastics such as PVC, PVAc and PA. They are therefore suitable for a variety of applications.

2.2.1.11. Water-based acrylic adhesive for PVC flooring

The adhesive is produced from a choice of base dispersion in the range of 20-40%, in this particular case at 29%. To suit the specific application, resins in the range of 10-30% are added (12% in this case), and fillers (usually chalk) are added at up to 60%. Additives present in only a few percent are typically surfactants, defoamers and wetting agents. This particular product is formulated with a high quantity of filler, just below 50% of chalk, in order to reduce cost and ease the processing.

The adhesive is used for PVC flooring.

2.2.1.12. Polyester hot-melt for the textile industry

The formulation is based on the adipic acid initially reacting with an excess of butanediol. The second step is a polycondensation using the PET, providing a high molecular polyester, typically 20-30000 g/mol with e.g. tetra isopropyl titanate as catalyst.

2.2.1.13. PVAc adhesive

Polyvinyl Acetate (PVAc) is manufactured by free-radical polymerisation of vinyl acetate. The PVAc polymer, or mix of polymers, is dissolved in a solvent such as e.g. an ester, ketone, aromatic hydrocarbon, or ether; in this particular case the solvents are methylene acetate and ethanol. Pyrogenic silica and water is added to adjust the rheology (viscosity).

The PVAc glue is used as a general-purpose adhesive with good bonding to cardboard, paper and wood, but with only moderate adhesion to plastics and low resistance to solvents as well as low impact strength.

2.2.1.14. UV-curing laminating adhesives

The adhesive mainly (>70%) consist of cyclo-aliphatic epoxy resin. For cost reduction and to increase flexibility, polyols or copolymerizable vinyl ethers are added up to 15%. The photoinitiator is a sulphonium salt that liberate protons/electrophiles when irradiated which initiates the cationic polymerisation.

The adhesive is recommended for varnish on metal, coatings on wood, paper, metals, plastics, glass and ceramic, and coatings requiring flexibility.

2.2.1.15. PUR dispersion adhesive

The PUR pre-polymer is produced with an NCO/OH relation of approx 1.5, equivalent to 100g of IPDI and 900g polycaprolactone, following this calculation:

$$\text{IPDI: } 9.009\text{mval/g} * 100\text{g} = 900.9\text{mval}$$

$$\text{Polycaprolactone: } 0.667\text{mval/g} * 900\text{g} = 600.3\text{mval}$$

$$\Rightarrow \text{NCO/OH} = 900.9/600.3 = 1.5$$

The quantity of the chain extender is usually in the same molar range as the polyol, i.e. at 1058g:

$$900\text{g caprolactone} / 114\text{g/mol} = 7.89\text{mol}$$

$$7.89\text{mol Dimethylol propionic acid} * 134\text{g/mol} = 1058\text{g}$$

Trimethylolpropane is used as proxy for dimethylol propionic acid.

Minor amounts of polyurethane thickener (modeles as IPDI) and water are added to the pre-polymer.

2.2.1.16.Solvent-based polyurethane adhesive for the shoe industry

The adhesive formulation represents a solvent-based, fast-crystallising adhesive for the shoe industry based on high crystalline polyurethane. The solids content is approx. 20%.

The data represents purchasing commercial polymers and additives, and dissolving them in the appropriate solvent, and hence not the method of synthesising the polymers in solution. The solvent combination used is ethyl acetate/methyl etkyl ketone. An alternative could be ethyle acetate/acetone.

Fumed silica is added to adjust the rheology (viscosity).

2.2.2. Finishing products

For all finishing products (lacquer, varnish, finish) foreground system boundaries are the same.

Technology description and included processes:

The system boundaries comprise the cradle to gate life cycle of a typical black PU lacquer in the year 2012. In case of specific electricity or steam supply, these systems are built up in GaBi models. The LCI dataset considers the production of the lacquer and its precursors and excludes any packaging material and transports of the finished product from the factory to subsequent users. Transportation processes for the raw materials are accounted for as far as data on average transport distances were available.

All relevant material and energy flows were included in the system. Life cycle impacts of production equipment and infrastructure were not included in the system as no evidence could be justified that these are to any extent relevant and thus fell under the cut-off criteria. In mass production the impact of production equipment and infrastructure normally is in orders of magnitude lower than the impacts of material and energy supply.

Data cut-off and completeness principles:

Coverage of at least 95% of mass and energy of the input and output flows, and 98% of their environmental relevance (according to expert judgment).

Data sources:

ULLMANN'S Encyclopedia of Industrial Chemistry

Individual industry data

2.2.3. Mix data

Mix data were created based on previous datasets:

- Mix varnish/lacquer maximum is based on the maximum LCIA of the following datasets : PU varnish, PU finish, Acrylic varnish, PU lacquer black
- Mix adhesive maximum is based on the maximum LCIA of the following datasets : 2-component PUR adhesive based on polyether and castor oil, Water-based acrylic adhesive for PVC flooring, Simple 2-component epoxy adhesive, Hot-melt based on EVA, PVC adhesive
- Mix adhesive PU maximum is based on the maximum LCIA of the following datasets : Solvent-based polyurethane adhesive for the shoe industry, 2-component PUR adhesive based on polyether and castor oil
- Finish maximum is based on the maximum LCIA of the following datasets : PU finish, Polyester finish

2.3. Background system boundaries

Electricity: Electricity is modelled according to the individual country-specific situations. The country-specific modelling is achieved on multiple levels. Firstly, individual energy carrier specific power plants and plants for renewable energy sources are modelled according to the current national electricity grid mix. Modelling the electricity consumption mix includes transmission / distribution losses and the own use by energy producers (own consumption of power plants and "other" own consumption e.g. due to pumped storage hydro power etc.), as well as imported electricity. Secondly, the national emission and efficiency standards of the power plants are modelled as well as the share of electricity plants and combined heat and power plants (CHP). Thirdly, the country-specific energy carrier supply (share of imports and / or domestic supply) including the country-specific energy carrier properties (e.g. element and energy content) are accounted for. Fourthly, the exploration, mining/production, processing and transport processes of the energy carrier supply chains are modelled according to the specific situation of each electricity producing country. The different production and processing techniques (emissions and efficiencies) in the different energy producing countries are considered, e.g. different crude oil production technologies or different flaring rates at the oil platforms.

Thermal energy, process steam: The thermal energy and process steam supply is modelled according to the individual country-specific situation with regard to emission standards and considered energy carriers. The thermal energy and process steam are produced at heat plants. Efficiencies for thermal energy production are by definition 100% in relation to the corresponding energy carrier input. For process steam the efficiency ranges from 85%, 90% to 95%. The energy carriers used for the generation of thermal energy and process steam are modelled according to the specific import situation (see electricity above).

Transports: All relevant and known transport processes are included. Ocean-going and inland ship transport as well as rail, truck and pipeline transport of bulk commodities are considered.

Energy carriers: The energy carriers are modelled according to the specific supply situation (see electricity above).

Refinery products: Diesel fuel, gasoline, technical gases, fuel oils, lubricants and residues such as bitumen are modelled with a parameterised country-specific refinery model. The refinery model represents the current national standard in refining techniques (e.g. emission level, internal energy consumption, etc.) as well as the individual country-specific product output spectrum, which can be quite different from country to country. The supply of crude oil is modelled, again, according to the country-specific situation with the respective properties of the resources.

C. DATA SOURCES AND QUALITY

1. Data quality requirements

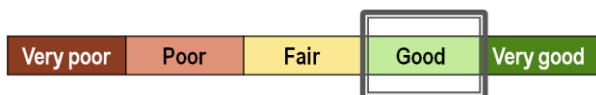
Quality requirements for Base Impacts® datasets are detailed in the general Base Impacts® documentation. No specific quality requirements were set for the plastic datasets.

2. Types and sources of data

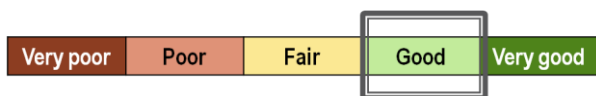
The data sources for the complete product system are sufficiently consistent: primary data from industry was supplemented and validated with different literature data (see technology description for references).

3. Data quality¹

3.1. Technological representativeness

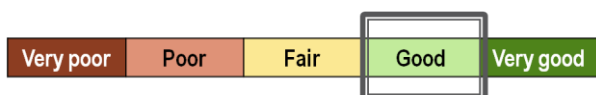


3.2. Time-related coverage

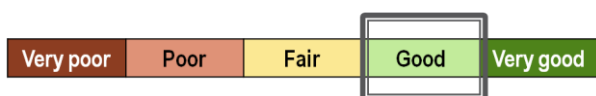


3.3. Geographical coverage

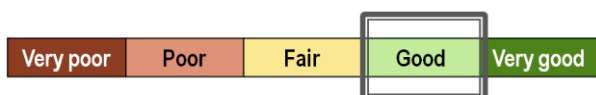
World exclusively



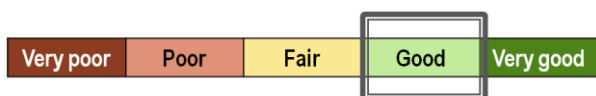
3.4. Precision



3.5. Completeness



3.6. Consistency



¹ May be updated on adhesive and finishing products

4. Multi-functionality and allocation procedure

4.1. Foreground system allocation procedure

These datasets do not require allocation procedures.

4.2. Background system allocation procedure

Background system allocation procedure follows the rules defined by PE International.

D. CRITICAL REVIEW

All Base Impacts® datasets follow the ILCD Entry Level requirements, which require a review either internal with public report or external.

The datasets were reviewed by internal critical review:

- Raw data : Validation of data sources, Sample tests on calculations, Cross-check with other source, expert judgment
- Unit process(es), single operation, black box: Energy balance, Element balance, Cross-check with other source, Cross-check with other data set, Mass balance, Compliance with ISO 14040 to 14044
- LCI results or Partly aggregated system: Energy balance, Element balance, Cross-check with other source, Cross-check with other data set, Expert judgment, Mass balance, Compliance with ISO 14040 to 14044
- Impact results : Cross-check with other source, Cross-check with other data set, Expert judgment, Compliance with ISO 14040 to 14044
- Documentation:, Compliance with ISO 14040 to 14044, Documentation
- Inventory methods : Compliance with ISO 14040 to 14044
- Impact results assesment : Expert judgement, Compliance with ISO 14040 to 14044
- Definition of the objectives and scope of the study: expert judgment, compliance with ISO 14040 to 14044
-

E. REPORTS FOR MORE INFORMATION

The following documents should be used for more information:

- Gabi Modelling Principles 2013 ;
- General Base Impacts® documentation
- Review report, available in the metadata of each dataset.

F. ADMINISTRATIVE INFORMATION

1. Commissioner

The datasets were modeled for the following commissioners:

- PE International
- ADEME

2. Dataset modeler

The datasets were modeled by the following modelers:

- PE International

APPENDIX: DATA NEED AND DATA SELECTION

The identified datasets are provided in Base Impacts®, with the following differences between consultation specifications and provided datasets:

Consultation specification	Available datasets	Justification
Adhesives		
Colle vinylique (1 composants)	PVC adhesive	
Colle vinylique (2 composants)	<i>Not provided</i>	
Colle thermofusible (éthylène vinyle acétate)	Hot-melt based on EVA	
Colle mélamine formaldéhyde (urée ou phénol)	<i>Not provided</i>	
Colle phénol formol	Phenolic resin adhesive modified with nitrile rubber	
Colle PU (1 composants)	Crystallising Polyurethane adhesive	
Colle PU (2 composants)	2-component PUR adhesive based on polyether and castor oil	
Colle époxy/polyépoxyde (1 composants)	Epoxy Adhesive Mix	
Colle époxy/polyépoxyde (2 composants)	Simple 2-component epoxy adhesive	
Colle polychloroprène (néoprène)	Solvent-based polychloroprene adhesive of good heat resistance	
Colle latex, base solvant	Pressure sensitive adhesive based on natural rubber	
Colle latex, base eau	Leather adhesive based on nitrile rubber	
Colle acrylique, base eau	Water-based acrylic adhesive for PVC flooring	
Colle polyester, base solvant (styrène)	Polyester hot-melt for the textile industry	
Colle PVA (1 composant)	PVAc adhesive	
/	UV-curing laminating adhesives	

Consultation specification	Available datasets	Justification
/	PUR dispersion adhesive	
/	Solvent-based polyurethane adhesive for the shoe industry	
Finishing products		
Urée formol	<i>Not provided</i>	
Laque PU - noir	PU Lacquer black	
Peinture PU avec solvant - noir	<i>Not provided</i>	
Peinture PU sans solvant - noir	<i>Not provided</i>	
Vernis acrylique	Acrylic Varnish	
Laque PU - vernis PU	PU Varnish	
Finition polyester	Polyester Finish	
Finition acrylique	Acrylic Finish	
Finition PU	PU Finish	