Facilitating Data Exchange between LCA Software involving the Data Documentation System SPINE

Report from Data Exchange Project, Phase 2000, involving:
The Centre for Environmental Assessment of Product and Material System (CPM),
ABB, Akzo Nobel, Assess, Chalmers Industriteknik (CIT), Nordic Port and Perstorp

Summary

This report present results from the first phase in the CPM project Data Exchange, which was initiated to facilitate environmental life cycle data communication within the documentation system SPINE and between LCA software. The aim of the project was to identify current problems related to the data exchange, and to focus on the most important issues to find consensus solutions involving both system developers and users.

The results consist of recommendations on common definitions, interpretations, and nomenclatures suited for LCA practitioners and system developers. The issues dealt with in this report are the technical specifications of the data communication file, called XFR file, nomenclatures, and minor technicalities. However, the nomenclatures and the XFR specification are considered to be the most important outcome of this project. In addition, the project group has discussed how to continue this collaboration in the future, in order to achieve further harmonisation in the system development.

The report contains a formal technical specification of the XFR file. The *nomenclatures* dealt with address *substances*, i.e. physical flows in terms of residue, natural resource, and emission, and descriptions of these in terms of *flow type*, and input or output *environment*. Other technicalities dealt with are *how to name objects of study, register addresses, specify dates*, and *manage empty fields*.

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1 Introduction

In the early 2000, CPM invited several life cycle assessment (LCA) system developers and users in order to arrange a joint problem-solving platform for data communication issues involving software developed from the SPINE concept and other LCA software. The aim was to facilitate the communication of SPINE formatted data sets among LCA system developers and users.

The data documentation system SPINE supports a common, well-structured, and flexible environmental information system that facilitates quality reviews e.g. in the documentation and communication phases. SPINE@CPM Data Tool is software developed at CPM and it may be used for LCA and documenting, storing and communicating life cycle inventory (LCI) data. Further, there are today three LCA calculation software based on the SPINE concept, EcoLab developed by Nordic Port, EPS Design System 4.0 developed at Assess, and LCAiT developed at Chalmers Industriteknik Ekologik (CIT).

During the last couple of years, the CPM network experienced issues frequently appearing in the practical data exchange between SPINE@CPM Data Tool and LCA calculation software. The aim of this project was to identify and compile all current problems related to the data exchange, and to focus on the most important issues to find consensus solutions involving both system developers and users. The results are recommendations on common definitions, interpretations, and nomenclature that will facilitate the data exchange and ideas on how to continue this work.

This report is the result from the project phase 2000 which was divided into two sub-projects, one involving nomenclature issues and minor technical issues, and the other technical specifications of the data communication file, called XFR. The XFR file is used for communication of LCA data between different databases and it can be communicated e.g. by diskette, through a local network or by e-mail. The first six chapters derive from the sub-project regarding nomenclature and minor technical issues, and the following chapter from the project handling the XFR specification.

The recommendations that result from this project are meant to be used by LCA practitioners and LCA system developers. The CPM intention is to let this project initiative lead to a continuous and international collaboration in the area of environmental data exchange. Interested parties are warmly welcome to join this collaboration during next year, when we will meet again in order to summarise the changed situation, discuss new solutions, and developments. The last chapter Future Work presents some issues that may be dealt with in future project phases.

Here are some reports that can give further information about the background of the SPINE concept etc:

"SPINE, A Relation Database Structure for Life Cycle Assessment"; Carlson R., Löfgren G., Steen B.; Göteborg; IVL-REPORT; September 1995
The original report documenting the SPINE structure.

"Establishment of CPM's LCA Database"; Carlson R., Pålsson A-C.; CPM report 1998:3, The report documents the CPM project establishing a Swedish national LCI database and its results, including the CPM data quality requirements and nomenclatures.

"Introduction and guide to LCA data documentation using the CPM data documentation criteria and the SPINE format"; Pålsson A-C; CPM report 1:1999
A report describing how to work with documentation of LCI data using SPINE, in correspondance with ISO and CPM data quality requirements (the report is a major revision and translation of CPM report 6:1997).

"An Assessment of the SPOLD format"; Erixon M., Ågren S.; CPM report 1998:5
A report describing method and result of the CPM assessment of the SPOLD format and comparison with the SPINE format.
Due to the obvious bias of our assessment from our previous experiences with working with SPINE, the SPOLD-group found reasons to respond to the result from our assessment. The response has been prepared by Bo P. Weidema in Brussels, January 1999: "*Response to the CPM assessment of the SPOLD format*".

"An interpretation of the CPM use of SPINE in terms of the ISO 14041 standard"; Arvidsson P. et al; CPM Internal Report 1999
The report is an adaptation and revisions of CPM report 1:1997. In this updated report, SPINE and the CPM LCI data documentation requirements is compared and interpreted with the final standard ISO 14 041:1998:

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2 Substance Nomenclature

2.1 Background

The substance nomenclatures addressed in this chapter are *Natural Resource, Emission,* and *Residue*, where the division only exists in order to present the groups of interest of this project. The substance groups were chosen because they were regarded as being important for the environmental impact assessment and the life cycle inventory. In addition, other groups of substances may be too business specific e.g. products and semi-manufactured components. The substance selection is acquired from the project participants, representing the most frequently used substances.

Notice that several substances may occur as different kinds of flow types, e.g. product or natural resource, and come from/go to different kinds of environments, e.g. water or land (see chapter 3). We recommend that such a substance not will be given different substance identities in the database, i.e. CO2 as an emission and CO2 as a raw material does not lead to double entry bookkeeping of CO2. The substance should be recognised by the combination of substance, flow type and environment, i.e. in regard of the example above CO2 is an *emission* to *air,* or a *refined resource* from the *technosphere*.

2.2 Recommendation for System Developers and Users of LCA Software

A substance, i.e. physical flow, should only be given one *reference* name, which describes the substance, material, or product as detailed as possible *in English*. In long run, the field *Substance Note*, addressed in connection with the substance nomenclature, should be used in order to describe the substance further and the function *Alternate Name*, not yet implemented in the SPINE tool, should be used to give the substance synonyms. In the meantime however, while the *Alternate Name* function is under development, all substance specifications, explanations, and synonyms should be given in the field *Substance Note*. This will guide the XFR file and LCA practitioner, so that the right interpretation is made in the data exchange.

2.2.1 Natural Resource

In this report substances that may occur as natural resources are presented in the four groups: *Elements in ore/metals, Minerals*, *Non-material energy resources* and *Other natural resources*, where the classification only exists in order to indicate which substance categories that are dealt with in this project. The principles of the nomenclatures are described in the following text and examples presented in table 1 further down.

1. *Elements in ore/metals* Elements in ore are in LCA contexts sometimes presented as the amount of e.g. metal extracted from ore, e.g. *Aluminium in ore, Copper in ore, Iron in ore*. However, this is not a comprehensive way of presenting the data, as it does not contain any information about the total amount of ore, including the rock that has been mined. The rest product from the mining may have to be added separately in the study, e.g. as *Rock*. Further, this presentation does not give any information about what kind of ore that are mined. Pure metals, e.g. aluminium, copper, and iron are considered to be *refined resources* and are not addressed in this project.
2. *Minerals* The total amount of mineral, including metals, rock etc. may be presented in two ways, where the first name structure is preferable:

2.1 Minerals should be described as detailed as possible, i.e. using the name of the specific type of ore, e.g. *Bauxite, Chalcopyrite, Magnetite*, see *2.1 Specific minerals* in table 1.

2.2 Minerals may also be named with respect to the content of main interest for the study, e.g. *Aluminium ore, Copper ore, Iron ore,* see *2.2 Non specific minerals* in table 1. However, this way of presenting data is not recommended, as it does not give any information about what type of ore that are mined.

3. *Non-material energy resources* The possible (theoretical) energy in natural resources shall be presented as e.g. *Nuclear energy, Hydro energy, Wind energy*, see *Non-material energy resources* in table 1. *Nuclear energy* may also be presented as *Uranium in ore*.
4. *Other natural resources* Examples of other natural resources are presented in table, e.g. *Clay, Hard coal, Raw rubber*. The substance can be given either in mass or energy units. Land use has not been dealt with in this project, as it is a difficult issue and the subject of many current projects. The humidity content of a substance or the fact that it is dry matter may be put in brackets after the substance name, e.g. *Peat (dry matter), Biomass (20% humidity), Wood (5% humidity)*. This structure may also be applied in regard of concentrations.

Table 1 Recommendations and examples of nomenclature for natural resources.

Default Name	*Alternate Name/ Reference Number*	*Explanation*	*Other Information/ Recommendations*
1. Elements in ore/metals			
Aluminium in ore		The amount of aluminium extracted from ore.	
Copper in ore		The amount of copper extracted from ore.	
Chromium in ore		The amount of chromium extracted from ore.	
Gold in ore		The amount of gold extracted from ore.	
Iron in ore		The amount of iron extracted from ore.	
Lead in ore		The amount of lead extracted from ore.	
Nickel in ore		The amount of nickel extracted from ore.	
Silver in ore		The amount of silver extracted from ore.	
Sulphur in ore		The amount of sulphur extracted from ore.	
Tin in ore		The amount of tin extracted from ore.	
Uranium in ore		The amount of uranium extracted from ore.	- Uranium in ore is also used to describe the energy content in nuclear power. - Presented as natural isotope composition.
Zinc in ore		The amount of zinc extracted from ore.	

Table 1 Continuation: Recommendations and examples of nomenclature for natural resources.

Default Name	*Alternate Name/ Reference Number*	*Explanation*	*Other Information/ Recommendations*
2. Minerals			
2.1 Specific minerals			
Anglesite			One of several lead ores
Bauxite		Composition varying between Al(OH)3 and AlO(OH)	One of several aluminium ores
Bentonite			
Carnotite			One of several uranium ores
Cerussite			One of several lead ores
Chalcocite	Copper glance	Cu2S	One of several copper ores
Chalcopyrite	Copper pyrite	CuFeS2	One of several copper ores
Chalk		CaCO3	
Chromite		FeCr2O4	
Cuprite			One of several copper ores
Dolomite		MgCO3+CaCO3	
Feldspar		Group of aluminosilicate minerals	Used in ceramic industries
Galena		PbS	One of several lead ores
Haematite		Fe2O3	One of several iron ores
Limestone		CaCO3	
Limonite			One of several iron ores
Magnetite		Fe3O4	One of several iron ores
Malachite			One of several copper ores
Olivine		A magnesium silicate	
Pitchblende		U3O8	One of several uranium ores
Rock salt	Sodium chloride	NaCl	
Siderite			One of several iron ores
Uraninite			One of several uranium ores

Table 1 Continuation: Recommendations and examples of nomenclature for natural resources.

Default Name	*Alternate Name/ Reference Number*	*Explanation*	*Other Information/ Recommendations*
2.2 Non specific minerals			
Aluminium ore			Aluminium ore can be Bauxite etc.
Copper ore			Copper ore can be Chalcopyrite, Chalcocite, Cuprite, Malachite etc.
Iron ore			Iron ore can be Haematite, Magnetite, Limonite, Siderite etc.
Lead ore			Lead ore can be Galena, Anglesite, Cerussite etc.
Oxide ore		Unspecific oxide ore	
Sulphide ore		Unspecific sulphide ore	
Uranium ore			- Uranium ore can be Pitchblende, Uraninite, Carnotite etc. - Uranium ore can be used to describe the energy content in nuclear fuel.
3. Non-material energy resources			
Geothermal energy	Geothermal	The energy content in geothermal energy	Prior to generation, transformation, and transportation losses.
Hydro energy	Hydro	The energy content (potential energy) in hydro power	Prior to generation, transformation, and transportation losses, i.e. not to be confused with electricity from hydropower.
Nuclear energy	Nuclear	The energy content in nuclear fuel	Prior to generation, transformation, and transportation losses, i.e. not to be confused with electricity from nuclear power.
Solar energy	Solar	The energy content in solar radiation	Prior to generation, transformation, and transportation losses.
Wind energy	Wind	The energy content (kinetic energy) in the wind	Prior to generation, transformation, and transportation losses.

Table 1 Continuation: Recommendations and examples of nomenclature for natural resources.

Default Name	*Alternate Name/ Reference Number*	*Explanation*	*Other Information/ Recommendations*
4. Other natural resources			
Biomass			E.g. used as biofuel
Clay			
Coal			Specify the type of coal if possible e.g. hard coal
Crude oil			
Gravel			
Ground water			
Hard coal	Stone coal		
Lignite			
Natural gas	Crude gas		
Peat			The humidity content or the fact that it is dry matter may be put in brackets after the substance name, e.g. "Peat (dry matter)" or "Peat (50% humidity)".
Raw rubber			
Sand			
Sea water			
Surface water			
Water			
Wood			

2.2.2 Emission

In table 2, a large number of substances that commonly act as emission flows are classified into four categories:

1) elements, cations and isotopes,
2) inorganic compounds and anions,
3) organic compounds, and
4) groups of substances (collective substances) and measured properties.

Note that this classification of substances is not necessarily the most logical one, but it was made for practical purposes.

For each substance in table 2, there may be a systematic name, one or two chemical formulas, one or more trivial or alternate names and a CAS (Chemical Abstract Service) registry number. In category 4), the substances have no individual chemical formula and no CAS Number. For organic compounds, there can be one chemical formula reflecting the structure of the compound (e.g. C6H5OH), and one formula that merely contains the total number of carbons, hydrogens, oxygens etc. in the molecule (e.g. C6H6O). The default name, i.e. the name recommended by the CPM project, is indicated by its **bold** text style. In the table, the substances are sorted in each substance category according to their default names.

Unfortunately, it was not possible to use a single principle for all four categories to establish which name should be the default name. For substances not included in the table, the following principles are recommended in order to find the default name:

For substances belonging to categories 1) and 2), use the chemical formula, if it is known. Use the simple element symbol (e.g. Cr) unless it is known that the substance is a specific ion (e.g.

Cr3+, CrO42-) or it is in a specific oxidation state (e.g. Cr(VI)). Also don't use the ion symbol or the oxidation state symbol unless this extra information is relevant.

For substances belonging to category 3), use the systematic name unless it is complicated and a trivial name is well-known; in that case, use the trivial name instead.

For substances belonging to category 4), use a well-known, not abbreviated name.

Table 2 is partially based on information (CAS numbers and synonyms) available at http://www.kemi.se, the web site of Kemikalieinspektionen (the Swedish National Chemicals Inspectorate). In Appendix, some background information for the discussion on emission nomenclature may be found.

Table 2 Nomenclature for a number of substances commonly occurring as emissions, and which were acquired by Data Exchange project participants.

Systematic Name	*Chemical Formula*	*Trivial or Alternate Names*	*CAS Number*	*Explanation*	*Other information/ Recommendations*
1) Elements, cations and isotopes					
Silver	**Ag**		7440-22-4		
Aluminium	**Al**	Aluminum	7429-90-5		Aluminum is Am. spelling
Arsenic	**As**		7440-38-2		
Arsenic(III)	**As(III)**			Trivalent arsenic	E.g. As2O3
Calcium	**Ca**		7440-70-2		
Cadmium	**Cd**		7440-43-9		
Cobalt	**Co**		7440-48-4		
Chromium	**Cr**		7440-47-3		
Chromium3+	**Cr3+**			Chromium(III) ion	
Chromium(VI)	**Cr(VI)**		18540-29-9	Hexavalent chromium	CrO42-, CrO3 etc
Caesium-137	**Cs-137**	Cesium-137	7440-46-2		Radioactive isotope
Copper	**Cu**		7440-50-8		
Iron	**Fe**		7439-89-6		
Mercury	**Hg**		7439-97-6		
Potassium	**K**		7440-09-7		
Magnesium	**Mg**		7439-95-4		
Manganese	**Mn**		7439-96-5		
Molybdenum	**Mo**		7439-98-7		
Nitrogen	N	**N total** Nitrogen total N-tot		Total nitrogen as N	Avoid Total nitrogen, Tot-N etc. See also NH4+ as N, NO3- as N!
Sodium	**Na**		7440-23-5		

Table 2 Continuation: Nomenclature for a number of substances commonly occurring as emissions.

Systematic Name	*Chemical Formula*	*Trivial or Alternate Names*	*CAS Number*	*Explanation*	*Other information/ Recommendations*
Nickel	**Ni**		7440-02-0		
Phosphorus	P	**P total** Phosphorus total P-tot	7723-14-0	Total phosphorus as P	Avoid Total phosphorus, Tot-P etc. See also PO43- as P!
Lead	**Pb**		7439-92-1		
Lead2+	**Pb2+**			Lead(II) ion	
Radon-222	**Rn-222**		10043-92-2		Radioactive isotope
Selenium	**Se**		7782-49-2		
Tin	**Sn**		7440-31-5		
Uranium-235	**U-235**		7440-61-1		Radioactive isotope
Zinc	**Zn**		7440-66-6		
2) Inorganic compounds and anions					
Chloride	**Cl-**		16887-00-6	Chloride ion	
Chlorine	**Cl2**		7782-50-5	Chlorine gas or dissolved chlorine	
Chlorine dioxide Chlorine(IV) oxide	**ClO2**		10049-04-4		
Hypochlorite Oxochlorate(I)	**ClO-**				
Cyanide	**CN-**		57-12-5	Cyanide ion	
Carbon monoxide	**CO**		630-08-0		
Carbon dioxide	**CO2**		124-38-9		CO2 (fossile) or in general
Carbon dioxide	CO2	**CO2 (renewable)**	124-38-9	CO2 from combustion or degradation of biomass or other renewable material	

Table 2 Continuation: Nomenclature for a number of substances commonly occurring as emissions.

Systematic Name	*Chemical Formula*	*Trivial or Alternate Names*	*CAS Number*	*Explanation*	*Other information/ Recommendations*
Chromium trioxide	**CrO3**		1333-82-0		A specific form of Cr(VI)
Chromate Tetraoxochromate(VI)	**CrO42-**		13907-45-4		A specific form of Cr(VI)
Carbon disulphide	**CS2**		75-15-0		Also spelled disulfide (Am.)
Fluoride	**F-**		16984-48-8	Fluoride ion	
Fluorine	**F2**		7782-41-4		
Hydrofluoric acid Hydrogen fluoride	**HF**		7664-39-3		
Hydrochloric acid Hydrogen chloride	**HCl**		7647-01-0		
Hydrocyanic acid Hydrogen cyanide	**HCN**		74-90-8		
Nitric acid	**HNO3**		7697-37-2		
Phosphoric acid	**H3PO4**		7664-38-2		Avoid Orthophosphoric acid
Hydrogen sulphide	**H2S**		7783-06-4		Also spelled sulfide (Am.)
Sulphuric acid	**H2SO4**		7664-93-9		Also spelled Sulfuric (Am.)
Ammonia	**NH3**		7664-41-7		
Ammonium	**NH4+**			Ammonium ion	
		NH4+ as N Ammonium as N NH4-N			Note that the quantity of NH4+ as N is smaller than the quantity of NH4+ by a factor 1,29
Dinitrogen oxide Nitrogen(I) oxide	**N2O**	Nitrous oxide	10024-97-2		
Nitrogen oxide Nitrogen(II) oxide	**NO**	Nitric oxide	10102-43-9		
Nitrogen dioxide Nitrogen(IV) oxide	**NO2**		10102-44-0		

Table 2 Continuation: Nomenclature for a number of substances commonly occurring as emissions.

Systematic Name	*Chemical Formula*	*Trivial or Alternate Names*	*CAS Number*	*Explanation*	*Other information/ Recommendations*
Nitrogen oxides	**NOx**			NO + NO2, as NO2	
Nitrite	**NO2-**		14797-65-0	Nitrite ion	
Nitrate	**NO3-**		14797-55-8	Nitrate ion	
		NO3- as N Nitrate as N NO3-N			Note that the quantity of NO3- as N is smaller than the quantity of NO3- by a factor 4,43
Phosphine	**PH3**		7803-51-2		
Phosphate	**PO43-**		14265-44-2	Phosphate ion	
		PO43- as P Phosphate as P PO4-P			Note that the quantity of PO43- as P is smaller than the quantity of PO43- by a factor 3,07
Sulphide	**S2-**			Sulphide ion	Also spelled Sulfide (Am.)
Sulphur hexafluoride	**SF6**		2551-62-4		Also spelled Sulfur (Am.)
Sulphur dioxide	**SO2**		7446-09-5		Also spelled Sulfur (Am.)
Sulphur trioxide	**SO3**		7446-11-9		Also spelled Sulfur (Am.)
Sulphur oxides	**SOx**			SO2 + SO3, as SO2	
Sulphite	**SO32-**			Sulphite ion	Also spelled Sulfite (Am.)
Sulphate	**SO42-**		14808-79-8	Sulphate ion	Also spelled Sulfate (Am.)
3) Organic compounds					
Ethanoic acid	CH3COOH C2H4O2	**Acetic acid**	64-19-7		
2-Propanone	CH3COCH3 C3H6O	**Acetone** Dimethyl ketone	67-64-1		
Ethyne	CHCH C2H2	**Acetylene**	74-86-2		

Table 2 Continuation: Nomenclature for a number of substances commonly occurring as emissions.

Systematic Name	*Chemical Formula*	*Trivial or Alternate Names*	*CAS Number*	*Explanation*	*Other information/ Recommendations*
2-Propenenitrile	CH2CHCN C3H3N	**Acrylonitrile**	107-13-1		
Benzene	C6H6		71-43-2		
Benzo(a)pyrene	C20H12		50-32-8		A polycyclic aromatic hydrocarbon (PAH)
Bromomethane	CH3Br	Methyl bromide	74-83-9		
Butadiene	CH2(CH)2CH2 C4H6		106-99-0		
Butane	C4H10	n-Butane	106-97-8		Liquefied petroleum gas (LPG) constituent
Butene	CH2CHC2H5 C4H8	Butylene	25167-67-3		
Trichlorofluoromethane	CCl3F	**CFC-11**	75-69-4		Avoid Freon 11, Arcton 11, Frigen 11, Genetron 11 etc
1,1,2-trichloro-1,2,2-trifluoroethane	CCl2FCClF2 C2Cl3F3	**CFC-113**	76-13-1		Avoid Freon 113 etc
1,2-Dichloro-1,1,2,2-tetrafluoroethane	CClF2CClF2 C2Cl2F4	**CFC-114**	76-14-2		Avoid Freon 114 etc
Dichlorodifluoromethane	CCl2F2	**CFC-12**	75-71-8		Avoid Freon 12 etc
Chloromethane	CH3Cl	Methyl chloride	74-87-3		
1,2-Dichloroethane	CH2ClCH2Cl C2H4Cl2	Ethylene dichloride	107-06-2		Avoid abbr. DCE, EDC
Dichloromethane	CH2Cl2	Methylene dichloride	75-09-2		
Di-(2-ethylhexyl) phthalate	C24H38O4	DEHP	117-81-7		A common plasticizer in PVC
2,3,7,8-tetrachlorodibenzo-p-dioxin	C12H4Cl4O2	**Dioxin (TCDD)**	41903-57-5		One of several Dioxins and Dibenzofurans
Ethane	C2H6		74-84-0		

Table 2 Continuation: Nomenclature for a number of substances commonly occurring as emissions.

Systematic Name	*Chemical Formula*	*Trivial or Alternate Names*	*CAS Number*	*Explanation*	*Other information/ Recommendations*
Ethanol	C2H5OH C2H6O	Ethyl alcohol	64-17-5		
Ethene	C2H4	Ethylene	74-85-1		
1,2-Ethanediol	(CH2OH)2 C2H6O2	**Ethylene glycol**	107-21-1		
Oxirane	(CH2CH2)O C2H4O	**Ethylene oxide** 1,2-epoxyethane	75-21-8		
Methanal	HCHO CH2O	**Formaldehyde**	50-00-0		
Bromochlorodifluoromethane	CBrClF2	**Halon-1211**	353-59-3		Used as fire extinguisher
Bromotrifluoromethane	CBrF3	**Halon-1301**	75-63-8		Used as fire extinguisher
1-chloro-1,1-difluoroethane	CClF2CH3 C2H3ClF2	**HCFC-142b**	75-68-3		"Soft freon". Avoid CFC-142b, Freon 142b etc.
Chlorodifluoromethane	CHClF2	**HCFC-22**	75-45-6		"Soft freon". Avoid CFC-22, Freon 22, R-22 etc.
Hexafluoroethane	C2F6	FC-116 Perfluoroethane PFC-116	76-16-4		Avoid Freon 116, CFC-116 etc
Hexane	C6H14	n-Hexane	110-54-3		
1,1,1,2-Tetrafluoroethane	CF3CH2F C2H2F4	**HFC-134a**	811-97-2		Avoid CFC-134a, Freon 134a etc
1,1-Difluoroethane	CHF2CH3 C2H4F2	**HFC-152a**	75-37-6		Avoid CFC-152a, Freon 152a etc
Methane	CH4		74-82-8		
Methanol	CH3OH CH4O	Methyl alcohol	67-56-1		

Table 2 Continuation: Nomenclature for a number of substances commonly occurring as emissions.

Systematic Name	*Chemical Formula*	*Trivial or Alternate Names*	*CAS Number*	*Explanation*	*Other information/ Recommendations*
Pentachlorophenol	C6Cl5OH C6HCl5O		87-86-5		
Phenol	C6H5OH C6H6O		108-95-2		
Propane	C3H8		74-98-6		Liquefied petroleum gas (LPG) constituent
2-Propanol	(CH3)2CHOH C3H8O	Isopropanol Isopropyl alcohol	67-63-0		
2-Propenal	CH2CHCHO C3H4O	Acrolein Acraldehyde	107-02-8		
Propene	CH2CHCH3 C3H6	Propylene	115-07-1		
Ethenylbenzene	C6H5CHCH2 C8H8	**Styrene** Vinylbenzene	100-42-5		
Tetrachloroethene	CCl2CCl2 C2Cl4	Perchloroethylene	127-18-4		Avoid abbr. PCE, Per
Tetrachloromethane	CCl4	Carbon tetrachloride	56-23-5		Avoid CFC-10
Tetrafluoromethane	CF4	FC-14 Perfluoromethane PFC-14 Carbon tetrafluoride	75-73-0		Avoid Freon 14, CFC-14 etc
Methylbenzene	C6H5CH3 C7H8	**Toluene**	108-88-3 108-88-3		
Tribromomethane	CHBr3	Bromoform	75-25-2		
1,1,1-Trichloroethane	CCl3CH3 C2H3Cl3	Methylchloroform	71-55-6		

Table 2 Continuation: Nomenclature for a number of substances commonly occurring as emissions.

Systematic Name	*Chemical Formula*	*Trivial or Alternate Names*	*CAS Number*	*Explanation*	*Other information/ Recommendations*
Trichloroethene	CHClCCl2 C2HCl3	Trichloroethylene	79-01-6		Avoid abbr. TCE, Tri
Trichloromethane	CHCl3	Chloroform	67-66-3		
Chloroethene	CH2CHCl C2H3Cl	**Vinyl chloride**	75-01-4		Avoid VCM, Vinyl chloride monomer
Dimethylbenzene	C6H4(CH3)2 C8H10	**Xylene**	1330-20-7		Note that there are three Xylene isomers: o-, m- and p-Xylene
4) Groups of substances and measured properties					
		Acid as H+ Acid (H+) H+ equivalents			Note that 1 g of Acid as H+ is equivalent to 1 mol of Acid as H+
Alkanols		**Alcohols**		Group of organic compounds containing -OH	
Alkanals		**Aldehydes**		Group of organic compounds containing -CHO	
Alkanes		Paraffins		Aliphatic hydrocarbons, saturated	Avoid CxHy, HxCy etc
Alkenes		Olefins		Aliphatic hydrocarbons containing double bonds	
		AOX		Adsorbable organic halogen, usually as Cl equivalents	Measured parameter, estimate of dissolved organic halogen
		Aromatics Aromatic hydrocarbons		Aromatic compounds including aromatic hydrocarbons	
		BOD		Biochemical oxygen demand, as O2 equivalents	Measured parameter, sometimes BOD5, BOD7

Table 2 Continuation: Nomenclature for a number of substances commonly occurring as emissions.

Systematic Name	*Chemical Formula*	*Trivial or Alternate Names*	*CAS Number*	*Explanation*	*Other information/ Recommendations*
		CFCs		Chlorofluorocarbons	Avoid Freons, Hard freons. See also individual CFCs.
		Chlorobenzenes Chlorinated benzenes			Includes chlorobenzene, dichlorobenzenes etc
		Chloroorganics Chlorinated organics Organo-Cl		Chlorinated organic compounds	
		Chlorophenols Chlorinated phenols			Includes chlorophenols, dichlorophenols etc
		Chlorinated VOC VOC-Cl		Chlorinated volatile organic compounds	
		COD		Chemical oxygen demand, as O2 equivalents	Measured parameter
		Detergents		Unspecified surface-active agents	
		Dioxin		Unspecified dioxin	Group including several "Dioxins". See also Dioxin (TCDD) above!
		Dissolved organics Dissolved organic compounds			Usually organics dissolved in water. Avoid if specific com-pounds are known. Avoid abbr. DSO.
		Dissolved solids Total dissolved solids			Measured parameter, usually salts dissolved in water. Avoid abbr. TDS, DSS.
		Dissolved organic carbon DOC		Dissolved organic carbon, as C equivalents	Measured parameter, usually emissions to water
		Dust		Particulate matter which does not come from a combustion process	See also Particles

Table 2 Continuation: Nomenclature for a number of substances commonly occurring as emissions.

Systematic Name	*Chemical Formula*	*Trivial or Alternate Names*	*CAS Number*	*Explanation*	*Other information/ Recommendations*
		HCFCs		Hydrochlorofluorocarbons	Avoid Freons, Soft freons. See also individual HCFCs.
		Hydrocarbons HC			Avoid abbr. CxHy, HxCy etc
		Metals		Unspecified metals	Avoid Metals if specific metals are known
		NMVOC		Non-metane volatile organic compounds, i.e. VOC except methane	Usually emission to air. Avoid NMVOC (coal combustion), NMVOC (diesel engine) etc.
		Oil		Unspecified oil	Oil is an unspecified mix of hydrocarbons
		PAH Polycyclic aromatic hydrocarbons		Group of aromatic hydro-carbons	
		Particles Particulate matter PM2.5, PM10		PM = Particulate matter	PM2.5 represents particles of a size <2,5 µm. See also Dust, Soot, which may be used to indicate origin or composition of particles.
		PCB Polychlorinated biphenyls		Group of chlorinated aromatic hydrocarbons	
		Petrol			Petrol is an unspecified mix of hydrocarbons
		Soot		Particulate carbon residue from combustion processes	Contains carbon formed in incomplete combustion. See also Particles.
		Suspended solids		Particulate matter suspen-ded (i.e. not dissolved) in water	Avoid abbr. Susp solids, SS, TSS
Thiols		Mercaptans		Group of organic com-pounds containing -SH	

Table 2 Continuation: Nomenclature for a number of substances commonly occurring as emissions.

Systematic Name	*Chemical Formula*	*Trivial or Alternate Names*	*CAS Number*	*Explanation*	*Other information/ Recommendations*
		Total organic carbon TOC		Total organic carbon, as C equivalents	Measured parameter, usually emission to water
		VOC		Volatile organic compounds	Usually emission to air. Avoid VOC (coal combustion), VOC (diesel engine) etc.

2.2.3 Residue

Residue nomenclature should include some words in connection with residue (e.g. waste, residue, scrap, sludge, ashes refuse etc.). Some common residue names are presented in table 3. The nomenclature used by the Association of plastics manufacturers in Europe (APME) is the base for the naming of residue.
For a more thorough nomenclature of different types of residue see European waste catalogue (E.g. presented in the Official Journal of the European Communities, 7.1.94, No L 5/15).

Table 3 Nomenclature for some residues, acquired by Data Exchange project participants

Name	*Explanation*	*Other Information/ Recommendations*
Non hazardous waste		One of the two categories that residue has to be devided into in an Environmental Product Declaration
Hazardous waste		One of the two categories that residue has to be devided into in an Environmental Product Declaration
Mineral waste	Waste earth and rock generated in mining operations	
Slags and ash	The solid waste produced by industrial boilers and furnaces	
Inert chemical waste	Waste from chemical processes that can be sent to landfill sites without further treatment	
Regulated chemical waste	The category of chemical waste that has to be sent to special storage sites because it is corrosive or toxic	
Mixed industrial waste	Usually consisting of waste such as discarded industrial packaging etc.	
Construction waste	Waste generated in building and plant construction operations	
Waste to incineration	Waste that is sent of site for incineration	
Waste to recycling	Materials that are collected by external operators and recycled	
Paper & board refuse		Is commonly collected by local authorities (or their commercial equivalents) and usually contains packaging materials
Plastics refuse		Is commonly collected by local authorities (or their commercial equivalents) and usually contains packaging materials
Metals refuse		Is commonly collected by local authorities (or their commercial equivalents) and usually contains packaging materials
Highly radioactive waste	Used fuel (including the sealing) from nuclear power generation	

3 Flow Type and Environment Nomenclature

3.1 Background

In order to facilitate the exchange of data, so that all users are familiar with similar nomenclature structures, the project participants decided on guidelines for a systematic approach when naming flow types and different environment types.

FlowType is a nomenclature defined according to the SPINE model. It is used for describing the different categories of flows coming into or out from a technical system, see figure 1. *Environment* is also a nomenclature defined according to the SPINE model and it is used for describing how the geographical area of origin or the recipient is connected to an input or an output flow.

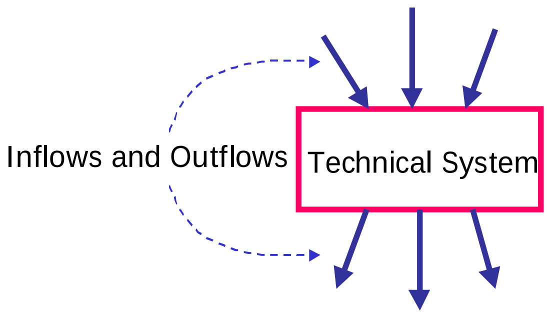

Figure 1 In the SPINE model the *Technical System* and the *Inflows* and *Outflows* are essential concepts when describing the data sets.

A combination of the two nomenclatures *FlowType* and *Environment* are usually required in order to define a flow, which is why these two nomenclatures are dealt with in the same section. There are of course several other flow properties that are needed in addition, when defining a flow properly, e.g. substance name (which is dealt with in a separate section), quantity, unit etc.

3.2 Recommendation for Users of LCA Software

For a user of an LCA software based on the SPINE model it is preferred to use the combinations of *FlowType* and *Environment* that are recommended in this document. This is because the *FlowType* and *Environment* combination often are used for sorting the inventory parameters in the result output table, see table 1, hiding flows from or to the environment in the graphical interfaces etc. If not using the recommendations, it will in some cases not be possible to use all features of the software properly. A user of the SPINE concept that is not using a software will also gain on using these recommendations, since he or she most likely will exchange data with another SPINE based software.

3.2.1 Definition of the FlowType and Environment nomenclatures

Table 4 Definition of the FlowType nomenclature.

FlowType	*Description*
Inputs	
Refined resource	Used for inputs of resources (raw material, energy etc) that have been processed in some way e.g. inputs of wood logs, steel, nitric acid, electricity or fuel oil.
Natural resource	Used for inputs of natural resources e.g. iron ore, bauxite, sea water, rock salt or crude oil.
Cargo (1)	Used for inputs of cargo to a transport activity.
Outputs	
Cargo (1)	Used for outputs of cargo from a transport activity.
Emission	Used for emissions e.g. CO_2, SO_2, COD or Fe^{3+}.
Residue (2)	Used for outputs that is without economic value and that is not air or waterborne e.g. the waste in a landfill site remaining at the end of the time period investigated or the residue that is collected for recycling.
Product	Used for the product of the studied system, which ends up somewhere else in the technosphere.
By-product	Used for an output to technosphere which has an economical value.

(1) The reason for using a flowtype for the cargo in a transport activity might not be “obvious”. There is an entity in SPINE called ActivityParameter, which can be used for defining the transport distance in a transport activity. The ActivityParameter is factor which all flows are multiplied with except for the input and output of cargo. Hence, the FlowType = Cargo is used in order to “earmark” these “cargo flows” so that the calculating software can increase all other flows in accordance with the transport distance.

(2) The word *Residue* was preferred prior to the more “specific” word *Waste*.

Table 5 Definition of the Environment nomenclature

Environment	*Description*
Air	Air is the environment for emissions from smoke-stacks and for diffuse airborne emissions such as methane from landfill sites.
Water	Water is the environment for most waterborne emissions. It is also the source of natural resources such as sea water. Water environment includes e.g. the sea, lakes, and creeks.
Ground	The flow Iron ore is a natural resource from the Ground environment.
Technosphere	Technosphere is the environment for all non-elementary flows. It is the source of refined resources such as steel and fuel oil. It is the recipient of products, by-products and non-elementary waste flows such as waste transported to landfill sites.
Other	The environment Other is suggested to be used only if the type of environment is unknown!

3.2.2 Combination of FlowType and Environment nomenclature

Table 6 Recommendations on which FlowType and Environment nomenclatures to use and how to combine them.

FlowType	*Environment*	*Comment concerning the combination*
Inputs		
Refined resource	Technosphere	Could by definition only be combined with Technosphere.
Natural resource	Air, Water or Ground	Could be combined with either Air, Water or Ground.
Cargo	Technosphere	Could by definition only be combined with Technosphere.
Outputs		
Cargo	Technosphere	Could by definition only be combined with Technosphere.
Emission	Air, Water, Ground or Technosphere (1)	Could be combined with either Air, Water, Ground or Technosphere.
Residue	Ground (2) or Technosphere (3)	Could be combined with either Ground or Technosphere.
Product	Technosphere	Could by definition only be combined with Technosphere.
By-product	Technosphere	Could by definition only be combined with Technosphere.

(1) This combination is used for emissions to technosphere e.g. emissions to a waste water treatment plant.

(2) This combination is used for a residue leaving the technosphere i.e. a solid or liquid output to nature that is without economic value and that is not air or waterborne e.g. the waste in a landfill site remaining at the end of the time period investigated.

(3) This combination is used for a residue output to the technosphere e.g. the waste, which is transported to a landfill site or the residue that is collected for recycling.

3.3 *Information for System Developers*

The table below presents the *translation key* regarding *FlowType* and *Environment* among the three SPINE software that was studied within the project (i.e SPINE@CPM Data Tool, EcoLab and LCAiT 4). In some situations a Specific Translation Key had to be defined, but most of the times the translation key between the software was obvious or not needed at all.

Table 7 Translation key between the FlowType and Environment combinations occurring in different software today.

FlowType in table 6	*FlowType* *SPINE@CPM Data Tool* [(1)]	*EcoLab* [(2)]	*LCAiT 4* [(3)]	*Environment* *For all software*	*Is the translation key OK or is a specific translation key between the software needed?* [(4)]
Inputs Refined resource	Resource	Raw material Energy Waste	Non-elementary	Technosphere	Specific Translation Key: CPM & LCAiT → EcoLab: FlowType = Raw material is choosen
Natural resource	Resource	Resource	Resource	Air, Water & Ground Exception [(5)]→ Resource is the only option in EcoLab	Specific Translation Key: EcoLab → CPM & LCAiT: Environment = Ground is choosen The transfer from CPM to EcoLab or LCAiT requires that CPM does not use any sub-levels in the Environment nomenclature e.g. Agricultural air.
Cargo	Cargo	Cargo	Cargo	Technosphere	---
Outputs Cargo	Cargo	Cargo	Cargo	Technosphere	---
Emission	Emission	Emission	Emission	Air, Water & Ground	The transfer from CPM to EcoLab or LCAiT requires that CPM does not use any sub-levels in the Environment nomenclature e.g. Agricultural air.
Emission	Emission	Emission	Non-elementary water emission	Technosphere	OK
Residue	Residue	Waste	Elementary waste	Ground	OK
Residue	Residue	Waste	Non-elementary waste	Technosphere	OK
Product	Product	Product	Product	Technosphere	---
By-product	By-product	Product	Co-product	Technosphere	Specific Translation Key: EcoLab [(6)] → CPM & LCAiT: The FlowType becomes Product

(1) SPINE@CPM Data Tool is software for documentation, storage, and communication of LCA data on the SPINE format. The software has been developed by CPM at Chalmers.

(2) EcoLab is an LCA calculation software, which is based on the SPINE format. Nordic Port AB has developed the software.

(3) LCAiT 4 is a LCA calculation software, which is based on the SPINE format. Chalmers Industriteknik Ekologik has developed the software.

(4) When it is not possible to find one single match between the FlowType/Environment definitions (in the different software) a “Specific Translation Key” between the software has to be defined (bold in the table). “OK” means that there is one single match between the definitions i.e. the translation key is obvioous *e.g. Residue/Ground in CPM = Waste/Ground in EcoLab = Elementary waste/Ground in LCAiT.*
--- means that the definitions are identical in all the software i.e. no translation at all is needed.

(5) EcoLab has the Environment = Resource, which might be a bit confusing. The reason though is to be able to distinguish between resource flows and emission flows (in the case they have the same name) in the impact assessment phase. The fact is that this has not been solved yet in the LCAiT software either. This can be solved by introducing FlowType when defining the impact assessment index in the impact assessment module. CIT suggests that both EcoLab and LCAiT implement this as soon as possible. This means that the translation key (defined above) between EcoLab and SPINE@CPM Data Tool & LCAiT will probably not be necessary in a near future.

(6) Not quite OK since the information about By/Co-products does not exist in EcoLab.

4 Naming Object of study

4.1 Background

There are various systematic approaches on naming *Objects of Study* today. The reason for this are e.g. depending on how the user organisations work with LCA, what data sets that are involved in the studies, and how the software interface presents the data. In order to facilitate the exchange of data, so that all users are familiar with similar name structures, the project participants decided on common guidelines for the systematic approach when naming an *Object of Study*.

4.2 Recommendation for Users of LCA Software

The *Object of Study* should be named after the process in focus, i.e. the name should describe the main activity and possibly give a short specification of the product in the same sentence, see examples in 4.3.

4.3 Examples

Examples of names of *Objects of Study* according to the user recommendation are:

Bending of steel plate <1mm
Cement production
Cold press forming with medium deformation
Combustion of waste
Drilling in mild steel
Electric welding
Extraction of crude oil and gas
Extraction of sulphur and production of sulphuric acid
Incineration of Epoxy
Landfill disposal
Manufacturing PU elastics
Mining of dolomite
Production of French electricity mixture
Treatment of hazardous waste

4.4 Recommendation for System Developers

It has come to hand that the software users often need comprehensive information in the name of the *Object of Study* in order to separate similar data sets, although this information already is given in the documentation of the data set. Examples of such information is if it is a unit process or a cradle-to-gate process (*Category*), the data source used (*Owner*, *Site*, or *Publication*), and the reference flow (*Functional Unit*). A solution to this problem is to make the software interface more users friendly by presenting relevant documentation fields in connection to the name field. This means all information necessary to the user may be displayed at the same time and long unpractical names of *Object of Study* will be avoided.

5 Address Registration

5.1 Background

The *JuridicalPerson* table in SPINE accommodate name, mail address, telephone number and so on for a person or an organisation. Juridical persons are referred to in other SPINE tables to represent sites, owners, commissioners, practitioners and reviewers.

There has been some confusion in how to use the name field; Is the name field reserved for personal names only, or may it also be used for the name of an organisation in cases where the organisation itself is the main issue?

5.2 Recommendation for Users of LCA Software

Name	Personal name should be documented in the order: family name, first name. The name field should be left empty if the record primarily specifies an organisation. A name *must not* use multiple lines.
MailAddress	The first line specifies the name of an organisation. Leave the first line empty if you want to emphasise the absence of an organisation name. The rest of the mail address is specified on the following lines. A mail address may well use multiple lines.
Empty values	The *Name* or *MailAddress* field may be empty for some juridical persons.

5.3 Examples

Name	*First line of MailAddress*
Andersson, Sven	*CPM*
CPM	*Chalmers University of Technology* *CPM* *Sweden*
Andersson, Sven	
Andersson, Sven	*Calm street 5*

5.4 Recommendation for System Developers

System developers can help its users to comply with the recommendation, e.g. by giving examples and prescriptions of explicit rules in manuals or directly in the software.

6 Date Specification

6.1 Background

There are many different date formats, and a correct interpretation of a date is not always possible without knowing exactly which date format has been used. SPINE stores dates as texts, not as neutral date values. Therefore the dates can not be presented according to the regional settings of each computer, they always appear exactly as the user entered them. To avoid date ambiguities, we recommend a common date format for all specification of dates.

SPINE contains two pure date fields: *Inventory/DateCompleted* and *QMetadata/DateConceived*. Dates may also be embedded in any text field where *Inventory/TimeBoundary* is the most obvious example.

6.2 Recommendation for Users of LCA Software

The following date formats are recommended for all specification of a single date:

- yyyy-mm-dd
- yyyy-mm
- yyyy

A time period is specified by a start date followed by the word *to* and an end date. The start date should be less than the end date.

6.3 Examples

2000-05-31
1997-12
1995
1995 to 2001
1999-12-24 to 2000-06-30

6.4 Recommendation for System Developers

Software could help its users to apply the recommended date format in the following ways:

- Show a date example where users are supposed to enter pure dates.
- Check the entered pure date values. Draw the user's attention to values that do not comply with this recommendation and explain what is wrong.

7 Managing Empty Fields

7.1 Background

Wen the fields are left empty in the data format, it is impossible to know the reason for this; has the data input practitioner forgot to document the accurate information or is it unknown? In order to clarify the reason for the missing information and avoid misinterpretations, some recommendations on how to express these circumstances are presented.

7.2 Recommendation for Users of LCA Software

Do not leave a text field empty if it is possible to express why the information is missing, see examples in 7.3. An empty text field should be interpreted as if the data input practitioner has not made up his or her mind about the information content.

7.3 Examples

Sometimes it is enough to use one or two words to clarify why the information is missing, see list of suggestion below. However, in some cases further explanations is crucial in order for the data user to make the correct interpretation.

Not known	The information is not known.
Not relevant	The information is not relevant.
Not applicable	The information is not applicable.
None	There is no information of this character in this data set.
Not applied	This procedure is not applied/used.

7.4 Recommendation for System Developers

Encourage the software users not to leave a text field empty. In this way the software will support a system with higher quality.

8 XFR Syntax Reference

This XFR syntax reference is produced at CPM, Chalmers, Sweden by Peter Forsberg.

Version 1.0, 15/6-2000
Version 1.1, 22/6-2000

8.1 Introduction

This reference defines the syntax for the data transfer format XFR, originally developed by Nordic Port, Sweden. The XFR format (SPINE Transfer Format) was intended to be a convenient and human readable format for exchange of environmental SPINE structured data. Since no inherent limitations of the structure exist, it can, however, be used for data following any kind of relational model and thus in particular those found in relational databases.

This reference describes, as the title suggests, the syntax of the XFR file. The aim of the syntax is to define valid sets of expressions, very much the way grammatical paragraphs define valid sentences in a natural language like English. In the same way the syntax does not deal with the contents of the expressions, that is, if they form something meaningful or not. It is thus possible to construct sentences that are perfectly grammatically correct, but doesn't make sense from the content point of view. To be able to know if a sentence is meaningful or not something else is needed; the conceptual structure. This structure, which must be hard to define for a normal spoken language, defines what makes sense according to the surrounding context of the sentence. In our case the conceptual format defines how certain fields should be interpreted. For data formats there is also a logical structure, which defines types for fields (text, integer, float, date etc) as well as primary and foreign key constraints. These structures are all dependent of each other, as indicated in figure 2.

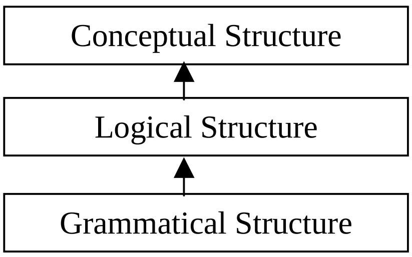

Figure 2 Data structures.

8.2 Definitions and Conventions

Terminals are endpoints in a syntax definition. No other resolution is possible. Terminals include the set of reserved words and user-defined identifiers.

Nonterminals are placeholders in the syntax and are defined elsewhere in this syntax summary. Definitions can be recursive.

An optional component is indicated by the subscripted $_{opt}$. For example,

{ *expression* $_{opt}$ **}**

indicates an optional expression enclosed in curly braces.

The syntax conventions use different font attributes for different components of the syntax. The symbols and fonts are as follows:

Attribute	**Description**
nonterminal	Italic type indicates nonterminals.
const	Terminals in bold type are literal reserved words and symbols that must be entered as shown. Characters in this context are always case sensitive.
$_{opt}$	Nonterminals followed by $_{opt}$ are always optional.

A colon (**:**) following a nonterminal introduces its definition. Alternative definitions are listed on separate lines, except when prefaced with the words "one of."

8.3 Elements of a XFR data set

This part describes the elements of the XFR data language, including the names, numbers, and characters used to construct a XFR data set.
The following topics are discussed:

- Tokens
- Comments
- Identifiers
- Constants
- String literals
- Punctuation

8.3.1 Tokens

In a XFR data set, the basic element recognised by the interpreter is the "token." A token is data source text that the interpreter does not break down into component elements.

Syntax

token :
identifier
constant
punctuator

Note The identifiers and constants described in this chapter are examples of tokens. Punctuation characters such as brackets (**[ ]**), commas (,) and dots (**.**) are also tokens.

White-Space Characters
Space, tab, linefeed, carriage-return, formfeed, vertical-tab, and newline characters are called "white-space characters" because they serve the same purpose as the spaces between words and lines on a printed page-they make reading easier. Tokens are delimited (bounded) by white-space characters and by other tokens, such as identifiers and punctuation. When parsing code, the XFR interpreter ignores white-space characters unless you use them as separators or as components of character constants or string literals. Use white-space characters to make a XFR data set more readable. Note that the interpreter also treats comments as white space.

Comments
A comment is text that the interpreter ignores but that is useful for understanding parts in the data set. Comments are normally used to annotate data sets for future reference. The interpreter treats them as white space. You can also use comments to make certain lines in the data set inactive.

A XFR comment is written in the following way:

The // (two slashes) characters in the beginning of a line, followed by any sequence of characters. A new line terminates this form of comment. Therefore, it is called a "single-line comment."

8.3.2 Identifiers

"Identifiers" are the names that are used for both table names and field names in the XFR data set. The syntax for identifier in XFR complies with the one used in SQL for table and field names.

Note Some databases allow whitespace characters in table and field names. To make the XFR data set compatible with as many databases as possible whitespace characters in table and field names are not allowed.

Syntax

identifier :
    nondigit
    identifier nondigit
    identifier digit
    identifier special-character

nondigit : one of
    _ a b c d e f g h i j k l m n o p q r s t u v w x y z
    A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

digit : one of
    0 1 2 3 4 5 6 7 8 9

special-character : one of
    # @

The first character of an identifier name must be a *nondigit* (that is, the first character must be an underscore or an uppercase or lowercase letter). SQL allows an identifier's name to be up to 64 characters long.

Note No special characters except **#** and **@** are allowed for identifiers.

The XFR interpreter does not distinguish between uppercase and lowercase letters. It is therefore important to know that identifiers that use the same spelling, regardless of upper or lower case letters, are treated as identical. For example, the following identifiers are treated as the same:

FlowNumber
flownumber
Flownumber
FloWNumBer

The following are examples of valid identifiers that conform to both SQL and XFR naming restrictions:

Table#32
Myself@mail_com
_Field_67

8.3.3 Constants

A “constant” is a number, character, or character string that is used as a data value in a XFR data set. Constants can represent floating-point, integer, strings, boolean or character values.

Syntax

constant :
floating-point-constant
integer-constant
string-literal-constant

Constants are characterised by having a value and a type.

Real Constants

A “real constant” or “floating-point constant” is a decimal number that represents a signed real number. The representation of a signed real number includes an integer portion, a fractional portion, and an exponent.

Syntax

floating-point-constant :
fractional-constant exponent-part $_{opt}$
digit-sequence exponent-part

fractional-constant :
digit-sequence $_{opt}$ **.** *digit-sequence*
digit-sequence **.**

exponent-part :
e *sign* $_{opt}$ *digit-sequence*
E *sign* $_{opt}$ *digit-sequence*

sign : one of
+ –

digit-sequence :
digit
digit-sequence digit

You can omit either the digits before the decimal point (the integer portion of the value) or the digits after the decimal point (the fractional portion), but not both. You can leave out the decimal point only if you include an exponent. No white-space characters can separate the digits or characters of the constant.

The following examples illustrate some forms of floating-point constants and expressions:

```
15.75
1,575E1   /* = 15.75   */
1575e-2   /* = 15.75   */
-2.5e-3   /* = -0.0025 */
25E-4     /* =  0.0025 */
```

Floating-point constants are positive unless they are preceded by a minus sign (–).

Integer Constants
An "integer constant" is a decimal (base 10) number that represents an integral value.

Syntax

integer-constant :
decimal-constant

decimal-constant :
nonzero-digit
decimal-constant digit

nonzero-digit : one of
1 2 3 4 5 6 7 8 9

digit : one of
0 1 2 3 4 5 6 7 8 9

Integer constants are positive unless they are preceded by a minus sign (–).

Note Only decimal integer constant are allowed.

No white-space characters can separate the digits of an integer constant. These examples show valid decimal constants.

```
/* Decimal Constants */
10
132
32179
```

String Literal Constants
A "string literal" is a sequence of characters from the source character set enclosed in double quotation marks (" "). String literals are used to represent a sequence of characters which, taken together, form a null-terminated string.

Syntax

string-literal :

"*s-char-sequence* $_{opt}$"

s-char-sequence :
s-char
s-char-sequence s-char

s-char :
any member of the source character set except the double quotation mark ("), backslash (\), or newline character
escape-sequence

escape-sequence :
simple-escape-sequence
octal-escape-sequence
hexadecimal-escape-sequence

simple-escape-sequence : one of
\a \b \f \n \r \t \v
\' \" \\ \?

octal-escape-sequence :
\ *octal-digit*
\ *octal-digit octal-digit*
\ *octal-digit octal-digit octal-digit*

hexadecimal-escape-sequence :
\x *hexadecimal-digit*
hexadecimal-escape-sequence hexadecimal-digit

The example below is a simple string literal:

```
"This is a string literal."
```

All escape codes listed in Table 1 are valid in string literals. To represent a double quotation mark in a string literal, use the escape sequence \". The single quotation mark (') can be represented without an escape sequence. The backslash (\) must be followed with a second backslash (\\) when it appears within a string. When a backslash appears at the end of a line, it is always interpreted as a line-continuation character.

Escape Sequences
Character combinations consisting of a backslash (\) followed by a letter or by a combination of digits are called “escape sequences.” To represent a new line character, single quotation mark, or certain other characters in a character constant, you must use escape sequences. An escape sequence is regarded as a single character and is therefore valid as a character constant.
Escape sequences are typically used to specify actions such as carriage returns and tab movements on terminals and printers. They are also used to provide literal representations of nonprinting characters and characters that usually have special meanings, such as the double quotation mark ("). Table 8 lists the ANSI escape sequences and what they represent.

Escape Sequence	**Represents**
\b	Backspace
\f	Formfeed
\n	New line
\r	Carriage return
\t	Horizontal tab
\v	Vertical tab
\'	Single quotation mark
\"	Double quotation mark
\\	Backslash
\?	Literal question mark
ooo	ASCII character in octal notation
\x*hhh*	ASCII character in hexadecimal notation

Table 8 Escape Sequences

8.3.4 Punctuation

The punctuation and special characters in the XFR character set have various uses, from organizing data structure to identify the tuples. They do not specify an operation to be performed.

Syntax

punctuator : one of
    [ ] : = ;

These characters have special meanings in the XFR syntax. Their uses are described throughout this reference.

8.4 XFR Format Structure

This chapter gives an overview of the XFR data set structure. Terms and features important to understanding XFR components are also introduced. Topics discussed include:

- XFR data set
- Data tables
- Data rows

8.4.1 XFR data set

The XFR data set represents the complete data set and is build up from a number of data tables. At least one data table must be present to form a complete XFR data set.

Syntax

xfr_data_set:
    data_tables

data_tables:
    data_table
    data_table data_tables

8.4.2 Data tables

The data table contains of a header, declaring the name of the table, and zero to many data rows. The header is enclosed in square brackets ([]). A table containing no data sets are consider valid to simplify the handling.

Syntax

data_table:
table_header
table_header data_rows

table_header:
[** table_name **]

table_name:
identifier

8.4.3 Data rows

A data row is made up from the field name in the particular table, the tuple number and the actual data associated with that field name. When the tuple number is omitted, 1 is assumed.

Syntax

data_rows:
data_row
data_row data_rows

data_row:
field_name = *field_value* ***;***
*field_name**: tuple_number* = *field_value* ***;***

field_name:
identifier

tuple_number:
integer

field_value:
integer
real
string_literal

8.5 XFR Format Syntax Summary

This part gives the full description of the XFR data set syntax.

Note This syntax summary is not part of the ANSI SQL standard, even though it complies to part of it.

8.5.1 Tokens

token :

identifier
constant
punctuator

8.5.2 Identifiers

identifier :

nondigit
identifier nondigit
identifier digit
identifier special-character

nondigit : one of

_ a b c d e f g h i j k l m n o p q r s t u v w x y z
A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

digit : one of

0 1 2 3 4 5 6 7 8 9

special-character : one of

 # @

8.5.3 Constants

constant :

floating-point-constant
integer-constant
string-literal-constant

floating-point-constant :

fractional-constant exponent-part $_{opt}$
digit-sequence exponent-part

fractional-constant :

digit-sequence $_{opt}$ **.** *digit-sequence*
digit-sequence **.**

exponent-part :

e *sign* $_{opt}$ *digit-sequence*
E *sign* $_{opt}$ *digit-sequence*

sign : one of

+ –

digit-sequence :

digit
digit-sequence digit

integer-constant :

decimal-constant

decimal-constant :
nonzero-digit
decimal-constant digit

nonzero-digit : one of
1 2 3 4 5 6 7 8 9

digit : one of
0 1 2 3 4 5 6 7 8 9

string-literal-constant :
"*s-char-sequence* $_{opt}$**"**

s-char-sequence :
s-char
s-char-sequence s-char

s-char :
any member of the source character set except the double quotation mark ("), backslash (\), or newline character
escape-sequence

escape-sequence :
simple-escape-sequence
octal-escape-sequence
hexadecimal-escape-sequence

simple-escape-sequence : one of
\a \b \f \n \r \t \v
\' \" \\ \?

octal-escape-sequence :
\ *octal-digit*
\ *octal-digit octal-digit*
\ *octal-digit octal-digit octal-digit*

hexadecimal-escape-sequence :
\x *hexadecimal-digit*
hexadecimal-escape-sequence hexadecimal-digit

8.5.4 Punctuation

punctuator : one of
[ ] : = ;

8.5.5 Structure

xfr_data_set:
data_tables

data_tables:
data_table
data_table data_tables

data_table:
table_header
table_header data_rows

table_header:
[** table_name **]

table_name:
identifier

data_rows:
data_row
data_row data_rows

data_row:
field_name **=** *field_value* ***;***
*field_name***:** *tuple_number* **=** *field_value* ***;***

field_name:
identifier

tuple_number:
integer

field_value:
integer
real
string_literal

9 Future

Some of the issues related to data exchange that came up in the discussion at the opening meeting of this project, were not dealt with in this project phase due to limited resources and in order to give priority to more important issues. These data exchange issues are shortly addressed in this chapter to be remembered in future projects.

The nomenclature problem is an extensive issue, which is not solved by the modest approach in this project. Experience show that in a well-defined, fairly small group, organisation, or network, it may be quite easy to agree on e.g. a nomenclature for substances. However, in a larger, international context it is a much more complex task to find *one* common way of naming and structuring matter, if not impossible. How can all these locally existing, well-defined groups or networks (like this project group) harmonise in this matter? A standardised way of dealing with hierarchical structures and nomenclatures needs to be developed on an international level, to support the common understanding of environmental information.

As a consequence of this, system developers need to be able to handle different nomenclatures. One way of doing this is by applying the SPINE structure regarding *alternate substance name*. This function supports the use and storage of synonyms and it may allow connections between substance names and different nomenclatures. SPINE also contains a structure that may be developed further and applied in order to *arrange and store the composition or content of a product or material*.

SPINE allows activities to contain other activities, i.e. several activities (sub-systems) may be aggregated into one activity (system) in order to make up to a product chain or a life cycle. It involves some technical issues when these composite data sets are imported and exported between software, which needs to be dealt with in the near future.

10 Appendix

10.1 Emissions - nomenclature in different data sources

Below, typical examples of emission names used in a number of different LCA data sources are listed. This document was used as a basis for the discussion on emission nomenclature in the CPM Data Exchange project.

10.1.1 Types of emissions

1. metals to air
2. other inorganic substances to air
3. organic substances to air
4. groups of substances (collective substances) to air
5. metals to water
6. other inorganic substances to water
7. organic substances to water
8. groups of substances (collective substances) to water

<u>APME (LCI data for production of plastics, latest version, 1999):</u>

1. Lead (Pb), Mercury (Hg)
2. Ammonia (NH3), Cl2, CO2, H2S, H2SO4, HCl, NOx, SOx
3. DCE, Methane, VCM
4. Aldehydes (CHO), Aromatic-HC, CFC/HCFC, Dust, Hydrocarbons, Metals, Organo-Cl
5. Al+++, CrO3, Cu+/Cu++, Hg, Na+, Ni++, Pb
6. Arsenic, CN-, Dissolved Cl2, F-, NH4, NO3-, Other nitrogen, Phosphate as P2O5, SO4--, Sulphur/sulphide
7. DCE, Phenol, VCM
8. Acid (H+), BOD, COD, Detergent/oil, Dissolved organics, Hydrocarbons, Metals - unspecified, Organo-chlorine, Suspended solids

(Comment: DCE=1,2-Dichloroethane, previously named EDC=Ethylene dichloride; VCM=Vinyl chloride (monomer), more accurately Chloroethene)

<u>CIT (according to Lisa's table):</u>

1. Cr, Cr3+, Hg, Hg+, Hg2+, Pb, Pb2+
2. Cl2, CO2, F-, H2S, H2SO4, NH3, NO2, SO2, SO42-
3. Benzene, C2F6, CH4, 1,2-Dichloroethane, Ethane, Formaldehyde, HCFC-22, Phenol, Vinylchloride
4. Aromatic VOC, CFC/HCFC, Chlorinated organics, Chlorinated VOC, Dioxin, Dust, HC, NMVOC, PAH, Particulates, VOC, VOC diesel engines
5. Cr, Cr3+, Hg, Hg+, Hg2+, Pb, Pb2+
6. Cl2, Dissolved chlorine, F-, H2S, H2SO4, NH3, NH4+, NH4-N, NO3-, NO3-N, Other nitrogen, PO43-, SO42-, Sulphide, Tot-N, Tot-P
7. Benzene, 1,2-Dichloroethane, Formaldehyde, Phenol, Vinylchloride
8. Acid as H+, AOX, BOD, BOD5, Chlorinated organics, COD, Dissolved organics, DOC, HC, Oil, PAH, Suspended solids, TOC

<u>CML (classification factors, 1992):</u>

1. Cr chromium, Cr3+ chromium(III), Cr6+ chromium(VI), Cu copper, Hg mercury, Pb lead

2. As arsenic, CO2 carbon dioxide, F- fluoride, HF hydrogen fluoride, NH3 ammonia, NO2 nitrogen dioxide, NOx nitrogen oxides, SO2 sulfur dioxide
3. C2F6 hexafluoroethane (CFC-116), CF3Br bromotrifluoromethane (HALON-1301), CH4 methane, CH2CHCl monochloroethene (vinylchloride), CHF2Cl chlorodifluoromethane (HCFC-22), CH2ClCH2Cl 1,2-dichloroethane, methane, 2,3,7,8-TCDD (dioxin)
4. aldehydes (average), alkanes (average), aromatics (average), chloro-PAH (general), chlorophenols (general), dioxin, halogenated hydrocarbons (average), hydrocarbons (average), non-methane hydrocarbons (average), petrol, xylenes
5. Cr chromium, Cr3+ chromium(III), Cr6+ chromium(VI), Cu copper, Hg mercury, Pb lead
6. As arsenic, CN- cyanide (free), F- fluoride, N nitrogen, NH4+ ammonium, NO3- nitrate, P phosphorus, PO43- phosphate
7. C6H6 benzene, CH2CHCl monochloroethene (vinylchloride), C6H5OH phenol, 2,3,7,8-TCDD (dioxin)
8. chloro-PAH (general), chlorophenols (general), COD chemical oxygen demand, crude oil, dioxin, petrol

<u>EAA (LCI data for aluminium production, 1996):</u>
1. -
2. ammonia, carbon dioxide, chlorine, fluorides (gas), fluorides (particulate), hydrogen fluoride, nitrogen oxides, sulphur dioxide
3. CF4 + C2F6
4. dust, hydrocarbon, PAH, VOCs
5. -
6. fluorides (total), sulphuric acid
7. -
8. chemical oxygen demand, organic C, PAH, suspended solids

<u>ETH (LCI data for energy production, 1994, in German):</u>
1. Cr Chrom, Cu Kupfer, Hg Quecksilber, Pb Blei
2. CN Cyanide, CO2 Kohlendioxid, HCl Salzsäure, NH3 Ammoniak, NOx Stickoxide als NO2, P Phosphor, SOx als SO2
3. Benzol, C2F6, CH4 Methan, Ethylen Dichlorid, Formaldehyd, R22 FCKW, Vinyl Chlorid
4. Alkane, Aromaten, NMVOC, PAH Polyzyklische aromatische HCs, Partikel, TCDD-Äquivalente
5. Ion Blei, Ion Chrom-III, Ion Chrom-VI, Ion Kupfer, Ion Quecksilber
6. Fluoride, Nitrate, Phosphate, Schwefelwasserstoff, Stickstoff gesamt, Sulfate
7. Formaldehyd in Wasser, Phenole, Xylol in Wasser
8. Alkane in Wasser, BSB5, COD, Fette und Öle gesamt, Kohlenwasserstoffe gesamt, Metallionen gesamt, Polyzyklische arom. KWe in Wasser, Säuren gesamt, TOC, Ungelöste Stoffe

(Comments: R22 FCKW=HCFC-22, a "soft" freon; BSB5=BOD5, KWe=Kohlenwasserstoffe=Hydrocarbons)

<u>ETH/BUWAL (LCI data for packaging materials, 1998):</u>
1. Lead (Pb), Mercury (Hg), Nickel (Ni)
2. Ammonia (NH3), Carbon dioxide fossil (CO2), Hydrofluoric acid (HF), Nitrogen oxides (NOx) as NO2, Sulphur oxides (SOx) as SO2
3. Benzene (C6H6), Methane (CH4), Halon H1301

4. Aldehydes, Aromatic HC, Dust/particulates, Halogenated HC, Hydrocarbons (HC), Metals, NMVOC non-methane HC, PAH policycl. arom. HC
5. Chromium (Cr), Iron (Fe), Lead (Pb), Mercury (Hg)
6. Ammonium (NH4+), Arsenic (As), Cyanide (CN-), Nitrate (NO3-), Nitrogen total, Phosphate (PO43-), Sulphate (SO42-)
7. Toluene (C7H8)
8. Aromatic HC, AOX as Cl-, BOD, Chlorinated HC, COD, DOC, Fats/oils, Metals, PAH policycl. arom. HC, Phenols, Suspended solids, TOC

IISI (LCI data for steel production, 1998):
1. -
2. Carbon Dioxide (CO2, fossil and mineral), Nitrogen oxides (NOx as NO2), Sulphur oxides (SOx as SO2)
3. -
4. Particulates - TOTAL
5. Chromium (Cr III, Cr VI), Lead (Pb++, Pb4+), Nickel (Ni++, Ni3+)
6. Ammonia (NH4+, NH3, as N), Fluorides (F-), Nitrogen - TOTAL (except Ammonia), Phosphates (PO43-, HPO4--, H2PO4-, H3PO4, as P), Phosphorous Matter (unspecified, as P)
7. Phenol (C6H6O)
8. COD (Chemical Oxygen Demand), Suspended Matter (unspecified)

MSR (Miljöstyrningsrådet, characterisation factors for EPDs, 1999):
1. -
2. CO2, HF, NH3, NO2, NOx, SO2
3. Benzene, Carbon tetrachloride, CH4, Formaldehyde, HCFC-22, Methane, Perfluoroethane, o-Xylene
4. Diesel car combustion emissions, Hydrocarbons (average), Non-methane hydrocarbons (average)
5. -
6. N to water, NH4+ to water, NO3- to water, P to water, PO43-
7. -
8. COD

UMIP (LCI database, 1996, in Danish):
1. Aluminiumoxid (Al2O3), Cr (chrom), Cu (kobber), Hg (Kviksölv), Pb (bly)
2. As (arsen), Carbondioxid (CO2), Fluorid (F-), Hydrogenfluorid (HF), Nitrogenoxider (NOx), Svovldioxid (SO2)
3. Methan (CH4)
4. Dioxin, PAH, Hydrogencarboner (HC), NMVOC, Uspec. aldehyd, Uspec. chlorholdige org. forb., Uspec. org. forbindelser, Uspec. partikler, VOC dieselmotorer
5. Cr (chrom), Cu (kobber), Pb (bly)
6. Fluorid (F-), Fosfat (PO4---), NH4-N, NO3-N, Sulfat (SO4--), Uspec.-N
7. Phenol
8. BOD, COD, DOC, H+ (hydrogenioner), Hydrogencarboner (HC), SS, Uspec. metaller, Uspec. olie, Uspec. stof