CHAPTER 6
PREPARING PROFILES

6.1 INTRODUCTION

In the context of the OECD Programme on the Cooperative Assessment of Existing Chemicals, *profiles* are succinct documents of a few pages in length that focus on the conclusions of the assessment, similar to an executive summary. They are agreed at periodic chemical assessment meetings or via written procedures. The profile is submitted for discussion along with the *assessment report* (a longer document focusing on discussion and interpretation of the hazard endpoints; see Chapter 5) and study summaries of underlying data for each endpoint (see Chapter 2) for each endpoint.

After review and revision at the assessment meeting or via written procedure, the profile is submitted for endorsement by the Task Force on Hazard Assessment and sent for consideration and approval by the Joint Meeting of the OECD Chemicals Committee and Working party on Chemicals, Pesticides and Biotechnology. When finalized, the profile and accompanying documents are made public.

Two main types of profiles may be prepared in the OECD Cooperative Chemicals Programme. Sponsors can prepare SIDS Initial Assessment Profiles (SIAPs) for chemicals that have full SIDS datasets (e.g., for high production volume (HPV) chemicals or categories). SIAPs would also be prepared for a category that is extended from a category that has already been agreed in the OECD Programme. For targeted assessments, an Initial Targeted Assessment Profile (ITAP) is prepared. Unlike assessment reports (which can either be prepared within the OECD programme or another programme), profiles are prepared specifically within the OECD Cooperative Chemicals Assessment Programme.

This chapter and the annex are organised as follows:

- ***Section 6.2:*** General guidance for preparing a profile
- ***Section 6.3:*** Endpoint-specific guidance for preparing a profile
- ***Annex:*** Format to be used when preparing a profile, with specific examples for SIAPs and ITAPs

Because other chapters focus on gathering data/elements within the Screening Information Dat Set (SIDS) (Chapter 2), grouping chemicals (Chapter 3) and data assessment (Chapter 4), this chapter focuses primarily on overall scope, content, and structure of the profile, with reference to specific aspects of data elements only as needed.

6.2 GENERAL GUIDANCE FOR PREPARING A PROFILE

Similar to the assessment report, there are a few guiding principles to consider that can be applied throughout the full profile.

6.2.1 Overall Scope and Length

The profile summarises the main conclusions on the hazards identified in the assessment report together with a brief summary of the exposure information necessary to put the hazards into context. The profile should describe endpoints with enough clarity and detail to be informative but should not repeat all the detailed information provided in the assessment report. In particular, the SIAP should present only the most important information about all SIDS elements and relevant non-SIDS elements, and the ITAP should briefly summarise the important studies from the ITAR.

The length, if for a single chemical with a full SIDS dataset and a moderate amount of data, might be a couple of pages long. The length will vary for other situations, of course, depending on the assessment. For example, a targeted assessment would likely be shorter whereas a category approach would require a longer profile.

The terminology and units of chemical concentrations and exposures or physicochemical and environmental fate properties found in the classification criteria of the Globally Harmonised System of Classification and Labelling of Chemicals should be used for consistency within the profiles. However, the actual classification of chemicals should be avoided.

Because assessments in the Cooperative Chemicals Assessment Programme are focused on hazard endpoints, references to risk assessment (e.g., margins of safety, PEC/PNEC ratio, etc.) should be avoided in the profile.

When preparing the SIAP, a standard format and structure should be used to allow for transparent communication of information and quick and efficient discussions when presented for agreement at SIAM. For ITAPs, standard language is also used for consistency. The Annex includes endpoint-specific language that can be used when preparing profiles.

6.2.2 Extent and Availability of Data

When several studies exist for the same endpoint and route of exposure, the key study should be reported in the profile with appropriate details (see Annex for examples). The rationale for selection of key studies is better placed in the SIDS dossier or the assessment report, including a justification in case of conflicting results. In addition, a very brief description of additional studies, their effects and associated doses/concentrations should be included for studies with reliability score of 1 or 2, especially if additional effects are identified.

6.2.3 Data Quality and Interpretation

Major deviations from OECD Test Guidelines should be reflected in the assessment report and dossier. However, the profile should include any deviations that might significantly affect results (e.g., administration of a test substance to rats on gestation days 7-20 versus 5-15).

In principle only reliable information should be used to describe the hazards of a substance within the profile, and any less reliable studies should generally be discussed only in the assessment report. Only in very rare circumstances should the data from less reliable studies be used (e.g., if a study is needed for a weight-of-evidence assessment or if it identifies significant results not seen in the key study and there is a good reason why details of the study cannot be obtained). If included, results from these less reliable studies should always be accompanied by caveats that describe their limitations. See Chapter 3, Section 3.1 for detailed guidance on data reliability, relevance and adequacy.

6.2.4 Analogues and Categories

For both analogue and category approaches, a rationale for using these data should be placed at the beginning of the profile. See Section 6.3 for preparing this section of the profile and the OECD Guidance Document on Grouping of Chemicals for more details on analogue and category approaches in general.

When using an analogue approach, the profile should clearly note for each endpoint where data are not available for the sponsored chemical and should clearly state the chemical name of the analogue that is used to fill the particular endpoint. This presentation approach can be used for both SIAPs and ITAPs.

When using a category approach, data for each endpoint should be provided together rather than providing all data for a single chemical before data for the next chemical are presented. In addition, for readability, a consistent order of presentation of the chemicals should be made. For example, a category might consist of chemicals A, B and C, and acute toxicity data are available for all three chemicals but repeated-dose toxicity data area available only for chemicals A and C. In this case, all acute data should be presented first, with the order, for example, of A, then B, then C. The profile should then discuss repeated-dose data for chemical A before presenting data on chemical C. This order (A,B,C) would be used for each of the endpoint sections. This rule can be applied whether preparing a SIAP or an ITAP.

For a category approach, especially for large categories, a concluding statement should be added at the end of each endpoint summary.

Hydrocarbon Solvents

As a result of discussions at SIAM, several specific items of information were agreed to include in the profiles that are prepared for hydrocarbon solvents. A list of identifiers is included in Section 6.3 below along with information on adding a caveat about the CAS number coverage, if needed. These identifiers and caveat should be used whether taking a a single "substance" or a category approach (which is more likely to be done) for hydrocarbon solvents. These identifiers are essential so that the category can be easily understood and evaluated. In addition to the identifiers noted in Section 6.3, it is essential that for the category as a whole, the carbon number range should identify at least 80% of the chemical constituents. For example, if the category is identified as UVCB substances in the range of C10-C13 aromatics, (as well as the individual UVCBs), then at least 80% of the constituents of the category should be within this range.

6.3 SECTION SPECIFIC GUIDANCE FOR PREPARING A PROFILE

The profile might include the sections indicated below. The SIAP needs to address all SIDS endpoints and may have additional entries for the category or analogue justification. There is more flexibility to the ITAP, but it should include some statndard language at the beginning to state the endpoints covered and reasons for targeting the assessment. Examples of the type of data and level of detail to be included in each of the sections discussed below are provided in the Annex.

6.3.1. Identification of the chemical(s)

This section, presented in a two-column format, indicates the chemical name(s), CAS number(s) and structure(s). When categories are presented, another line indicating category name should also be included and each chemical and CAS number should be identified. If there are many substances within a category, molecular structures (and other identifiers, if necessary) should be shown in the Chemical Identity section of the assessment report only in order to keep the profile as simple as possible; in these cases, an appropriate note should be placed in this section of the profile to indicate where to find the

details. For substances that are not pure (e.g. non isolable substances, complex mixtures, substances supplied as aqueous solutions), their composition should be summarized briefly. Similar considerations should be made for other UVCBs or complex mixtures produced from variable feedstocks.

Hydrocarbon Solvents

As a result of discussions at SIAMs, several specific identifiers were agreed as necessary to include in the profiles for hydrocarbon solvents. These are:

- CAS number
- Carbon number range
    - The range should include at least 80% of the chemical constituents found in the UVCB;
    - Further, the percent of indicated carbon number range should be specifically noted (e.g., C10-C13 > 90%)
- Content of: benzene, n-hexane, sulphur or other components with specific toxicities
- PINA (paraffins, isoparaffins, naphthenes [cyclics] and aromatics) distribution
    - Indicate first three if between 10-80% and indicate aromatics as < or > 2%
- Boiling point range

Because CAS numbers used for hydrocarbon solvents may include a wider range or higher percentages of certain constituents for other uses (e.g., fuel vs. solvent uses), a note should be added specifically to the profile for any hydrocarbon solvents to indicate that other streams with the same CAS number might not be covered in the assessment if they don't meet the identification criteria described in the assessment.

6.3.2 Introductory Note Regarding Targeted Assessments (ITAP only)

At the beginning of the ITAPs, a note should be included to indicate which endpoints are assessed. The Annex also includes standard language to be used in this note stating that the evaluation is not a full SIDS assessment and that the endpoints are agreed by member countries. Also, the availability of any assessment reports prepared in other programmes with links to appropriate websites as needed should be noted here.

6.3.3 Rationale for Targeting the Assessment (ITAP only)

This section should be added for any single chemical or category assessment that targets certain endpoints. The rationale will by necessity vary depending on the purpose of the assessment. If the targeted endpoints are evaluated within a certain regulatory context, some background on the regulatory programme can be added. Alternately, a rationale could simply be that the targeted endpoints/related effects are known toxicities of concern for a given chemical or category; in this case it must be remembered that there could be other toxicities associated with the chemical that have not been tested.

6.3.4 Analogue/Category Rationale

This section should be included for assessments that rely on data from analogues or uses a category approach to fill data gaps. Detailed information on concepts related to building categories, category and analogue justifications and issues related to read-across is available in the OECD Guidance

Document on Grouping of Chemicals.

Analogue Rationale

Within this section, assessments that rely on analogue data to fill SIDS endpoint datagaps for a full SIDS assessment should include a description of the analogue, a brief overview of the SIDS datagaps, and a justification for read-across of the data for these endpoints from the analogue to the sponsored chemical. For a targeted assessment, it is also possible that analogues might be used. Thus, a similar approach should be taken for this section for the ITAP as is used for the SIAP.

If information from a chemical that has a previous OECD assessment is being used as an analogue, it should be specifically stated and a link or a reference to the assessment should be included in the profile. See the Annex for an example.

Category Rationale

This section should provide an overview of the basis for the full SIDS or targeted category, including the reason the chemicals can be assessed together as a group and how data from the tested chemicals can be used for untested chemicals within the category. Although the section should be succinct, it should be detailed enough for readers to clearly understand the rationale and read-across/trend-analysis approach to filling data gaps. If any of the category members have been already assessed in the OECD Programme, a link or a reference to the previous assessment should be included in the profile.

6.3.5 Physical-chemical Properties

The SIAP should always include this section, and it is recommended that the ITAP also include a physical-chemical property section with the understanding that ITAPs may not present all the properties typically included in a SIAP.

In the profile, the most relevant basic physical/chemical property information on the chemical should be presented first in this section. For the SIAP, the properties should be presented in the order indicated in the Annex. A similar order can also be followed for ITAPs where such data are available.

Endpoint values should be specified as to whether they have been estimated (e.g., via (Q)SARs) or measured experimentally. Any other useful information (e.g., pKa for ionisable substances) should be reported.

6.3.6 Human Health

Results of toxicity tests and human data should be summarized and presented in the order specified in the Annex. SIDS endpoints should be summarized for the SIAP along with any important non-SIDS endpoints without including all details from the assessment report. For targeted assessments, SIDS or non-SIDS endpoints may be included. Lists of both types of endpoints are included in other chapters (see Chapters/Sections 2.2.1 and 5.3). In the SIAP and for any of the endpoints that are included within an ITAP, the order of the additional endpoints should reflect the IUCLID format (e.g., toxicokinetics before all endpoints; skin irritation, eye irritation and skin sensitisation after acute toxicity; carcinogenicity after genetic toxicity).

This section should include the actual doses at which adverse effects were observed along with a description of the adverse effects, as well as conclusive statements that support the results, for example statements on whether the substance is to be regarded as likely to result in reproductive toxicity, genotoxicity, etc.

Care should be taken to use consistent language for endpoints. For example, for irritation or sensitization, it is recommended that adjectives to qualify the severity of the observed effect should match the classification terminology of the GHS.

Although there are likely to be additional important considerations within the human health section, a couple of end-point specific ones are noted here.

For example, where a toxicokinetic study is not available, it is possible to make general observations regarding absorption and metabolism, taking account of the chemical structure, physicochemical and available toxicodynamic information. See Annex to Chapter 4 for information on assessing toxicokinetics data.

Where there is evidence of mutagenicity *in vivo* (e.g., chromosome aberrations, micronuclei) but no information on carcinogenicity, the profile should include a statement in the carcinogenicity section indicating a potential concern for this endpoint. However, expert judgement should be applied in making such a statement.

Conclusion

A sentence that describes the overall conclusions of the assessment should be included in the human health section and should be included in bold (see examples in the Annex). The concluding sentence indicated whether the chemical(s) present a hazard or not and what the identified hazards are. For SIAPs, this is accompanied by standard language stating that the SIDS endpoints have been met. For ITAPs, a similar conclusion can be included, without the need for stating that SIDS endpoints have been met.

The criteria described in the GHS may be used as a general background reference for judging the hazard of a substance for the purpose of deriving consistent conclusions for substances assessed in the OECD Cooperative Chemicals Assessment Programme. However, it should be kept in mind that no classification is performed in the context of the this Programme.

6.3.7 Environment

When preparing a SIAP, data for all SIDS endpoints should be presented or discussed in the order presented in the Annex using standard language. Examples of this standard language are also in the Annex. Key studies should be chosen .

Environmental Fate

For some compounds, it also may be important to include certain non-SIDS endpoints as discussed below. Regardless of whether a SIAP or ITAP is prepared, the test substance (e.g., the parent compound or a hydrolysis product) and all products analysed during the test should be specified. The profile should also indicate whether endpoint values were estimated (e.g., via (Q)SARs) or measured experimentally.

Details and proposed text that should be included in the profile are provided in the Annex and cover the following endpoints: degradation (hydrolysis half-life, photodegradation half-life), biodegradation, distribution and transport between environmental compartments, and bioaccumulation.

Ecotoxicity

Results for ecotoxicity tests and other relevant information should also be summarised and presented in this section. The key study should be reported in the profile with details listed below. In addition, a very brief description of additional studies, their effects and associated doses/concentrations should be included for studies with reliability score of 1 or 2, especially if additional effects are identified. The following results from ecotoxicity tests can be noted:

- Aquatic Toxicity:
  - *Acute toxicity* to fish, aquatic invertebrates and aquatic plants:
    - Report available LC_{50}/EC_{50} values, indicating study duration and species.
  - Available chronic toxicity data on fish, aquatic invertebrates and aquatic plants
    - Report the NOEC values.

It is important to indicate whether reported values represent measured or nominal concentrations. In the case of unstable test substances or substances tested as mixtures, the chemical identity on which the result is based should be clearly stated. For substances with very low solubility and difficult to test substances (e.g. substances that are not stable under test conditions), a brief reference to the preparation of the test solution is useful (e.g. type and concentration of dispersant used, loading rate, or WAF, etc.). For substances that ionise appreciably at environmentally relevant pHs, the measured pH of the test solution should be included or a statement describing any buffering conducted during testing.

Additional information on known toxicity or effects in other environmental compartments may be added to the profile if relevant for the overall assessment.

Conclusion

A brief conclusion section should be included in the environment section in bold (see examples in the Annex). For SIAPs, this should address aquatic toxicity. Statements about biodegradation and bioaccumulation should also be included when LC/EC_{50}s are below 100 mg/L, or occasionally when there are other indications of the potential for chronic effects. The conclusion in the SIAP should be accompanied by standard language stating that the SIDS endpoints have been met. A similar section can be included for ITAPs without the need for stating that SIDS endpoints have been met..

The criteria described in the GHS are usually used as a reference for judging the hazard of a substance for the purpose of deriving consistent conclusions for substances assessed in the OECD Cooperative Chemicals Assessment Programme. However, it should be kept in mind that no classification is performed in the context of the this Programme.

6.3.8 Exposure

The SIAP should summarize the exposure information presented in the SIAR, and at a minimum should include information on production volume and major use functions/categories. Additional information might include sources of potential exposure, including environmental releases and occupational/consumer exposure. As in the SIAR, it is necessary to transparently describe and qualify the

scope of the available exposure information to the extent possible. It is important not to provide overreaching conclusions if the available data do not allow such conclusions.

Exposure information from the sponsor country (or the country where the lead company is located) is sufficient to fulfill the SIDS elements. Therefore, it is important to highlight the uncertainty behind the exposure data when available for only a limited area. When data are available for countries other than the sponsor country, the origin of production/import volume, use pattern and any other exposure information should clearly be specified as to whether it is for the sponsor country or alternately, whether it pertains to other countries or regions.

If targeted assessments include exposure data, similar recommendations can be followed for the ITAP as used for the SIAP.