

Customisation Opportunities of IUCLID 6 for the Management of Chemical Data



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Customisation Opportunities of IUCLID for the Management of Chemical Data

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Foreword

The Organisation for Economic Co-operation and Development (OECD) member countries, the European Commission, partner countries and other stakeholders including international organisations, industry, and non-governmental organisations work together in the OECD chemicals safety programme (The OECD Environment, Health and Safety Programme [www.oecd.org/chemicalsafety/]) to develop and co-ordinate activities on chemical safety and biosafety on an international basis. The OECD Joint Meeting of the Chemicals Committee and Working Party on Chemicals, Pesticides and Biotechnology (Joint Meeting) manages this work. In order to achieve efficiencies in chemical management, part of this work is dedicated to the development and/or promotion of information technology systems, including the software application, IUCLID (International Uniform Chemical Information Database), of the European Chemicals Agency (ECHA).

In 1999, the OECD Task Force on Existing Chemicals, a subsidiary body of the OECD Joint Meeting, recommended the use of the IUCLID software for the collection and distribution of data under the OECD High Production Volume (HPV) Chemicals Programme. The Joint Meeting established the IUCLID User Group Expert Panel (the Expert Panel) under the auspices of the OECD to oversee and provide a catalyst for further development of IUCLID and to identify world-wide IUCLID user needs, particularly those identified by users in regulatory settings. The European Commission, which owned IUCLID, committed to consult the Expert Panel on all further developments of IUCLID in order to assure full compatibility between the European Union programme on existing chemicals and that of the OECD.

The ownership of IUCLID was transferred to ECHA in 2008. ECHA, as the implementing body of the European Regulation on Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), as well as the Regulation on the classification, labelling and packaging of substances and mixtures (CLP Regulation) and the Biocidal Products Regulation, has the task to develop and maintain IUCLID and the underlying format in collaboration with the OECD.

The IUCLID software was developed further to comply with the EU regulations, the OECD HPV Chemicals Programme, and with developments in international harmonisation, especially the OECD Harmonised Templates.

The version of IUCLID software released in 2016 allows for greater customisation of IUCLID.

The IUCLID User Group Expert Panel developed this document in collaboration with ECHA to outline the possibilities for customising IUCLID for use in different jurisdictions and for extension and integration with other tools.

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Abbreviations and acronyms

API	Application Programming Interface
CLP	Classification, Labelling and Packaging
EC	European Commission
ECHA	European Chemicals Agency
GHS	Globally Harmonized System of Classification and Labelling of Chemicals
IMG	ECHA IUCLID Management Group
ITEM	IUCLID Template Manager
IUCEF	IUCLID Extension Framework
IUCLID	International Uniform Chemical Information Database
OECD	Organisation for Economic Co-operation and Development
OHTs	OECD Harmonised Templates for Reporting Chemical Test Summaries
(Q)SARs	Quantitative Structure-Activity Relationships
REACH	European Regulation on Registration, Evaluation, Authorisation and Restriction of Chemicals
TGs	OECD Test Guidelines
TOC	Table of Contents
UI	User interface
XML	eXtensible Mark-up Language

Executive summary

The IUCLID (International Uniform Chemical Information Database) can be customised to manage chemical data in different contexts and is a platform employing globally harmonised data elements pertinent to chemicals.

IUCLID, available for free download from the website of the European Chemicals Agency (ECHA), is a computer software used by regulatory bodies and industry to record, store, maintain and exchange data on chemicals. A variety of countries currently use IUCLID in various regulatory contexts.

ECHA develops and maintains the IUCLID software and the underlying format in collaboration with the OECD. This collaboration allows international experts to identify world-wide IUCLID user needs, particularly those identified by users in regulatory settings. IUCLID is part of an “ecosystem” of IT tools developed and promoted by the OECD and its member countries around common harmonised electronic formats, the OECD Harmonised Templates for Reporting Chemical Test Summaries (OHTs), to support regulatory activity on chemicals and data sharing.

The version of IUCLID software released in 2016 allows for greater customisation of IUCLID and for extension and integration with other tools. For example, the standard IUCLID data elements can be extended to capture specific information for specific legislative data needs before they are added to the OHTs.

This document describes four main elements related to the customisation of IUCLID including how the IUCLID format can be configured and customised, the main IUCLID features and add-ons, integration with other systems and development of alternative user interfaces.

The document also outlines how customisation of these different elements requires different expertise and resources. It incorporates user stories regarding customisation of and data migration to IUCLID from ECHA, Australia, and Canada.

Chapter 1. Introduction

1.1. Objective of this document

The objective of this document is to outline what IUCLID (International Uniform Chemical Information Database) offers to regulatory bodies and industry as a key application to record, store, maintain and exchange data on chemicals.

IUCLID is currently used in a variety of countries and regulatory contexts. A central aspect of IUCLID is therefore the extent to which it is customisable and facilitates the management of chemical data across these different contexts. In outlining what IUCLID offers as an international chemicals management tool, this document focuses on describing the customisable features of IUCLID illustrated with real-life use cases. From this document, the reader should gain an understanding of how IUCLID can be adapted to different regulatory scenarios, what is involved in the customisation of IUCLID, what expertise is required, and where to find more detailed information.

There are four main elements to the customisation of IUCLID described in this document:

1. the IUCLID format
2. IUCLID's features and add-ons
3. the integration of other systems with IUCLID
4. the development of alternative user interfaces on top of IUCLID.

It is important to make a special note concerning the first of these elements: the IUCLID format, the specification and organisation of data elements in IUCLID. The IUCLID format has a crucial role in supporting the global harmonisation of data standards and data exchange and is the foundation for all the customisable elements of IUCLID listed above. The specification and organisation of some data elements in IUCLID come from the work of other entities to harmonise and/or define and manage data elements for specific types of information or purposes. The chief engine of the IUCLID format are data formats established by the Organisation for Economic Co-operation and Development (OECD). The purpose of these formats, the OECD Harmonised Templates for Reporting Chemical Test Summaries (OHTs), is to harmonise the reporting of chemical test summaries. Taking this into consideration, the document also describes the management and procedures surrounding the development of the OHTs as well as other parts of the IUCLID format.

1.2. Overview of IUCLID

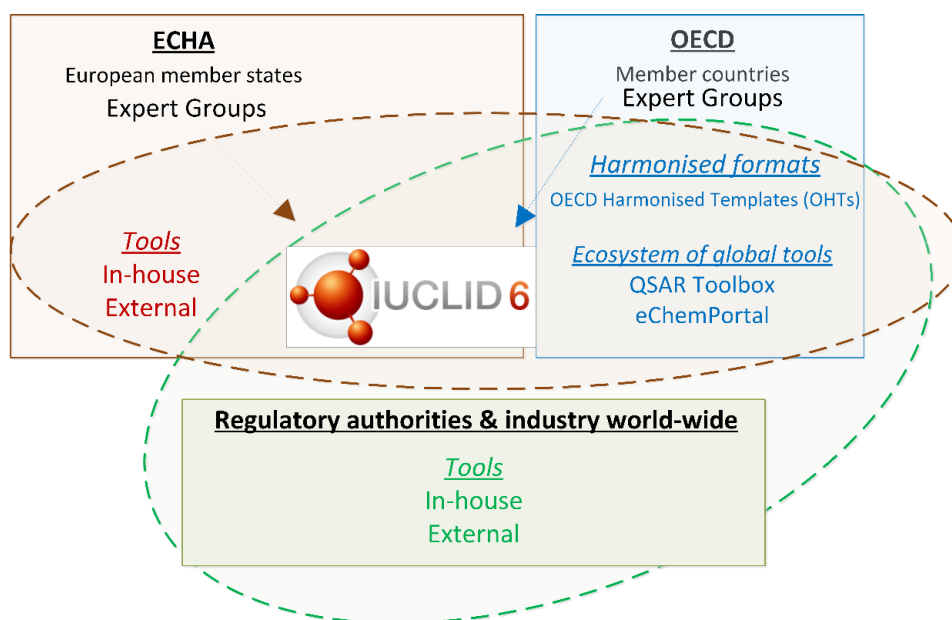
IUCLID is a software application designed to record, store, maintain and exchange data on the intrinsic and hazard properties of chemical substances or mixtures, as well as the uses of these substances and the associated exposure levels. It is a key software application for both regulatory bodies and the chemical industry where it is used in the implementation of

various regulatory programmes. Its principal function is to capture and make available data on chemicals, in a structured and harmonised way.

IUCLID supports international cooperation regarding the management of chemicals. Its format captures information which comply with the reporting requirements of the OECD Test Guidelines, as well as other national/international methods used for chemical studies. The OECD Test Guidelines¹ play a role in the system of mutual acceptance of chemical safety data among OECD countries² which supports international harmonisation, reduction of duplicative testing of chemicals and the minimisation of barriers to trade.

The move to IUCLID version 6 (IUCLID 6) in 2016 introduced IUCLID as a platform allowing extensions and integrations with other tools in a way that is beneficial to experts using the format for their processes and analyses. The development of the application benefits from international input at the OECD.

Figure 1.1. IUCLID in the scope of international cooperation regarding the management of chemicals



1.3. Strength of Global harmonisation

One of the great strengths of IUCLID is that it provides a platform and a process for global harmonisation of data elements pertinent to chemicals, thus providing a means to promote and support global data standards and data sharing. The standard IUCLID data elements can be extended for capturing information from new approach methodologies or non-standard data generation methods. This provides some flexibility for customisation of IUCLID for users who, for example, need to capture specific information before it has been added to the OHTs or have specific legislative data needs. A balance is required to ensure that the harmonisation strength of IUCLID is not diluted through too much individual customisation. The OECD IUCLID Users Group Expert Panel acts as a forum for discussion on proposed IUCLID customisations with a goal of promoting/sharing new

templates and providing a means to move a customisation into the standard IUCLID data definition, where appropriate.

1.4. Overview of the OECD Harmonised Templates for Reporting Chemical Test Summaries (OHTs)

The OECD Harmonised Templates for Reporting Chemical Test Summaries (OHTs)³ are standard data formats for reporting information on chemical properties or their effects on human health and the environment and to describe their use and related exposure to workers, consumers and the environment. They are usually designed to report test summaries related to a particular endpoint (e.g. chemical properties such as boiling point or water solubility, environmental characteristics such as biodegradation in soil or toxicity to fish, health features such as skin irritation or genetic toxicity), for studies conducted according to OECD Test Guidelines and other national and international methods. To date, over 120 OHTs cover physico-chemical properties, degradation and accumulation of chemical substances in soil, the water or air, toxicity to wildlife or human health, pesticide residue chemistry, analytical methods, efficacy, emissions from treated articles, intermediate effects, and information on chemical use and exposure.

The OHTs' specifications are used by chemical test specialists and information technology developers to identify the relevant elements and necessary data to include in the reporting of a chemical study summary in harmonised nomenclature. It also specifies the structure and format in which the information should be provided and exchanged.

The OHTs are available in a readable format (Word file) and include:

- structured elements (i.e. fields, picklist items, free text prompts, predefined tables and executive summaries)
- picklists for specific test guidelines which contain the most often cited guidelines
- help texts and guidance notes which explain what kind of data entry is expected in a given field.

Each template is associated with its corresponding XML Schema file (eXtensible Mark-up Language), an export format in a common computer language which facilitates the electronic exchange of data across different systems for data entry, storage and management.

The data elements included in the OHTs are generally grouped as follows:

- Administrative data
- Data source
- Materials and methods
- Results and discussions
- Overall remarks, attachments
- Applicant's summary and conclusion.

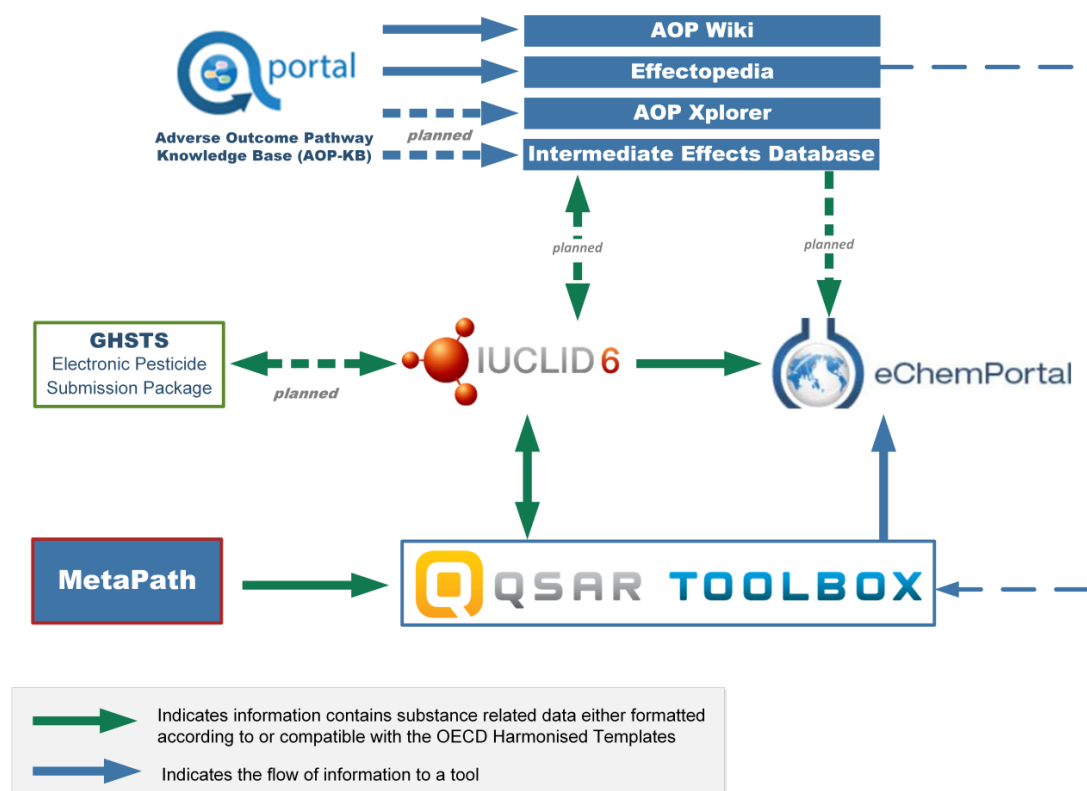
... and include generic elements for all OHTs:

- Literature reference
- Test material information
- Reference substance
- Chemical inventory.

The OHTs should not be seen as constituting OECD data requirements. Different data elements may be relevant in different contexts, for example for the legislative requirements of different regulatory authorities. The OHTs are also not prescriptive as to how the fields are technically implemented. However common practices in chemical test reporting (use or compatibility with the harmonised and agreed upon data exchange format) allow for exchange of data.

OECD and its member countries have developed and promoted specific IT tools around these common harmonised electronic formats to build an “ecosystem of tools” to support regulatory activity on chemicals. This ecosystem of tools includes IUCLID, the OECD QSAR Toolbox, eChemPortal (the Global Portal to Information on Chemical Substances), and MetaPath⁴. These tools can potentially be used by other systems employing the OHTs, expanding the ecosystem beyond the OECD context.

Figure 1.2. Interlinkage of tools developed to support chemical management in OECD countries



Notes

¹ The OECD Test Guidelines

[www.oecd.org/env/ehs/testing/oecdguidelinesforthetestingofchemicals.htm]

² Mutual Acceptance of Data (MAD)

[<http://www.oecd.org/env/ehs/mutualacceptanceofdatamad.htm>]

³ The OECD Harmonised Templates for Reporting Chemical Test Summaries (OHTs)

[www.oecd.org/ehs/templates]

⁴ Ecosystem of OECD supported or promoted tools: <https://oe.cd/it-tools>

Chapter 2. IUCLID (what comes with IUCLID by default)

2.1. Features of IUCLID

IUCLID is made available, for free, from the IUCLID website (<http://iuclid.eu>).

IUCLID users can benefit from the following:

- off-the shelf software: IUCLID 6 database, server (API) and client (Java swing user interface and a web interface introduced in 2018), Desktop and Server versions. Examples of available features are: substance management, dossier creation and comparison, validation, printing, user and role management, report generation, basic searches
- IUCLID 6 exchange format, which includes the OECD Harmonised Templates: <https://iuclid6.echa.europa.eu/format>
- Helpdesk support: <https://echa.europa.eu/contact>
- maintenance service (bug fixes, improvements relevant for the whole user community, format update¹).

Users can also benefit from new features, extensions, and add-ons developed by third parties:

- Text analytics
- Report templates
- Provider Agent (provision of data to eChemPortal).

2.2. Organisation of the information in IUCLID

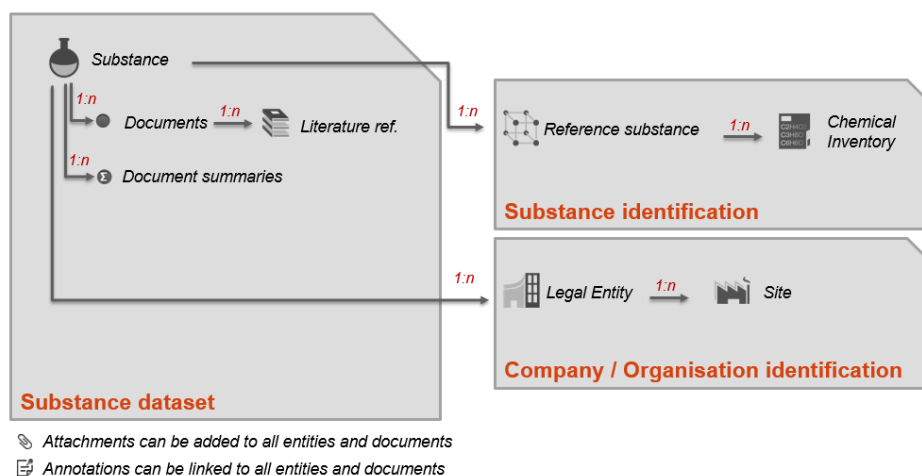
Information is structured in IUCLID according to the following concepts:

- Data entry in IUCLID is done in *entities* and *documents*.
 - Entities are data elements that can be re-used in different contexts and are usually managed in inventories, for example *Substance* entity, *Legal Entity*.
 - The information in IUCLID is also organised in documents that gather all relevant data fields for a specific type of information, for example classification and labelling, and boiling point study summary.

Some entities can link to other entities and contain documents; this is the case of the main IUCLID entities, the *Substance* and the *Mixture / Products* entities. A *Category* entity describes chemical categories.

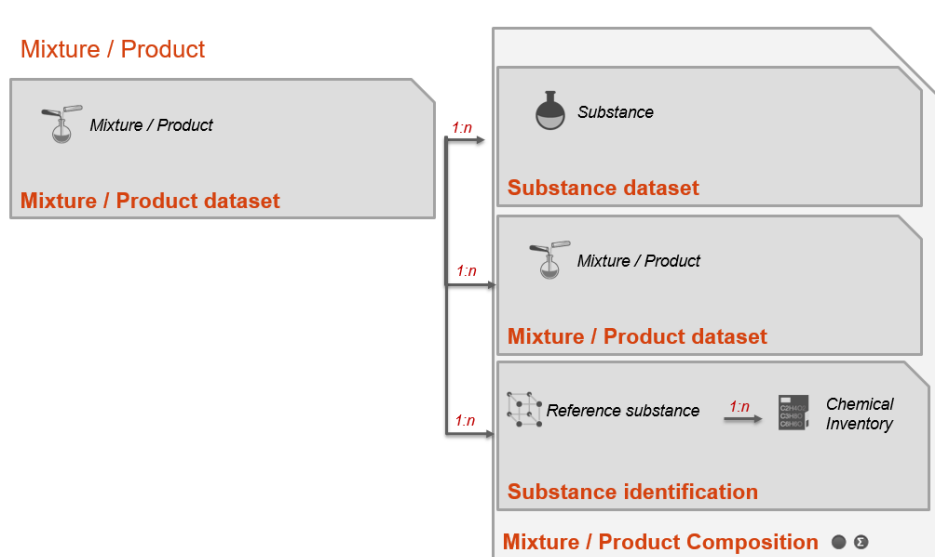
In the figure below, a substance is created and data relevant to this substance is entered in a series of sub-documents and entities. The main chemical identifiers are stored in *Reference Substances* and *Chemical Inventory* entries while the information on manufacturing sites and chemical companies are recorded in a *Site* entity and a *Legal Entity*, respectively.

Figure 2.1. Main IUCLID entities and relationships (substance)

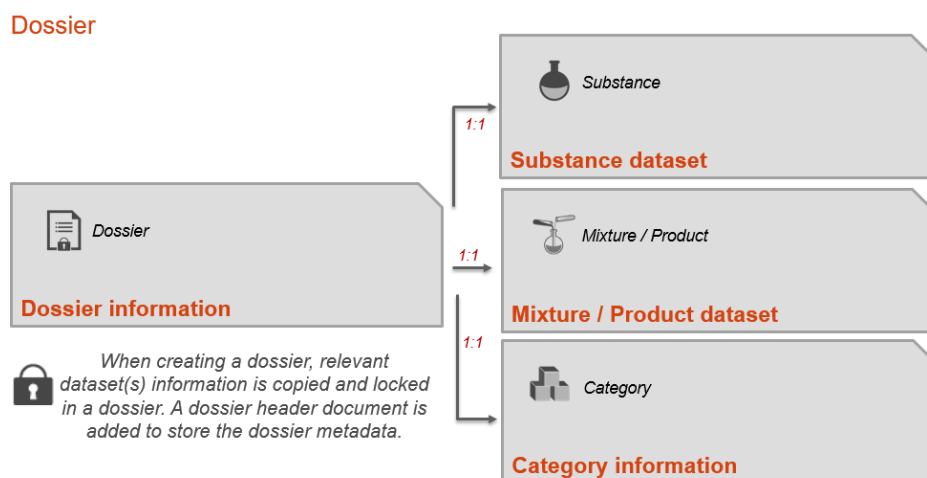


The following figure represents the data organisation for a mixture.

Figure 2.2. Main IUCLID entities and relationships (mixture)



- All the data are entered and stored in logical datasets containing documents and entities. When all the necessary data relevant for a specific (regulatory) context is available, it can be copied and packaged in a *Dossier*. A Dossier is a write-protected copy of the data stored in a Substance, a Category or a Mixture/Product. The dossier concept is detailed in the next section of this document.

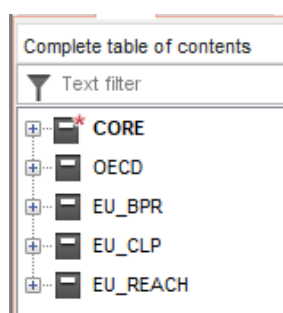
Figure 2.3. Organisation of the information in an IUCLID dossier

2.3. The IUCLID Table of Contents, submission types and dossiers

For each substance or mixture created, the information that can be viewed and managed in IUCLID is displayed according to different pre-defined Table of Contents (TOC) in the *TOC* tab of a navigation panel. The TOC view has three main functions:

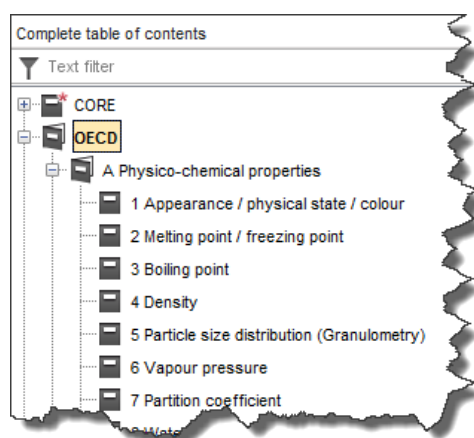
1. provides access to specific documents in an entity for creation, editing, viewing, export, etc.
2. displays the structure of the documents in an entity in a particular regulatory context
3. indicates whether a document is mandatory for a particular type of data submission made for regulatory purposes.

The user can choose to view a generic list of all the available type of information that is supported by the IUCLID format, the “Complete table of contents”, in order to manage the information in a way that is independent of a given regulatory context and only focused on the type of information maintained in the system.

Figure 2.4. Pre-defined TOC: The “Complete table of contents” view

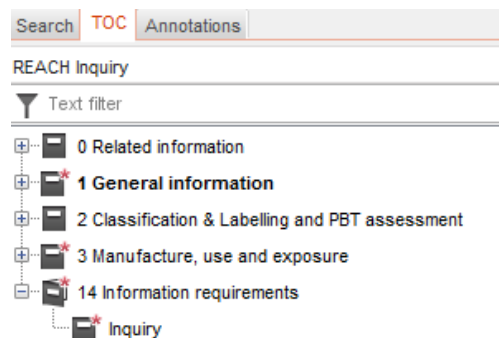
Source: Screenshot of IUCLID 6 2.0.0. build: 30/10/2017

In the view below, all OHTs, managed at the OECD level, will appear under the node “OECD” of the “Complete table of contents”.

Figure 2.5. Pre-defined TOC: View of all OHTs

Source: Screenshot of IUCLID 6 2.0.0. build: 30/10/2017

By selecting a different view from the pre-defined list of TOC, the user can display the IUCLID data in a way that matches the name of the information requirement set in a legislation (section and document names) and that indicates whether information is required by distinguishing between mandatory and optional sections. The screenshot below shows an example of the specific table of contents created to represent the information requirements related to the Inquiry process under the EU REACH regulation.

Figure 2.6. Pre-defined TOC: View related to the EU REACH regulation Inquiry process

Source: Screenshot of IUCLID 6 2.0.0. build: 30/10/2017

The TOC / views related to a regulatory process can be associated with *Submission Types*. Submission types do not only provide IUCLID users with a way to display the relevant table of contents but also to create IUCLID *Dossiers* containing this relevant information. During the dossier creation process in IUCLID, the user may enter additional administrative data related to the dossier in the “dossier header” associated to the selected submission type. The following screenshot displays the steps of the IUCLID dossier creation where the user selects the submission type to be applied and enters the additional information in the corresponding dossier header.

Figure 2.7. Steps of the IUCLID dossier creation

The figure consists of two screenshots from the IUCLID software interface, illustrating the steps of dossier creation.

The top screenshot, titled "Substance", shows a selection screen for the submission type. The options are:

- CLP Regulation - CLH dossier
- EU_REACH**
 - REACH Annex XV - Restriction
 - REACH Annex XV - SVHC
 - REACH Application for authorisation
 - REACH Downstream user notification of authorised use
 - REACH Downstream user report
 - REACH Inquiry
 - REACH Notification of substance in article
- B...

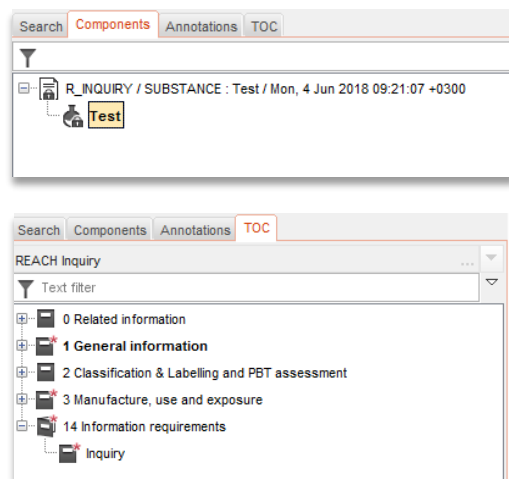
The bottom screenshot, titled "Dossier creation wizard", shows a form for entering administrative information. The submission type is "REACH Inquiry". The form includes the following fields:

- Dossier name (given by user)
- Dossier submission remark
- Dossier specific information**
 - Remarks
 - Document

Source: Screenshots of IUCLID 6 2.0.0. build: 30/10/2017

Once created, the dossier displays the relevant IUCLID data in a context-specific way. As an example, a REACH Inquiry notification dossier is represented below.

Figure 2.8. REACH Inquiry notification dossier



Source: Screenshots of IUCLID 6 2.0.0. build: 30/10/2017

IUCLID can be configured to adapt the default table of contents to a specific regulatory context; this is done by creating a submission type (see section Submission types).

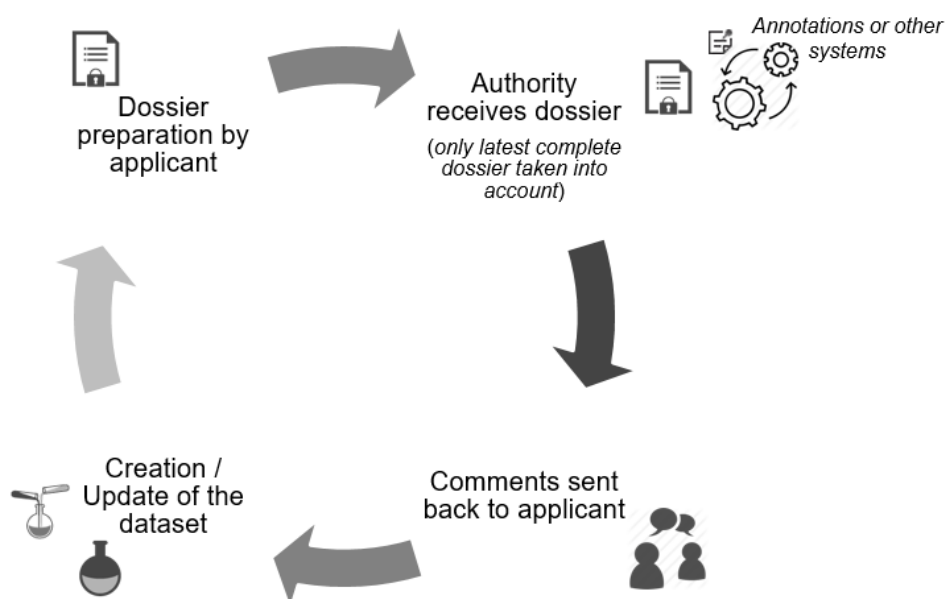
2.4. IUCLID and regulatory data submission

IUCLID is a tool that supports chemical data management and exchange of this information in regulatory contexts. One of the main use cases is the transfer of information from the data provider to the organisation requiring the data to be provided. Typically, a *Dossier* is used to submit data to a regulatory authority to satisfy a legal obligation arising from a legislation, for example the European Union regulation for the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH).

Two different approaches can be defined in order to describe the IUCLID data flow between the data providers and the receiving organisations:

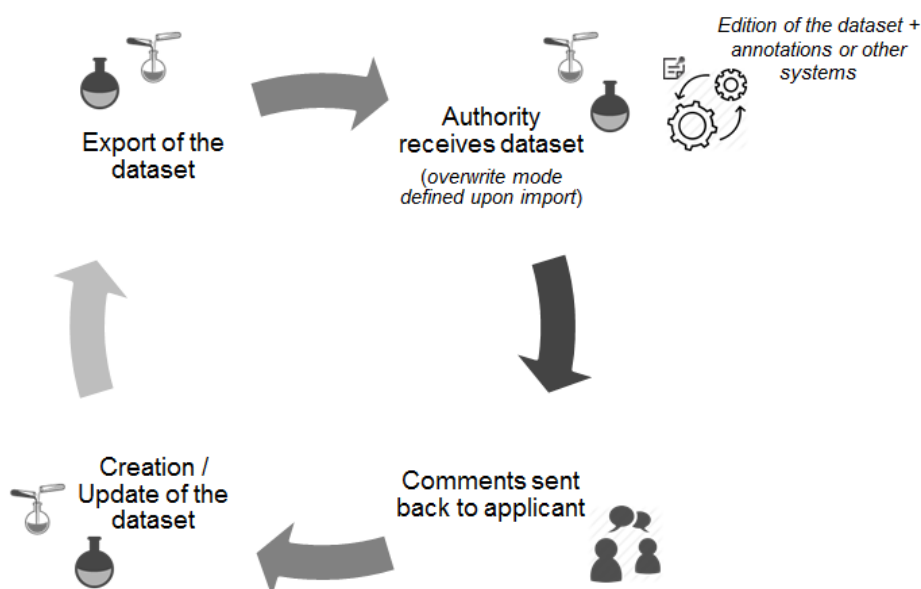
1. The review approach: In this first approach, the data provider submits the data to the regulatory organisation which oversees the review and evaluation of the submitted information. If some elements need to be corrected or new data must be submitted, the regulatory organisation asks the data provider to send an update of the initial submission. In this case, management of the submission content is the responsibility of the data provider. On the authority side, the data collected are processed and reviewed using IUCLID features, such as data aggregation, in combination with other tools and data sources.

Figure 2.9. IUCLID data submission, the review approach



2. The collaborative approach: In the second approach, the regulatory organisation manages the data and combines different sources of information into its repository of chemicals information. The data provider can submit data that then are reviewed and added by the regulatory experts into a main chemical dataset that they maintain.

Figure 2.10. IUCLID data submission, the collaborative approach



Note

¹ For more information on IUCLID and OECD formats, refer to Management of the IUCLID format, in this document.

Chapter 3. Management of the IUCLID format

3.1. Introduction

A fundamental aspect of the IUCLID application is the format of the chemical data. The format is managed by a dedicated tool: The IUCLID Template Manager (ITEM). The structure of the IUCLID format is based on the level of harmonisation that has been reached internationally at the level of the OECD, as well as between regulatory programmes. The management of the IUCLID format reflects this structure, which means that each level of harmonisation is represented by a type of definition provider. The definition provider is responsible for managing the IUCLID format as well as the business processes for changing the format for which it provides the definition, a so called *Definition Provider*. One of the key elements assigned to a Definition Provider is the IUCLID *document* where chemical data is entered, such as endpoint study records, the substance composition, etc.

The principal Definition Provider types are the OECD and IUCLID CORE, in which agreement has been reached across regulatory jurisdictions and/or programmes as to what data are required under these definitions. There are also individual definition providers of the IUCLID format, which reflect an individual regulatory programme such as the EU's REACH regulation. All elements of the IUCLID format are grouped under and assigned to one of these Definition Providers types:

- **OECD:** This Definition Provider includes all the OECD Harmonised templates (OHTs) which are covering the following areas:
 - Study summaries (based on the requirements of the OECD test guidelines or other recognised testing protocols)
 - Substance information (e.g. reference substance containing the main substance identifiers)
 - Uses and exposure information
 - Annotations (to store the outcome of an assessment of the available data).
- **DOMAIN:** In IUCLID there is a distinction between documents and entities which are independent elements that can be managed in inventories. In IUCLID, the following entities are provided in the DOMAIN Definition Provider: Substance, Mixture, Legal Entity, Site, Template, Reference Substance, Literature Reference, Chemical Inventory, Annotations, Contact, Category.
- **CORE:** The elements of the IUCLID format stored under this Definition Provider have been developed as part of the IUCLID project and have been agreed at the level of the OECD IUCLID Users Group Expert Panel, but are not (though they could potentially be) officially harmonised at the OECD level, i.e. part of the OHTs. In general, IUCLID documents that are identified as being useful for more than one regulatory-specific Definition Provider (see below) but not (yet) part of the OHTs, are stored in the CORE Definition Provider.
- **Regulatory-specific Definition Providers:** The elements of the IUCLID format stored under this Definition Provider type are not harmonised at the level of the

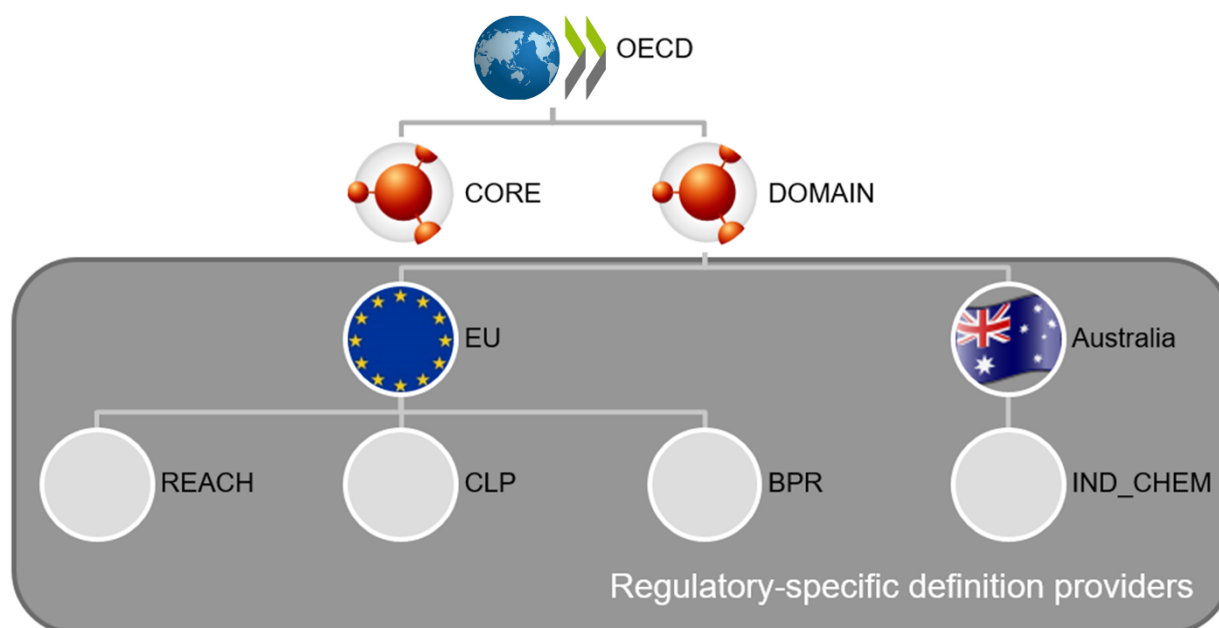
IUCLID project or the OHTs. These elements are designed to capture data specific to a certain regulation and are unique to that regulation, such as the EU's REACH Inquiry process.

The first three IUCLID Definition Providers above have a specific status as they represent the highest levels of harmonisation that can be reached by the data format. The data elements stored under these Definition Providers are agreed at the OECD level either by the OECD Expert Group on the OECD Harmonised Templates (OHT Expert Group) or by the OECD IUCLID Users Group Expert Panel. They are available to be used by all IUCLID users and their content should, in principle, not be duplicated in other Definition Providers. For example, if there is a need as part of a regulatory process to collect data on the flash point, the relevant OECD or CORE documents should be used instead of duplicating the format in other regulatory-specific Definition Providers.

The regulatory-specific elements of the Regulatory-specific Definition Providers are not precluded from harmonisation and can be proposed to the OECD IUCLID Users Group Expert Panel or the OHT Expert Group for inclusion into the CORE or OECD definition providers respectively. At the time of publication of this document, the following regulatory-specific definitions are available:

- EU_REACH, that includes all regulatory specific information needed as part of the EU REACH regulation
- EU_CLP, containing specific information for the EU CLP regulation
- EU_BPR, containing specific information for the EU Biocidal Products Regulation
- prototypes are being developed for Australia,

Figure 3.1. Representation of the hierarchy between Definition Providers



3.2. Building blocks of the IUCLID format

The IUCLID format is primarily based around document definitions, such as all the Endpoint Study Record documents and Endpoint Summary documents in IUCLID. In defining the IUCLID format, the ITEM tool provides the following building blocks to structure and define documents for a particular legislation:

- **Phrases** are picklist options, e.g. “experimental study”.
- **Phrasegroups** contain Phrases and are displayed as picklists in IUCLID. Phrasegroups can re-use existing Phrases.
- **Text templates** are pre-defined texts which appear in IUCLID text fields to guide users on what information to enter and act like a guidance template.
- **Entities** are the re-usable/linkable elements of IUCLID, such as reference substances, legal entities, test materials etc. These entities, once entered in IUCLID, are stored in an inventory and can be re-used and linked to documents.
- **Blocks** are ITEM specific and do not have an IUCLID equivalent. They are designed to help re-use sets of fields in two or more documents. For example, the Administrative record block in ITEM is a set of standardised OHT fields re-used in many OHTs.
- **Documents** contain a collection of IUCLID fields where data can be entered and stored inside the IUCLID database. Each field has a number of components. The primary component is the datatype, which governs what type of IUCLID fields it is. Based on the datatype, documents can re-use Entities, Text templates and Phrasegroups (and their Phrases). Documents can also directly re-use Blocks.
- **Submission Types** are regulatory specific contexts or related to a specific data collection process, and contain the IUCLID section tree which organises the information requirements for that regulation or process, and provides entry points to the documents IUCLID users will need to complete.

- **Definition Providers** are the highest part of the IUCLID hierarchy in terms of format management and act as a “parent” or “provider” to all the above building blocks. Every building block, whether Phrase, Block or Entity et al., will have a Definition Provider. Definition Providers have the additional function of grouping documents in a hierarchy.
- **Application Tag** is the container of the Definition Providers to be added to a specific IUCLID release. They establish the contract between the format managed at the OECD level and an IUCLID distribution. For example, IUCLID 6.1 included the following definition providers: CORE v2.25, OECD v2.20, EU_REACH v.2.5, EU_CLP v2.5 and EU_BPR v2.6. IUCLID 6.3 includes the following definition providers: CORE v4.13, OECD v.4.7, DOMAIN v.1.5, EU_REACH v4.8, EU_CLP v.4.12, EU_BPR v.4.9 and AU_IND_CHEM v.1.8.

3.3. Update and extension of the IUCLID format

3.3.1. Changes to the IUCLID format

A change to the IUCLID format can either be major or minor.

A major change is when, due to this change, there would be a loss of compatibility with the next version of IUCLID. Major changes to the IUCLID format often affect the transfer of data between versions and require migration rules to ensure compatibility between versions. Migration rules can be defined in ITEM to prevent data loss. A major change to IUCLID typically happens once a year, in the third or fourth quarter. The prioritisation of changes to the IUCLID format begins in February of the same year. Non-backwards compatible changes which require migration of data should be avoided when possible due to the impact on systems integrated with IUCLID and the burden created for the management of those systems.

A minor change, on the contrary, does not need a new major version of IUCLID. A minor change, such as a field label change or a change to the help text, does not require migration rules.

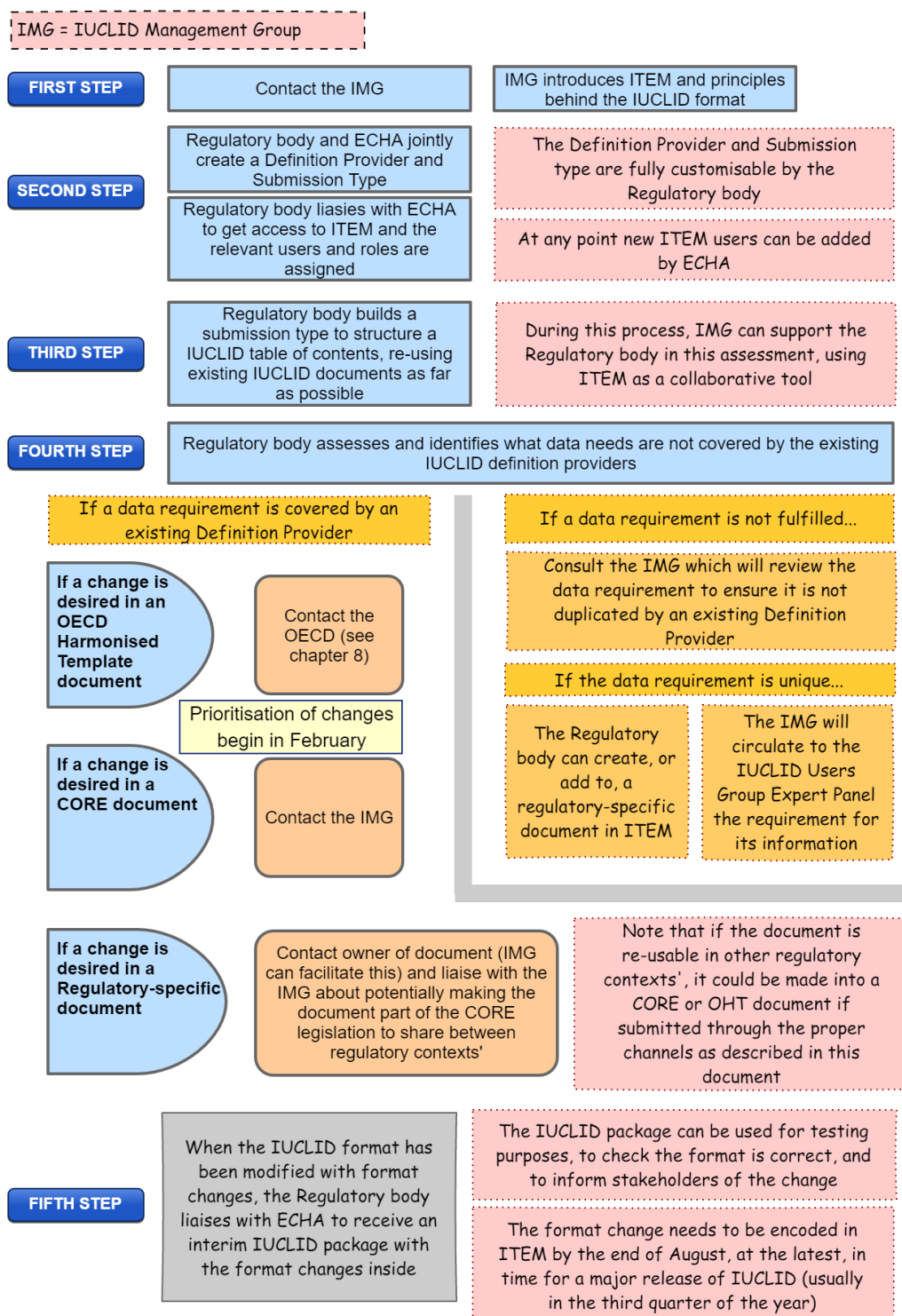
There are specific processes for changing the format according to the Definition Provider type. This is elaborated below.

3.3.2. Customising IUCLID for a new regulatory-specific format

When a regulatory body or organisation wishes to receive, exchange or create data in the IUCLID format, such as the case with Australia (See Section 6.2), then an extension to the current IUCLID format may be required. Below is a general outline of the steps a regulatory body should take towards extending the IUCLID format. The hierarchy of Definition Providers types described above must always be kept in mind when updating the IUCLID format.

The IUCLID Management Group (IMG) referred to in the illustration below is comprised of the ECHA IUCLID team and coordinates with the IUCLID Users Group Expert Panel and the OECD Secretariat.

Figure 3.2. Process for defining a new Definition Provider, Submission Type, and associated documents in the IUCLID format



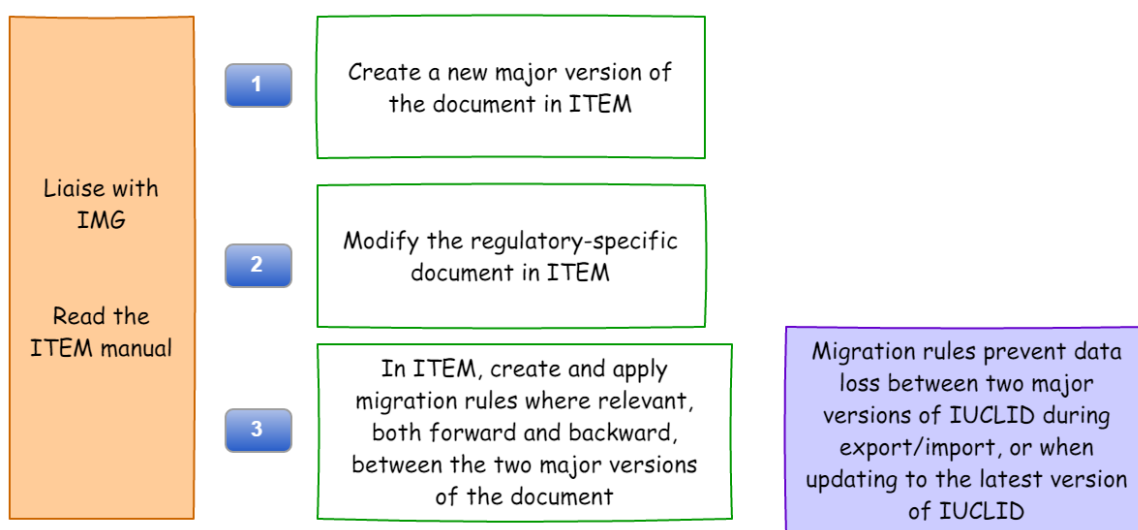
If a Regulatory body already has a Regulatory-specific Definition Provider defined in the IUCLID format but wishes to add a new regulatory-specific document to its Regulatory-

specific definitions or propose changes to existing OECD, CORE or other Regulatory-specific documents, then it should follow the fourth and fifth steps in the diagram above.

3.3.3. Update of IUCLID documents (regulatory-specific data formats)

If the Regulatory body wishes to update a Regulatory-specific document under a definition which it has provided, the changes should also be checked according to the fourth and fifth steps in the diagram above to assess whether the update of the document does not include data already collected by other documents. The regulatory body can inform and discuss with the IMG to check if its new data requirements have already been captured by another definition provider.

Figure 3.3. Process for changing a regulatory-specific document



3.3.4. New IUCLID documents (OECD and IUCLID formats)

New IUCLID documents can also be proposed to be developed in the OECD and CORE Definition Providers. In that case, the relevant coordinating bodies should be consulted in order to reach an agreement, respectively the OHT Expert Group and the OECD IUCLID Users Group Expert Panel.

3.3.5. Update of IUCLID documents (OECD and IUCLID formats)

Existing Document formats, for example for "Boiling point", cannot be customised; an update to an existing Document format is officially proposed and agreed through the existing processes and governance (OHT Expert Group and the OECD IUCLID Users Group Expert Panel).

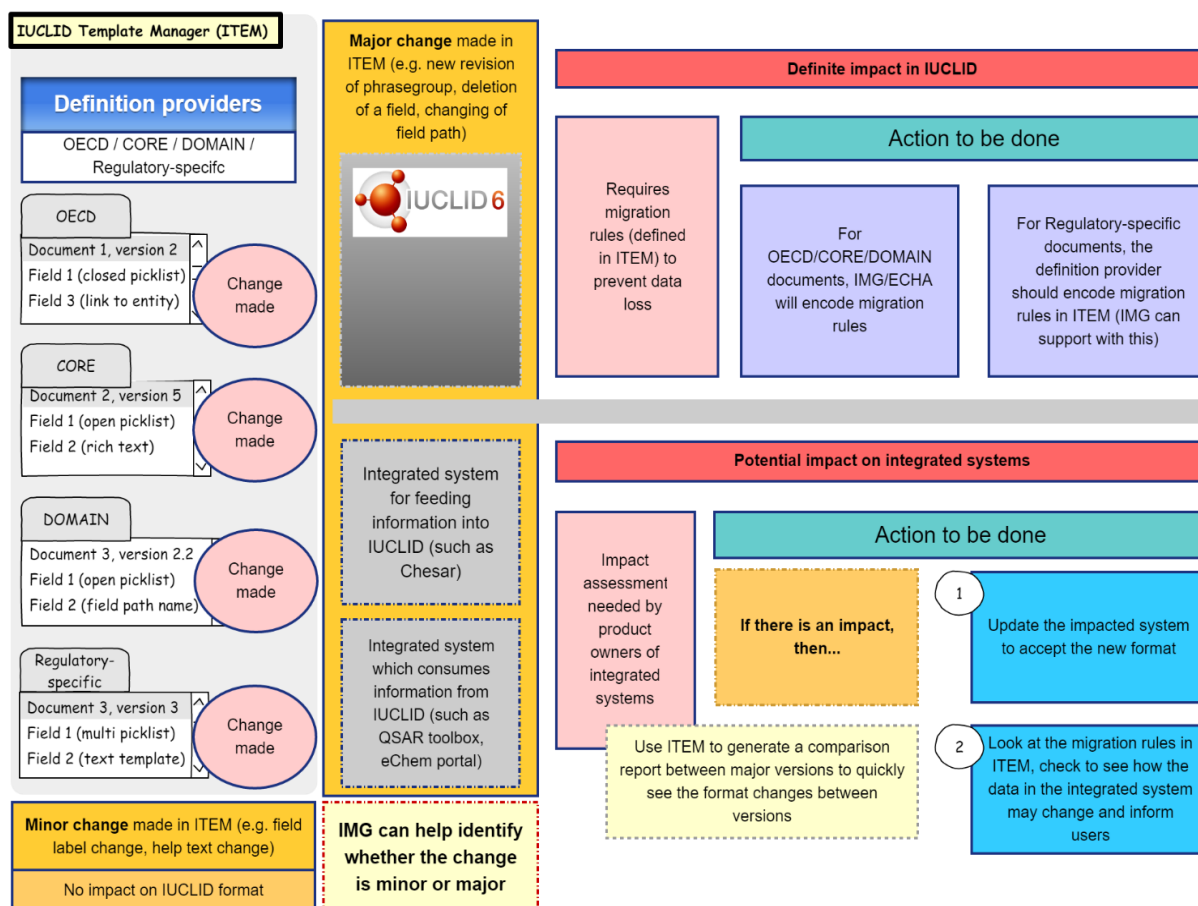
3.3.6. The impact of changing the IUCLID format

When changing the IUCLID format through one of the routes above, there is potentially:

- Impact on the next major version of IUCLID
- Impact on systems integrated with IUCLID
- Impact on business processes in which IUCLID is involved
- A need to create migration rules to prevent data loss between major versions.

The illustration below captures the broad process of how to manage a major change to the IUCLID format:

Figure 3.4. Major and minor changes to the IUCLID format and follow-up actions



Chapter 4. IUCLID customisable elements

As presented earlier in this document, the main purpose of IUCLID is to facilitate the management and processing of chemicals information. To achieve this, several components of IUCLID are customisable and, therefore, can be adapted to different regulatory contexts.

- The **IUCLID format** allows for the structuring of the information available on chemicals in a standardised way. As mentioned before, the OECD Harmonised Templates (OHTs) are all available in IUCLID to record substance properties (physico-chemical, fate and behaviour, toxicological and eco-toxicological properties) and use and exposure information. As well, the IUCLID format covers additional information areas such as the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) or the endpoint summaries which capture information about a grouping of endpoint study records. This format can be further extended with the addition of regulatory or process-specific documents in Definition Providers.
- **Submission types** can be created in order to indicate to the data providers the information requirements that are set by a specific regulatory context or data collection process. These requirements are identifiable in the TOC views of substance and mixture datasets in IUCLID.
- The **validation** feature of IUCLID can verify the completeness of the data stored in the application. Available validation rules can be re-used and new ones can be developed.
- Once the data are collected, **reports** can be generated by dataset. This is done by the reporting engine which can accept customised report templates.
- If the data have to be published or disseminated, there might be a need to **filter** out some confidential or non-public information. The filtering engine supports this and can be configured depending on user needs.
- Finally, IUCLID provides different levels of **help systems** and supports **translation**.

4.1. IUCLID format (using ITEM)

4.1.1. IUCLID documents

The IUCLID Template Manager (ITEM) has been developed by the European Chemicals Agency (ECHA) to support the specification, development and testing of the IUCLID format. It is remotely available and provides a collaborative online space where users within or between organisations can share specifications, work simultaneously on the data format, and approve one another's work. ITEM was designed to be a user-friendly application and a bridge between the business and the IT developers.

It is recommended to first work on an ITEM document template (using a text editor such as Word) together with the relevant business persons in order to define the content of the

format and to agree on the type of information collected. Once the agreed content has been entered into ITEM, the specifications can be implemented in IUCLID with minimum effort as ECHA and its contractors have automated most of the conversion process from ITEM's specifications to their implementation in IUCLID.

Technically, documents relevant to the same context are packaged in an IUCLID Definition Provider module that can be added to any IUCLID installation in order to extend its format and submission types according to the context-specific needs. The IUCLID developers use the specifications created in ITEM to automatically generate the JAVA code needed to bring the specifications to IUCLID.

It should be noted that the creation of new documents and the extension of existing ones (adding new fields for example) is supported by ECHA as part of the standard maintenance service provided with IUCLID and based on the fact that this process has been largely automated and does not require many resources from the IT developers. However, more complex document updates, associated with advanced migration rules (e.g. merging fields, removing fields and keeping the content) cannot be supported by the standard maintenance service, except for the documents which are part of the CORE, DOMAIN and OECD Definition Providers. In these more complex cases, a specific agreement needs to be found between the definition provider and the IUCLID Management Group (IMG) in order to move forward with the implementation step. However, more and more support is provided for the development of migration rules and, as in the case of the format definition, their logic is progressively automated, thus reducing the associated coding effort and resources.

4.1.2. Submission types

ITEM also provides the user with a way to identify which IUCLID documents are relevant for a specific regulatory context or data collection process. This is done via the creation of Submission Types.

Submission Types are used to configure the Table of Contents (TOC) to be used by the data provider in order to easily identify the relevant information requirements.

While creating a submission type, the user will have the possibility to use existing documents from the OECD, CORE and DOMAIN Definition Providers together with the specific documents eventually also provided by a custom Definition Provider.

The documents selected by the user to be part of the submission type can be organised in sections and sub-sections (of the TOC) and have an indication of whether they are optional or mandatory.

The submission type can then be used in IUCLID to display the information sorted according to the TOC corresponding to the information requirements set by a data collection process. They can also be used to package the information in IUCLID dossiers.

Table 4.1. Support for creation and modification of submission types

IUCLID document management task	Definition Provider	Support
New Submission types	All	Standard IUCLID support provided by ECHA
Extension of Submission types	All	Standard IUCLID support provided by ECHA
Modification of Submission types involving migration	OECD CORE DOMAIN	Standard IUCLID support provided by ECHA
Modification of Submission Types involving migration	Regulatory-Specific Definition Providers	Although ECHA has started to automate simple migration rules, more advanced migration operations need to be discussed before any development is done.

More information about the IUCLID Template Manager (ITEM), including a user manual, can be found on the IUCLID website: <https://iuclid6.echa.europa.eu/template-manager>

4.2. Validation

IUCLID has a tool called the “Validation Assistant”. This tool validates the quality, consistency and accuracy of the data entered inside a substance dataset or dossier. The tool provides a user with a guiding message on how to correct an error or improve the quality of data and warns the user of the severity of the issue found. There are two levels of checks: “Submission checks” (a severe or potentially severe issue) and “Quality checks” (less severe, but requires checking). Within these two levels, the severity of the issue is further elaborated by distinguishing the validation checks between “failure” (must be checked and corrected) and “warning” (potentially needs correcting).

The Validation Assistant contains a number of validation rule scenarios. Each scenario contains a combination of triggers which, if activated, run a particular set of validation rules on an IUCLID dataset or dossier.

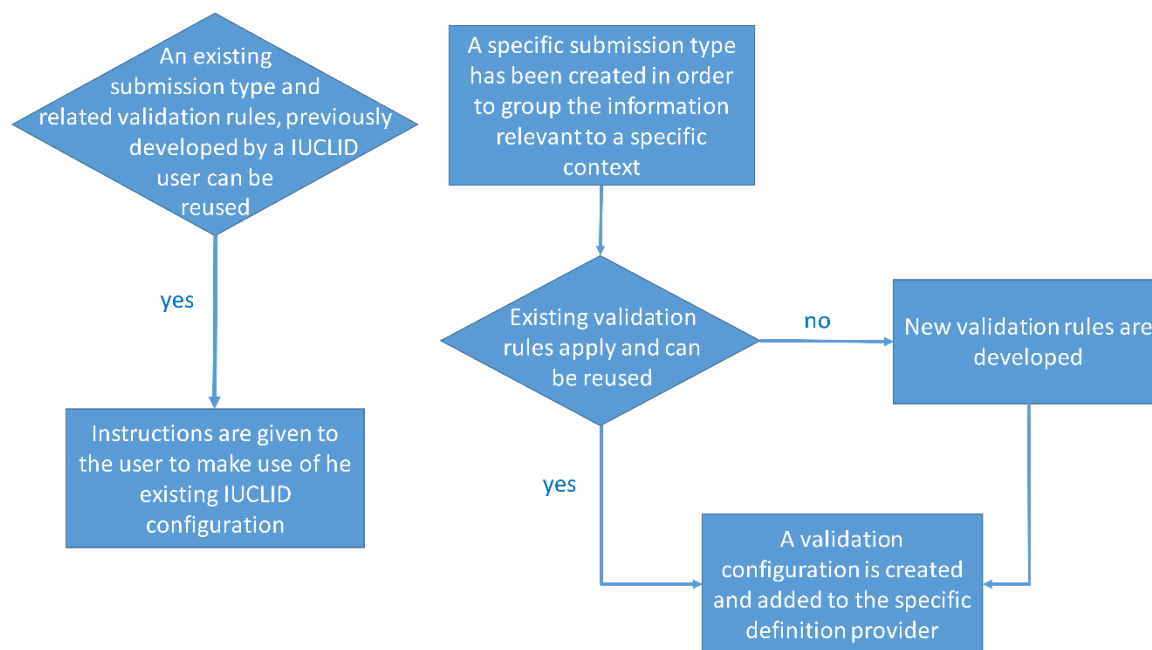
Regarding the customisability of the Validation Assistant, the existing validation rules and scenarios can be reused by organisations which would like to customise IUCLID by providing their own validation configuration to be included in a Definition Provider. There are several ways in which this can happen:

1. Another IUCLID user directly reuses the existing scenarios and associated rule sets that are applied to check the completeness of specific dossiers. In that case, the user will simply reuse the information requirements and associated verification rules defined by another IUCLID user.
2. An IUCLID user who has already defined his own information requirements by selecting the relevant IUCLID documents from the OECD, IUCLID and/or his own Definition Provider, and has created the corresponding Submission Types can select the rules that apply from the list of existing validation rules. This selection, in combination with the necessary triggers will form the validation scenarios that are used to check the completeness of the datasets prepared by the users entering the information to comply with a specific regulatory context. The newly developed configuration will have to be loaded, in an IUCLID release, inside the relevant Definition Provider.
3. A third scenario also exists in which the user will not only select rules from the existing catalogue but also specify his own rules. This step requires the involvement of a developer who will write the rules code to be added to the specific Definition

Provider. The IUCLID developers can support the development of a small set of additional simple rules if needed.

These different scenarios are illustrated by the following flowchart.

Figure 4.1. Different scenarios for the customisation of the Validation Assistan



Note: More information on the data validation can be found on the IUCLID website: <https://iuclid6.echa.europa.eu/data-validation>.

4.3. Reporting

IUCLID comes with a feature called the “Report Generator”. This feature allows an IUCLID user to extract data from an IUCLID dataset or dossier and generate a readable, user-friendly, customised report of IUCLID information in different output formats, for example RTF or PDF. The Report Generator can also be used to facilitate the exchange of IUCLID data with other data management systems. This is done by using the Report Generator to generate an XML or CSV file of IUCLID data to populate another system with this information.

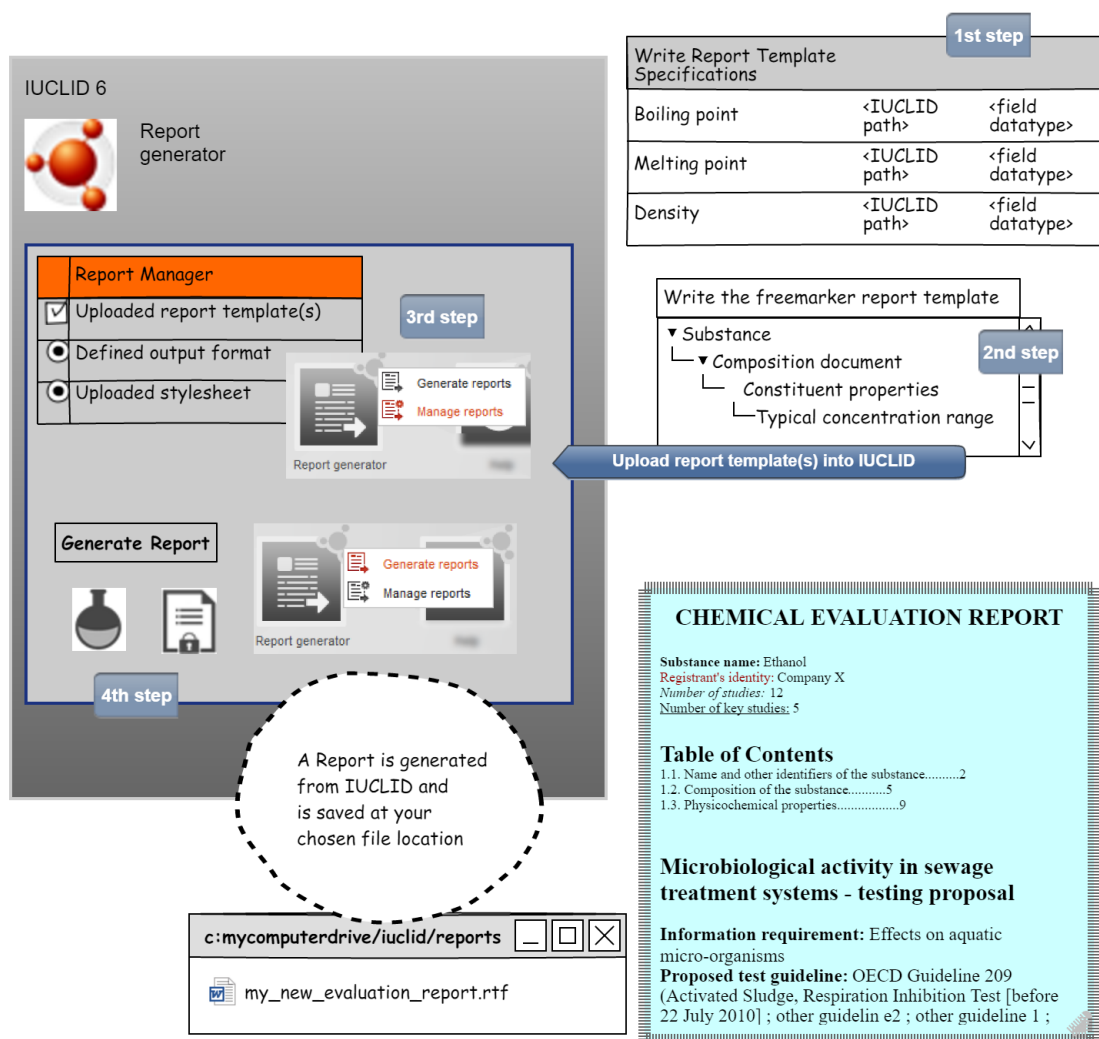
The IUCLID information which a report contains and the format of the report is fully customisable by any IUCLID user. To customise the information a report contains, the user writes what is called a Freemarker Report Template (FTL file) and uploads it into IUCLID's Report generator manager by selecting to “Manage reports” in the Report Generator. The report can then be generated at any time from IUCLID in a file format of the user's choice. Some IT skills are required for writing an FTL file, but a novice can learn the basics relatively quickly.

The potential usage of the Report generator can be summarised in the following four steps illustrated by the figure below.

- Step 1: The user writes the report specifications, i.e. the IUCLID information that should be extracted and how it should be presented to the end user.

- Step 2: A corresponding report template (FTL file) is written. This step requires some IT skills which can easily be learned.
- Step 3: The report template is loaded in an IUCLID installation.
- Step 4: The report feature is applied to the selected dataset (either a substance, a mixture or a dossier).

Figure 4.2. Process for writing and generating a customised report



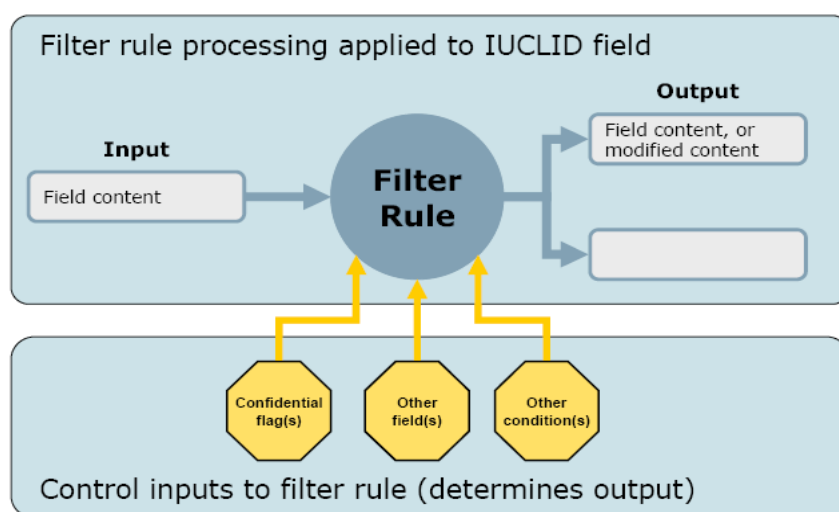
The IUCLID website (<https://iuclid6.echa.europa.eu/reports>) provides the following documentation and examples to help a user get started with customising a report template for extracting IUCLID data:

- an introductory guide to creating customised reports
- step-by-step instructions on how to use the Report Generator
- examples of customised report templates which are compatible with a range of file formats.

4.4. Filtering

Filtering rules are used by several IUCLID features (export, create dossier, printing, reporting) to filter non-public information from dossier datasets according to three generic rules, (1) always publish, (2) publish unless claimed as confidential, (3) never publish the fields, for example the content of the field “Confidential details on test material”. There are also eight more specific additional rules, for example, filter out the IUPAC name if the IUPAC name was claimed as confidential.

Figure 4.3. Filter rule logic

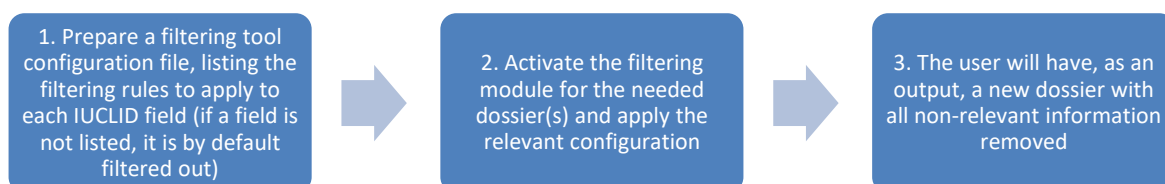


These existing filtering rules are provided by the IUCLID filtering module and can be re-used in a customised way for example, to remove from a dossier all data which is not relevant for a specific purpose, such as to exchange data with a third party or to make the data publicly available.

A configuration file (TXT file) can be customised and then either applied manually by the user or added to IUCLID within a Definition Provider. IUCLID generates a report of the outcome of the filtering and can create a new filtered dossier.

To summarise, a user who would like to filter out specific information from a dossier would proceed as follows:

Figure 4.4. Procedure to customise filtering



Note: More information can be found on the IUCLID website: <https://iuclid6.echa.europa.eu/data-filtering>.

4.5. Help System

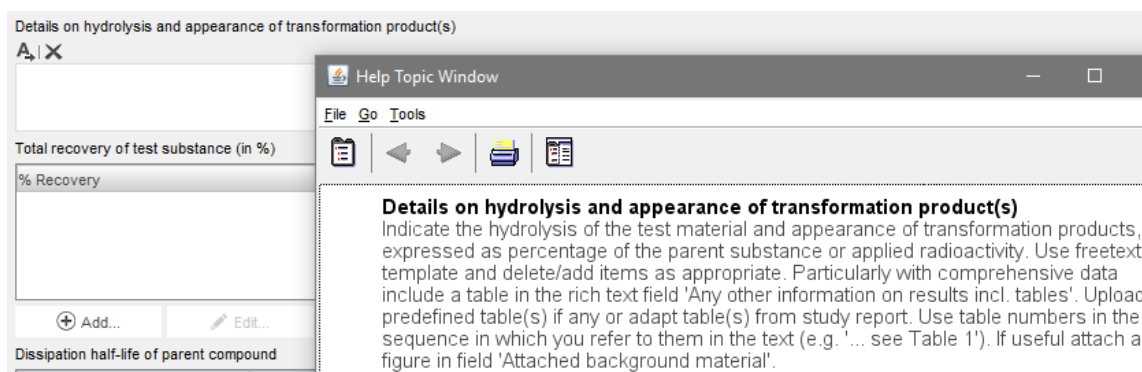
The IUCLID Help System is organised in three different layers.

The first layer consists of help information, provided together with the format itself, which explains the meaning of specific IUCLID fields and the kind of data to be stored there. This information is part of the IUCLID format specification and managed in the IUCLID Template Manager (ITEM). The following image is an example of the help associated with a field located in the OHT for Hydrolysis.

Figure 4.5. Example Help text for an IUCLID field

Field name	Help text
Details on hydrolysis and appearance of transformation product(s)	<p>Indicate the hydrolysis of the test material and appearance of transformation products, expressed as percentage of the parent substance or applied radioactivity. Use freetext template and delete/add items as appropriate.</p> <p>Particularly with comprehensive data include a table in the rich text field 'Any other information on results incl. tables'. Upload predefined table(s) if any or adapt table(s) from study report. Use table numbers in the sequence in which you refer to them in the text (e.g. '... see Table 1').</p> <p>If useful attach a figure in field 'Attached background material'.</p>

This first layer of help information is provided in the format specification and is available to all users accessing the relevant IUCLID documents. The following screenshots show how this help text is displayed to the users of the IUCLID application and in the IUCLID web interface.

Figure 4.6. Display of Help Topic Window in the IUCLID application

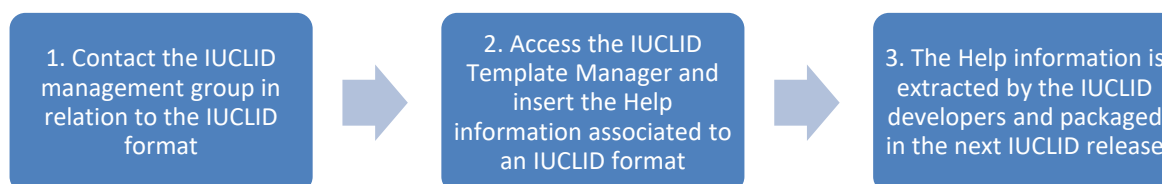
Source: Screenshot of IUCLID 6 2.0.0. build: 30/10/2017.

Figure 4.7. Display of Help Topic Window in the IUCLID web interface**Details on hydrolysis and appearance of transformation product(s) ? A Insert existing templates**

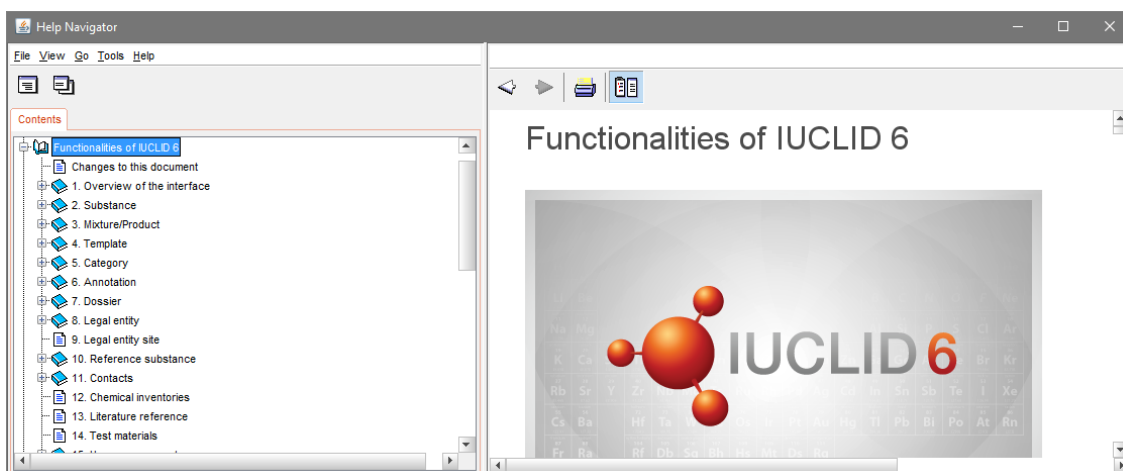
Indicate the hydrolysis of the test material and appearance of transformation products, expressed as percentage of the parent substance or applied radioactivity. Use freetext template and delete/add items as appropriate. Particularly with comprehensive data include a table in the rich text field 'Any other information on results incl. tables'. Upload predefined table(s) if any or adapt table(s) from study report. Use table numbers in the sequence in which you refer to them in the text (e.g. '... see Table 1'). If useful attach a figure in field 'Attached background material'.

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The update process for this information is linked to that of the documentation of the IUCLID format as described in the figure below.

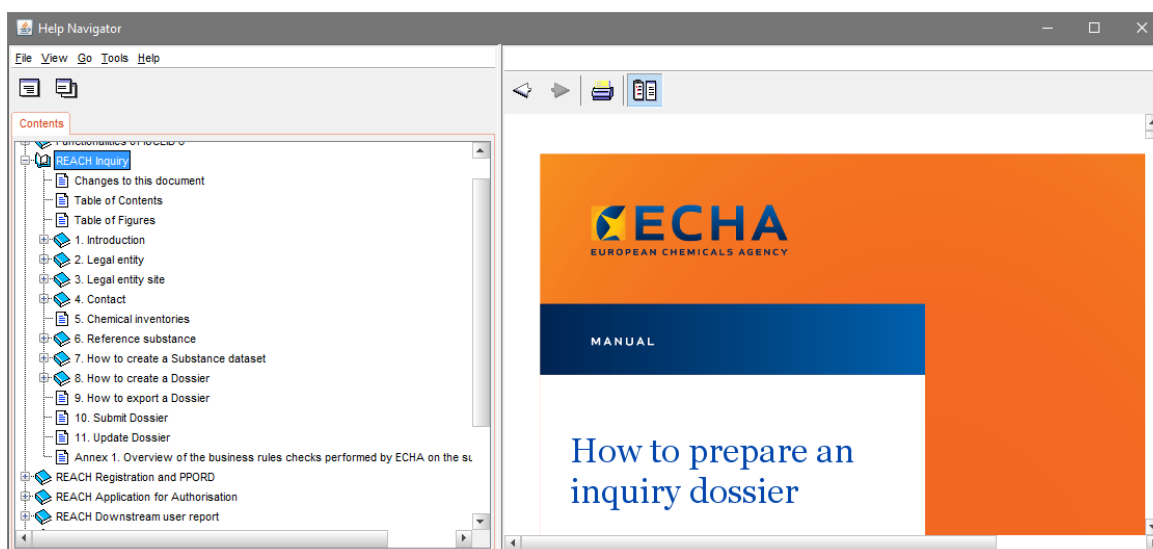
Figure 4.8. Procedure to customise Help information as part of the IUCLID format specification

The second layer of help information is provided in the IUCLID functionalities manual which describes the main features available in IUCLID. It is distributed on the IUCLID website¹ but is also accessible directly from the IUCLID application itself. ECHA maintains the manual taking into account the adaptations made to the IUCLID application and agreed at the level of the OECD IUCLID Expert Panel.

Figure 4.9. IUCLID functionalities manual

Source: Screenshot of IUCLID 6 2.0.0. build: 30/10/2017.

The third layer of help information differs from the previous two in the sense that it is linked to a specific context under which the IUCLID application is used. The information is usually provided in the form of manuals addressing one specific need, and the content is managed by the organisation responsible for the specific use of IUCLID. These manuals can be distributed from a website and also can be integrated in the standard IUCLID distribution. For example, the manual on how to prepare an Inquiry notification under REACH is created by the European Chemicals Agency and made available on the ECHA website.

Figure 4.10. Display of Help information in IUCLID addressing the use of IUCLID for a specific purpose

Source: Screenshot of IUCLID 6 2.0.0. build: 30/10/2017.

In order to integrate this help layer to a planned release of the IUCLID application, the organisation responsible for the information should provide the content to the IUCLID Management Group in an agreed format.

4.6. Translation

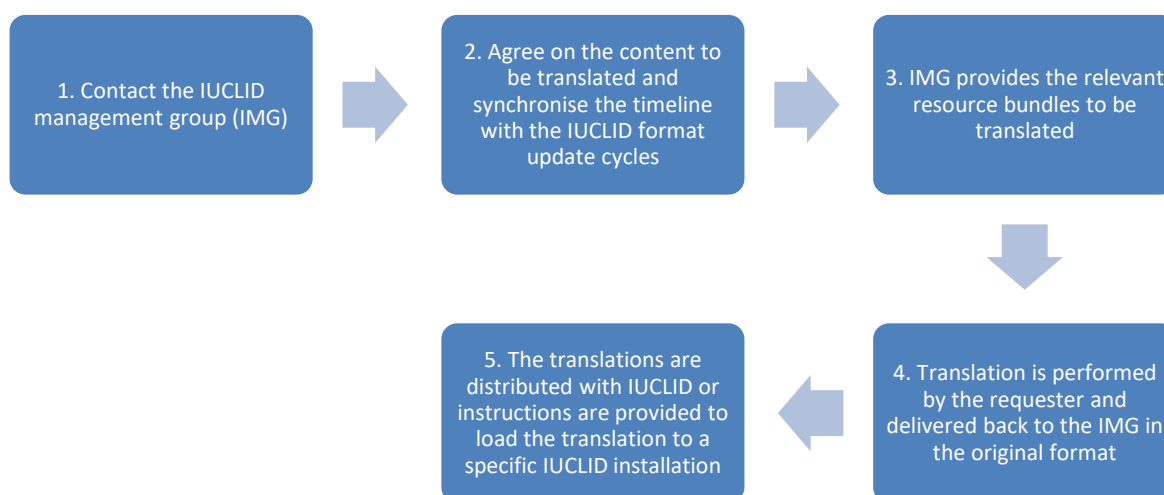
Some elements of IUCLID can be translated at the technical level. The values of all IUCLID elements that can be potentially translated in different languages are maintained in resource bundles.

The following elements of IUCLID may be translated:

- IUCLID document names and section names displayed in Table of Contents
- field labels
- phrases (included in IUCLID picklists)
- free text templates (to support data entry in free-text fields)
- help text.

Currently only the English version is available. However, the following process can be used in order to translate all or parts of the IUCLID translatable elements:

Figure 4.11. Procedure to translate the IUCLID translatable elements



If the translation of some elements is missing, the English version, provided in the resource files, will remain and be used by the application, by default.

In the case of an update of the source of previously translated elements, in a Definition Provider, the resource files will be regenerated and made available by the IUCLID developers. The elements that have been updated in the Definition Provider will be in their English version and made available by the IMG for a translation if needed.

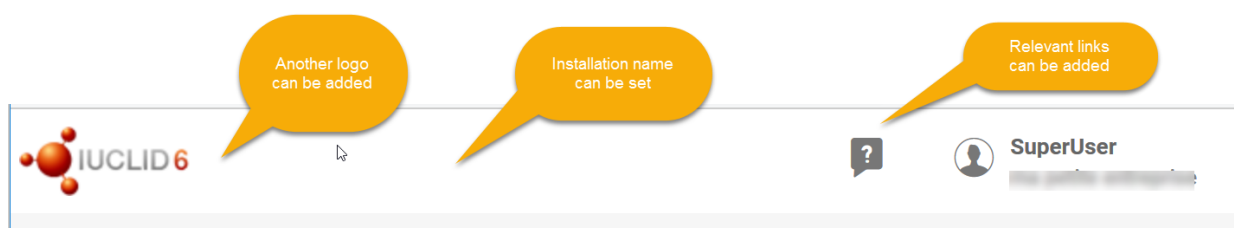
The IUCLID user manual is currently available in all EU languages through the IUCLID interface, and the Help Topic Windows are provided only in English.

4.7. Web interface

Since the introduction of the web interface in IUCLID version 6.3, some customisable elements are also available at this level.

The first customisation element is the top bar of the user interface. By configuring an IUCLID installation, the system administrator can control the following elements: the installation name, the installation logo and a list of links relevant to the specific installation.

Figure 4.12. Customisation of the top bar of the IUCLID web interface



The second customisation element is the configuration of users that can login automatically, using a specific user account, by accessing a customised URL. This can be useful when providing a public access to an IUCLID installation.

Note

¹ The website of the European Chemicals Agency on documentation regarding IUCLID 6 [<https://iuclid6.echa.europa.eu/documentation>]

Chapter 5. System to system integration

5.1. Integrating with IUCLID using the IUCLID Public API

IUCLID can be used in connection with other tools. This can be achieved by different means:

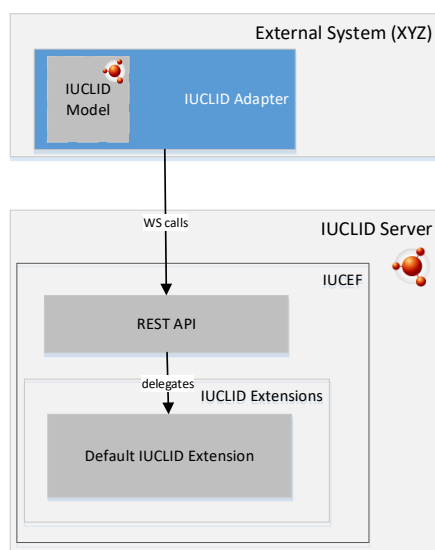
- exchange of data in an agreed format (e.g. the i6z IUCLID files)
- extraction at the database level
- use of the IUCLID REST Public API.

The IUCLID public REST Web Services API (IUCLID 6 Public REST API), the recommended approach, allows integration to external systems.

Integration of IUCLID with other systems allows automation of data processing, data entry or data exchange, as well as use of data stored in IUCLID to perform specific operations in another system. For example, the Chesar tool (see section 5.4.2.1.) uses some key chemical properties to calculate the fate of the substance in the environment and then sends the calculation back to IUCILD to be stored in the relevant use and exposure IUCLID documents.

The IUCLID Public API exposes as web services the most common functionalities on the user interface: searching, document handling, importing and exporting, sharing entities, executing the Validation Assistant. It also exposes utility operations to retrieve information about the available Definition Providers, the available Submission Types and Tables of Content, the IUCLID document definitions, and phrase groups and phrases.

Figure 5.1. Public API



The prerequisite for use of the Public API is familiarity with the IUCLID data model, for example, how the information is organised in IUCLID, and with the REST API syntax.

This API is maintained, and backward compatibility ensured.

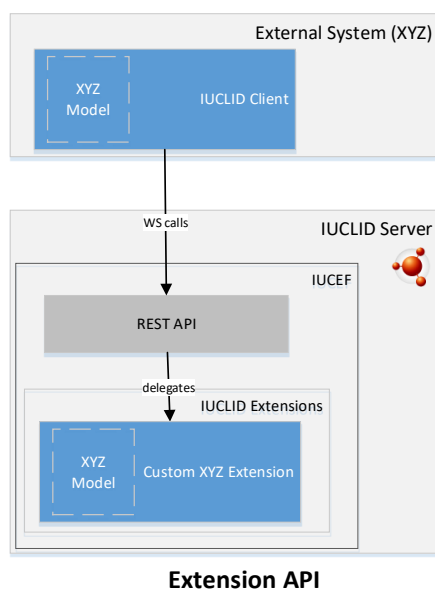
Documentation of the IUCLID 6 REST Public API can be found at <https://iuclid6.echa.europa.eu/public-api>

5.2. Integrating with IUCLID using the IUCLID Extension Framework (IUCEF)

The IUCLID Extension Framework (IUCEF) is a component of IUCLID which further facilitates the integration of external systems with IUCLID. It enables the deployment of “IUCEF” extension modules that extend or customise the default URL resources and operations provided by the IUCLID API.

IUCEF provides the possibility to register custom extension modules that enable the:

- registration of custom queries
- conversion of IUCLID dossiers, entities and documents to custom (own) data structure, back and forth
- registration of custom HTML or DocBook report templates for printing,
- implementation of custom pre-import checks
- registration of import/export configurations
- conversion of job execution reports to custom format.

Figure 5.2. Extension API

The prerequisite for use of the IUCEF, in addition to the prerequisite for the Public API, is familiarity with the IUCLID extension Java API (IUCEF) in order to build a custom extension module to be deployed with an IUCLID installation.

5.3. Differences between the Public API and the extension API

The IUCLID Public API supports document-oriented operations, which means that a single web service call can retrieve data from a single document, and a single call can write data to a single document.

In comparison, with the extension API, the scope of operations can be customised, which means that a single web service call can retrieve data from multiple documents and write data to multiple documents belonging to the same dataset.

The drawback with the extension API is that it requires slightly longer development as the developer has to prepare a custom extension module in IUCLID and a client module in the integrated system. However, it has the advantage of having the flexibility to use a custom syntax during the data exchange.

The development is faster using the IUCLID Public API. Only an adapter needs to be deployed on the integrated system. However, the syntax is restricted to use the IUCLID data model.

5.4. Examples of tools integrating with IUCLID

The tools presented in the following sections offer a certain level of IUCLID system to system integration.

5.4.1. Tools in the OECD ecosystem

Since the publication of the first OHTs, OECD has focused the development and promotion of IT tools around these formats to address in a systematic way the whole range of needs regarding the regulation of chemicals. eChemPortal and the QSAR Toolbox are part of this OECD ecosystem of tools.

5.4.1.1. eChemPortal - The Global Portal to Information on Chemical Substances (via the IUCLID Provider Agent)

eChemPortal, the Global Portal to Information on Chemical Substances, is a web application that facilitates access to information on chemicals to support health and environment decisions concerning chemicals.

Users can search by substance identity, classification, or property and effects criteria on data from multiple data sources. Search results give direct web links to information submitted to government chemical programmes at national, regional, and international levels. The information is focused on hazard and risk assessments, chemical property datasets, classification results, and exposure and use of existing and new industrial chemicals, pesticides, and biocides.

To allow searches by property and effects criteria, data are submitted by data sources in OHT compatible formats. Data sources storing summaries of the results of chemical tests in the OHTs formats, such as IUCLID, can more easily submit data and be linked to from the eChemPortal. An IUCLID provider agent web application is available to this end. The IUCLID Provider Agent has been designed in order to extract relevant data from IUCLID and create and post XML files with the data in the eChemPortal format.

Information on eChemPortal can be found at <http://www.oecd.org/ehs/eChemPortal>.

For more information on the IUCLID Provider Agent for the eChemPortal, contact the IUCLID Management Group.

5.4.1.2. Hazard assessment - QSAR Toolbox

The QSAR Toolbox is a software application which contains a wide collection of scientific information, data and models, as well as scientific procedures that together allow users to predict the properties of a chemical based on the experimental evidence available for similar chemicals. It facilitates the practical application of grouping of chemicals and read-across approaches for data gap filling and serves as a platform that incorporates various modules and databases from other sources, including IUCLID.

Data can be imported from IUCLID to a newly created database in the QSAR Toolbox via a direct transfer using Web Services. The import of study results from any type of chemical into the QSAR Toolbox increases the possibilities for read-across, category building and (Q)SAR model building. As well, predicted endpoint data can be exported from the QSAR Toolbox and assigned to a substance in IUCLID by directly connecting to an IUCLID server (via Web Services).

Information on the QSAR Toolbox can be found at <http://www.oecd.org/env/hazard/qsar>.

5.4.2. Tools in other ecosystems

5.4.2.1. Chemical safety assessment and review - ECHA - Chesar

Chesar (CHEmical Safety Assessment and Reporting tool) is an application that helps companies carry out their chemical safety assessments and prepare their chemical safety reports and exposure scenarios for communication in the supply chain.

Chesar enables registrants to carry out their safety assessments in a structured, harmonised, transparent and efficient way. This includes the importing of substance-related data directly from IUCLID, describing the uses of the substance, carrying out exposure assessment including identifying conditions of safe use, related exposure estimates and demonstrating control of risks. Based on this, Chesar automatically generates the chemical safety report and exposure scenarios for communication as a text document, and export information on use and exposure to IUCLID. Chesar also facilitates the re-use (or update) of assessment elements generated in a single Chesar instance or imported from external sources.

Further information on Chesar is available on the following website: <https://chesar.echa.europa.eu/>

5.4.2.2. Chemical safety assessment and review - ECHA - Odyssey

Odyssey is an application intended for internal ECHA use. Odyssey is built with the purpose of performing as an expert system supporting dossier evaluation and inquiry dossier assessment by providing efficient instructions, consistency and reporting tools for the assessment tasks carried out by the scientific officers. As a rule-based decision support application, Odyssey enables the standardisation and traceability of the scientific decision making within the dossier evaluation and inquiry processes.

5.4.2.3. Submission system - ECHA - REACH-IT

REACH-IT is the central IT system delivered as a web portal that supports Industry, European Union Member State competent authorities and ECHA to securely submit

process and manage data and dossiers. Member States competent authorities, ECHA and Industry actors have access to specific functions of REACH-IT to fulfil their requirements under the REACH and CLP regulations. REACH-IT also provides a secure communication channel between these three parties to help them coordinate the processing and evaluation of data and dossiers.

Further information on REACH-IT is available on the following website:
<https://echa.europa.eu/support/dossier-submission-tools/reach-it>

Chapter 6. User stories about customisation

6.1. ECHA

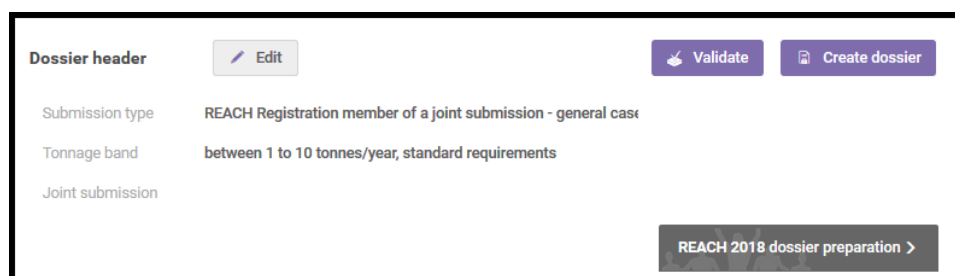
6.1.1. Alternative user interfaces

In addition to the IUCLID standard user interface (UI), ECHA is progressively developing an IUCLID web interface. In the first phase of this development, ECHA customised several elements of the web interface. These are good examples of how alternative user interfaces can be built on top of an IUCLID database and server to help users enter data and fulfil information requirements under different regulatory contexts.

6.1.1.1. Dossier header editing and storage

In the standard UI, when running the Validation Assistant or creating a dossier, the user is asked for certain information to identify the regulatory context for which he is entering data, for example on the Submission Type or the tonnage band. With the web user interface, this process was streamlined by collecting and storing this information in a “Dossier header” at the top of the substance dataset so users do not have to repeatedly enter the same information when re-running the Validation Assistant or creating a dossier.

Figure 6.1. Dossier header view in the web user interface



Source: IUCLID Cloud v6.2

6.1.1.2. Validation Assistant – sticky message

In the web user interface, the Validation Assistant message was made more usable and prominent by showing the validation message when the user goes to the document which needs to be corrected. This was a purely web user interface customisation by using the web browser to store the validation message when going into a document from the validation report.

Figure 6.2. Validation Assistant report and sticky message

Validation report containing all validation messages

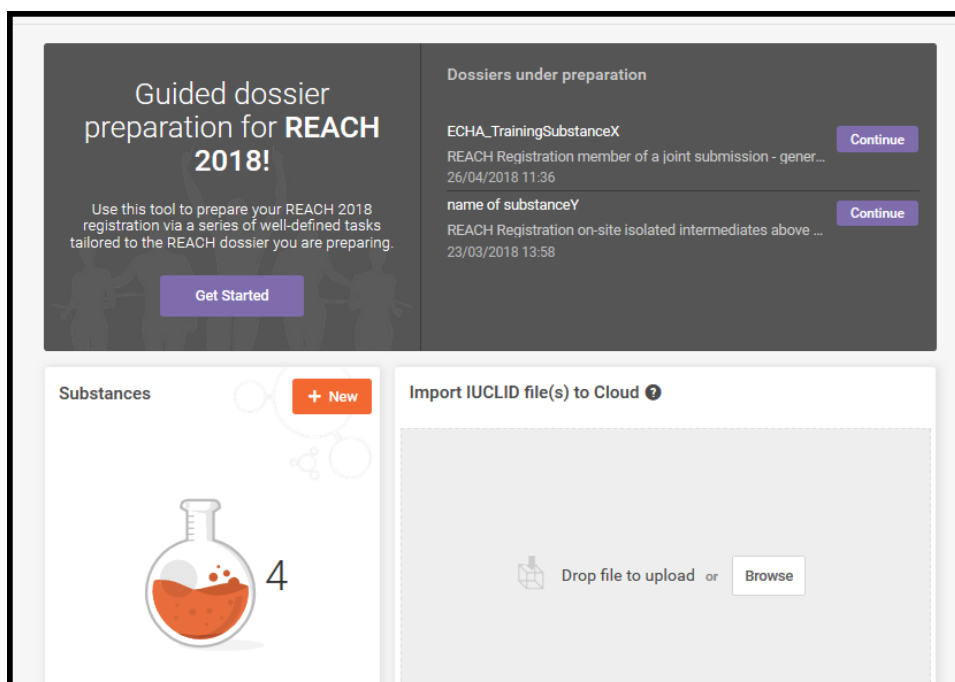
Sticky validation message inside document

Document: Manufacture

Source: IUCLID Cloud v6.2

6.1.1.3. Guided dossier approach

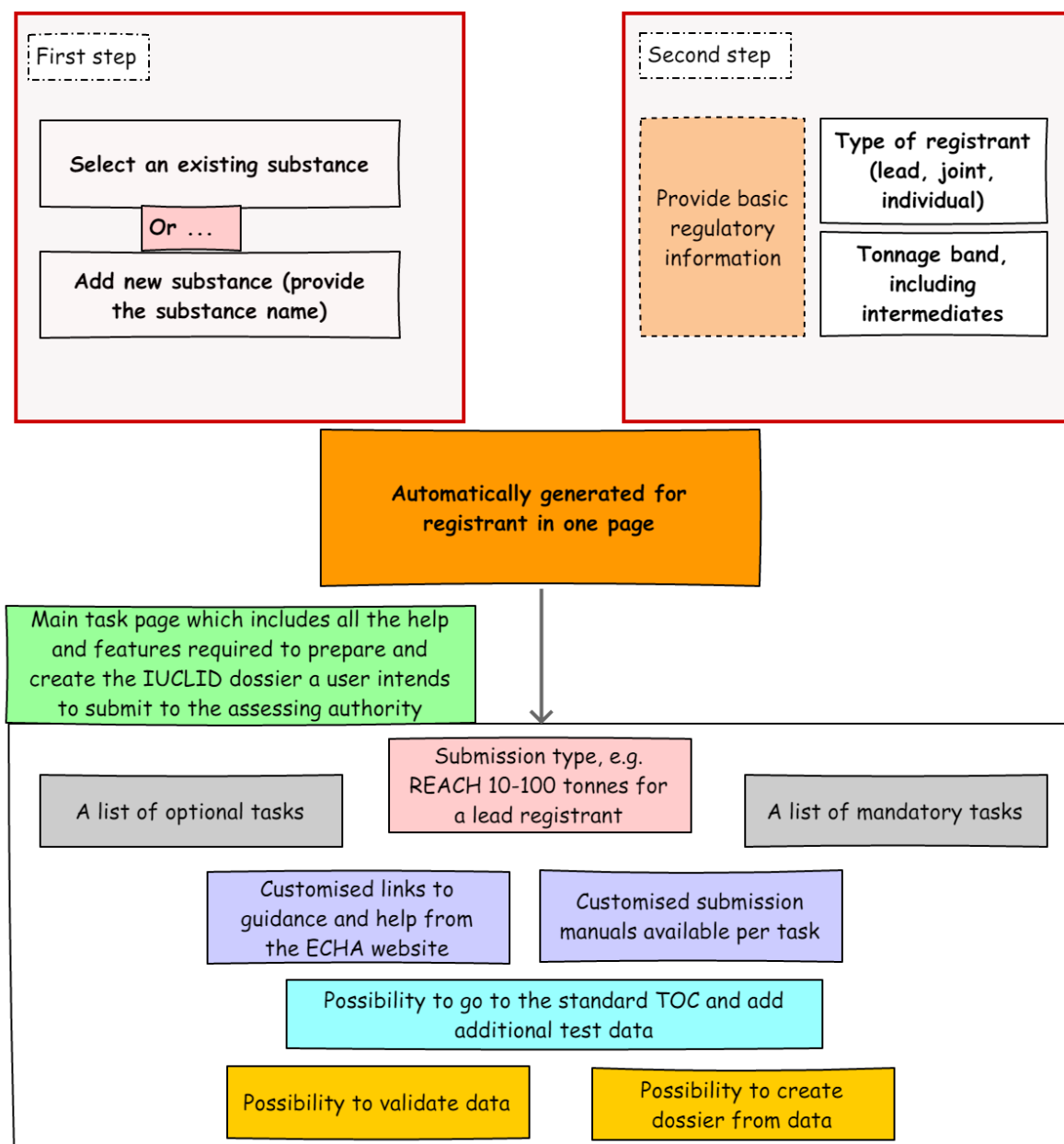
A task-based tool, “Guided Dossier Preparation Tool”, implemented in the web user interface, helps infrequent users of IUCLID complete information requirements in a dossier. This UI customisation introduced a dashboard widget as an entry point into the tool and a UI customisation to display the tasks that users should complete to prepare, validate and create a dossier.

Figure 6.3. Dashboard widget for the Guided Dossier Preparation Tool

Source: IUCLID Cloud v6.2

When starting the Guided Dossier Preparation Tool, users are first presented with a two-step wizard to collect the necessary information concerning a user's regulatory-situation, the purpose of which is to automatically generate a main task page which they use to prepare their dossier. The wizard flow and the contents of the main task page are illustrated in the diagram below.

Figure 6.4. Two-step wizard and the contents of the main task page

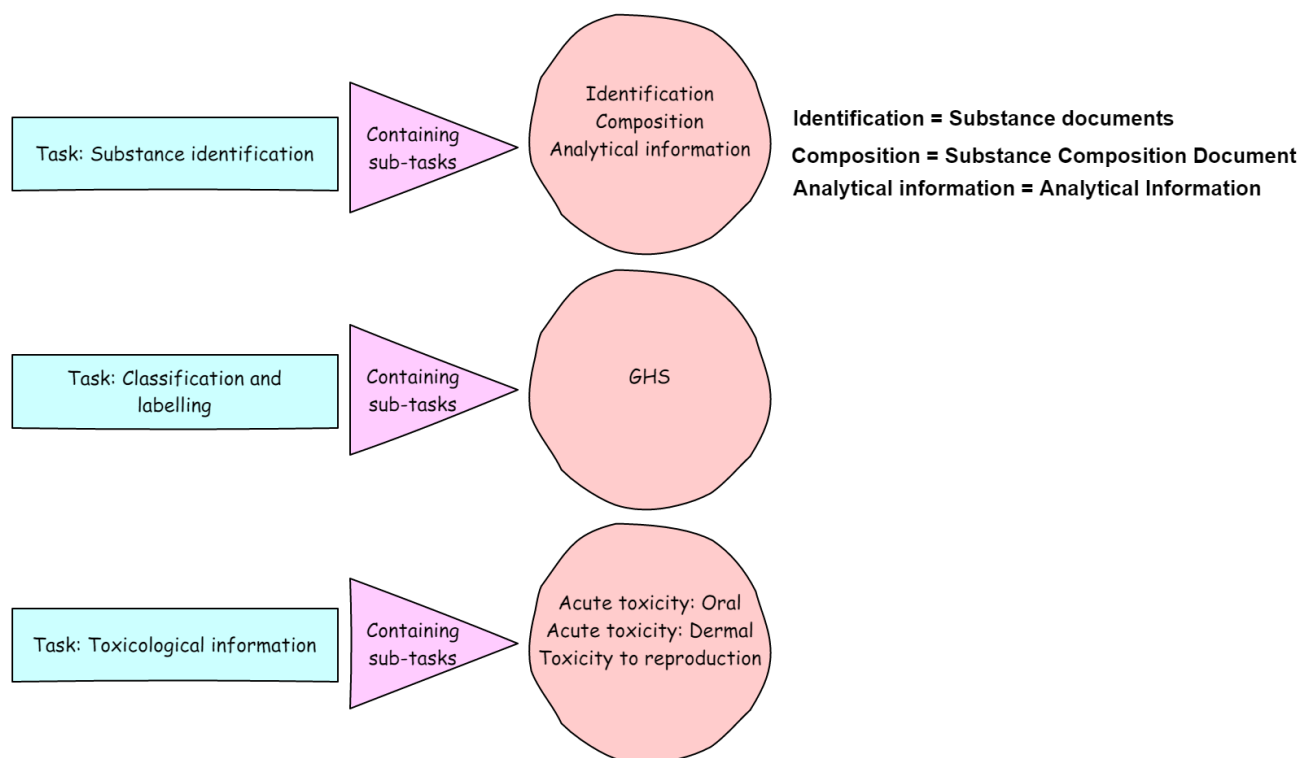


As shown above, the tasks that a user should complete are split between mandatory and optional tasks so that the user understands what information must be provided, and what information is conditional. This split in the mandatory and optional tasks is based on the Submission Type which is automatically generated for the user. How the Submission type is defined was calculated in a separate regulatory-analysis exercise by ECHA.

Each task is named and organised by the type of data expected to be entered for that task. Then, within each task, for example “Toxicological information”, there are a series of sub-

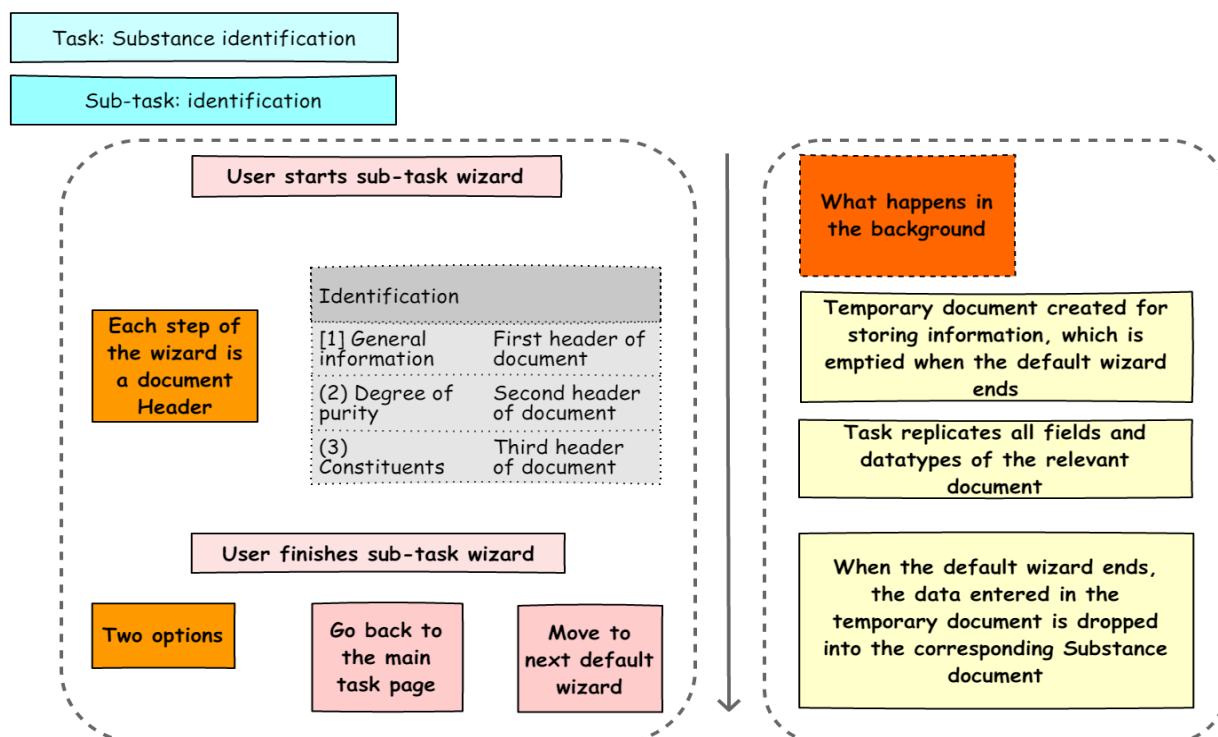
tasks to complete in order to complete the main task. Each sub-task maps directly to one IUCLID document. The task and sub-task structure used is outlined below:

Figure 6.5. Organisation of the tasks in the Guided Dossier Preparation Tool



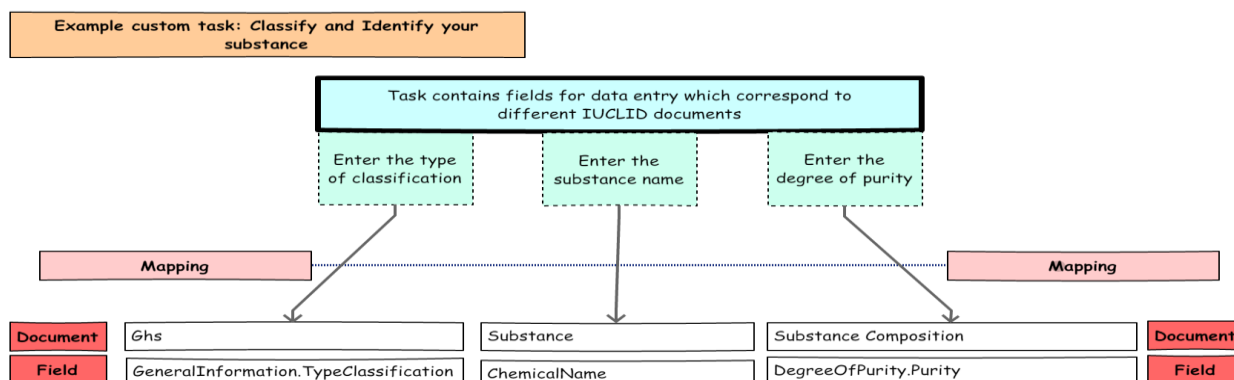
Each sub-task is a wizard-style approach to data entry with each wizard step corresponding to a header of a main section (a “level 1” header) of the IUCLID document on which the sub-task is based. The following diagram illustrates what users see and what happens in the background when a sub-task wizard begins, using the example of the task “Substance identification” and the sub-task “Identification”.

Figure 6.6. How the sub-task works for the user and what happens in the background



As indicated in the diagram above, the information entered in a sub-task is stored in an additional layer between the IUCLID client and the IUCLID database and, when the sub-task is finished, is then sent to and stored in the relevant document in the IUCLID database. This approach to capturing IUCLID data in a temporary task and mapping this data to a relevant IUCLID document, allows for more intelligent customisation in the task. The data entered in a task could have its own data structure and be mapped across different IUCLID documents. For example, a single task could be created which captures substance identification, classification and compositional information, and this data then mapped to the relevant IUCLID documents, as illustrated in the following diagram.

Figure 6.7. Customised tasks example



When the tasks have been completed, the Guided Dossier Preparation Tool allows the user to launch the Validation Assistant (to check data consistency, accuracy and quality) and to create a dossier (read-only snapshot) from the data that has been entered using the task-based approach.

6.1.2. Report Generator templates

ECHA has developed a number of report templates designed to extract IUCLID data and to generate a report to be used in various work processes. Three examples of report templates based on requests from authorities and industry are described below.

6.1.2.1. Example 1: Confidentiality Report (BPR Article 66) (in PDF/RTF/CSV formats)

The Confidentiality Report (BPR Article 66) extracts the confidentiality claims made by companies submitting IUCLID dossiers under the European Union's Biocidal Products Regulation. The report facilitates a regulatory obligation for ECHA and the European Union Member States to process and evaluate the confidentiality claims and follow up the evaluation, if needed, with individual registrants.

6.1.2.2. Example 2: Summary of Product Characteristics (in XML format)

The Summary of Product Characteristics report extracts mixture/product information from IUCLID and generates an XML file. This XML file is compatible with a separate system and is uploaded into this system to help an industry user prepare a Summary of Product Characteristics which is then attached to the IUCLID registration dossier.

6.1.2.3. Example 3: Classification and Labelling report (in RTF/PDF formats)

The Classification and Labelling report extracts information about the classification and labelling of a substance and generates a report which a lead registrant under REACH can circulate to co-registrants to inform them of the classification and labelling of the substance, and to initiate feedback on this classification from co-registrants.

6.2. Australia

6.2.1. Alternative user interface

Australia is developing the capability for importers or manufacturers (introducers) of industrial chemicals to create and submit an application for an assessment certificate (for industrial chemicals not already listed on Australia's Inventory) through a business services portal. Applications through the portal will include administrative information (including fee payments) and an interface for submitting chemical data in a format compatible with IUCLID. The user will enter chemical data into the online form (including the ability to upload documents) which will be converted into a dossier when the completed form is submitted to the regulatory authority.

The risk assessment of industrial chemicals in Australia is managed by the regulatory authority and not industry. The regulator will use the submitted dossiers to create the complete dataset for the assessment. Therefore, it is not a requirement for every available field in a particular document (e.g. flammability) to be completed by the user in the portal. The user interface will show the subset of fields that need to be completed.

Figure 6.8. Screenshot of web user interface data submission prototype

The screenshot displays a web user interface for data submission. At the top, there are three navigation tabs: Administration, Participants, and Chemical data. On the left, a document structure is visible, with 'Flash point.001' selected under the 'Physical and chemical properties' section. The main content area is titled 'Administrative data' and contains several form fields: Confidentiality (Please select), Justification (text input), Endpoint (Please select), and Type of information (Please select). Below this is the 'Data source' section, which includes a 'Reference' table with columns for Id and Name, and a 'Flash point' table with columns for Flash point and Atm. press. A callout box points to the 'Flash point' table with the text: 'Custom interface only shows fields applicant may need to complete.'

For each application type, the mandatory chemical data are prescribed through legislation (while any other data available to the applicant must also be provided); this determined the format of the Submission Type developed in ITEM.

As a consequence, each IUCLID document that is in the application Submission Type needed to be examined to determine the minimum sections/fields which are required for an application to proceed. In turn, this informed the rules that needed to be written for the Validation Assistant to enable the creation of a dossier.

To facilitate the certificate application Submission Type to be able to accommodate different application types and occasions where multiple parties are contributing information, a dossier header was created. The dossier header allows sets of validation rules to be applied that check broad data requirements (such as when toxicological data are not prescribed) or allow the various parties to an application provide their information while maintaining protection of confidential business information. This allows a user to

successfully submit data that would otherwise be required but are being provided by another party.

6.2.2. Design considerations

Australia has data requirements for industrial chemicals that are currently not covered by documents in IUCLID, for example, polymer characterisation data. To enable these data to be stored in IUCLID, a custom document was created in ITEM. The data are currently captured in forms in .doc format. However, as IUCLID stores structured data, a direct replication of the current forms was not an optimal approach. Multiple revision cycles were required to develop the data structure for the document that was fit for purpose. For example, early drafts of a block of fields for reactive functional groups initially comprised a single table covering all levels of concern (high, medium and low). However, it was more effective to separate these into individual tables due to the different regulatory treatment of chemicals with reactive functional groups in each level of concern (e.g. low concern groups do not required an FGEW calculation). This in turn affected other design decisions such as the content of picklists for particular fields.

Figure 6.9. Evolution of polymer characterisation block

Prototype – based on paper form

Reactive functional groups ^

Functional group	Level of concern	FGEW	Remarks
Carboxylic acid	Low	n/a	
epoxides	moderate	5800	End group analysis

+ Add... Edit... Delete Move up Move down

final

Reactive functional groups ^

Polymer contains only low concern reactive functional groups

Reactive functional groups - moderate concern ^

Reactive functional group

Functional group	Functional group equivalent weight (FGEW)	Remarks
epoxides	5800	calculated usi

+ Add... Edit... Delete Move up Move down

Reactive functional groups - high concern ^

Reactive functional group

Functional group	Functional group equivalent weight (FGEW)	Remarks

+ Add... Edit... Delete Move up Move down

Combined functional group equivalent weight ^

Combined functional group equivalent weight (FGEWcombined)

5800

Remarks

Reactive functional group only terminates one end of the polymer.

Chapter 7. Migration of legacy data

7.1. Australia

The introduction of industrial chemicals in Australia relies upon a chemical inventory to differentiate industrial chemicals that are new (requiring assessment, permits or exemptions) or existing (listed on the inventory). The Australian regulator currently uses an internal chemical register which contains the record of all chemicals and links them to business activities including assessments, permits and inventory processes. The register is built on an SQL Server database.

The development of new IT systems for reforms to the regulatory scheme requires data to be linked between the administrative/workflow systems and IUCLID which will be used as a chemical data repository.

The data model of the regulator's database is different to the IUCLID data model. The IUCLID logical model breaks down data based on "how" IUCLID organises them whereas, in the Australian system, it is broken down based on "what" those data are.

Chemical inventories can be imported with an IUCLID chemical inventory archive file. This file could not be generated from the current Australian IT system. Therefore, Altova® MissionKit® was purchased so that the Altova® MapForce® module could be used to map chemical data from the SQL Server databases into the required XML files. The XML files needed to follow the specific XML format as described by the IUCLID XML schema definition files (xsd files)¹.

In a new mapping design file, a "Database" component was connected to the chemical table in the SQL database. Then "XML Schema/File" components were connected to the inventory Schema files (inventory.xsd and manifest.xsd). A "Text File" component for holding the UUID value was generated by Altova® MapForce® function "create-guid". This value was used in the *.i6d file name. Each column from the source SQL table was mapped to the two XML components.

The *i6d* and *manifest.xml* files were automatically generated using Altova® MapForce® for each chemical in the register. They were then packaged into an *i6z* archive file. Over 42,000 chemicals were successfully imported into IUCLID as chemicals on the Australian inventory. A similar process was used to create Reference Substances for all the chemicals and import them into IUCLID. Reference substances were then linked to chemicals on either (or both) the EC inventory (installed by default in IUCLID) and the Australian inventory.

7.2. Canada

In 2013, Canada installed its first IUCLID instance. As part of the initial work, a project was initiated to migrate data from legacy databases into the new instance of IUCLID.

In total, over 86,000 records needed to be migrated from the legacy systems. Flat files (XLS format) were exported from the two legacy systems (an Oracle database and an Access database). A separate Microsoft Excel™ with SMILES data was also available. With the help of a consultant, a script was created to insert the data from the flat files into IUCLID. The biggest challenge was mapping data elements from the legacy systems to the IUCLID fields, as well as describing logic to create Reference Substances/Substances versus just updating existing IUCLID Reference Substances/Substances.

The mapping of data elements involved identifying data in the legacy systems and determining how it should map to IUCLID fields and also included the challenge that sometimes there was not always a "one to one" relationship. Further, as Canada migrated the data, it wanted to transform some of the data to create more standard entries in IUCLID. For example, previous system IDs were migrated into the "Other IT System Identifiers" field, and, the "Regulatory program" field "Other" option was used to add legislative specific chemical identifiers.

Regarding the challenge of "create vs update", this logic was followed: the order of insert/update was to first address the Reference Substance data, so that when Substance data was added, links to existing Reference Substances could be created. As such, the first step for the Reference Substances, so that duplicate records for the same chemical were not created, was to have the script first query IUCLID to determine if a Reference Substance already existed for data that was being migrated (by comparing CAS numbers). If a Reference Substance already existed in IUCLID, then some fields of the Reference Substance were simply updated using key migration data (e.g. adding a name, adding a SMILES). However, if the Reference Substance did not exist, then the Reference Substance was created and the data were migrated into the new Reference Substance. Once the Reference Substances were created or updated, Canada could then begin the migration of key Substance data by creating new Substance records and then linking them to the related Reference Substances.

Note

¹ The website of the European Chemicals Agency regarding the IUCLID format [<https://iuclid6.echa.europa.eu/et/format>]

Chapter 8. OECD activities and procedures related to IUCLID

8.1. Overview of the collaboration of the OECD IUCLID Users Group Expert Panel and ECHA

Several regulations in Europe state that the development of IUCLID is a way to support the regulatory processes in terms of collection and management of data on chemicals, and the European Union law stipulates the need to work in collaboration with the Organisation for Economic Co-operation and Development (OECD) to reach greater harmonisation of the data format¹. The European Chemicals Agency (ECHA), as the implementing body of the European Regulation on Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), Regulation on the classification, labelling and packaging of substances and mixtures (CLP Regulation) and the Biocidal Products Regulation, has the task to develop and maintain IUCLID and the underlying format in collaboration with the OECD.

This collaboration takes place in the OECD IUCLID User Group Expert Panel. The Expert Panel identifies worldwide business requirements for enhancement of IUCLID independent of the context, but giving priority to needs identified by users in regulatory settings. The Expert Panel discusses the relevance of any new OECD Harmonised Template Reporting Chemical Test Summaries (OHTs) for the IUCLID user community and recommends whether to implement it as part of the IUCLID format. It is also consulted for the prioritisation of changes to IUCLID, the impact of those changes, and at times testing of implemented changes prior to release, as well as collecting and setting priorities for user needs on related tools which support the use of IUCLID.

ECHA takes the recommendations of the Expert Panel into consideration and manages the actual implementation of changes to address the identified user needs. ECHA guarantees the maintenance of the application and plug-ins allowing the addition of specific features to the application enabling customisation (extension points), and manages a Helpdesk that can be contacted in case of issues in the standard use of the application. The IUCLID Management Group (IMG) at ECHA is responsible for this work.

8.2. Procedure of the OECD IUCLID Users Group Expert Panel

The OECD IUCLID Users Group Expert Panel is composed of members nominated by governments and stakeholders of the OECD Joint Meeting of the Chemicals Committee and Working Party on Chemicals, Pesticides and Biotechnology (Joint Meeting) and its subsidiary bodies. It is co-chaired by a representative of ECHA, on behalf of the European Commission, and a staff member of the OECD Secretariat. The work of the Expert Panel is carried out via web conferences and an annual meeting. Workshops or web conferences can be organised on specific projects involving the relevant parties. At a minimum, a report on these parallel activities takes place each year during the plenary session of the Expert Panel.

8.3. Procedure for developing/revising the OECD Harmonised Templates

Proposals to create new OHTs, or revise existing OHTs, come from different avenues:

- As most templates are built to cover the reporting needs of tests made according to the OECD Test Guidelines (TGs), the OHTs need to be adapted to updates of the existing TGs and new TGs that are issued every year.
- Proposals can come from other subsidiary bodies or expert groups to the OECD Joint Meeting to cover specific reporting needs not yet included in the OHTs or suggest necessary revisions.
- Proposals for improvements may be received from stakeholders who use systems based on the OHTs.
- Stakeholders may also see a need or opportunity to further harmonise data formats so that they are made applicable across different regulatory contexts. This harmonisation may be for existing OHTs or for templates that are not yet official OHTs.

The OECD Expert Group on the OECD Harmonised Templates (OHT Expert Group) supports the creation and revision of the OHTs. Experts are nominated by national authorities, industry and observer organisations interested in chemical test reporting issues and the interface between Test Guidelines and related databases. The drafts of new or revised templates undergo a thorough review process before their publication:

1. Pre-draft (new or revised) documents are usually developed in Word format by *ad hoc* experts (usually from national authorities) of the test guidelines and endpoint covered by the Template. The OECD Secretariat co-ordinates this development.
2. Draft documents are circulated for comments and suggestions under written procedure to the OHT Expert Group, as well as other OECD bodies such as the IUCLID Users Group Expert Panel, the Expert Group on the Electronic Exchange of Pesticides Data where relevant, and the authorities developing the OECD Test Guidelines.
3. Comments received are considered by the *ad hoc* experts and the OECD Secretariat for finalising the draft templates. Depending on the nature and the extent of the changes brought to the initial drafts, further round(s) of comments by the OHT Expert Group might be necessary.
4. Draft templates are then entered in the IUCLID Template Manager (ITEM) in order to produce the (final) draft technical package for the OHTs (Word format, XML Schema file, etc.) and allow to test their implementation and analyse their impact in IUCLID.
5. The (final) draft templates are submitted to the OECD Joint Meeting for comments and endorsement under written procedure.
6. The revised and new OHTs are published on the OECD Website.

8.4. Coordination of activities between the Expert Panel and ECHA to vet changes to the IUCLID formats

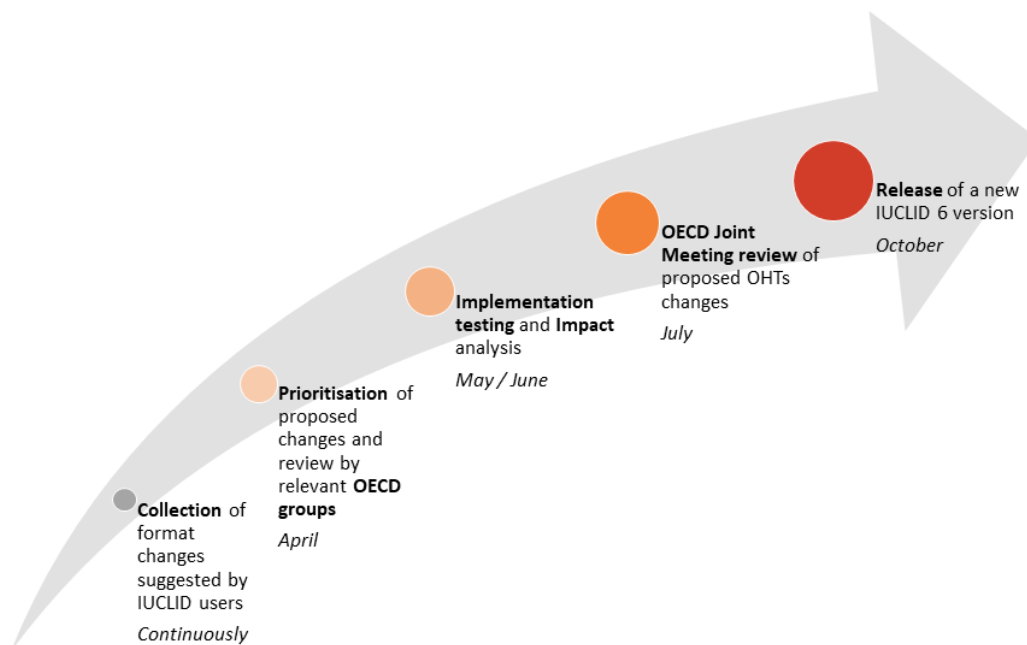
The updates of the OHTs and the associated changes to the underlying IUCLID format are synchronized, when possible, in a review and agreement cycle. The aim is to publish one set of updated and/or new OHTs per year and release one major version of IUCLID with updated formats per year. In addition to the OHTs, there may be other updates brought to

IUCLID such as adapting it to specific formats, like the Globally Harmonized System of Classification and Labelling of Chemicals².

The OECD Expert Panel takes part in this review cycle for major releases of IUCLID.

1. Information is continuously collected in a **requirements inventory** (*backlog*) from different sources including the Expert Panel, the OHT Expert Group, and the IUCLID Helpdesk.
2. A **prioritisation** is proposed by ECHA (changes to OHT are automatically prioritised) for a commenting period by the Expert Panel at the beginning of the year.
3. An updated list of changes is shared with the Expert Panel for **review and agreement**. The OHT Expert Group (and other relevant groups) are also consulted on the changes affecting the OHTs.
4. An **impact analysis** is performed based on feedback from the Expert Panel and other IUCLID users on integration points between the latest version of IUCLID and IUCLID modules (report templates, Derived No-Effect Levels [DNEL] tool) and for other applications integrated with IUCLID, documenting the following dependencies:
 - integration scenarios (why?)
 - dependencies to the IUCLID format (list of paths)
 - dependencies on IUCLID modules (IUCLID public Application Programming Interface (API), filtering, reporting, validation assistant)
 - dependencies on service interfaces (Java API and web services API).
5. The format changes are then **implemented** in the system for testing before release of the next version of IUCLID. Migration functionality between the previous format and the updated format (backward and forward migrations) are implemented at the same time as the format changes in order to facilitate testing.
6. When relevant, the (final) revised OHTs are submitted to the OECD Joint Meeting for comment and endorsement under written procedure, as necessary for substantial changes (not for small editorial improvements).
7. The release of the major version of IUCLID with format changes is targeted for the beginning of the fourth quarter of each year.

Figure 8.1. Targeted yearly schedule for IUCLID (IUCLID CORE, DOMAIN and OECD) format changes



Developments of formats for specific legislations can be released when needed as part of an IUCLID update, not necessarily the major release, since this will impact solely the users of the specific legislation and not all IUCLID users.

For authorities who have customised IUCLID for specific legislations, the timing of the first implementation is most important and needs to be planned carefully as it is usually driven by a legislative deadline. Later updates may be easier to align with the standard ECHA IUCLID cycle for major releases.

Notes

¹ e.g. article 111 of EU regulation (EC) 1907/2006 - REACH

² The website of the United Nations Economic Commission for Europe regarding the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) [http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html]

Annex A. Glossary

Block	A Block is specific to the IUCLID Template Manager (ITEM). It is designed to help re-use sets of fields in two or more documents.
Dataset	All the data are entered and stored in IUCLID in logical datasets containing <i>documents</i> and <i>entities</i> .
Definition Provider	The IUCLID format is separated in different groups of defined data formats depending on the source of the definition of the format. A group is expressed as a <i>Definition Provider</i> . The name of a Definition Provider often reflects the name of the source, an organisation (e.g. OECD), a legislation (e.g. EU_REACH), or an element which provides the definition of the format as well as the business processes for changing the format for which it is responsible..
Definition Provider Type	A <i>Definition Provider Type</i> indicates the level of harmonisation that a <i>Definition Provider</i> has reached. The management of the IUCLID format reflects this structure. At the time of publication of this document, there are three different levels of harmonisation represented by Definition Provider Types. The principal three Definition Provider types are the OECD, IUCLID CORE (CORE), and IUCLID DOMAIN (DOMAIN) in which agreement has been reached across regulatory jurisdictions and/or programmes as to what data are required under these definitions. The Regulatory-specific Definition Provider Type covers Definition Providers which reflect individual regulatory programmes such as the EU's REACH regulation.
Document (IUCLID document)	Documents are a collection and container of IUCLID fields for a specific type of information where data can be entered and stored inside the IUCLID database. Each field has a number of components. The primary component is the datatype, which governs what type of IUCLID fields it is. Based on the datatype, documents can re-use Entities, Text templates and Phrasegroups (and their Phrases). Documents can also directly re-use Blocks.
Endpoint study record	An Endpoint study record is a <i>document</i> (template) in IUCLID in which data is entered to describe a study, for example Melting point / freezing point.

Endpoint summary	An endpoint summary provides a <i>document</i> (template) in IUCLID in which information is entered about a grouping of endpoint study records.
Entity (IUCLID entity)	Entities are the re-usable/linkable elements of IUCLID, such as reference substances, legal entities, test materials etc. These entities, once entered in IUCLID, are stored in an inventory and can be re-used and linked to documents.
IUCLID format	The format is expressed in the general-purpose mark-up language XML, and XML Schema definition files (.xsd) for all IUCLID 6 entities and documents. In addition, the format is made available in a more readable version (.doc).
Phrasegroups	Phrasegroups are displayed as picklists in IUCLID and contain Phrases.
Phrases	Phrases are items which make up a picklist.
Submission types	Submission Types are defined in the IUCLID Template Manager (ITEM) to identify which IUCLID documents are relevant for a specific regulatory context or data collection process and are used to configure the Table of Contents (TOC) to be used by the data provider in order to easily identify the relevant information requirements.
Table of Contents (TOC)	A Table of Contents (TOC) is an IUCLID section tree which organises the information requirements, and provides entry points to the documents IUCLID users can create, edit, view, and export.
Text templates	Text templates are pre-defined texts which appear in IUCLID text fields to guide users on what information to enter and act like a guidance template.
<end of document>	

The IUCLID (International Uniform Chemical Information Database) can be customised to manage chemical data in different contexts and is a platform employing globally harmonised data elements pertinent to chemicals.

The version 6 of IUCLID software released in 2016 allows for greater customisation of IUCLID and for extension and integration with other tools. For example, the standard IUCLID data elements can be extended to capture specific information for specific legislative data needs before they are added to the OHTs.

This document describes four main elements related to the customisation of IUCLID including how the IUCLID format can be configured and customised, the main IUCLID features and add-ons, integration with other systems and development of alternative user interfaces.

The document also outlines how customisation of these different elements requires different expertise and resources. It incorporates user stories regarding customisation of and data migration to IUCLID from ECHA, Australia, and Canada.

oe.cd/iuclid

