Customisation Opportunities of IUCLID 6 for the Management of Chemical Data - 2nd edition

Series on Testing and Assessment

No. 297

OECD

BETTER POLICIES FOR BETTER LIVES

Series on Testing and Assessment
No. 297

Customisation opportunities of IUCLID for the Management of Chemical Data – 2nd edition

OECD

About the OECD

The Organisation for Economic Co-operation and Development (OECD) is an intergovernmental organisation in which representatives of 38 industrialised countries in North and South America, Europe and the Asia and Pacific region, as well as the European Commission, meet to co-ordinate and harmonise policies, discuss issues of mutual concern, and work together to respond to international problems. Most of the OECD's work is carried out by more than 200 specialised committees and working groups composed of member country delegates. Observers from several countries with special status at the OECD, and from interested international organisations, attend many of the OECD's workshops and other meetings. Committees and working groups are served by the OECD Secretariat, located in Paris, France, which is organised into directorates and divisions.

The Environment, Health and Safety Division publishes free-of-charge documents in twelve different series: **Testing and Assessment**; **Good Laboratory Practice and Compliance Monitoring**; **Pesticides**; **Biocides**; **Risk Management**; **Harmonisation of Regulatory Oversight in Biotechnology**; **Safety of Novel Foods and Feeds; Chemical Accidents; Pollutant Release and Transfer Registers; Emission Scenario Documents; Safety of Manufactured Nanomaterials;** and **Adverse Outcome Pathways.** More information about the Environment, Health and Safety Programme and EHS publications is available on the OECD's World Wide Web site (www.oecd.org/chemicalsafety/).

This publication was developed in the IOMC context. The contents do not necessarily reflect the views or stated policies of individual IOMC Participating Organizations.

The Inter-Organisation Programme for the Sound Management of Chemicals (IOMC) was established in 1995 following recommendations made by the 1992 UN Conference on Environment and Development to strengthen co-operation and increase international co-ordination in the field of chemical safety. The Participating Organisations are FAO, ILO, UNDP, UNEP, UNIDO, UNITAR, WHO, World Bank and OECD. The purpose of the IOMC is to promote co-ordination of the policies and activities pursued by the Participating Organisations, jointly or separately, to achieve the sound management of chemicals in relation to human health and the environment.

IOMC

INTER-ORGANIZATION PROGRAMME FOR THE SOUND MANAGEMENT OF CHEMICALS

A cooperative agreement among **FAO, ILO, UNDP, UNEP, UNIDO, UNITAR, WHO, World Bank and OECD**

Photo credit: Cover © Egorov Artem/Shutterstock.com

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[1] to develop and co-ordinate activities on chemical safety and biosafety on an international basis. The Chemicals and Biotechnology Committee manages this work[2]. 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 then OECD Joint Meeting of the Chemicals Committee and Working Party on Chemicals, Pesticides and Biotechnology (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 for a number of EU regulations and Directives, has the task to develop and maintain IUCLID and the underlying format in collaboration with the OECD.

After 2008, 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 the 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. This is the second version of the document.

This document is published under the responsibility of the Chemicals and Biotechnology Committee of the OECD.

Note

[1] The OECD Environment, Health and Safety Programme [www.oecd.org/chemicalsafety/]

[2] The mandate and name of the OECD Joint Meeting of the Chemicals Committee and Working Party on Chemicals, Pesticides and Biotechnology (Joint Meeting) was revised to become the OECD Chemicals and Biotechnology Committee (CBC). The change entered into force on 1 January 2021.

Modification history

Version	Date	Modification
1	February 2019	First version of this document.
2	June 2021	*1. Introduction* • Updated text and figure on interlinkage of tools developed to support chemical management in OECD countries *2. IUCLID (what comes with IUCLID by default)* • New information on the IUCLID *Working Context* and *Table of Contents*, replacing information on the *Guided Dossier Approach* *3. Management of the IUCLID format* • New Definition Providers: NZ and EU_PPP *4. Configuring IUCLID* • New table representing the scope of the maintenance and configuration possibilities of IUCLID • Updated information on reporting • New information on how multilingualism (data entry in multiple languages) works and is configured • Updated information on translation of the user interface (internationalisation) with an updated process graph *5. System to system integration and the migration of data to IUCLID* • Additional information on means to connect other tools with IUCLID • Addition of Text analytics and Data extractor as new examples of tools integrating with IUCLID *6. User stories about customisation* • New Matrix view of the use of IUCLID in OECD countries • Updated user story from ECHA regarding alternative user interfaces • Updated user story from Australia • New user story from New Zealand *7. Coordination of activities between the Expert Panel and ECHA to vet changes to the IUCLID formats* • Updated targeted yearly schedule for IUCLID (IUCLID CORE, DOMAIN and OECD) format changes • Updated schedule and text on coordination of activities for changes to the formats for specific legislations

Table of contents

Tables

Figures

Abbreviations and acronyms

API	Application Programming Interface
CLP	Classification, Labelling and Packaging
EC	European Commission
ECHA	European Chemicals Agency
FTL	FreeMarker Template Language
GHS	Globally Harmonized System of Classification and Labelling of Chemicals
IMG	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 worldwide 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 configuration and for extension and integration with other tools. For example, the standard 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, Canada, and New Zealand.

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:

- the IUCLID format
- IUCLID's features and add-ons
- the integration of other systems with IUCLID
- 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 complying with the reporting requirements of the OECD Test Guidelines, as well as other

national/international methods used for chemical studies. The OECD Test Guidelines[1] play a role in the system of mutual acceptance of chemical safety data among OECD countries[2] 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
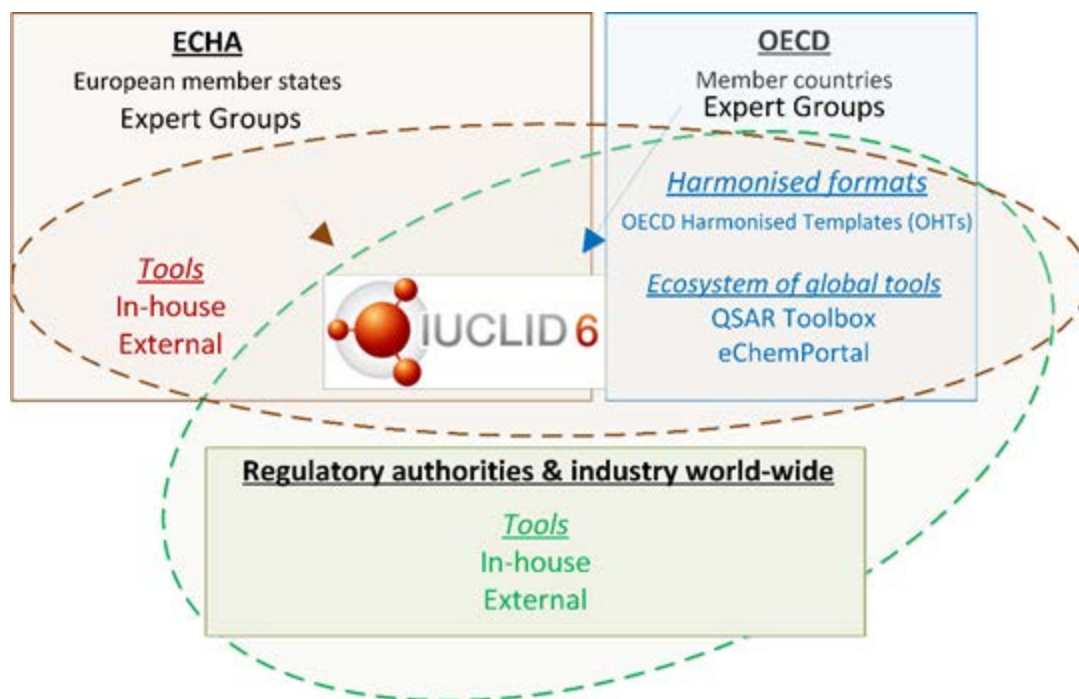
1.3. Strength of Global harmonisation

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. For example, IUCLID export files can be considered as a reference implementation of the OHT export format.

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, and eChemPortal (the Global Portal

to Information on Chemical Substances)[4]. 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
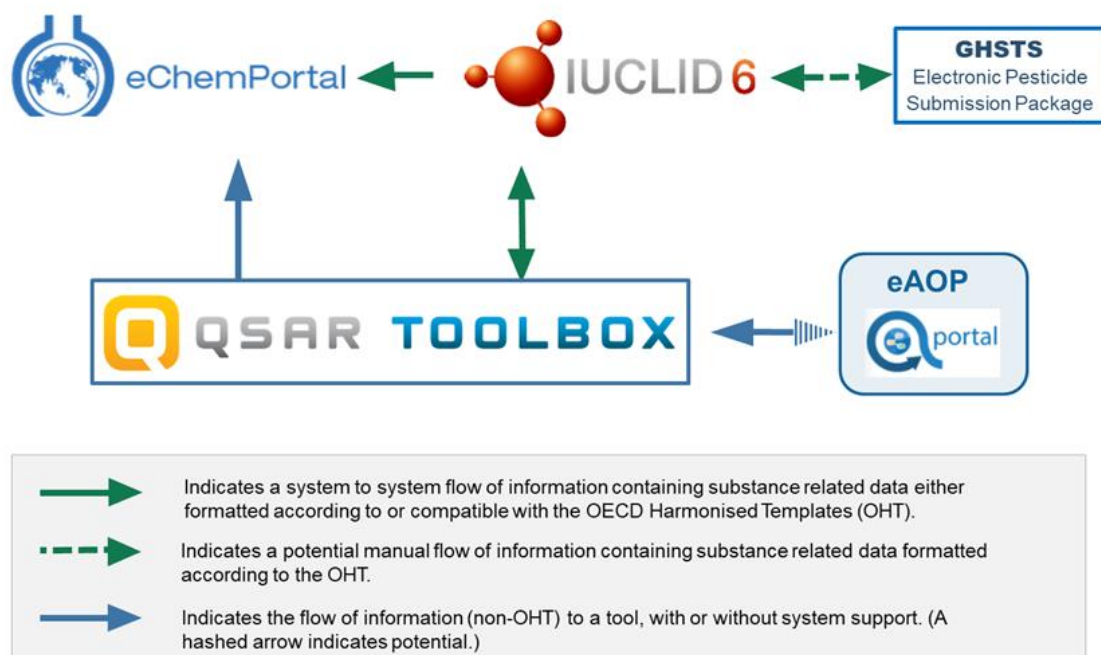
Notes

[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 web interface, available in 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 for the use of the IUCLID interface, independently of the context in which the tool is used, while questions on the use of IUCLID in a specific context are addressed by the relevant organisations: https://echa.europa.eu/contact

- maintenance service (bug fixes, improvements relevant for the whole user community, format update[1])

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

- Text analytics (see 5.5.2)

- Data Extractor (see 5.5.2)

- Report templates, (see 4.3)

- Provider Agent - submits data stored in IUCLID to the eChemPortal (see 5.5.1).

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 and are usually managed in inventories, for example *Substance* entity, *Legal Entity*, *Literature Reference* 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 or 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*, *Mixture / Products*, and *Template* entities. In addition, a *Category* entity describes and references categories of substances or mixtures, and an *Article* entity contains information about manufactured articles.

In the figure below, a substance is created and data relevant to this substance are entered in a series of linked documents and entities. The main chemical identifiers are stored in *Reference Substances* while the information on organisations or chemical companies are recorded in a *Legal Entity*.

Figure 2.1. Main IUCLID entities and relationships (substance)
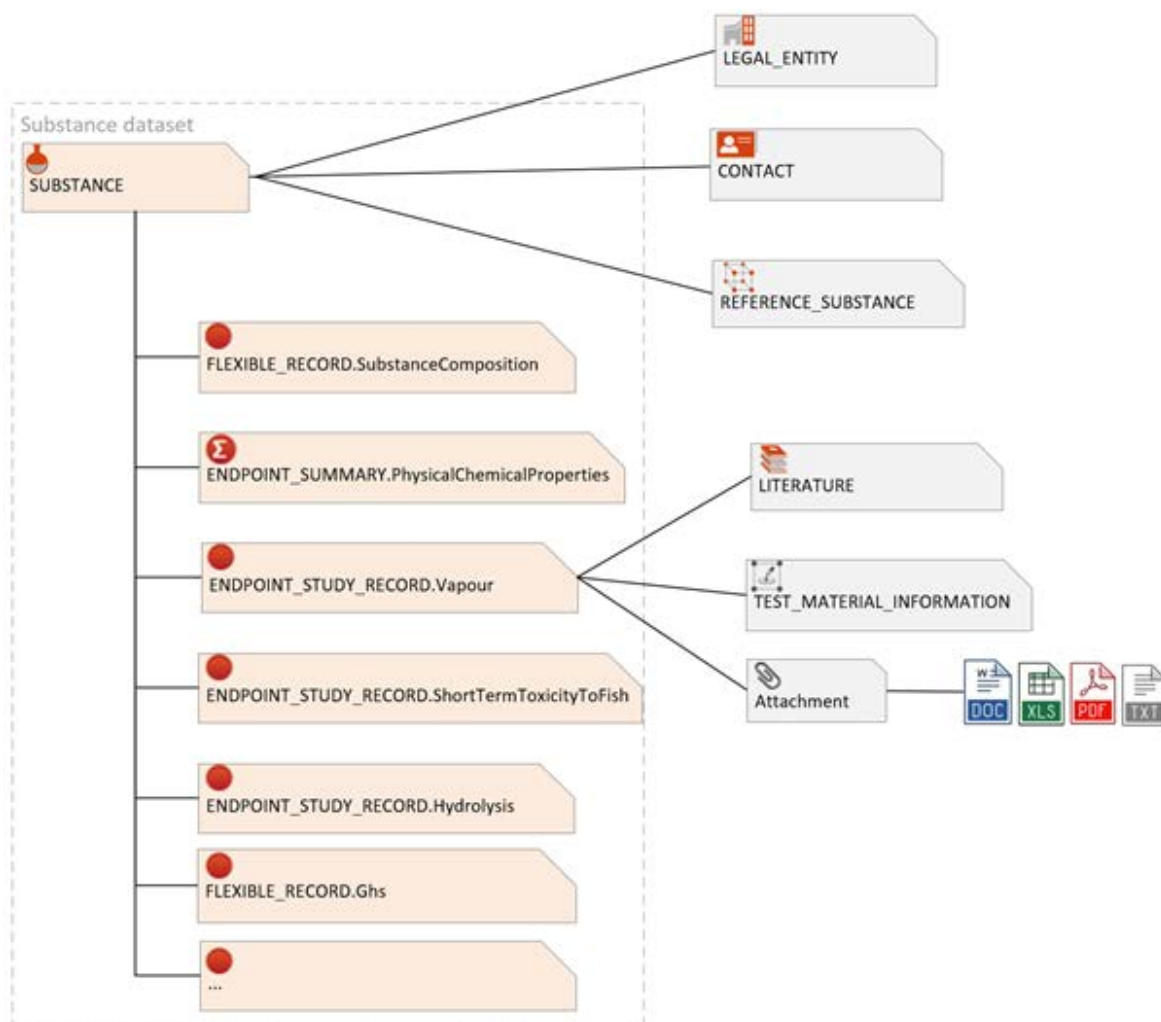
The following figure represents the data organisation for a *Mixture/Product*.

Figure 2.2. Example of the main IUCLID entities and relationships (for a main mixture/product and two components)
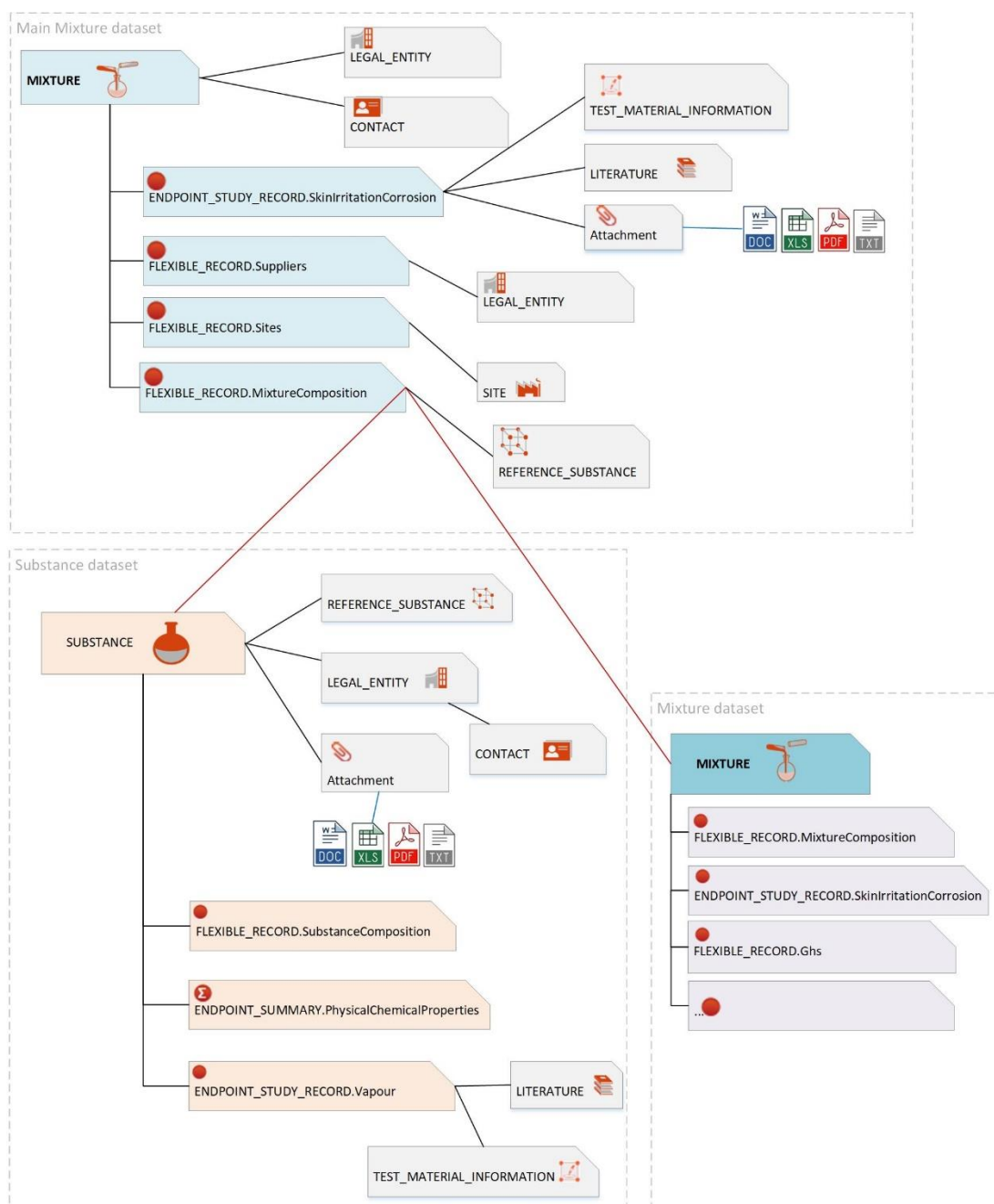
When all the necessary data relevant for a specific (regulatory) context are available, they can be packaged in a read-only *Dossier*.

A *Dossier* is a write-protected copy of the data stored in a *Substance*, a *Category*, a *Mixture/Product* or an *Article*. The *Dossier* concept is detailed in the next section of this document (see 2.3.4).

Figure 2.3. Organisation of the information in an IUCLID dossier
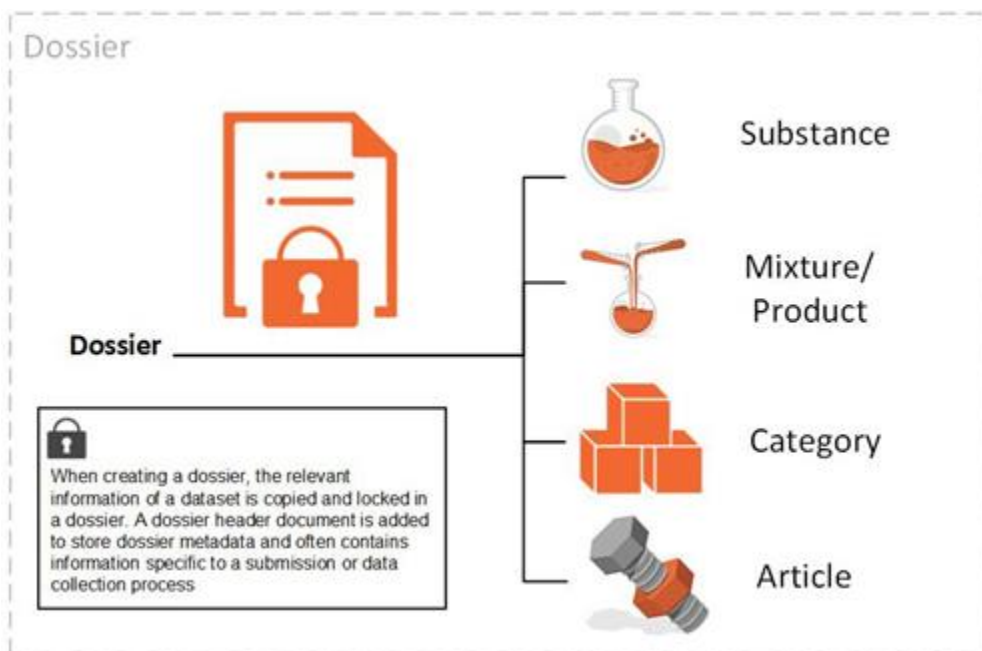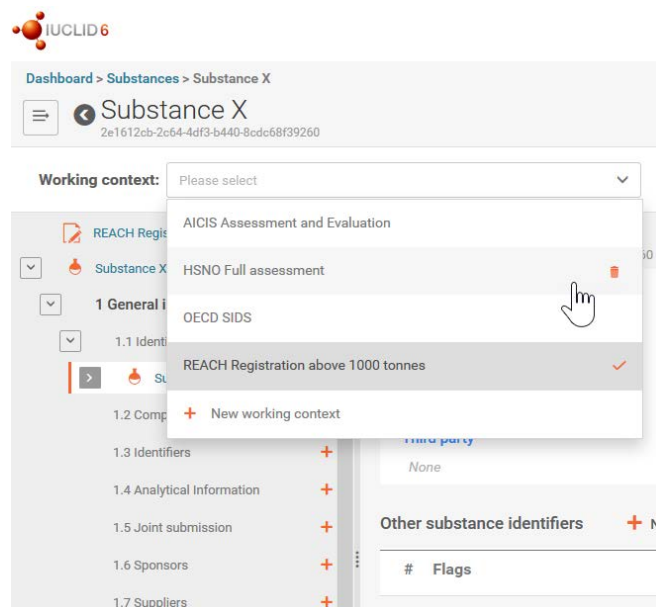

2.3. The IUCLID Working Context, Table of Contents and Dossiers

For each *Substance*, *Mixture/Product*, *Category* and *Article* entity, there are a number of pre-defined Working Contexts' (see section Chapter 3.) which provide IUCLID users with a visual context for the preparation and management of their data. The Working Contexts:

- associate a unique Table of Contents (TOC) to the Working Context. The Table of Contents lists the information requirements for that Working Context by organising a view of IUCLID data according to a specific regulatory programme or data collection process.
- provide a unique sub-Table of Contents per component of a main entity, in order to provide a complete view of the information requirements and to visualise all the data provided in Substance or Mixture datasets used as children of a main Substance or Mixture
- provide a unique dossier header for that Working Context (if a *Dossier* can be generated) which contains a relevant set of fields to be completed prior to the submission of data
- can also provide simplified views of documents and entities (so-called custom documents and entities) limited to regulatory-specific set of fields to complete.

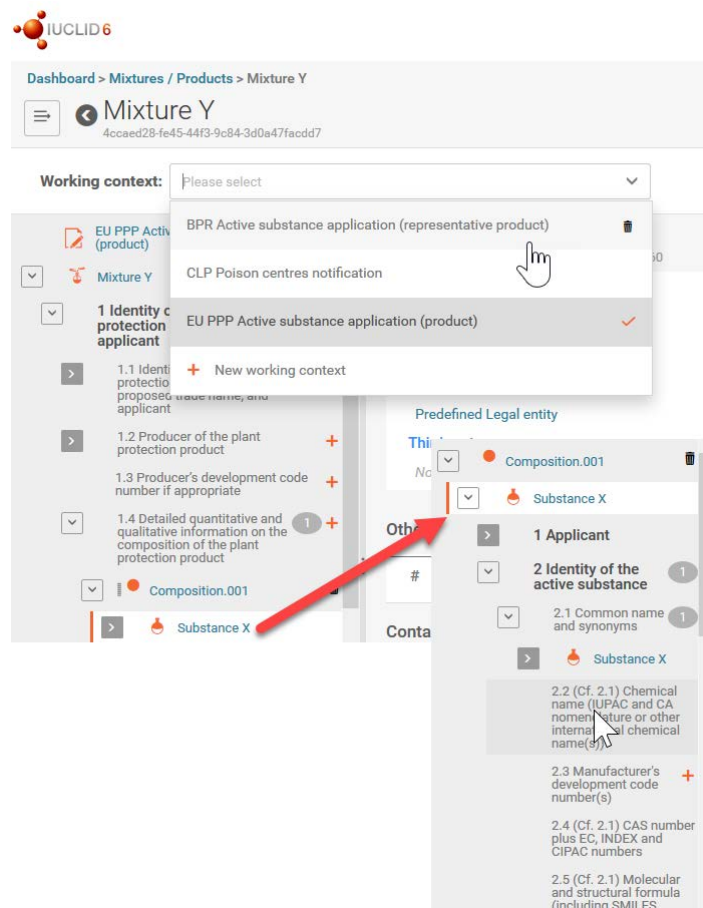### *2.3.1. Example of viewing a Substance-based Working Context and TOC*

Figure 2.4. Substance-based view of a working context

Source: Screenshots of IUCLID 6 5.1.2. build: 28/10/2020

2.3.2. Example of viewing a Mixture-based Working Context and TOC

Figure 2.5. Mixture-based view of a working context

Source: Screenshots of IUCLID 6 5.1.2. build: 28/10/2020

2.3.3. Complete table of contents

The user can choose to view a generic list of all the available structured information that is supported with 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 or data collection process and only focused on the type of information maintained in the system.

Figure 2.6. Pre-defined TOC: The "Complete table of contents" view

Source: Screenshot of IUCLID 6 4.14.1. build: 24/04/2020

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

Figure 2.7. Pre-defined TOC: View of all OHTs

Source: Screenshot of IUCLID 6 4.14.1. build: 24/04/2020

2.3.4. Dossiers

As mentioned, the Working Context not only provides IUCLID users with a way to display the relevant TOC but also, if relevant, to create IUCLID Dossiers containing this information.

The user may enter additional administrative data related to the dossier in the "dossier header" associated with the selected TOC. The following screenshot displays the steps of the IUCLID dossier creation in which the user has selected a Working Context and enters the additional information in the corresponding dossier header.
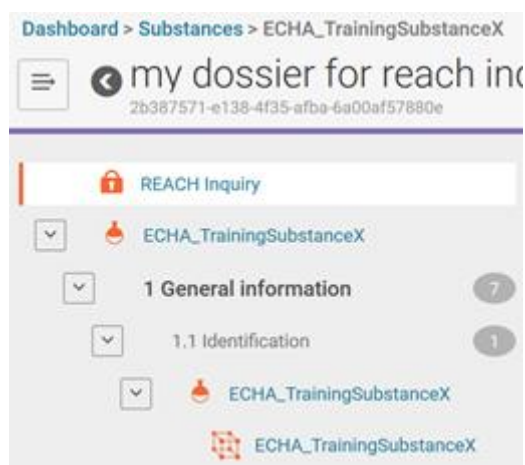
Figure 2.8. Steps of the IUCLID dossier creation
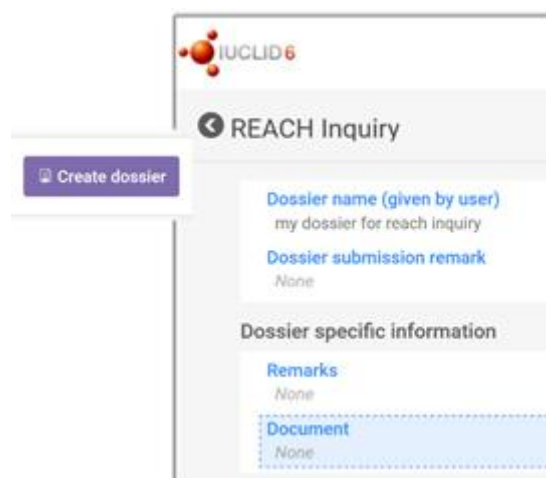
Source: Screenshots of IUCLID 6 4.14.1. build: 24/04/2020

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

Figure 2.9. REACH Inquiry notification dossier

Source: Screenshots of IUCLID 6 4.14.1. build: 24/04/2020

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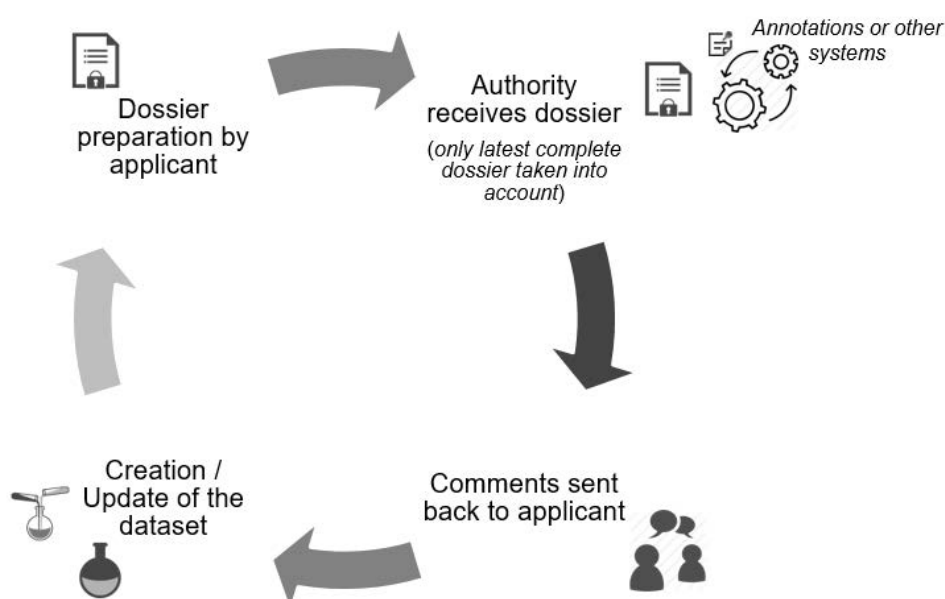
2. The collaborative approach: In the second approach, the regulatory organisation manages the data and combines different sources of information into its repository of chemicals information. The data provider can submit data that then are reviewed and added by the regulatory experts into a main chemical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

Figure 2.11. IUCLID data submission, the collaborative approach
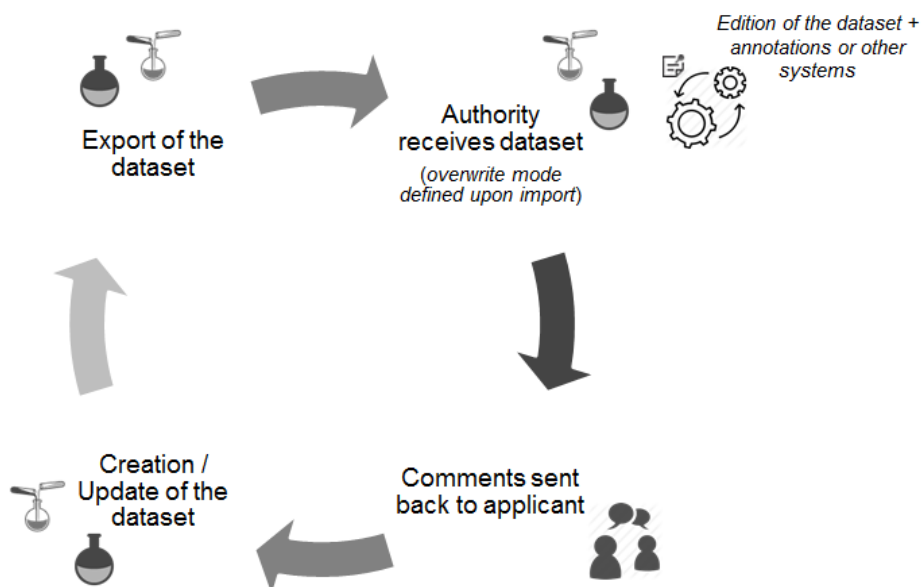
Note

[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 defined by a chief provider of its format, and as such is known as a *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. One of the key elements assigned to a definition provider is the IUCLID *document* where chemical data are entered, such as endpoint study records, the substance composition, etc.

3.1.1. Definition Providers

The main Definition Providers are the OECD, (IUCLID) Domain and (IUCLID) CORE, in which agreement has been reached across regulatory jurisdictions or programmes as to what data are required under these definitions. There are also additional definition providers of the IUCLID format, which reflect an individual regulatory programme such as the EU 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 cover 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/Product, Article, 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 a regulatory-specific Definition Provider.

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, including 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

- AU_IND_CHEM containing specific information for Australia's Industrial Chemicals Introduction Scheme

- NZ_HSNO containing specific information for the New Zealand Hazardous Substances and New Organisms programme

- EU_PPP containing specific information for the EU Plant Protection Products Regulation

- EU_SCIP containing specific information for the needs of the database that contains the information submitted on substances of concern in articles

Figure 3.1. Representation of the hierarchy between Definition Providers
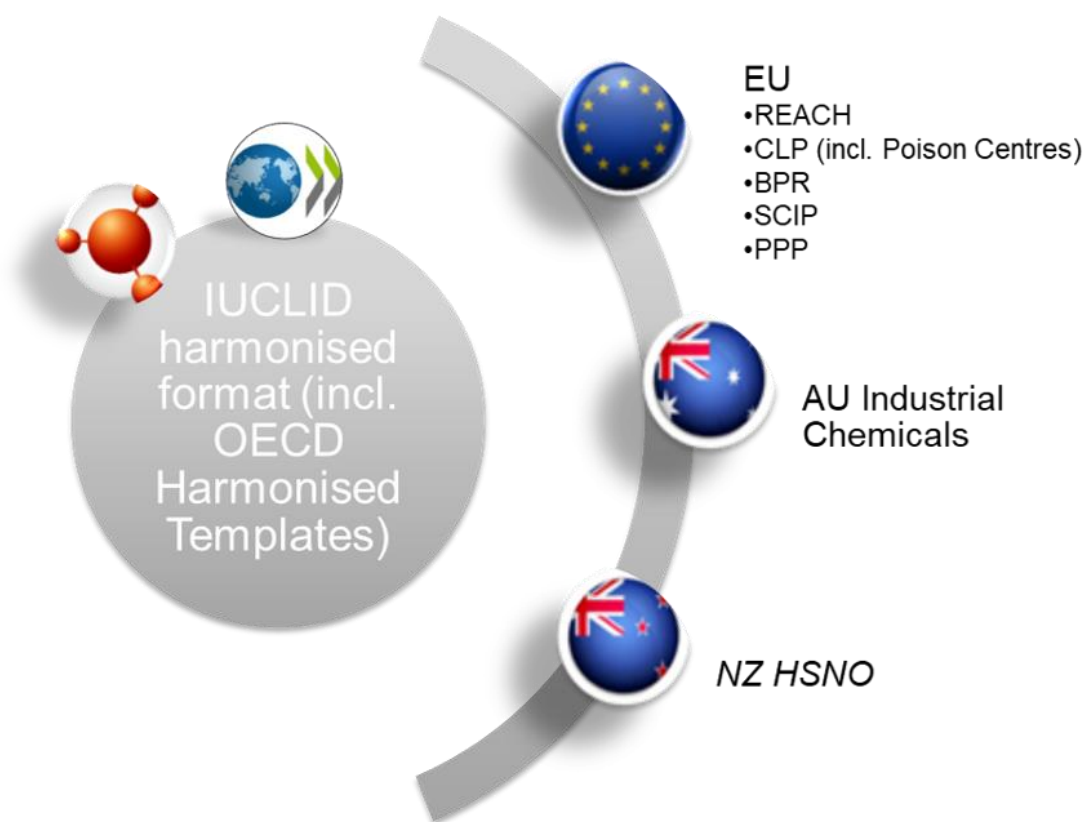
3.2. Building blocks of the IUCLID format

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.

Table of Contents (TOC): provides access to specific documents in an entity (Substance, Mixture, Article) for operations such as creating and editing documents. The TOC allows the format provider and owner to:

- display and organise IUCLID documents corresponding to a set of information requirements and is used as part of a Working Context. The TOC is organised as a hierarchy so that sections and their documents can be nested together, for example, Section 7 (document: Ecotoxicological Summary) / Section 7.1 (document: Biodegradation Summary) / Section 7.1.1 (document: Biodegradation products)

- define the section names as well as the name of the documents which are nested under the relevant sections

- indicate whether a document is mandatory or optional

- Indicate and define whether a customised view of a standard IUCLID document should be displayed to the user.

Working Contexts define a specific regulatory context or a specific data collection process. The Working Context has the following main functions:

- indicates which main entity is applicable in the Working Context, such as Substances, Mixtures, Articles or Categories

- defines which Table of Contents' (TOC) and sub-TOCs (for example of a Mixture component) are to be used

- indicates whether a dossier can be created, and which dossier header is applicable, in the Working Context

- indicates if a customised view of a standard entity, should be displayed to the user (See section 0).

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 etc., 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 6.5 included versions of the following definition providers: AU_IND_CHEM, CORE, DOMAIN, EU_BPR, EU_CLP, EU_PPP, EU_REACH, OECD, and NZ_HSNO.

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 between versions 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 (see 7.4). 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.
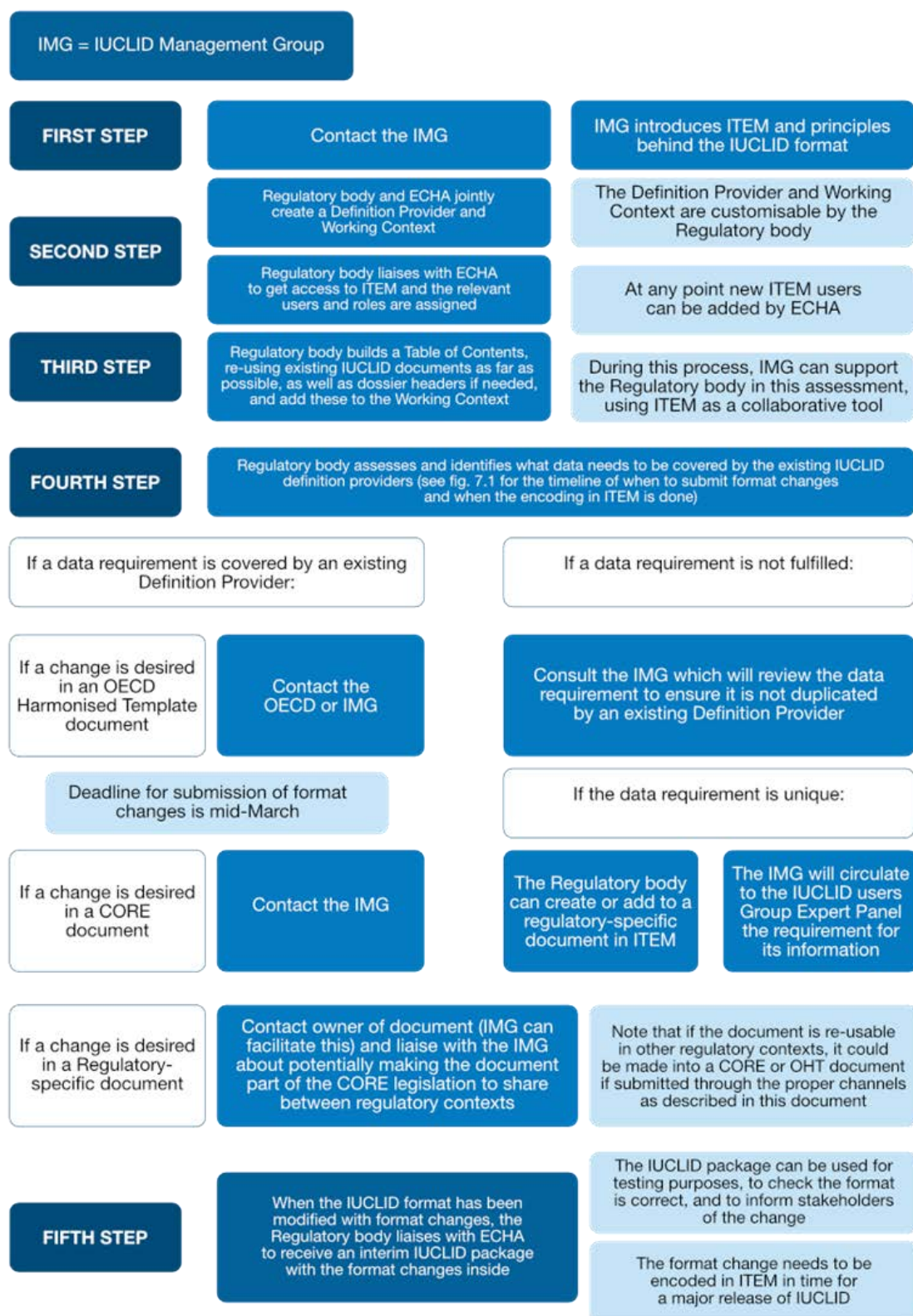
There are specific processes for changing the format according to the Definition Provider type. This is elaborated below.

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 6.3), 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, Working Context, and associated documents in the IUCLID format

IMG = IUCLID Management Group

FIRST STEP — Contact the IMG — IMG introduces ITEM and principles behind the IUCLID format

SECOND STEP
- Regulatory body and ECHA jointly create a Definition Provider and Working Context — The Definition Provider and Working Context are customisable by the Regulatory body
- Regulatory body liaises with ECHA to get access to ITEM and the relevant users and roles are assigned — At any point new ITEM users can be added by ECHA

THIRD STEP — Regulatory body builds a Table of Contents, re-using existing IUCLID documents as far as possible, as well as dossier headers if needed, and add these to the Working Context — During this process, IMG can support the Regulatory body in this assessment, using ITEM as a collaborative tool

FOURTH STEP — Regulatory body assesses and identifies what data needs to be covered by the existing IUCLID definition providers (see fig. 7.1 for the timeline of when to submit format changes and when the encoding in ITEM is done)

If a data requirement is covered by an existing Definition Provider: | If a data requirement is not fulfilled:

If a change is desired in an OECD Harmonised Template document — Contact the OECD or IMG | Consult the IMG which will review the data requirement to ensure it is not duplicated by an existing Definition Provider

Deadline for submission of format changes is mid-March | If the data requirement is unique:

If a change is desired in a CORE document — Contact the IMG | The Regulatory body can create or add to a regulatory-specific document in ITEM | The IMG will circulate to the IUCLID users Group Expert Panel the requirement for its information

If a change is desired in a Regulatory-specific document — Contact owner of document (IMG can facilitate this) and liaise with the IMG about potentially making the document part of the CORE legislation to share between regulatory contexts | Note that if the document is re-usable in other regulatory contexts, it could be made into a CORE or OHT document if submitted through the proper channels as described in this document

FIFTH STEP — When the IUCLID format has been modified with format changes, the Regulatory body liaises with ECHA to receive an interim IUCLID package with the format changes inside | The IUCLID package can be used for testing purposes, to check the format is correct, and to inform stakeholders of the change

The format change needs to be encoded in ITEM in time for a major release of IUCLID

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
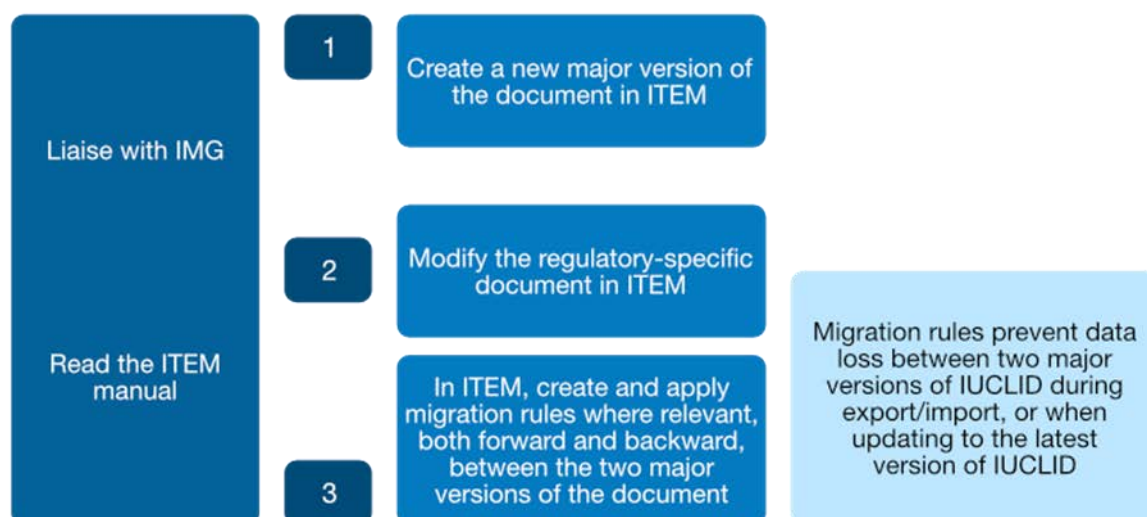
3.3.4. New IUCLID documents (OECD and IUCLID formats)

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 though 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
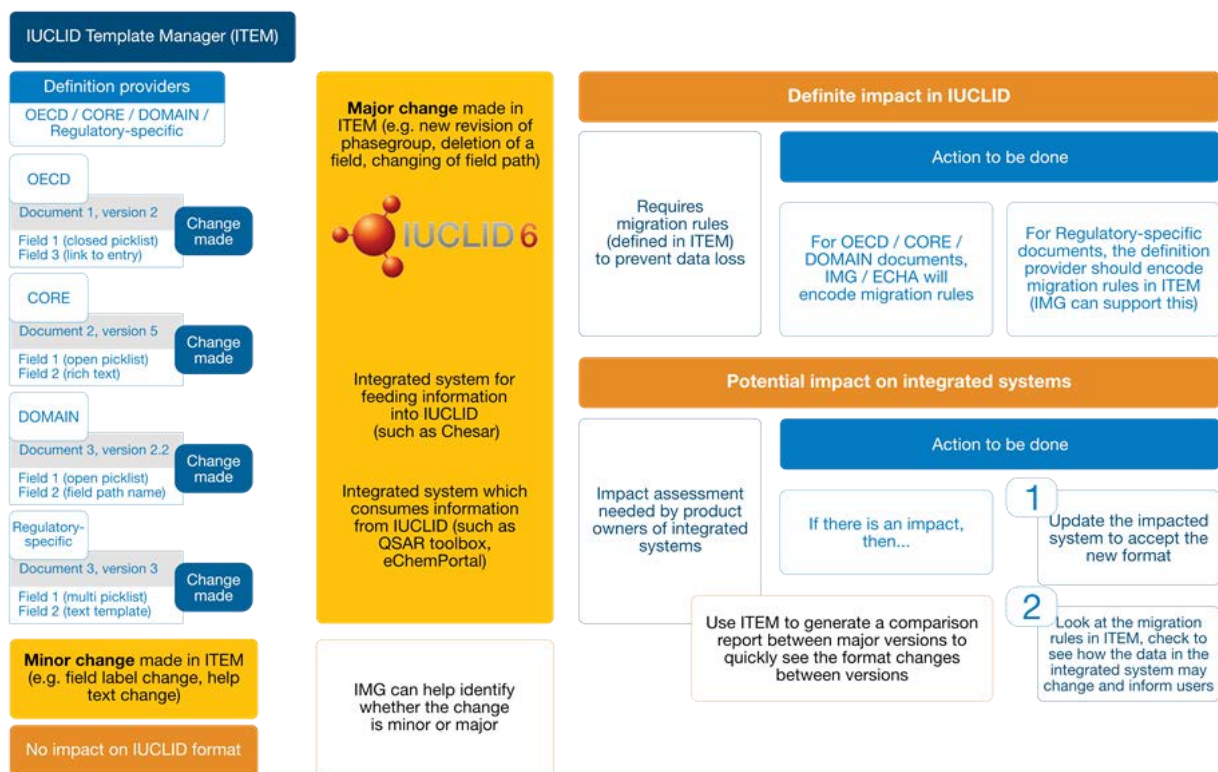
Chapter 4. Configuring IUCLID

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 configurable 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.

Working contexts can be created in order to indicate to data providers and assessors a regulatory context or data collection process which is specific to them. This entails a definition of regulatory or data collection process specific TOC views of substance and mixture datasets, an indication that a dossier can be created and the provision of dossier headers, as well as governance on whether a customised view of a document should be displayed.

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** and **multilingualism**.

The table below summarises what aspects of IUCLID are part of the **standard maintenance** of the application, secondly what can be **easily configured by users** and is supported by the application and processes during development and thirdly, what aspects largely reside **outside the scope of routine configuration** (although still possible but requiring special agreement with the IMG).

Table 4.1. Scope of IUCLID configuration

Scope of IUCLID Configuration	Additional information on the configuration	Standard maintenance by the IUCLID team	Configurable by users with IUCLID team support	Configuration options which require specific agreement
OECD/CORE/DOMAIN Formats				
Update to OECD / CORE / DOMAIN Definition Providers and related format		✓		
Implementation of the latest format in IUCLID for all Definition Providers		✓		
Migration rules for the OECD / CORE / DOMAIN formats		✓		
Update to the format for existing report templates		✓		
Update to the format for existing validation scenarios and rules		✓		
Field help text		✓		
Regulatory-specific Formats				
Own Definition provider (a regulation or data collection process owner)	Create a definition provider which contains the regulatory-specific Working Context format and table of contents.		✓	
	Compare versions of the Definition Provider using ITEM to track format changes		✓	
	Show and export (XML) migration rules underneath the Definition Provider using ITEM		✓	
	Export Help content using ITEM		✓	
	Export structure of the content underneath the Definition Provider (XML)		✓	
	Validate that the Definition Provider's content is consistent and without conflict in versions history		✓	
Own Working Context				
	Define the related entities which the Working Context will apply to		✓	
	Select the relevant dossier header which will be used when creating dossiers from the Working Context		✓	
	Select the sub-TOC(s) and related conditions to view a specific sub-TOC		✓	
	Select a custom document to be viewed for the entities view as part of the Working Context		✓	
Own Table of Contents				
	Order of sections and documents		✓	
	Name sections		✓	
	Name documents		✓	
	Define a section or document as mandatory or optional to complete		✓	
Data fields and documents				
	Create new section documents if not already provided by the OECD/CORE definition providers		✓	
	Create custom documents which provide a simplified view of existing IUCLID documents (and define the migration of data from the custom document view to the source IUCLID)		✓	
	Create new phrasegroups and phrases (picklist items) for fields in		✓	

Scope of IUCLID Configuration	Additional information on the configuration	Standard maintenance by the IUCLID team	Configurable by users with IUCLID team support	Configuration options which require specific agreement
	regulatory-specific documents			
	Create new text templates to guide users on the input for a specific text field			
Migration rules				
	Create migration rules to migrate IUCLID data from one major version to another using the set of existing migration rule logic			
Dynamic content rules				
	Create dynamic content rules to enable/disable hide/unhide fields using the set of existing dynamic rule logic			
Custom migration rules for regulatory-specific definition providers				
Help				
Technical questions about IUCLID answered				
IUCLID Functionalities manual				
Customise the top bar of the web interface to add links to specific manuals or web pages				
Regulatory/submission questions answered by the Definition provider of the Working Context (in collaboration with the ECHA Helpdesk)				
Filtering				
Filtering applied to specific IUCLID operations, export, dossier creation				
Configure TXT file for filtering for individual dossiers (e.g. when exporting or creating a dossier) or filtering in bulk a set of dossiers				
Validation				
Re-use existing validation rules and scenarios directly				
Define own Validation scenario and configuration file (setting rule level/warning/message), and use existing validation rules to validate against certain Working Contexts				
Reporting				
Re-use report template modules and other report FTLs				
IUCLID API				
IUCLID REST API is maintained throughout IUCLID versions				
Multilingualism				
Enable specific fields to be entered in two or more different languages				
Translation of interface				
Enable field labels and phrases (picklist items) to be translated in another language than the default				
Top bar of IUCLID				
Configure the logo in the top-left hand corner of the web interface				

4.1. IUCLID format (using ITEM)

4.1.1. Guidance on creating IUCLID documents

When creating an IUCLID document, it is recommended to first export a related ITEM document template in Word format, and together with the relevant business persons, use this 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 that can be added to any IUCLID installation in order to extend its format and Working Contexts according to the regulatory-specific or data collection needs. The IUCLID developers use the specifications created in ITEM to automatically generate the JAVA code needed to bring the specifications to IUCLID.

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 message to the user of the validation assistant with guidance 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 by users in organisations implementing their own set of validation rules, 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. An organisation directly reuses the existing scenarios and associated rulesets that are applied to check the completeness of specific dossiers. In that case, the organisation will simply reuse the information requirements and associated verification rules defined by another IUCLID user customisation.

2. An organisation which has already defined its own information requirements by selecting the relevant IUCLID documents from the OECD, IUCLID and/or its own Definition Provider, and has created the corresponding table of contents 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 an organisation will not only select rules from the existing catalogue but also specify its 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.

With these options come additional configuration possibilities to support users in organisations implementing their own set of validation rules who wish to further modify elements of their Validation rulesets. They can customise themselves, at the level of the Validation scenario, the following elements using a configuration Excel (XLSX) and Text (TXT) files:

   a. Rules can be activated or deactivated by users (using the provided XLSX file).

   b. Rule levels (failure, warning, reminder) can be changed by users per rule (using the provided XLSX file).

   c. The rule identity name can be modified by users. For example, TCC_0102_02 can be changed to OECD_TCC_0102_02 to designate the organisation which is running the validation scenario. This helps users identify rules according to their own submission and validation processes (using the provided XLSX file).

   d. A customised rule message can be provided for the rules triggered in the Validation scenario. This helps users shape the message according to the rule's regulatory purpose and context (using the provided TXT file).

These different scenarios are illustrated by the following flowchart.

Figure 4.1. Different scenarios for the customisation of the Validation Assistant
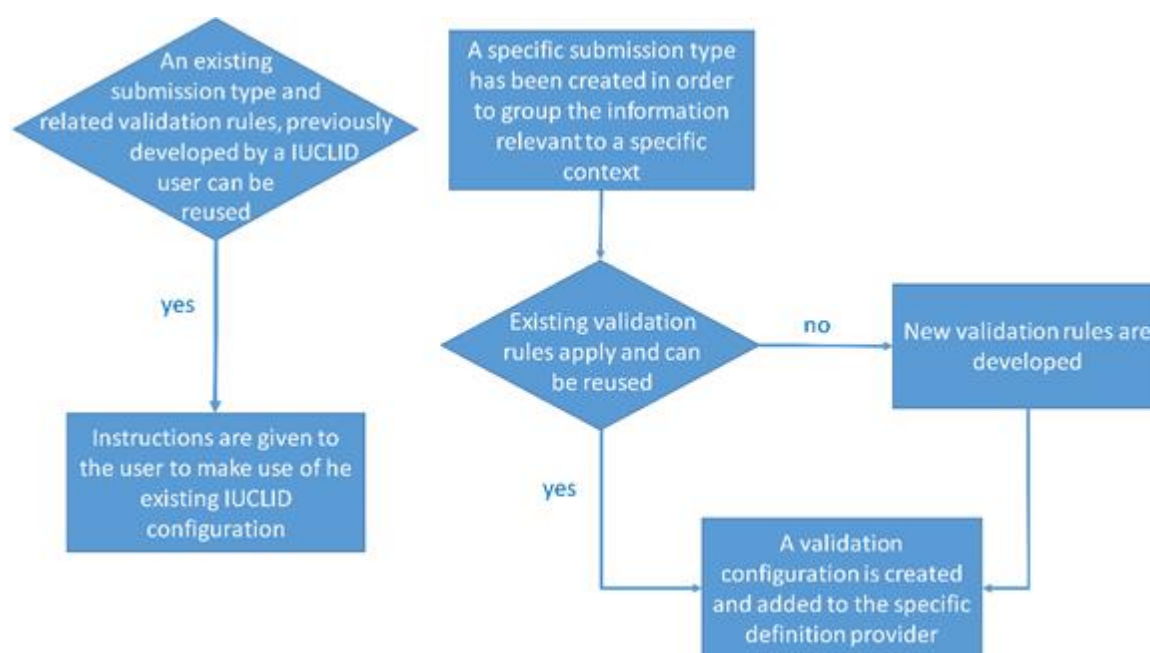
More information on the data validation can be found on the IUCLID website: https://iuclid6.echa.europa.eu/data-validation.

4.3. Reporting

IUCLID comes with a feature called the "Report Generator". This feature allows an IUCLID user to extract data from an IUCLID Substance, Mixture or Article dataset or dossier, and generate a readable, user-friendly, customised report of IUCLID information in different output formats, for example, RTF, PDF, CSV and HTML. 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 are fully customisable by any IUCLID user. To customise the information a report contains, the user writes what is called a FreeMarker Template Language (FTL) file and uploads it into IUCLID's Report Manager. 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.

To support the re-use of FreeMarker code for IUCLID and to help report-builders of hazard assessment reports, a set of common FTL modules are provided on the IUCLID website: https://iuclid6.echa.europa.eu/reports. The modules can be used to extract the major robust summary studies and endpoint summaries from IUCLID, as well as classification and labelling information, physical-chemical summaries, and chemical structure identity and composition information. Contact the IMG for more information on the exchange and update of available FreeMarker code for IUCLID.

The steps to create and generate a report 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: The user writes a corresponding report template (FTL file). This step requires some IT skills which can easily be learned. Alternatively, you can re-use the common modules to avoid writing full templates, for example, if you want to extract the classification and labelling information. (The IUCLID team can facilitate users with this work by showing examples and answering questions).

- Step 3: The user uploads the report template in a IUCLID installation, with the appropriate output types selected (for example, PDF, RTF) and associated to a relevant main entity (for example, a Substance entity).

- Step 4: The user generates the report from a Substance, Mixture, Category or Article dataset or dossier.

Figure 4.2. Process for writing and generating a customised report
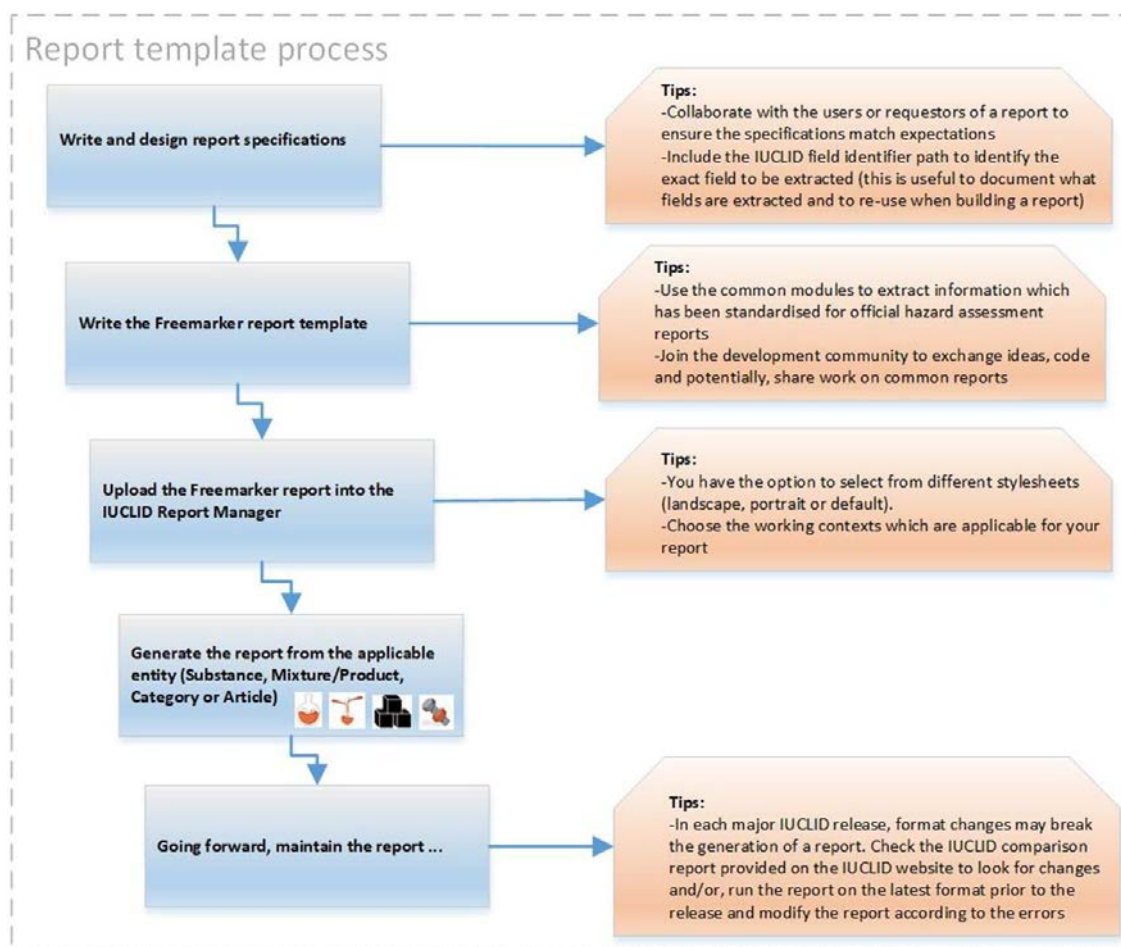
The IUCLID website (https://iuclid6.echa.europa.eu/reports) provides the following documentation and examples to help a user get started with customising a report template for extracting IUCLID data:

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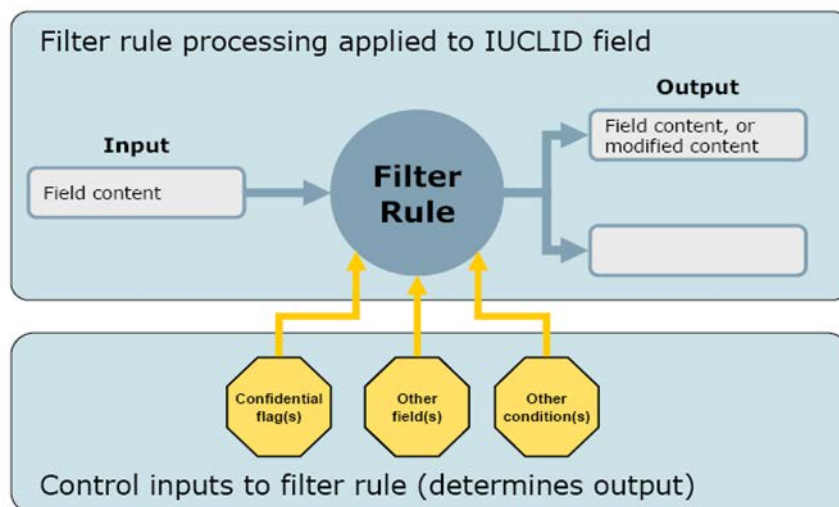
These existing filtering rules are provided by the IUCLID filtering module and can be re-used in a customised way for example, to remove from a dossier all data which is not relevant for a specific purpose, such as to exchange data with a third party or to make the data publicly available.

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 shown in the following figure.

Figure 4.4. Procedure to customise filtering
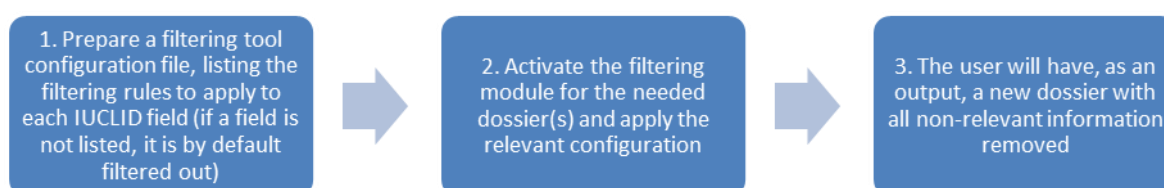
More information can be found on the IUCLID website: https://iuclid6.echa.europa.eu/data-filtering.

In addition to the above, a bulk dossier filtering tool is also available. The tool sends a request to a IUCLID instance where the dossiers to filter are located, applies a custom filtering configuration file (TXT file) to these dossiers and exports the filtered dossiers to a folder location specified by the user. The filtering file can be customised by any IUCLID user to match the filtering configuration required. Typically, the bulk filtering tool is used to move a subset of data from a large IUCLID instance to a file for publication or dissemination. To use the bulk filtering tool, contact the IMG and the tool can be shared.

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)	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'.

Source: Screenshot of ITEM 2.6.26.

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 web interface

Study design

Analytical monitoring ❓ ^

Indicate whether test substance was monitored in the test solutions. For robust study summaries or as requested by the regulatory programme, provide further details on sampling and analytical methods in the corresponding freetext fields.

Please select ⌄
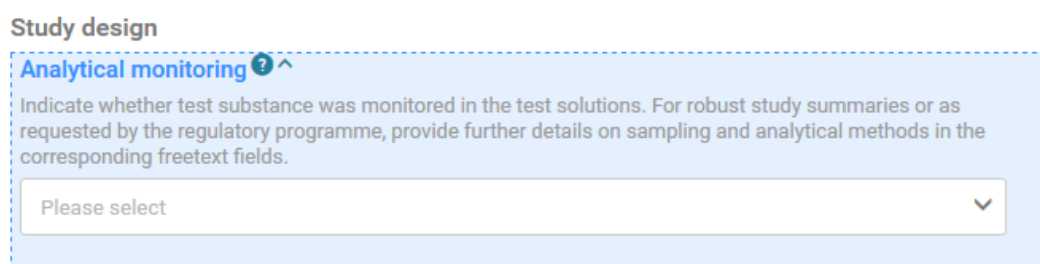
Source: Screenshots of IUCLID 6 5.1.2. build: 28/10/2020

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

Figure 4.7. Procedure to customise Help information as part of the IUCLID format specification
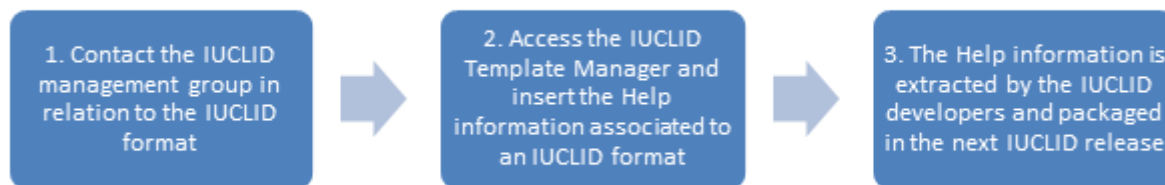
The second layer of help information is provided in the IUCLID functionalities manual which describes the main features available in IUCLID. It is distributed on the IUCLID website[1] but is also accessible directly from the IUCLID application itself. In the web interface, you can access the manual in different languages by clicking on the question-mark in the top left-hand corner of the page. ECHA maintains the manual taking into account the adaptations made to the IUCLID application and agreed at the level of the OECD IUCLID Users Group Expert Panel.

Figure 4.8. IUCLID functionalities manual

Source: Screenshot of IUCLID 6 4.14.1. build: 24/04/2020.

The third layer of help information is provided in the configurable top bar of the IUCLID web interface, which can provide links to relevant Help documents stored on Internet websites. The information is usually in the form of manuals addressing one specific need, and the content is managed by the organisation

responsible for the specific use of IUCLID. 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, and is made reference to in the IUCLID web interface under "Dossier preparation manuals"'.

Figure 4.9. Display of Help information in IUCLID addressing the use of IUCLID for a specific purpose
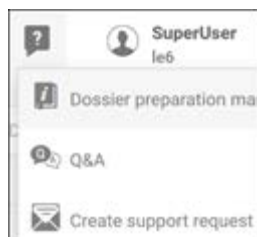
Source: Screenshot of IUCLID 6 4.14.1. build: 24/04/2020.

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. Multilingualism (data entry in multiple languages)

You can enter any language into most IUCLID text fields (marked as 'Multilingual' in an ITEM field), such as Japanese or Turkish, and this will be saved and displayed correctly in the dataset and dossier views, in the Print and Reporting generation outputs, as well as the Validation Assistant.

If the user is expected to enter one language only, such as Japanese, then the multilingual fields do not need to be activated. If a user is expected to enter information in two or more languages in the same text field, for example, in English, Bulgarian, Spanish and French, IUCLID provides this possibility, if activated.

By default, text fields marked 'Multilingual' in ITEM are enabled to permit entries in multiple languages. The user interface will only show a field in multiple languages when it is defined and configured as such in ITEM, and uses the:

> 1. Specific working context, e.g. "Poison Centre Notifications [PCN]"
> 2. Respective dossier header to specify the languages to select.

Here is an example of how multilingual fields for Bulgarian, French and German have been activated for the PCN working context in the Toxicological summary document.

Figure 4.10. Example of multilingual fields
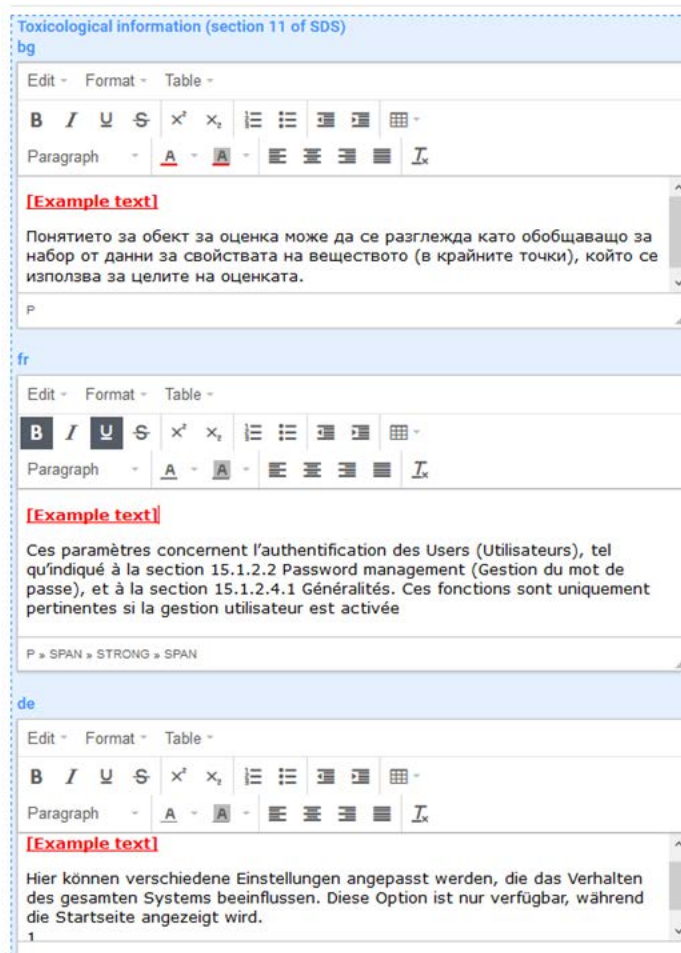
Source: Screenshots of IUCLID 6 5.1.2. build: 28/10/2020

As shown above, every language entered for the toxicological summary field will be displayed with its respective language code, for example BG for Bulgarian, FR for French and so on.

To configure ITEM and activate multilingual fields, contact the IMG.

4.7. Translation of the user interface (internationalisation)

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 have been tested and can be translated:

- field labels
- phrases (included in IUCLID picklists).

The following elements of IUCLID could potentially be translated, but have not yet been tested:

- IUCLID document names and section names displayed in the Table of Contents
- free text templates (to support data entry in free-text fields)
- help text.

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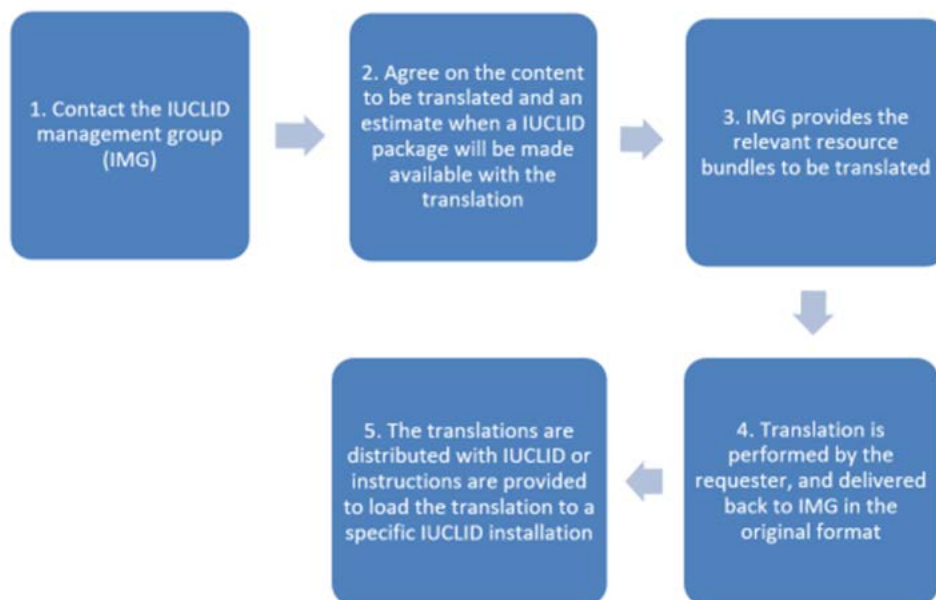
If the translation of some elements is missing, the English version, provided in the resource files, will remain and be used by the application by default.

Below is a proof of concept for translating the IUCLID interface, using a Finnish translation of the Product Information document: *FLEXIBLE_RECORD.ProductInfo.*

Figure 4.12. Example (proof-of-concept) translation of the IUCLID interface
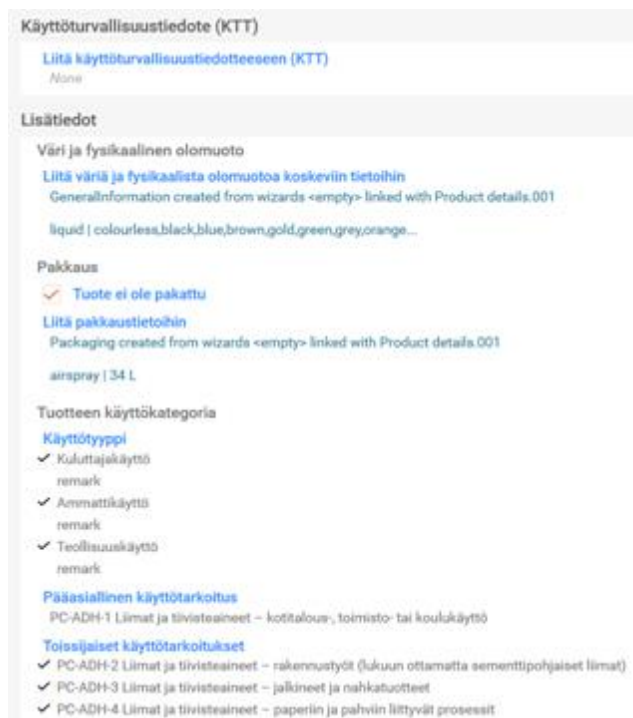
Source: Screenshots of IUCLID 6 5.1.2. build: 28/10/2020

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.

4.8. 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 4.13. 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 and the migration of data to IUCLID

5.1. The migration of non-IUCLID data to the IUCLID format

Newcomers to IUCLID often have data stored in a non-IUCLID format which they wish to migrate to the latest IUCLID format. This can be legacy data from an old system, or data which are actively being collected and modified.

In the section below, two established methods are documented for migrating large amounts of data to IUCLID, with a focus on the IUCLID public REST API.

An alternative approach to migrating non-IUCLID data to an IUCLID instance is to use the IUCLID Uploader tool, which at the time of writing is in a prototype stage and will be further enhanced over the coming years. The Uploader tool makes use of the Knime Analytics Platform® to transform chemical data into exportable i6z (IUCLID) files. Knime offers the following technical advantages:

- helps to visually identify the IUCLID elements (documents, fields) that should be populated
- simplifies the format to which the existing non-IUCLID data should be transformed
- offers the features of KNIME to build the migration logic from an external source to the IUCLID format
- requires less technical IT knowledge to build the migration workflow.

Users wishing to migrate data in bulk to the IUCLID format are advised to contact the IMG to discuss which method is best suited to the type of data being migrated, the objective of the migration in terms of the entities to be created in IUCLID, and if the migration is a one-time migration, or an ongoing migration.

More information on the Uploader tool can be found on the IUCLID website: https://iuclid6.echa.europa.eu/data-uploader.

5.2. Integrating with IUCLID and the IUCLID Public API

IUCLID can be used in connection with other IT systems/tools. This can be achieved by two different means: building custom scripts, or taking advantage of the IUCLID public REST API. Some of the technical advantages and disadvantages of the two methods are highlighted below, followed by more information on the IUCLID public API.

- Building a **custom script/application** that generates i6z files for import into IUCLID:
  - Technical advantages:
    - Independent i6z files can be generated that represent full datasets/dossiers.

- – Migration can be re-executed for problematic i6z files only.
  - o Technical disadvantages:
    - – i6z file generation is considered sometimes more complex (e.g. due to additional administrative technical data like the manifest.xml).
    - – If certain inventory documents (like Reference Substance) are reused, they must be included in different i6z files. The user has to make sure that they are always the same data, so that they do not overwrite each-other during importing the i6z file.
    - – The approach is slightly harder to do manual verification as the user needs to import the generated i6z file to an IUCLID instance to see the result.
- Building a custom script/application that writes to a IUCLID instance via the **IUCLID public REST API**:
  - o Technical advantages:
    - – It is easier to reuse inventory documents (e.g. Reference Substances).
    - – It is easier to test, as data are generated directly in a IUCLID instance, where they can be checked manually.
  - o Technical disadvantages:
    - – Individual IUCLID documents are created/filled in during one transaction. It could be harder to ensure the business consistency of a full dataset/dossier.
    - – If there are failing migrations, some clean-up (deleting invalid data) might be needed before re-running the migration.

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 5.5.2) 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 Tables of Content, the IUCLID document definitions, and phrase groups and phrases.

Figure 5.1. Public API
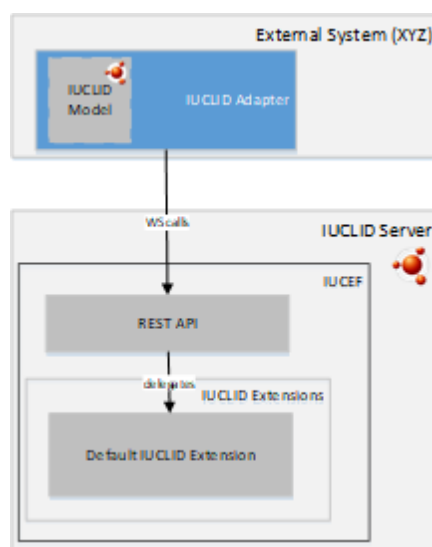
The prerequisite for use of the Public API is familiarity with the IUCLID data model, for example, how the information is organised in IUCLID, and with the REST API syntax.

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.

5.3. 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
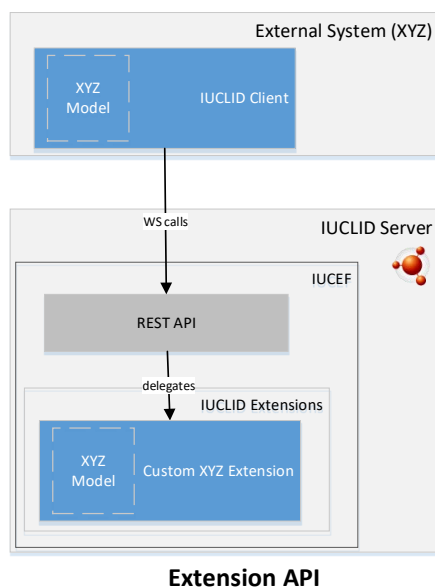
Extension API

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.

5.4. 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.

5.5. Examples of tools integrating with IUCLID

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

5.5.1. 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.

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.echemportal.org.

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

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.

5.5.2. Tools in other ecosystems

Text analytics

Text analytics is a search engine built for IUCLID and provides a high level of performance using elastic search. It is installed separately from, but connected to, an instance of IUCLID.

Text analytics allows a user to rapidly search all IUCLID fields including the text content of attachments. Therefore, searches can be performed on both structured data, such as picklists and dates, as well as on unstructured data, such as free text fields and attachments.

Text analytics uses the latest IUCLID document definitions, and therefore will be compatible with the latest version of IUCLID.

A Text analytics installer is available for download from the IUCLID website, which also provides installation instructions, a user manual, and key hardware requirements:

https://iuclid6.echa.europa.eu/text-analytics.

Data extractor

The IUCLID Data Extractor is an advanced tool that permits the mass extraction of IUCLID dossiers and documents across an IUCLID database (using their UUIDs). A user can create and save extraction jobs for re-use later, as well as exchange these extraction jobs with other users.

The Data Extractor is installed separately from, but connected to, an instance of IUCLID and has its own web user interface modelled on the IUCLID data structure. The Data Extractor has its own database, and it is possible to extract data from an IUCLID running on the same machine or, on a separate machine.

The Data Extractor installer is available for download from the IUCLID website (for MS Windows), as well as installation instructions, a user manual, and key hardware requirements: https://iuclid6.echa.europa.eu/data-extractor.

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. 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/.

Chemical safety assessment and review - ECHA - Odyssey

Odyssey is an application intended for internal ECHA use. Odyssey is built with the purpose of performing dossier assessment, as an expert system supporting dossier evaluation and inquiry, 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.

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. Overview of the use of IUCLID in OECD member countries

IUCLID is used in multiple regulatory contexts. The table below represents an overview of how IUCLID is used at the date of this publication by different regulatory jurisdictions, regulatory programmes, international and supranational bodies, with an emphasis on IUCLID's format, engines, modules, and API. The table is in the form of a matrix. The left-hand side column represents the different stages of the regulatory process in which IUCLID is used (which can repeat at different points in the process). The top row indicates, at a high level, the regulatory jurisdiction and/or context in which IUCLID is used. The latest overview is available on the IUCLID site at https://iuclid6.echa.europa.eu/project-iuclid-6.

Table 6.1. Matrix view of the use of IUCLID in OECD countries

Key:
Areas where IUCLID is used (●) or considered for use (○)

	AU (AICIS)	CA (existing chemicals)	CA (new chemicals)	NZ (Hazardous substances)	CH (biocidal products)	CH (new substance notification and further obligations for substances)	US (OCSPP)	US (NCCT)	US (RAD)	EU PCN (CLP_ECHA)	EU WFD (ECHA)	EU REACH (ECHA)	EU BPR (ECHA)	EU CLP (ECHA)	EU PPP (EFSA)	EU EASIS (JRC)	OECD (SIDs)
Dossier preparation																	
Enter data in a structured format	●	●	●	○	●	●			●	●	●	●	●	●	●	●	●
Perform presubmission quality checks	●			○	●	●				●	○	●	●	●	○		
Reporting generator for dossier preparation	○			○		●				●	○	●	●		○		
Previewing publicly disseminated data	○												●		○		●
Submission process																	
Format check	●				●	●				●	●	●	●	●			
Validation	●			○		●				●	○	●		●	○		
IUCLID Extension modules										●	○	●	●	●			
Dissemination																	
Filtering												●			○		
Aggregation												●					
Provider agent												●			○	○	●
Post submission work (analysis/assessment)																	
IUCLID for searching dossier contents	●	●		○	●	●	●	●	●			●	●	●	○	○	●
IUCLID for entering additional assessment information	●	●		○			●	●	●								
IUCLID reporting engine in assessment/evaluation	●			○		●						●	●	○	○		

Key (icons): 🔴 = Areas where IUCLID is used; ⚫ = or considered for use

Key: Areas where IUCLID is used or considered for use	AU (AICIS)	CA (existing chemicals)	CA (new chemicals)	NZ (Hazardous substances)	CH (biocidal products)	CH (new substance notification and further obligations for substances)	US (OCSPP)	US (NCCT)	US (RAD)	EU PCN (CLP_ECHA)	EU WFD (ECHA)	EU REACH (ECHA)	EU BPR (ECHA)	EU CLP (ECHA)	EU PPP (EFSA)	EU EASIS (JRC)	OECD (SIDs)
IUCLID annotations in assessment/evaluation	⚫			⚫	🔴	🔴							🔴				
IUCLID aggregation engine for assessment/evaluation												🔴					
IUCLID for data analysis by other, integrated systems	⚫	⚫		⚫			🔴	🔴	🔴			🔴	🔴	🔴		⚫	🔴

6.2. ECHA

6.2.1. Alternative user interfaces

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.

Dossier header editing and storage

When running the Validation Assistant or creating a dossier, the user is asked for certain information to identify the regulatory context for which the user is entering data, for example on the Table of contents or the tonnage band. With the web user interface, this process is 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
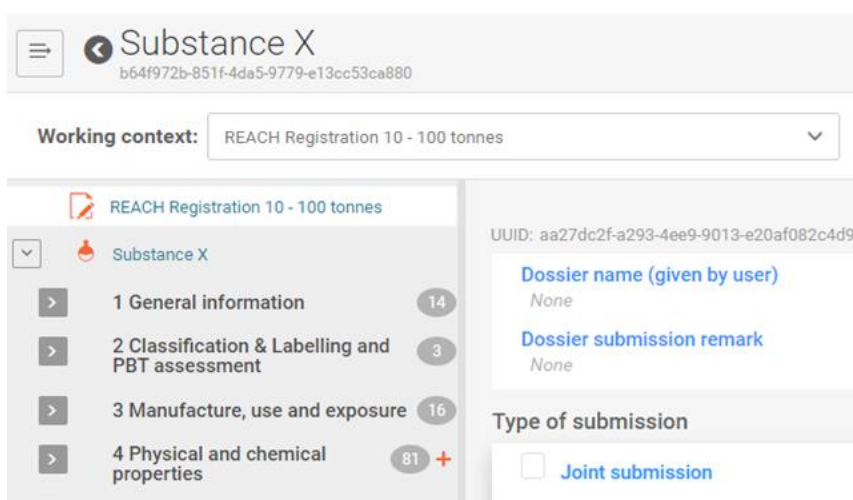
Source: Screenshots of IUCLID 6 5.7.0. build: 28/10/2020

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
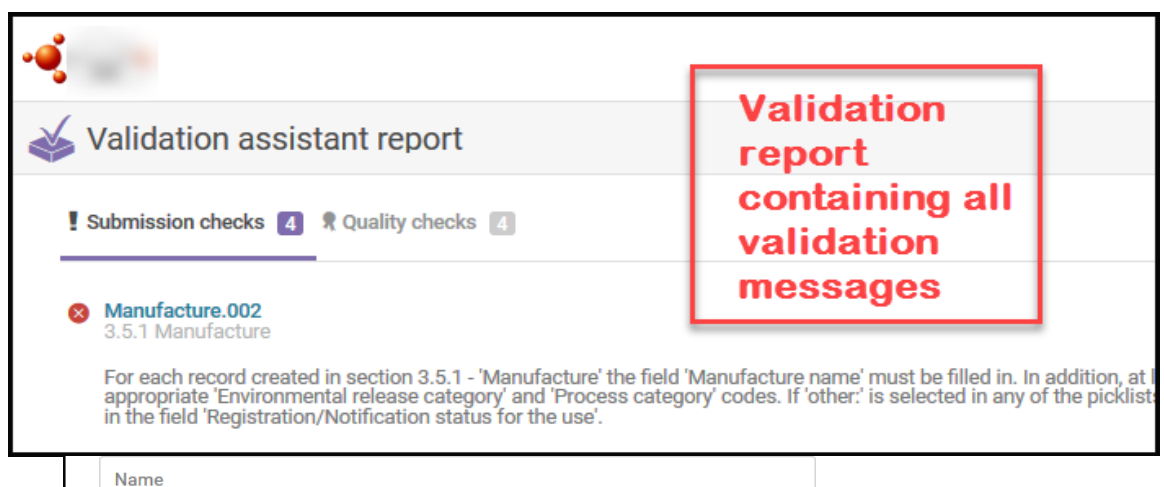
Source: IUCLID Cloud v6.2

6.2.2. 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.

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.

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.

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.

6.3. Australia

The Australian Industrial Chemicals Introduction Scheme (AICIS), within the Australian Government Department of Health, regulates the importation and manufacture (introduction) of industrial chemicals, including cosmetic ingredients, in Australia. AICIS replaced the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) on 1 July 2020.

AICIS has developed a new IT system that enables importers or manufacturers (applicants) of industrial chemicals to create and submit an application for an assessment certificate (for industrial chemicals not

already listed on Australia's Inventory). The AICIS Business Services portal is the external user interface that connects to internal databases including AICIS' IUCLID instance (refer to Figure 6.3).

Custom online forms exposed on the portal enable applicants and other participants (agents or chemical data providers) of a certificate application to provide administrative (including fee payments) and chemical information. Business-related information received from applicants or other participants is stored in Microsoft Dynamics Customer Relationship Management (CRM), whilst chemical-related information is stored in AICIS' IUCLID instance. CRM is also used to manage AICIS workflows.

Figure 6.3. AICIS IT System components
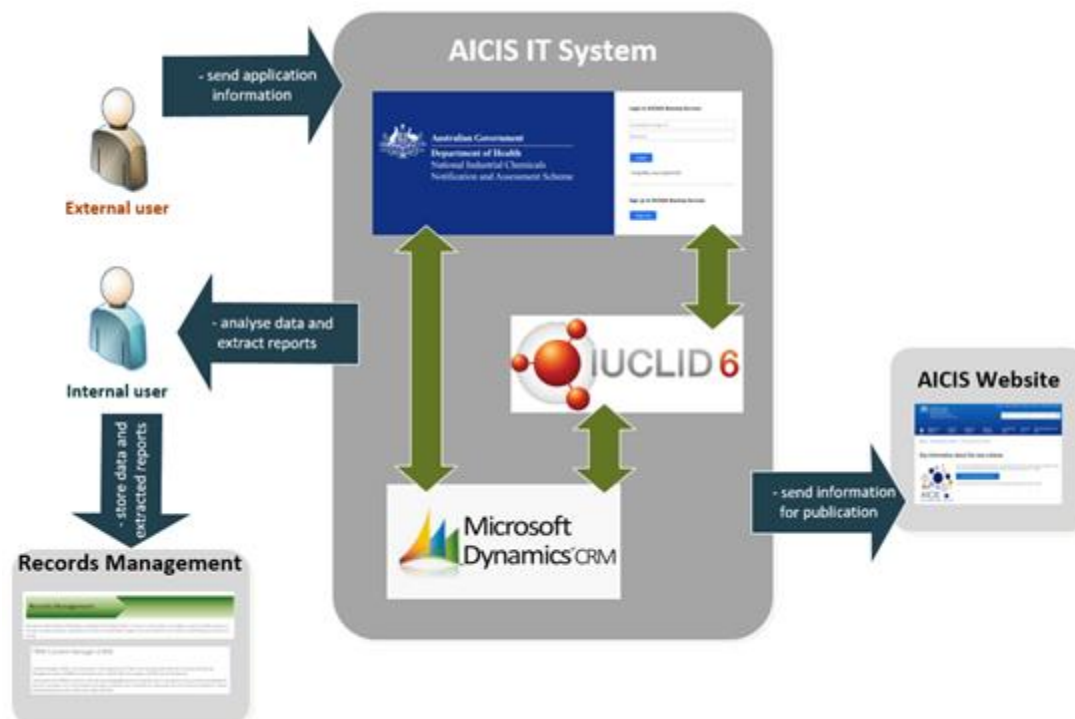
6.3.1. Alternative user interface

Integrating AICIS Business Services with IUCLID

Applicants and other participants of a certificate application (portal users) can provide chemical-related information via an upload feature (a portal user can directly upload a dossier that was validated using the Australian ruleset) or by completing the custom online forms (portal forms).

The portal forms utilise the numerous features of IUCLID Public REST API (refer to section 5.2 for further details). Information received from the IUCLID Public REST API is used to render portal forms and to expose the common functionalities and utility operations of IUCLID on AICIS Business Services (refer to Figure 6.4).

Figure 6.4. Overview of AICIS portal forms
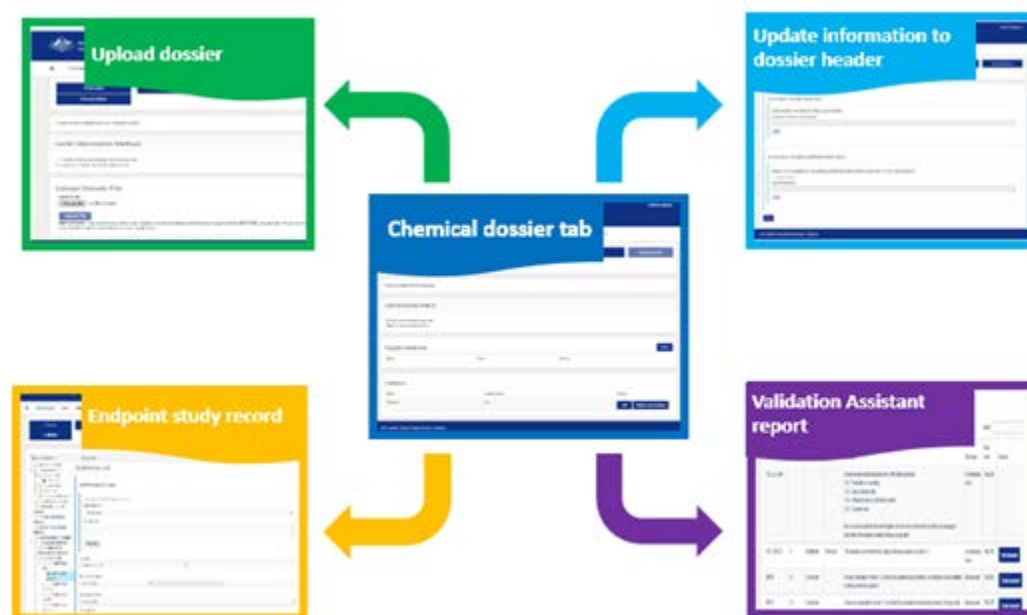
Source: Screenshots of 'Chemical dossier' tab from AICIS Business Services portal for assessment certificate application; build 01/07/2020

Through the portal forms users can create and update reusable references (inventory documents such as reference substances, literature references and sites) and substance datasets. Information entered by users is written/passed to related records (e.g. inventory documents and endpoint summary records) in AICIS' IUCLID instance during the creation and update of the portal form.

Once chemical information has been received by AICIS for a certificate application the data contained in the dossier(s) will be copied to create a complete dataset in AICIS' IUCLID instance for AICIS assessors to conduct the risk assessment.

Additional features have been included in a number of portal forms to assist users with providing chemical-related information to AICIS. These features include the automatic generation of dossiers when a user submits their chemical-related information to AICIS and exposing a subset of IUCLID fields on certain types of portal forms (such as endpoint study records). The additional filters applied during the rendering of portal forms expose fields to capture the basic information required for a certificate application. As the risk assessment of industrial chemicals in Australia is managed by AICIS and not by industry, the remainder of the information will be entered by AICIS assessors during the risk assessment.

Integrating CRM with IUCLID

AICIS employs two databases, CRM and IUCLID, to manage business-related and chemical-related information, respectively. A number of applications related to the introduction of an industrial chemical into Australia require information to be linked between the two databases.

Universal Unique IDentifier (UUID) generated in AICIS' IUCLID instance are used to link the two databases. The UUIDs are stored in CRM at the business, chemical and application level. For certificate applications, the related substance dataset URL is stored in CRM, enabling AICIS assessors to launch the substance dataset in IUCLID from CRM.

6.3.2. Validation

AICIS worked with the IUCLID Management Group (IMG) to select rules from the existing library of validation rules that catered for the information requirements of AICIS. The majority of rules configured for certificate applications are from the existing library with minor modifications to the message content and how the rules were configured (failure vs warning). In addition, four new custom rules were developed with the assistance of IMG.

Additional features incorporated into the portal

The new customisation available in the web user interface for showing the Validation Assistant message on documents (that require correction) was incorporated into the portal forms. A user can navigate to documents requiring correction from the validation report and once the document has loaded, they will be able to view the validation message at the top of the document.

6.3.3. Design considerations

Australia has information requirements for industrial chemicals that are currently not covered by documents in IUCLID. To enable this information to be stored in IUCLID, AICIS worked with the IMG to customise a number of documents in ITEM.

Dossier header editing and storage

To accommodate the different certificate application types and occasions where multiple participants (applicants, agents and chemical data providers) are contributing information, a customised dossier header was created. This dossier header enables each applicant or participant of an application to provide information about the chemical that they are in possession of, whilst protecting confidential business information. The dossier header also enables validation rules to be configured to reflect the information requirements based on the certificate application type selected. Additionally, the dossier header for the Australian-specific TOC AICIS assessment and evaluation was customised to identify key administrative aspects of the assessment/evaluation (e.g. purpose, type, focus).

Polymer characterisation

Identification of reactive functional groups (RFGs) to aid in the characterisation of polymers are separated into individual tables based on the level of concern. Included in the design consideration is the content of picklist values for particular fields and regulatory treatment of low concern RFGs (e.g. those do not require functional group equivalent weight [FGEW] calculation).

PBT document

The CORE PBT document has been slightly modified in the Australian-specific TOC. The concept of vP (very Persistent) and vB (very Bioaccumulative) does not exist in Australian legislation and as such was removed from the flexible record.

Assessment and Evaluation Statements

A new document has been designed in an existing Australian-specific TOC to record risk assessment information, recommendations to Australian prescribed bodies, and high-level summaries of assessments/evaluations. Majority of the fields included in this new section would otherwise come from existing IUCLID fields that would be re-purposed or from an external system (e.g. customised CRM fields or documents stored in local/shared drive). This document will enable risk assessments to be written directly to IUCLID. Consideration in the design of this section was based on the ability for information to be disseminated easily using IUCLID, especially in the Australian context. Additionally, the inclusion of this

new section greatly assists in the publication of AICIS Assessment/Evaluation Statements following completion.

Commercial Evaluation Authorisation (CEA) and Pre-introduction Report (PIR)

The CEA TOC is similar to the certificate application working context with an additional section on the additional information required for this application type. This TOC has no portal component and will be used mostly for internal purposes.

A prototype of a PIR is available to AICIS and has been implemented with an initial attempt to apply dynamic content rules. Further development of this TOC will be considered in the future.

6.3.4. Data entry

AICIS' certificate application working context have alternative user interfaces consistent with the information requirements relevant to each type. When applicants submit their chemical-related information through the portal forms, dossiers are generated per participant (applicant or chemical data provider) in AICIS' IUCLID instance. These dossiers are then converted to datasets which AICIS assessors/evaluators can then screen and update during the risk assessment of the chemical. AICIS plans to maintain one dataset for an assessment/evaluation. Where additional information has been gathered from literature reviews or further information obtained from applicants, these will be added manually by internal users as separate documents to the dataset.

For assessments and evaluations conducted by AICIS outside of the certificate application process new datasets will be created and the Australian-specific TOC AICIS assessment and evaluation will be used for internal assessments/evaluations. Naming conventions are adopted to distinguish for example, datasets created for other processes; or datasets created for the same Reference Substance. A similar process to updating datasets related to certificate applications will be followed for these other applications and evaluations. Internal users will manually add information gathered from literature reviews or obtained from specific stakeholders that provided information as part of a voluntary or mandatory call for information. The AICIS' IUCLID instance has the ability to preview publicly-disseminated dossiers, and information from these dossiers can be utilised in subsequent assessments/evaluations. There is opportunity to merge datasets once the outcomes have been determined.

Upon finalisation and publication of the assessments/evaluations, the datasets will then be converted into dossiers and saved in the Australian Government Department of Health's records management system.

6.3.5. Reporting

AICIS will customise several reports using the Report Generator feature. Examples of generated reports include assessments/evaluations for internal peer review, screening reports of hazards by way of GHS classifications, AICIS Assessment and Evaluation Statements, and reports to facilitate data exchange/dissemination to other risk assessment agencies or regulators. Reports will be generated from Substance and Category datasets.

Specific to the AICIS Assessment and Evaluation Statements, the output (PDF or RTF) is designed ready for publication in the AICIS website. The output file in XML and/or CSV formats will be further investigated.

AICIS prepared the report specifications of the output file and associated IUCLID field identifiers and sought advice from ECHA in writing the report template (FTL format). "Common modules" were re-used in the FTL formats for ease of designing the report templates and to be consistent with the IUCLID-default chemical safety report (CSR) format. The generated FTLs are then loaded in IUCLID for report generation.

6.3.6. Data migration

Inventory/Reference substance

The Inventory is a regulatory tool that differentiate industrial chemicals as unlisted or listed. AICIS currently uses an internal chemical register which contains the record of all chemicals and links them to business applications including certificates, authorisations and inventory processes. The chemical register is maintained in CRM which is built on an SQL Server database. AICIS will manage reference substances in IUCLID to maintain alignment with the chemical register.

IUCLID's data structure (modular approach) and functionality provides an effective means of sharing data internationally and as such, AICIS imported its register into its instance of IUCLID. To facilitate this process, third party software Altova® MissionKit® (Altova® MapForce®) was utilised to map chemical data from the SQL Server database into the required XML files, following the specified XML format described by the IUCLID XML schema definition files (xsd files). These were then packaged into an i6z archive file. As a result, approximately 40,000 chemicals on the register were imported into AICIS' IUCLID instance as reference substances.

Legacy assessments

AICIS has legacy systems, built on Access and SQL Server databases, which contain assessment information for more than 20,000 chemicals. The information can be exported as flat files (XLS format). Most of the fields are in free text format and do not align with the structured data format of IUCLID. Mapping of the source datatypes to the identified IUCLID fields are planned to transform the information for eventual migration. ECHA presented options for the migration activity including the development of the IUCLID Uploader tool.

6.3.7. Other functionality

Category entity

AICIS will be using the Category entity to manage the assessment and evaluation of groups of chemicals from consolidated assessment certificate applications or evaluations initiated by the AICIS Executive Director. Working context for Category and dossier headers to facilitate this work in IUCLID have been implemented.

Template entity

The Template entity will be used for several purposes which include: inserting data in multiple sections to be copied/inherited to Substance or Category datasets and creating a standard set of preferred text to be used in internal risk assessments and evaluations.

Data extractor and Text Analytics

The IUCLID add-ons, Data Extractor and Text Analytics, are planned to be used in the future.

6.4. Canada

6.4.1. Migration of legacy data

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 were 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 were 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.

6.5. New Zealand

New Zealand is in the process of updating its hazardous substance classification system to the GHS version 7 and is taking the opportunity to upgrade its end of life sql visual basic bespoke application hazardous substance database (HSDB) as part of this. The decision was made to move to IUCLID for global alignment and anticipated opportunities for the easy import of data on hazardous substances and data sharing.

In New Zealand, hazardous substances are primarily regulated under the Hazardous Substances and New Organisms (HSNO) Act administered by the New Zealand Environmental Protection Authority (EPA). Other legislation and agencies also have roles across the regulatory landscape of hazardous substances, including the Health and Safety at Work Act administered by WorkSafe New Zealand. The HSNO Act requires that all hazardous substances (including both individual compounds and mixtures) imported or manufactured, must be done so in accordance with an approval issued under the Act. The majority of hazardous substances are regulated under approvals called group standards which contain conditions relating to a set of related substances, hazards and uses. The remainder, mostly agrichemical and pesticide products have individual approvals covering specific substance risk assessment and risk management measures.

6.5.1. Migration of existing data

The EPA's existing hazardous substance database contains around 45,000 chemicals and mixtures and their related data. This will be migrated to IUCLID using Microsoft® Azure® data/integration pipelines to extract, transform and load the existing database records into staging tables and then into the final i6d/i6z file structures for loading into IUCLID using the import functionality.

Mapping of the existing fields in the current HSDB to IUCLID was carried out so that a home could be found for each piece of information. Where homes could not be found, new NZ-specific documents were designed. A challenge was the need to record the HSNO approval number (unique identifier) in the new Regulatory History document, whilst also requiring it to be searchable within IUCLID. The solution was to create a link to the Regulatory History document field from the Regulatory Identifiers, which is a searchable field.

6.5.2. Data entry

The NZ EPA will maintain a single dataset for each hazardous substance, and data for new substances and mixtures will be entered manually. The EPA would like to receive dossiers for the more complex data-rich applications and intends to trial this with industry. This will greatly improve efficiency and reduce the likelihood of transcription errors by introducing a degree of automation.

Developing a custom user interface (UI) was discussed initially but quickly discounted as the ECHA team demonstrated the new web UI and the improved ease of data entry.

6.5.3. Design of new documents

The NZ EPA database project team has been working with ECHA to customise IUCLID for NZ-specific use. This has meant the design of a number of new documents to record NZ regulatory information, risk assessment information and the HSNO classification and controls. The team has also been working with EFSA on updating IUCLID to hold pesticide information, particularly ecotoxicology and environmental-fate information in OHTs and Endpoint Study Summaries.

This process has highlighted challenges in trying to keep IUCLID as a global system, so that it is applicable to a variety of regulatory contexts, and to help users determine when a document can be utilised or repurposed and when a new document is required.

6.5.4. Other functionality

The NZ EPA intends to use the category functionality to manage its group standards and the substances and mixtures that are linked to them. This will require an update by ECHA to allow categories to include mixtures.

The NZ EPA also intends to use the validation assistant to ensure dossiers are submitted with all the required information and implement internal data quality checks to support this.

6.5.5. Reporting

NZ EPA will make use of the Report Generator within IUCLID to provide the basis of our science memo (a staff assessment report) and other reports based on single substances/mixtures such as a "mixture spreadsheet" (a summary of the hazard profiles of the components in a mixture to allow the mixture hazard profile to be calculated). Reports will also be created to allow a user to view summary information for a substance without needing to open all the documents involved, such as a GHS classification summary or a summary of the key regulatory information for a substance.

In addition to creating new DocBook reports for use within IUCLID, NZ EPA will also use Microsoft® Power BI® to develop reports requiring data frommultiple substances/mixtures.

IUCLID data will be presented as a tabular model to Microsoft® Power Bi® via a lightweight modern data architecture running in the Microsoft® Azure® cloud. This will be updated with deltas from IUCLID via a custom API based on the IUCLID API Extension Framework.

Figure 6.5. Reporting solution of New Zealand
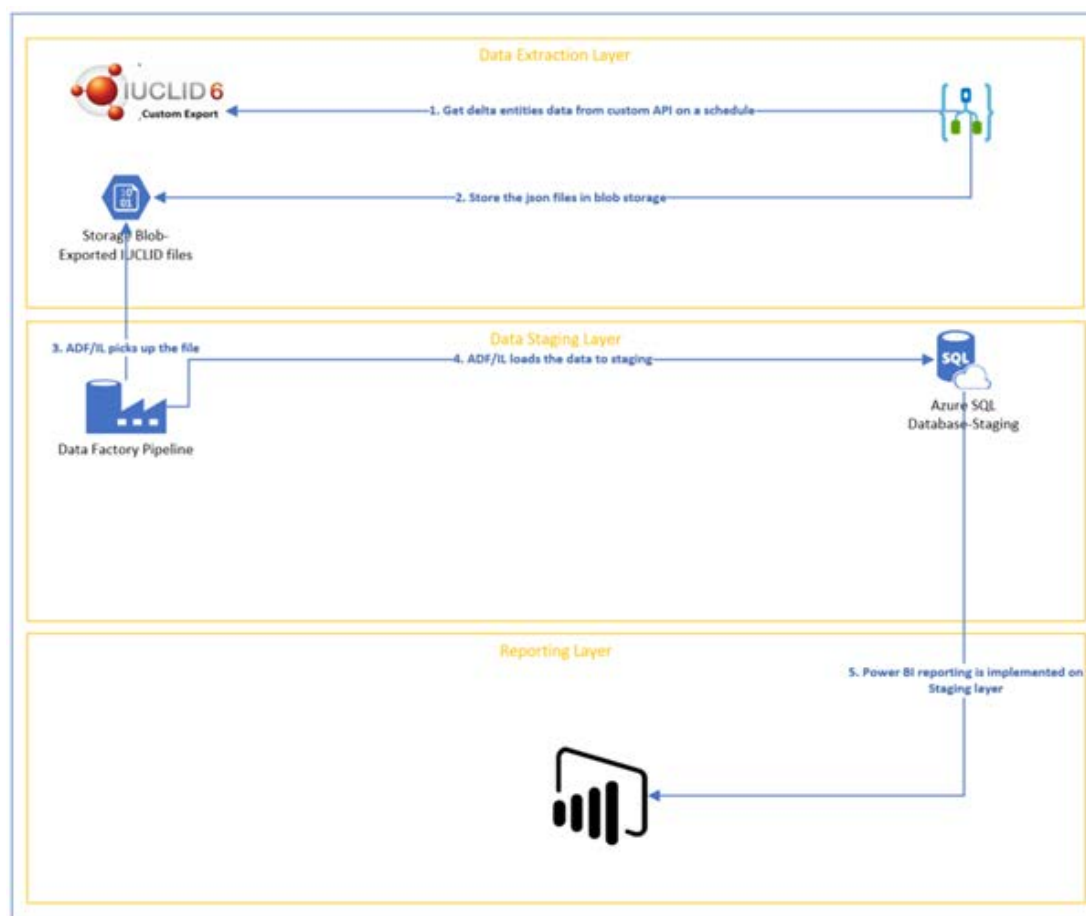
6.5.6. Web publishing

The NZ EPA publishes data on approved chemicals and mixtures and their controls (Approved Substances with Controls web search), on the classifications of chemicals (Chemical Classification and Information Database search) and on its inventory of substances (NZ Inventory of Chemicals). The CCID web search is on the eChemPortal.

The publishing solution will leverage the custom API and Data Mart used for reporting, with Microsoft® Azure® API Manager providing the endpoint for connectivity to the NZ EPA web hosting partner's API.

Figure 6.6. Web publishing solution of New Zealand
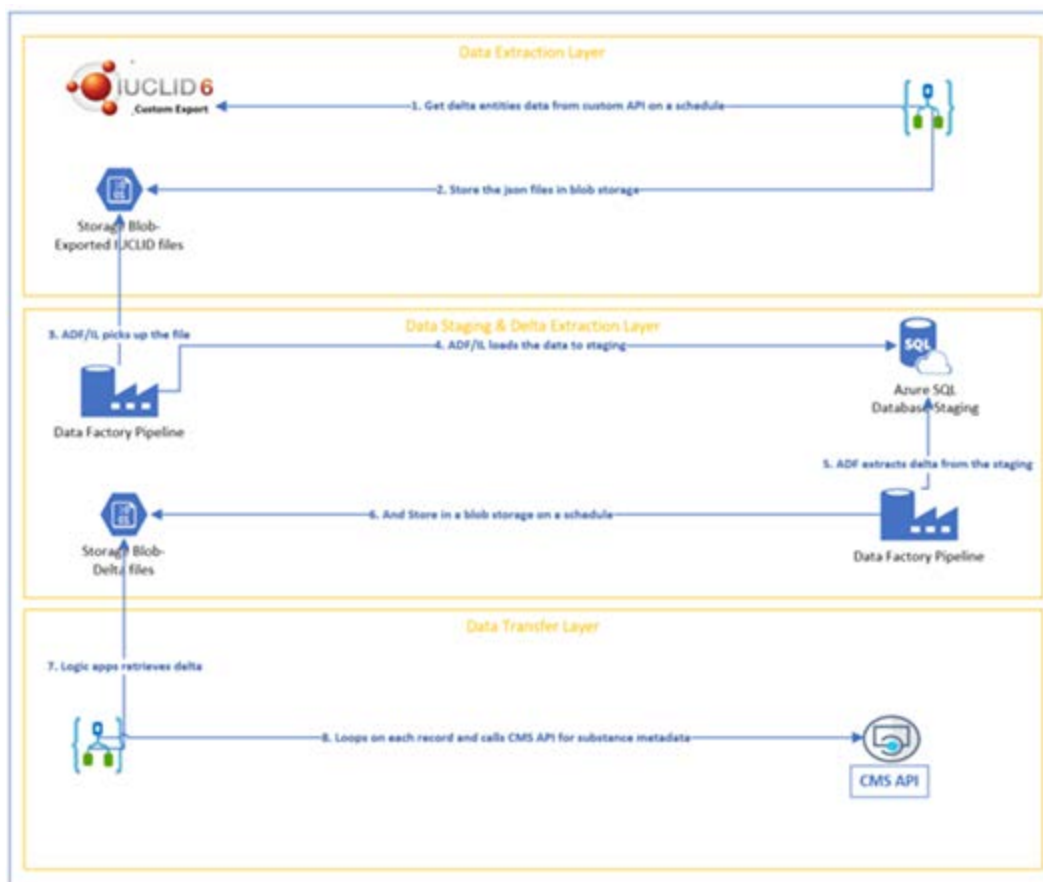
Chapter 7. OECD activities and procedures related to IUCLID

7.1. 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 format[1]. The European Chemicals Agency (ECHA), as the implementing body for a number of EU regulations and Directives and in partnership with European Food Safety Authority (EFSA) to support the use of IUCLID for the Plant Protection 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, 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.

7.2. 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 Chemicals and Biotechnology Committee 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.

7.3. 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 Chemicals and Biotechnology Committee 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.

3. 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.

4. 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.

5. 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.

6. The (final) draft templates are submitted to the OECD Chemicals and Biotechnology Committee for comments and endorsement under written procedure.

7. The revised and new OHTs are published on the OECD Website.

7.4. 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 release one major version of IUCILD with updated formats, including updated and/or new OHTs, per year. In addition to the OHTs, there may be other updates to IUCLID, such as adapting it to specific formats, like the Globally Harmonized System of Classification and Labelling of Chemicals[2].

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. Proposed changes are **encoded in ITEM** together with the associated migration rules and dynamic content rules.

3. Draft changes are shared with the Expert Panel and other IUCLID users (the OHT Expert Group and other relevant groups on the changes affecting the OHTs) for **review and impact analysis** 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:

   o integration scenarios (why?)

   o dependencies to the IUCLID format (list of paths)

   o dependencies on IUCLID modules (IUCLID public Application Programming Interface (API), filtering, reporting, validation assistant)
   o dependencies on service interfaces (Java API and web services API).

4. 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.

5. When relevant, the (final) revised OHTs are submitted to the OECD Chemicals and Biotechnology Committee (CBC) for comment and endorsement under written procedure, as necessary for substantial changes (not for small editorial improvements).

6. The release of the major version of IUCLID with format changes is targeted for the beginning of the fourth quarter of each year.

Figure 7.1. Targeted yearly schedule for IUCLID (IUCLID CORE, DOMAIN and OECD) format changes
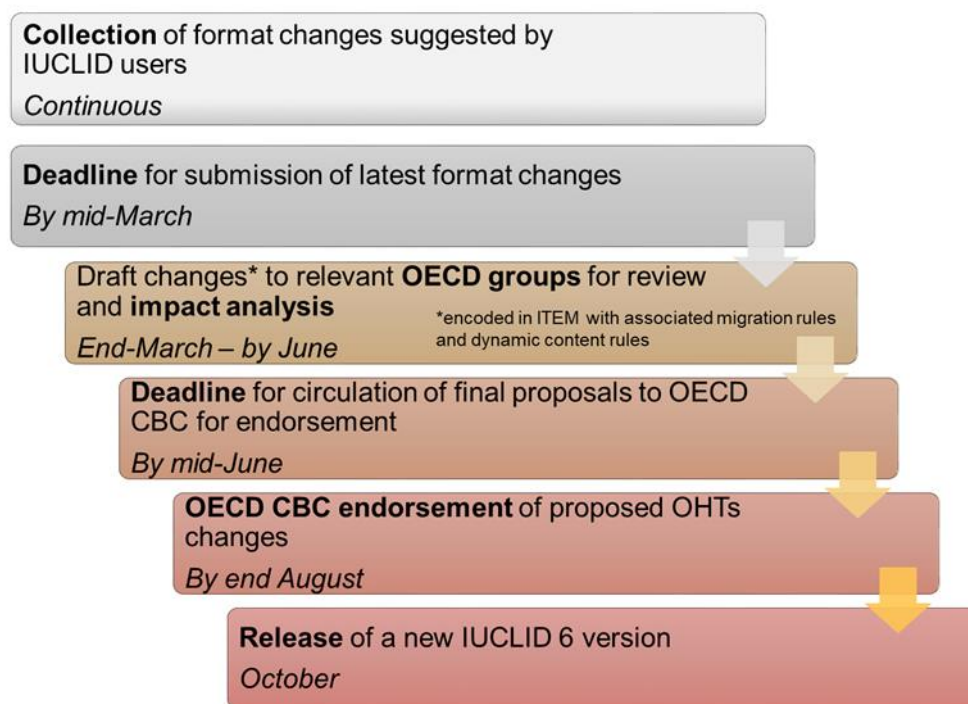
Not all harmonised documents have the same usage level. A change to a harmonised document, requested after the proposed deadline, could be implemented if all impacted organisations approve the change and there is still a possibility to perform the circulation and endorsement processes.

7.5. Coordination of activities for changes to the formats for specific legislations

Developments of formats for specific legislations or data collection processes can be released when needed as part of an IUCLID update, 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.

Each year, owners of Definition Providers should define a deadline for changes to be implemented for their specific Definition Providers. The deadline should be **no later than 15 August** to be included in the standard ECHA IUCLID cycle for the major release of the year. However, it is always recommended to inform the IMG as early as possible in order to identify timely changes that could be implemented at a more harmonised layer of the IUCLID format.

In order to prepare for a major IUCLID release, Definition Provider owners who have integrated IUCLID within their organisations, and possibly with other integrated applications as well, should:

- Regularly check the draft formats of others Definition Provider owners.
- Understand the impact of an IUCLID format change on their system.
- Identify the tasks needed for an update, explore possibilities to streamline them, plan for the adaptation tasks to be performed every year.

- Inform the IMG about the fields used by their applications, particularly if only a subset of the fields are used, so that the IMG can upload this list in ITEM to be added to the comparison reports and facilitate the impact assessment.

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]

Chapter 8. Annex I: 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.
Custom Document Definition	A special IUCLID document that has the only purpose to define an alternative UI form for another document definition.
Dataset	All the data are entered and stored in IUCLID in logical datasets containing *documents* and *entities*. Datasets contain editable data.
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 *Definition Provider*. 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 *Definition Provider Type* indicates the level of harmonisation that a *Definition Provider* 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.

Dossier	A Dossier is a read-only snapshot of a dataset and includes a dossier header containing information on the intended submission.
Dossier header	A IUCLID document that represents the root document of a dossier.
Endpoint study record	An Endpoint study record is a *document* (template) in IUCLID in which data are entered to describe a study, for example Melting point / freezing point.
Endpoint summary	An endpoint summary provides a *document* (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.
Working Context	Working Context is defined in the IUCLID Template Manager (ITEM) to identify and define a regulatory context or data process. The Working Context contains key elements of the IUCLID interface, including the Table of Contents (TOC) and sub-TOC, to be used by the data provider in order to easily identify the relevant information requirements, the associated dossier header and custom entities.
Table of Contents (TOC)	A Table of Contents (TOC) is a IUCLID section tree which organises the information requirements of a particular working context, 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.

IUCLID (International Uniform ChemicaL Information Database) is a software application designed to record, store, maintain and exchange data on chemicals. 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. IUCLID can be customised and configured to manage chemical data in different contexts and is a platform employing globally harmonised data elements pertinent to chemicals. It is continuously updated to provide greater customisation, extension and integration with other tools. This second edition provides the latest updates on IUCLID features and processes, including visual "working" contexts for the preparation and management of data according to regulatory contexts or data processes, possibilities for data entry in multiple languages, and a matrix view of the use of IUCLID in OECD countries.

oe.cd/iuclid