EnviroInfo 2000: Umweltinformatik '00 Umweltinformation für Planung, Politik und Öffentlichkeit

Sound Management of Chemical Information via Internet

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Abstract

The chemical industry worldwide has released millions of chemical products to date. As EU plants tend to "go east", governments are going to support the establishment of EU law pursuant to national chemical control regulations. This specific scenario can also be applied to many other regions in the world. The large number of chemical products, the numerous international chemical control regulations (Feierl 1998) and the need for international cooperation make the sound management of chemical information a key success factor. This is true for both industry and controlling authorities. This contribution describes the requirements for sound management of chemicals and the recent developments in the IGS (Information and communication system on hazardous substances). IGS is a well established, Internet based and multilingual substance information system relying on close cooperation between a powerful network of data providers.

1. Requirements for the sound management of chemical information

1000 to 2000 chemicals are produced or imported into the EU in quantities over 10 tonnes per year. Around 80,000 chemicals are produced or imported in quantities under 10 tonnes per year or not traded at all. The number of preparations (mixtures) on the European market is estimated to be between 1 and 2 million (Donker, 2000).

Companies as well as public organisations incur considerable expenses in collecting, evaluating, validating, exchanging and distributing information on these substances and preparations (called substance information throughout this paper).

High data volume: Databases with ten of thousands of substances and about 100 to 400 properties each (e.g. CAS-number, flashpoint, toxicology, first aid, ...) are not unusual. This means a typical volume of about 1 million items of information to handle.

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High data quality requirements: Data quality must be high in all respects since it is important in gaining users' acceptance. However, data quality is often poor. Important information such as test conditions may be missing. Legal information such as classifications and limit values are often not up to date. Substances are not properly identified. For instance, the substance information on "Benzol" may be else scattered in the records for "Benzol", "Benzen", and "1,3,5 Cyclohexatrien". Or records of different substances are merged – so you may find all information on "Schwefelsäure rauchend (smoking)" and "Schwefelsäure 10%ig" under "Schwefelsäure".

Meeting the demands of specific user groups: Substance information has to be prepared for specific user groups. For instance, firemen need precise instructions on how to act and not physical, chemical and toxicological numbers. For people at the workplace the MSDS (Material Safety Data Sheet) information has to be summarized in such a way that even a untrained worker is aware of the hazards and the safety precautions to be taken.

Legislation and different languages must be incorporated to serve users in different countries.

The **fundamental requirements** for software supporting the sound management of chemical information can be derived from the demands described above. They are:

1. Efficient and high quality substance data management with low costs of ownership (tools for operating centres)
    - Generic data structure for handling all types of substance information (properties) as well as that related to national regulations
    - Flexible tools to integrate newly collected information with existing information
    - Quality assurance methods and tools
    - Easy to explain and easy to implement data exchange interfaces permitting cooperation with other data providers

2. Flexible services for users (user applications)
    - Access via Intranet/Internet to minimize administration costs at users' sites (low cost of ownership)
    - Standard and multilingual user interfaces with access to all substance databases of interest
    - Efficient preparation of user specific information (considering the users' information requirements, local legislative background and language)
    - Flexible reporting features to meet national reporting obligations
    - Individual authorisation of user access to specific information
    - Billing of users for access to specific substance information

2. IGS – a Toolset for Sound Management of Chemical Information via the Internet

The IGS was initiated in 1988 by the Ministry of Environment of North Rhine-Westphalia and implemented with a budget of about 8 million Euro. Today IGS is available at more than 3000 workplaces. IGS is the German de facto standard for the management and retrieval of the public substance information pools with more than 150,000 substances and up to 400 items of information on each substance.

The National Operation Emergency Centre (NOEC), Zurich, supplies all Swiss cantons with IGS-substance information in 3 languages.

In industry IGS is widely used to ensure safety at the workplace as well as environmental protection and, last but not least, to assist fire brigades.

As figure 1 shows, the IGS system can be used in two different user environments, namely public authorities and companies.

Public authorities monitor companies to ensure that they comply with all legal requirements concerning the use of hazardous substances. In order to collect information on the most relevant substances and chemical products on the market authorities build cooperation networks and share work. One example is the GSBL project operated by all German federal states and the Federal Environmental Agency (Umweltbundesamt).

Companies have to assure legal compliance with respect to (only) those substances and intermediate products they produce and market. That may be one hundred or up to several thousand. However, data quality is vital and specific reports and documents have to be provided for internal purposes, customers and inspection authorities.

- Notification of new products according to chemical control legislation for all countries where they are to be sold
- Classification of company products (e.g. transport regulations ADR, IMDG, IATA; chemical control legislation based on EU directive 88/379/EEC and its amendments)
- Specific labelling of packaging for all countries where the products are sold
- Issue of Material Safety Data Sheets (MSDS)
- Specific instructions for workers (in Germany e.g. handling instructions according to TRGS 555)
- Exchange of substance information with customers, other sites and associated companies

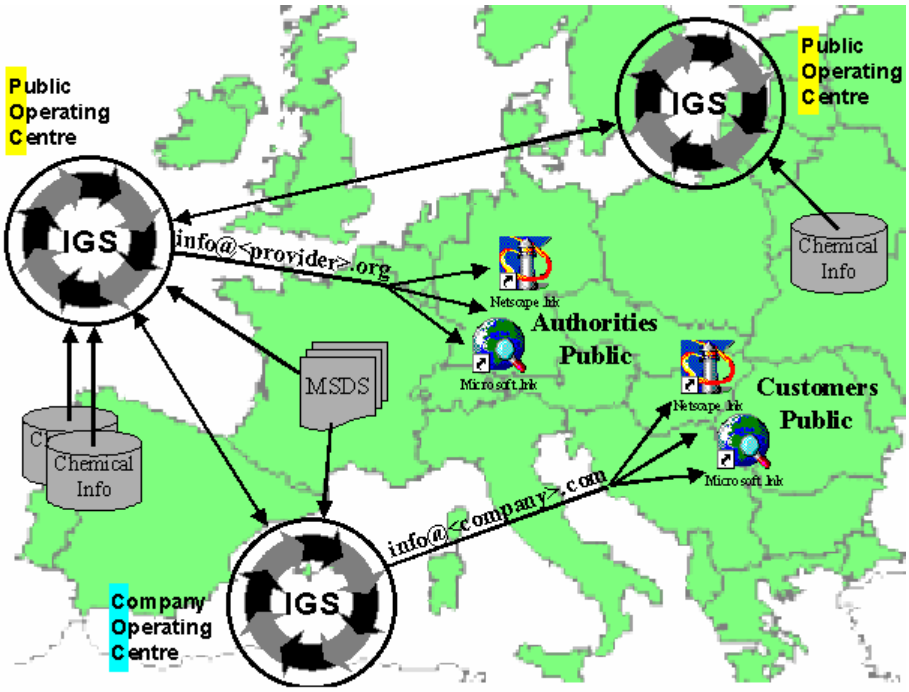

Figure 1
Central quality assurance of substance information via IGS operating centres and its distribution by the IGS user applications via Intranet/Internet

3. The IGS-Operating Centre Toolkit - in Brief

With respect to figure 1 the IGS-software serves two different purposes:

1. The IGS operating centre tool set supports the process of integration of substance information into a consistent database, its quality assurance and the compilation of user-specific databases.
2. The IGS user applications IGS-check and IGS-fire permit the retrieval of substance information at users' sites (more in section 4.).

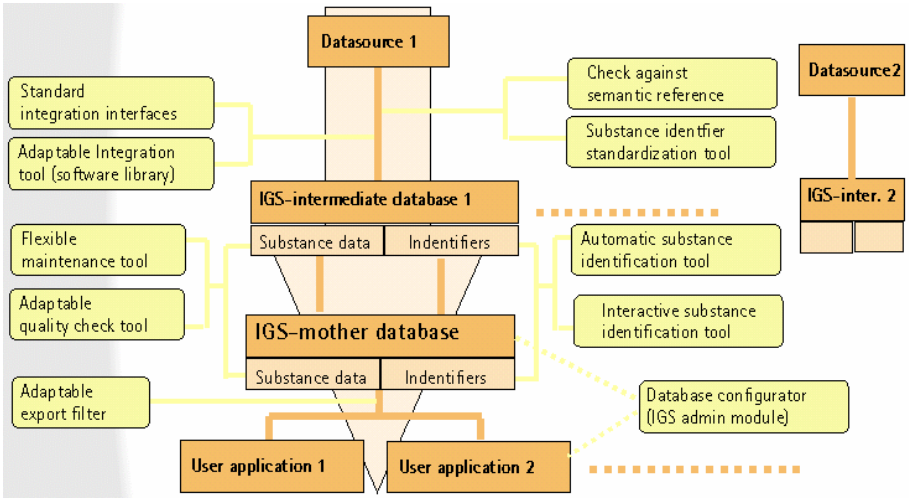

Figure 2
Information flow and tools within the IGS operating centre tool kit

The IGS operating centre toolset supports the integration of one or more external substance databases into one consolidated database ("IGS parent database") and via this into standard user-specific databases which are used for substance information retrieval (figure 2) The IGS concept satisfies the basic requirements for the sound management of chemical information as stated in section 1.

4. The Internet/Intranet User Application IGS-Check 4.0

More emphasis will be placed on the IGS-check 4.0 user application (Herrmann, 1998). This tool allows data retrieval from one or more substance databases provided by the IGS operating centres.

IGS-check 4.0 is based on a 3-tier architecture. Access to the substance databases is provided by the IGS servlet and ODBC or JDBC, respectively.

At the client sites the IGS-check 4.0 applet can be run with standard browsers. The required plug in with the "swing classes" can either be downloaded from the SUN Server or, more efficiently, from the users' in-house IGS Server. IGS-check 4.0 is also available with pure HTML output for organisations and companies with high Internet security requirements.

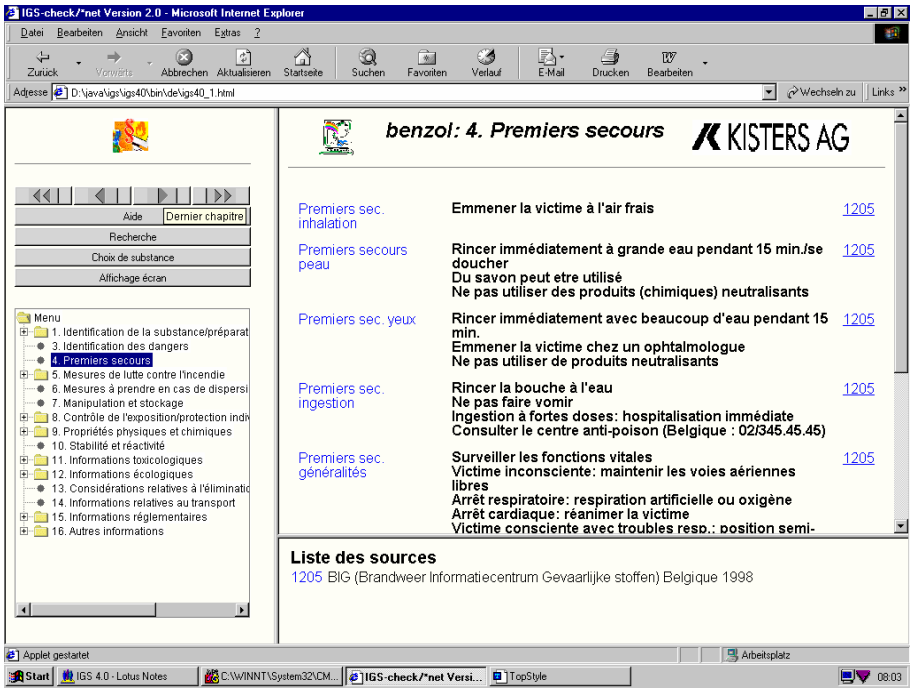

Figure 3
Dialogue box from the IGS check 4.0 Internet/Intranet user application (language flag set to French)

As figure 3. shows, IGS check 4.0 can access substance information in different languages. It is aimed to provide IGS-check 4.0 in up to 12 languages. Translation of the user interface and approximately 400 technical terms takes about 30 hours for each language.

The end user is thus able to switch between different substance databases and to set different views of the selected database. Each view may serve a specific type of user or a specific task, one of the requirements set out in section 1.

By using the GUI Builder PowerJ 3.0[3], trained users can implement separate windows for the presentation of substance information. The resultant JAVA classes can be easily integrated.

[3] PowerJ is a trademark of Sybase.

5. Recent Developments

Recent developments will make IGS-check more suitable for use in companies producing or processing substances or preparations. The following specific features already outlined in section 2 will be implemented in IGS.

- Issuing of Material Safety Data Sheets (MSDS) with any content, language and format
- Specific labelling of packaging with any content, language and format
- Specific instructions for workers with any content, language and format
- Exchange of substance information with any content, language and format

The implementation of these features is straightforward since the IGS database as well as the data IGS exchange interface have a generic design, resulting in a uniform information structure for each substance property (e.g. lethal dose or flashpoint).

The country-specific variations in content, language and format can be implemented by defining specific information profiles with aid of the IGS admin tool and appropriate HTML/XML frames or MS Word macros.

Despite the fact that MSDS information is stored in relational databases, electronic exchange of MSDS between producer and customer is still the exception. Therefore, hundreds of thousands of MSDS are released on paper and afterwards keyed in manually by the recipients. This underlines the need for an efficient integration toolset. According to figure 4 the integration process consists of 4 steps:

- Step 1: Registration of the MSDS by manually entry of about 10 parameters such as e.g. trade name, producer/importer, date of release. Based on this information, IGS-check will permit the existence of MSDS to be queried from remote sites via the Intranet/Internet.
- Step 2: Scanning and OCR (Optical Character Recognition) will permit an picture of the MSDS to be stored and allow full-text retrieval to a certain extent. This service can be charged e.g. at an annual flat rate.
- Step 3: Additional brief substance properties of high information value should be typed in. They may be legal classifications, limit values or physical properties. This information can be automatically transformed into user-specific statements.
- Step 4: More information is extracted to prepare instruction sheets for workers such as the German handling instructions according to TRGS 555. These documents offer high added value and may be charged per document.

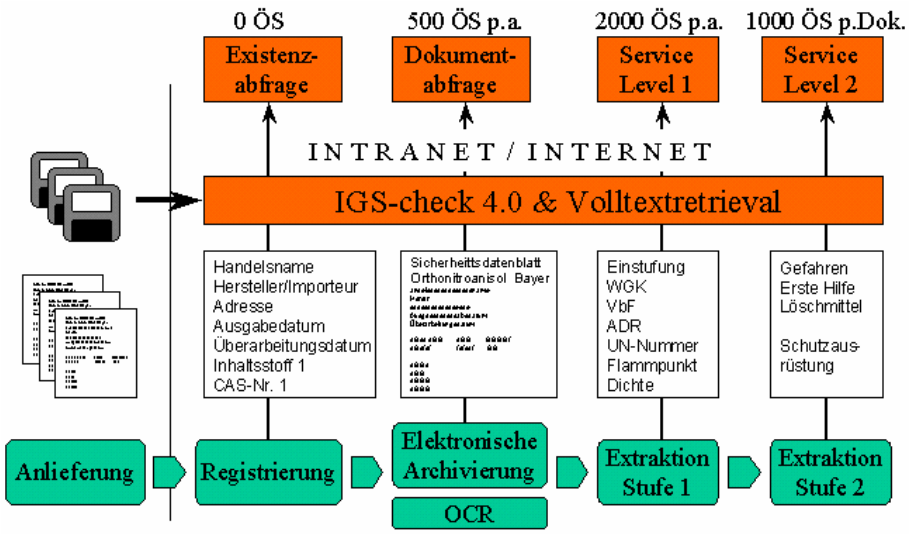

Figure 4
Concept for the integration of information from paper based MSDS

6. References

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