The NESSHY Hydrogen Sorption Properties Database

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1   Introduction

The final aim of NESSHY project is to identify the most promising solid storage solutions for such applications. To assess the potential of the various materials as hydrogen stores and to identify the most promising storage systems, it is important to have access to materials respective hydrogen sorption performance data and related information, and also to means for their comparison and evaluation. This is the need that the NESSHY hydrogen sorption properties database (NESSHY-DB) came to fulfil. It was built by the JRC-IE, as a tool to manage, store and exchange data and information from researchers between the different NESSHY laboratories.

Moreover, NESSHY-DB meets also a requirement of DG RTD, to have a permanent repository of the experimental results acquired by NESSHY, which could guarantee their availability beyond the time frame of the project.

1.1   State-of-the-art

To our knowledge there is only one other database dedicated to hydrogen solid-state storage publicly available on the internet. In 1995, G. Sandrock at the Sandia National Laboratory started a "On-line Hydride Database", in the frame of the Task 12 of the Hydrogen Implementation Agreement of the International Energy Agency (IEA-HIA) [1].The database was created as a literature reference service for the scientists in Task 12 and has grown up to almost 2000 hydride alloys and 1200 references. The Sandia database has not been updated in the last years, and its structure is optimised for classic metal hydrides only [2,3].

The NESSHY-DB is not in competition with the Sandia one. Objectives and structure differ considerably. This will appear clear in the detail in the following chapters. To mention here just some of these differences, NESSHY-DB can accommodate primary experimental data such as pcT, TPD and kinetics curves, and to respect intellectual property rights (IPR) issues, it offer scientists different access levels.

2   Description of the NESSHY-DB

2.1   Overview

The NESSHY-DB was built for the archiving, exchange and comparison of experimental results and material properties data generated in the NESSHY laboratories. The main driver was to ensure that all scientific and research data are available within the NESSHY Consortium .Therefore all data are organised centrally for maximising their usability, efficient management, exploration and ultimately conservation for the future. In addition, the tool had to facilitate the data exchange without compromising the confidentiality of the information. These requirements dictated the actual structure and functionalities of the database.

The NESSHY-DB is based on the JRC portal ODIN (On-line Data Information Network, https://odin.jrc.ec.europa.eu), which provides web-enabled access to a number of engineering and materials databases. These applications share fast cabling, firewall, secure connection, redundancy to guarantee high availability, central data and user management, common hard- and software infrastructure in order to facilitate maintenance and further development (see Figure 1). Further details on the JRC databases hardware and software system and structure can be found in general in references [4 and 5], while [6] describes the content of HIAD, the Hydrogen Incidents and Accidents Database developed in the frame of Network of Excellence HySafe.

The NESSHY-DB has been designed with an appropriate interface for data content, entry, retrieval and reporting. The database contains public and restricted data and has the necessary access control implemented via a central registration and login procedure. It offers also the possibility for data evaluation employing special graphical development environments. It is dedicated to experimental hydrogen sorption and thermo-physical properties data obtained on mainly new materials generated by the NESSHY participating laboratories. It also includes already published hydrogen storage material data and results from inter-laboratory comparison exercises run within the project for the data harmonisation and the development of testing protocols. The NESSHY-DB is currently restricted to partners only. It serves for data organisation, comparison, reporting and ultimately for the material down-selection, which feeds in the engineering task of the programme of work of NESSHY.
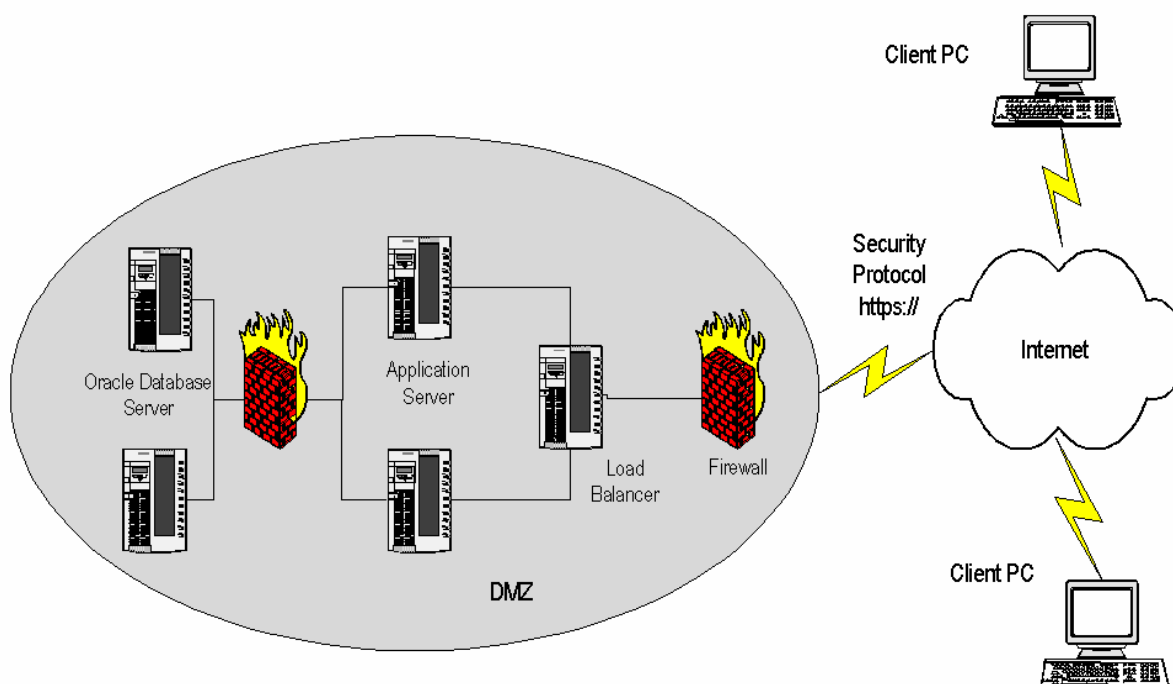
Figure 1:   Structure of the web-enabled JRC ODIN portal.

2.2   Database structure

The NESSHY-DB has basically three modules. The first two modules focus on experimental data produced in the various NESSHY laboratories. They comprise an experimental data retrieval module and a data upload module with a web-enabled interface for the direct remote upload of data. The third module serves as repository for the physical and engineering data as well as a structured collection of engineering data necessary for the design and construction of the solid-state storage tanks.

2.3   Access rights and handling of data

The database is built in such a way to ensure that different levels of access rights are possible and implemented to separate the confidential/restricted data from public data. The data owner decides which parties can access and enter data. There is also an option for the so-called 'power users' allowing them to manage their own sources. A method for "de-classifying" parts of data, as opposed to the whole source, to change from confidential to restricted or public has also been introduced. By default, all authorised users belong to the "NESSHY_Public Group". These members have "read rights" (can retrieve but neither write new data nor edit existing data) to all data sources that are identified as "read-accessible". If a data source is identified as "restricted" then no one apart from the data owner (or specific users following data owner's authorisation and an action by the administrator) can see its content. A "source" is visible to a user only if the user has read rights for this source. There is also a possibility for restricted write access rights, enabling the users retrieval and modification of data. For a group of users (for instance work package leaders within NESSHY) specific access rights/characteristics can be created. Every user can also belong to certain (sub)group(s) with extra privileges and access rights to restricted sources of data, which can be set as required and authorised by data owners. Access permissions apply to the whole (sub)group allowing for easier management.
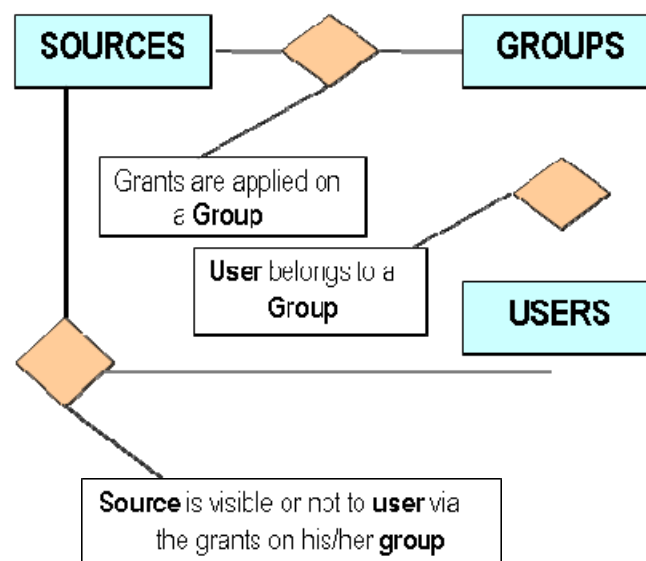

Figure 2:   Entity/relation diagram for NESSHY user authorisation.

Every organisation gets by default two data source folders/source identifiers for entering data – one where data which will be viewed by all authorised NESSHY users are placed and another source folder for confidential/restricted data. More Source folders can be created as required and following approval of organisation/company main contact person in NESSHY and their request to the DB administrator. Users belonging to one organisation are linked to the respective sources through confirmation by their organisation's main contact person in NESSHY. One or more users per organisation may also be assigned as data validators to control the quality of the data entered.

2.4   Intellectual property rights

Scientific data sharing and access to collectively generated data sets constitute important knowledge and their dissemination and management are essential for scientific progress but can also be quite sensitive and subject to Intellectual Property Rights. As stated earlier, for the time being the NESSHY-DB is restricted within the NESSHY Consortium. The platform, under which the database runs, its structure and operation, are JRC property. The general rules described under Article 9 on Intellectual Property Rights of the NESSHY Consortium Agreement hold for the access to, use and exploitation of the NESSHY DB. Ownership of and access to the data, information and knowledge entered in the NESSHY DB lie with the Contractor (Laboratory) that has generated the data. Any use or exploitation of these data must be directly requested from the respective Laboratory. In the near future, and pending the Consortium members' agreement, the NESSHY-DB will be released for use by the European research community.

2.5   Functioning of the NESSHY-DB

The NESSHY-DB database consists of a web enabled interface and three modules for remotely uploading, retrieving & managing data. The entry module allows uploading hydrogen sorption materials data, which can be retrieved via the retrieval module. The third module is dedicated to Physical & Engineering Parameters. The DB has an 'import/export' data feature and an elaborated 'advanced selection' option for retrieval, and good graphical data presentation. Introductory manuals dedicated to each module have been uploaded, along with online help screen shots with detailed instructions for every step.

3   Summary and Follow-up

The Novel Efficient Solid Storage for Hydrogen Database (NESSHY-DB) is a web-enabled tool designed and running under the JRC ODIN platform and it is currently at the disposal of the NESSHY Consortium. It was developed for storing hydrogen sorption test data generated on new materials, as well as literature available data and the results of inter-laboratory comparison exercises. A part from exchanging and conserving data and knowledge, it is a flexible and robust tool for managing and fully exploring experimentally derived information for assessing the performance of materials as potential hydrogen stores.

At the moment, the database is populated only with results from JRC and from the three NESSHY Round Robin Exercises. It has been made publicly available and is waiting for input from partners.

References

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