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The Web-enabled ODIN Portal Useful Databases for the European Nuclear Society

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ABSTRACT

Materials databases (MDBs) are powerful tools to store, retrieve and present experimental materials data of various categories adapted to specific needs of users. In combination with analysis tools experimental data are necessary for e.g. mechanical design, construction and lifetime predictions of complex components. The effective and efficient handling of large amounts of generic and detailed materials properties data related to e.g. fabrication processes is one of the basic elements of data administration within ongoing European research projects and networks.

Over the last 20 years, the JRC/Institute of Energy of the European Commission at Petten has developed and continuously improved a database for experimental materials properties data (Mat-DB). The Mat-DB database structure is oriented to international material standards and recommendations. The database and associated analysis routines are accessible through a web-enabled interface on the *On-line Data Information Network* (ODIN: http://odin.jrc.nl). ODIN provides controlled access to Mat-DB and other related databases (e.g. the document database DoMa) and thus allows European R&D projects to securely manage and disseminate their experimental test data as well as any type of supporting documentation (e.g. unfiltered raw data, reports, minutes, etc). Using the Internet project partners can instantly access and evaluate data sets entered and validated by one of the members.

This paper describes the structure and functionality of Mat-DB and gives examples how these tools can be used for the benefit of European nuclear R&D community.

1 INTRODUCTION

Fast access and exchange of materials data between research, design and manufacturing teams working on different sites worldwide is a challenging issue to be addressed during the product cycle in materials engineering [1]. Another important issue is safeguarding high investments made into materials research, which means that experimental data must be properly conserved, easily located and quickly retrieved. Materials databases (MDBs) are powerful tools to address these problems. Various categories of MDBs exist for different requirements, for example containing standards data on metallic alloys [2,3] and plastics [4]

or more complex database applications needed for the design analysis [5]. MDBs are also basic elements for establishing knowledge based and expert systems-

With the emergence of the Internet, the capability of MDBs has further increased. Webenabled MDBs provide a more centralized management and conservation of the data. Finding and accessing the required data is much faster than to search for them in a traditional manner, e.g. from handbooks or Microsoft Excel files. In particular the dissemination of research results has improved significantly, as the data are accessible over the World Wide Web. However, only few web-enabled materials applications exist at present on the market. Examples are the Materials databases of NIMS (National Institute for Materials Science) in Japan [6], which contain a lot of data but their web interfaces for data retrieval are still very limited. Currently, acceptance and use of web-enabled, publicly available MDBs is still hindered by problems such as lack of standardization, ease of handling and availability of free qualified data.

The JRC was considering these problems in the development of the database applications to support in particular European R&D projects in storing, accessing and evaluating materials data together with related documentation.

It is the objective of the paper to describe in detail the present status of JRC MDBs and planned activities to establish a European data network. Details of the features of the JRC MDBs have been described recently elsewhere [7]. Emphasis of this paper will be the introduction into the JRC Petten database applications for use in European R&D projects.

2 DATABASE FEATURES

The JRC has been developing two material databases for safeguarding and managing its experimental materials data resulting from in-house research some 20 years ago [8,9]: Alloys-DB and Corrosion-DB. Alloys-DB covers mechanical and thermo-physical properties data of engineering alloys at low, elevated and high temperatures for base materials and joints [10]. It includes e.g. irradiation materials testing in the field of fusion and fission, tests on single crystals with thermal barrier coating for gas turbines and mechanical properties testing on a corroded specimen. Corrosion-DB refers to weight gain/loss data of high temperature exposed engineering alloys, ceramics and hot isostatic pressed powder materials and covers corrosion tests such as oxidation, sulfidation and nitridation. The extension to other types of corrosion is under consideration. Alloys-DB and Corrosion-DB have been recently merged to Mat-DB. The database structure of Mat-DB has continuously grown and the application developed from the initial mainframe database without graphical user guidance, over stand-alone PC and client/server applications to the new web-enabled application (see section 3). All current applications use an identical database structure simplifying data exchange between the JRC and its external MDB partners. The commercially available Mat-DB is being used as standalone PC or client/server applications by a number of European industry and research organizations to manage their in-house experimental test results. The Web-application is at present installed only at the Petten Server. Updates and further developments are presented and discussed during annual user meetings with these customers.

Mat-DB is designed for experimental data, which is delivered by the laboratories in defined formats and quality. The emphasis is on data from tests, which comply with existing or pre-normative standards. The data can be entered, stored and accessed with typical database routines and can be evaluated with integrated analysis tools.

The Mat-DB entities (see Table 1) contain detailed meta-information and entry of many fields is mandatory to increase data quality. Thesauri are provided for many text and image

fields facilitating and improving standardization during data entry and retrieval. All entities contain additional fields (customer internals), which can be used for company-specific purposes. In addition to the numerical and alphanumerical data, any type of binary files can be stored within the database, for example final reports of R&D activities, drawings or large amounts of raw data (unfiltered curve data, basic output of strain gauge measurements). In total, the database structure for base materials contains more than 130 tables and 1850 fields, which are grouped into logical entities: *data source*, *material*, *specimen*, *test condition* and *test result* (see Table 1). The entity 'test result' is divided into different areas, which contain tables for storing test type specific mechanical (23) and thermo-physical (10) properties and corrosion data (see Table 2).

Table 1: Description of Mat-DB entities

Entity	Meta-information for e.g.
Data Source	Organization, laboratory, scientist, R&D project
Material	Material characterisation, chemical composition, heat treatment, process data, microstructure (joinings need a 2 nd material entity)
Specimen	Sampling, orientation, type of specimen, geometry, coating layers
Test condition	Test environment, mechanical or thermal pre-exposure, irradiation
Joining	Process method, joining parameters, joining geometry, filler metal
Test result	See table 2

Table 2: Mat-DB test result entity

MECHANICAL PROPERTIES	• IRRADIATION
• CRACK GROWTH & FRACTURE	Irradiation creep
Creep crack growth	Swelling
Cyclic creep crack growth	• TENSILE
Fatigue crack growth	Compression
Fracture toughness	Multiaxial tensile
Impact	Uniaxial tensile
• CREEP	Small punch tensile
Cyclic creep	THERMO-PHYSICAL PROPERTIES
Multiaxial creep	Density
Torsional creep	Electrical resistivity
Uniaxial creep	Emissivity
Small punch creep	Linear thermal expansion
• RELAXATION	Poisson's ratio
Multiaxial relaxation	Specific heat
Uniaxial relaxation	Shear modulus
• FATIGUE	Thermal conductivity
High cycle fatigue	Thermal diffusivity
Low cycle fatigue (load control)	Young's modulus
Low cycle fatigue (strain control)	CORROSION
Thermal fatigue	High temperature corrosion
Thermo-mechanical fatigue	

3 WEB-ENABLED MAT-DB

The emergence of the Internet created new opportunities for materials databases. Therefore the JRC has recently ported Mat-DB to the Internet. Objectives of the web-enabled application are:

- Facilitating data management, exchange and dissemination within European R&D projects,
- Providing a data pool which contains public and restricted data for use in industry, research and education,
- Providing the web-enabled Mat-DB to interested multi-national organizations and customers for exchanging confidential data to authorised members via their Intranet.

The final goal of JRC is to provide the full cycle of data entry, retrieval and analysis over the Internet, as it is available in the PC and client/server applications. Furthermore it is planed to network with partners in order to increase both, the amount of available data and the tools for analysing the data. The following sections describe in detail the features of the webenabled Mat-DB.

3.1 Data entry and exchange

Mat-DB provides web-enabled data entry from the machine into the database for European project and network partners (see figure 1) by using XML (eXtensive Mark-up Language). XML is an established standard to exchange data over the Internet between organisations having dissimilar structured databases or between machines and databases. Data are not only assigned by their values but also by their names and units. The nomenclature of the field names within Mat-DB is compatible with the standard MATML (www.matml.org), a library developed by the international materials society and maintained by NIST (US: National Institute of Standards and Technology).

Post processing tools of the machines, which are extended to export into the defined XML format, can transfer the test data in a random order into Mat-DB because the application recognises and applies the data to the assigned database fields. Source, material, specimen, test condition and joining meta-information can be completed within separate steps. The whole data sets can be checked, updated and validated before they are uploaded into the relational database part and released for clients. Such an XML based data entry procedure [11] with a user-interface similar to the PC client is pilot tested within the running European R&D project "TMF-Standard" [12].

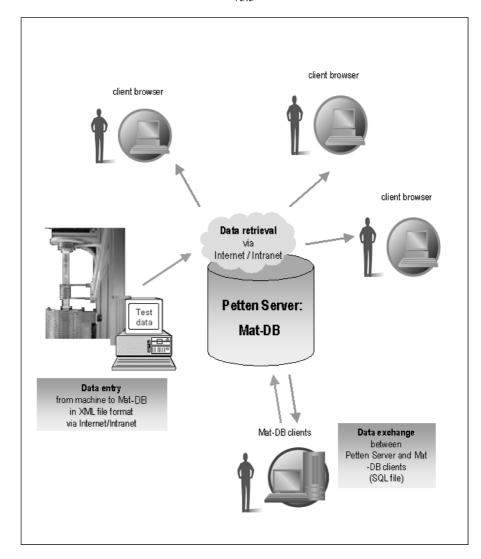


Figure 1: Data flow from machine into Mat-DB

3.2 Data retrieval and analysis

The user interface for web-enabled data retrieval follows the lines of the well-established stand-alone PC and client/server applications, although it is slightly less sophisticated due to the limitations of the HTML protocol [13]. It allows constructing a query to retrieve the test results in three sequential levels. The first level starts with mandatory selections on *source*, *test type* and *material* following a hierarchical order. Data retrieval can then be continued with optional selections of a so-called *combined material*, which characterizes special features of the material such as service exposed, irradiated, low carbon, etc., *batch identifier*, *specimen* (type) and (test) *environment*. Retrieval can be finished with optional selections on test type specific fields such as *time at rupture*, *test temperature*, *elongation* in the case of *uniaxial creep*.

After the mandatory fields have been specified the *Generate report* button is active allowing the user to create an overview report on the selected material tests. The report contains links to detailed information on e.g. source (including documentation), heat treatment, chemical composition, raw data sets or numerical and graphical curve information. Furthermore the report screen allows exporting the selected test data to pre-defined EXCEL charts or starting routines for analysing the test data.

Mat-DB contains a number of the test-type specific analysis routines, which allow a fast evaluation of the retrieved data. The evaluation programme library (see table 3) contains mathematical models, constitutive equations, parametric expressions and regression functions. The analysis routines allow a comparison of data sets against each other. Database customers often use the analysis results for their publications and reports [14]. For the web-enabled application the analysis routines are re-programmed and implemented as Java applets, i.e. the analysis routines together with the selected data are downloaded onto the client PC and then run locally as fast and highly interactive desktop programmes. They allow user specified extrapolations and interactive manipulations to add or delete data points. Currently, only the Larson-Miller analysis routine is implemented. Within 2005 most of the other analysis routines shown in table 3 will be implemented into the web-enabled Mat-DB as Java applets. The materials parameters calculated by the analysis routines are necessary for inelastic analysis calculations of high temperature exposed components. Figure 2 shows a 2nd order polynomial Larson-Miller extrapolation. Triangular symbols belong to the dissimilar welded joint X10 CrMoVNb9 1/ X20 CrMoV12 1 – dj, the rectangular symbols to the similar welded joint X10 CrMoVNb9 1 – sj.

Table 3: JRC Petten MDBs evaluation programme library

Creep

Creep relations: Norton creep law, Prandtl creep law, Soderberg creep law, Monkman-Grant relation, Dobés-Milîcka relation

Extrapolation methods: Larson-Miller, Manson-Haferd, Manson-Brown, Orr-Sherby-Dorn, Spera, Minimum commitment method

Constitutive creep equations: Theta projection, Mc Vetty equation, Kachanov equation

Interpolation routines: Polynomial creep curve fit, Polynomial stress dependence, Isochronous & isostrain determination

Fatigue

Ludvik law, Manson-Coffin relation, Basquin analysis, Frequency modified Manson-Coffin relation

Crack growth

ASTM compliant creep crack growth analysis, Creep crack growth plot, Fatigue crack growth analysis

HT Corrosion

Weight gain/loss analysis: Power law, Power law-time, Parabolic $\Box m^2$, Parabolic $t_{1/2}$, Kp(t), Breakaway

In addition to the existing database analysis routines, the JRC is currently integrating **Fitit**, - proprietary software of the Fraunhofer Institute in Germany designed for the calculation of complex material models. **Fitit** can be used for models defined as a set of differential equations and analytic functions, e.g. Chaboche and Kachanov. Data selected within the web-enabled Mat-DB can be sent to **Fitit**, which then fits the data to a selected model. Once the model parameters have been calculated, they are returned to Mat-DB and the user can apply them for Finite Element (FE) lifetime calculations of high temperature exposed components with commercial codes like ABAQUS or ANSYS [15], which improves safety and reliability and saves costs.

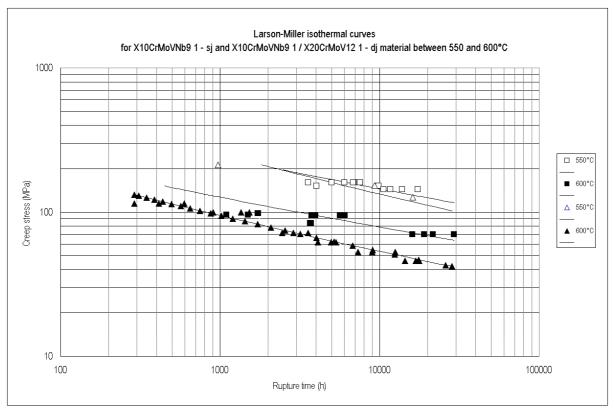


Figure 2: Larson-Miller extrapolation of a Siempelkamp data set: Similar (X10 CrMoVN b9 1 – sj: triangular symbols) and dissimilar (X10 CrMoVNb 9 1/ X20 CrMoV 12 1 – dj: rectangular symbols) welded joints

4 DOCUMENTATION DATABASE DOMA

The web-enabled Mat-DB is deployed to the ODIN portal (http://odin.jrc.nl), which provides access to various web-enabled database applications for engineering and nuclear safety. In order to facilitate maintenance and further development the applications share central data and user management, professional hard- and software infrastructure and powerful, redundant and secure database servers for the storage of data and documents. They are continuously maintained and updated to the need of customers.

One of the ODIN applications which complements Mat-DB by providing controlled access to any kind of supporting documents is the documentation database (DoMa). DoMa is a web-enabled digital document repository designed to enhance the dissemination of information amongst the R&D community in the energy sector. Any type of electronic record (i.e. publications, minutes, spreadsheet, graphic, etc.) may be stored. Documents are organized in a hierarchical structure as in any standard file system with folders and subfolders and document retrieval is controlled through access rights: a public document can be retrieved by any registered user, a confidential document requires that the user has been granted specific access rights for the document. Document upload and administration of access rights is delegated to the responsible persons of the various projects, i.e. each project can upload their documents and control the access their area remotely via the DoMa web-interface.

Since Mat-DB and DoMa share a common user management, it is possible to synchronise access to protected areas in both databases, i.e. a user who has access to protected numerical data in Mat-DB can transparently access the corresponding documentation in DoMa and vice-versa.

5 BENEFIT FOR EUROPEAN MATERIALS PROJECTS

The intention of JRC as a supra-national institution is safeguarding high investments made into European materials research and to conserve the knowledge. As one way in achieving this goal, the JRC offers Mat-DB and DoMa to European R&D projects and other European groups and committees as a free tool to manage and exchange their experimental data and documentation, similar to the Japanese 'Data Freeway', which was set up to exchange data between several research centres [16]. European R&D participants, who are supported by public funding, are encouraged to release their data for public access at the end of the project. Thus, the project benefits from a sophisticated web-enabled database for the management and conservation of materials data and related documentation. The European research community may benefit from the availability of valuable data and analysis routines.

Mat-DB contains the experimental properties data, which are filtered, smoothed, reduced, etc. A complex thermo-mechanical fatigue test for instance could run depending on the loading conditions several hundred or thousands cycles. To store all of them would slow down even the most powerful database. Therefore usually only some specific cycles together with hysteresis information (usually reduced to 200-300 data points per hysteresis) are stored in a database. But, if necessary, also the raw data sets can be stored as binary objects in Mat-DB. A project partner can conserve for example his original EXCEL file and all other partners who have access rights can then open this file within a Mat-DB retrieval session. Moreover documentation related to the data sets such as final reports can be stored directly in Mat-DB. On the other hand project related information such as publicly available project description, e.g. a link to the website and confidential documentation such as reports accessible only for a chosen group of customers (confidentiality level 1) and minutes of project meetings (confidentiality level 2) can be stored in DoMa. Project coordinator can enter the documentation in DoMa and determines the access rights. If somebody would request any access to the confidential parts the project responsible receives a mail and can make his decision. DoMa and Mat-DB are linked with each other. Having logged-in in Mat-DB the user can retrieve documentation from DoMa and vice versa. The access rights together with password and user identification are administrated in the ODIN application server.

The web-enabled Mat-DB provides access to public, restricted and confidential materials data and documentation from former and current European R&D activities and from extensive material programmes, e.g. the German High Temperature Reactor Programme [17]. It currently contains a pool of public and restricted data with approximately 25000 materials tests. Public and restricted data sets are released only after agreement by the data owner; confidential data sets are accessible by the project participants only. The quality of data is the responsibility of the laboratory where they have been generated. JRC does not take any liability for the data. Offering a broad range of materials data together with the analysis options and related documentation would make the ODIN platform a an address of interest both for research and industry. However, proprietary data are often very sensitive and/or the data owners invested significant resources for testing the materials. Therefore they do not want to release the data without any return. In such a case, the ODIN portal may act in future as a tool for exchange of materials data and documentation over the Internet or could act as data warehouse [18] for European groups and committees, which retain full control over their own data.

6 SUMMARY AND CONCLUSION

Material databases (MDBs) are important and powerful tools for the conservation, exchange and dissemination of data. The potential has even further increased with the emergence of the Internet. The availability of experimental materials data in a defined and traceable quality is necessary for structural integrity and inelastic analysis calculations or complex materials modelling. In combination with FE calculations lifetime predictions can result in a much better use of high temperature exposed components, which improves safety and reliability and saves costs. Therefore the European engineering community should be very interested in conserving valuable data and documentation and in establishing an evergrowing data pool promptly accessible via the Internet.

The JRC has a long history of developing material databases and can offer a mature web-enabled Mat-DB to manage mechanical, thermo-physical and corrosion properties data. The database has a complex structure and includes detailed meta-information on the *material*, *test condition*, *data source* etc. Mat-DB and the related analysis routines are installed on a powerful and secure server within the On-line Data Information Network (ODIN: http://odin.jrc.nl). The application is offered at no charge to support European R&D activities as well as European groups and committees for the management and conservation of their experimental materials data and the project participants are encouraged by the EU to release their data for public access at the end of the project. Data owners who invested a lot of money for testing the materials and intend to sell restricted materials data and documentation over the Internet could use ODIN to form a materials data warehouse.

Since ODIN is a central portal to a series of its activities, the JRC intends to ensure a long-term continuation of the related applications including maintenance and further development of the web-enabled Mat-DB and DoMa. The structure of Mat-DB, for instance could be upgraded to include additional material groups such as polymers, ceramics and composites. New test types will be added as required. The web-enabled Mat-DB will be further developed to include the entire cycle of data entry from machine to database, data retrieval and analysis.

REFERENCES

- [1] Advanced Engineering Materials Vol. 4, 2002, Nr. 6, pages 317-416: Special Issue "Materials and Process Selection", WILEY-VCH Verlag GmbH &Co KgaA, Weinheim
- [2] Plantfacts Database of the German VDEh (Verein Deutscher Eisenhüttenleute German Iron and Steel Institute): http://www.vdeh.de/deutsch/arbeit/informat/plantfe.htm
- [3] WIAM®-METALLINFO database, IMA-Dresden: http://www.ima-dresden.de/deutsch/startde.htm
- [4] Materials Databases of MBase, Aachen, Germany: http://www.m-base.de/main/en/index.html
- [5] MSC.Mvision Databanks, USA: http://www.mscsoftware.com
- [6] Materials Databases of NIMS National Institute for Materials Science, Japan: http://mits.nims.go.jp/db top eng.htm

- [7] H.H. Over, E. Wolfart, W. Dietz, L. Toth, "A web-enabled materials database to support European R&D projects and network activities", Advanced Engineering Materials, August, 2005
- [8] R.C. Hurst, H. Kröckel, H.H. Over, P. Vannson, "The Use of Models in Materials Databanks", Materials 88 Materials and Eng. Design, The Institute of Metals, London 1988
- [9] H. Kröckel, H. H. Over, "The Need for an European Approach to Materials Characterisation and Data Management", International Symposium on Advanced Materials for Lightweight Structures, ESA –ESTEC, Noordwijk, Netherlands, March 1994
- [10] H.H. Over, J. H. Rantala N. Taylor, W. Dietz, "A materials properties database approach to cover welded joints", 2nd International Conference on Integrity of High Temperature Welds, London, UK, 10th 12th November, 2003
- [11] M. Nagy, H.H. Over, A. Smith, "XML related Data Exchange from the Test Machine into the Web-enabled Alloys-DB", 19th International CODATA Conference, "The Information Society: New Horizons for Science", Berlin Germany, 7th - 10th November 2004
- [12] Thermo-mechanical fatigue the route to standardisation', CORDIS R&D project no. GRD2-2000-30014
- [13] H.H. Over, E. Wolfart, E. Veragten, "Data Retrieval and Evaluation within the Webenabled Alloys-DB", 19th International CODATA Conference, "The Information Society: New Horizons for Science", Berlin, Germany, 7-10 November 2004
- [14] P.J. Ennis, "Candidate Materials for a Modular High Temperature Reactor Power Plant in Engineering Issues in Turbine Machinery, Power Plant and Renewables", editors A Strang, R.D. Conroy, W.M. Banks, M. Blackler, J. Leggett, G.M. McColvin, S. Simpson, M. Smith, F. Starr, R. Vanstone, Maney, IoM3 Publications, Book Number B0800, ISBN 1-904350-20-8, 2003, pp 1029 – 1037
- [15] R. Mohrmann, V. Denner, T. Hollstein, "'Zur Lebensdauervorhersage von Austenit-Ferrit-Mischverbindungen"', Tagungsband FDBR Düsseldorf (2003) Teil 4
- [16] M. Fujita, Some Trials on WWW Servers in the "Data Freeway", Scientific Data in the Age of Networking, 15th International CODATA Conference, 29 September - 3 October 1996, Tsukuba, Japan
- [17] Endbericht zum Verbund-Forschungsvorhaben des BMFT, "Auslegungskriterien für hochtemperaturbelastete metallische und keramische Komponenten sowie des Spannbeton-Reaktordruckbehälters zukünftiger HTR-Anlagen", Teil B: Metallische Komponenten, KFA Jülich, August 1988
- [18] Y. Li, "Building The Data Warehouse For Materials Selection in Mechanical Design", Advanced Engineering Materials 2004, 6, No. 1 2, pp 92 95