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The web-enabled database of JRC-EC, a useful tool for managing European Gen IV materials data

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Abstract

Materials and document databases are important tools to conserve knowledge and experimental materials data of European R&D projects. A web-enabled application guarantees a fast access to these data. In combination with analysis tools the experimental data are used 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 data with regard to properties related to e.g. fabrication processes, joining techniques, irradiation or aging is one of the basic elements of data management within ongoing nuclear safety and design related European research projects and networks. The paper describes the structure and functionality of Mat-DB and gives examples how these tools can be used for the management and evaluation of materials data of European (national or multi-national) R&D activities or future reactor types such as the EURATOM FP7 Generation IV reactor types or the *heavy liquid metals cooled reactor*.

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 [6].

With the emergence of the Internet, the capability of MDBs has further increased. Web-enabled 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 EXCEL files. In particular the dissemination of public 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 National Institute for Materials Science (NIMS) in Japan [7], which offer a lot of data but their interface guidance is still very limited. Currently, acceptance and use of (web-enabled) MDBs is still hindered by the following problems:

1. Many organizations use proprietary MDBs, which are customized to their requirements and internal practices. The structures of the databases are not standardized and therefore interoperability and data exchange between different organisations is difficult.
2. Data entry and validation are necessary but time-consuming tasks in order to ensure high-quality data. Often, scientists do not invest the required time to store the data in MDBs, instead they keep them in simple EXCEL sheets or other customised formats.

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3. Materials data from publicly funded R&D projects are not sufficiently made available in electronic format. Therefore immediate access to free, public data sets is limited.
4. Industrial companies often hesitate to make their experimental data freely available; publications often contain limited information (e.g. on material processing details) and experimental information on product specific features is difficult to retrieve.
5. It is the objective of the paper to describe in detail the present status of the JRC MDB and the aim to establish a European materials database for future reactor types such as the EURATOM FP7 Generation IV reactor types or the *heavy liquid metals cooled reactor*.

2. Database description and structure

The JRC has been developing the material database Mat-DB for safeguarding and managing its experimental materials data resulting from in-house research some 20 years ago [8,9]: Mat-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 irradiation materials testing in the field of fusion and fission, tests on thermal barrier coating for gas turbines and mechanical properties testing on a corroded specimen. Corrosion part 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. The database structure 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. All current applications use an identical database structure simplifying data exchange between the JRC and its external MDB partners. Mat-DB is being used as stand-alone PC or client/server application by a number of European industry and research organizations to manage their in-house experimental test results. 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.

In order to conserve as much information as possible, the database contains detailed meta-information and entry of many fields is mandatory to increase data quality (see Table 1). Thesauri are provided for many text and image fields facilitating and improving data entry and retrieval. All entities contain additional fields (customer internals),

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
Specimen	Sampling, orientation, 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

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 also Table 1). The entities are linked within a relation table. For tests on dissimilar joints, e.g. weldments a *joining* and also a second *material* entity are added. 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).

3. Web-enabled Mat-DB

Mat-DB of JRC Petten is deployed to the secure ODIN (*O*n-line *D*ata *I*nformation *N*etwork) Portal: (http://www.odin.jrc.ec.europa.eu). The ODIN portal provides access to various web-enabled database applications for engineering and nuclear safety. The applications share fast cabling, firewall, secure connection, redundancy to guarantee high availability, central data and user management, professional hard- and software infrastructure in order to facilitate maintenance and further development, e.g. ORACLE as a powerful RDBMS, and professional database servers with high capacity Raid Arrays for the storage of data and documents. They are continuously maintained and updated.

Final reports of R&D projects, drawings of any format and the whole project documentation including minutes of meetings can additionally be stored in a structured manner (e.g. public and confidential areas) in the related web-enabled documentation database DoMa and linked to project specific data sets.

One of the motivations for developing Mat-DB and DoMa was to provide fast access to public and confidential data sets together with other documentation on the Petten Server and help to conserve, manage and analyze data of

Table 2
Mat-DB test result entity

Mechanical properties
Crack growth and fracture
Creep crack growth
Cyclic creep crack growth
Fatigue crack growth
Fracture toughness
Impact
Creep
Cyclic creep
Multiaxial creep
Torsional creep
Uniaxial creep
Small punch creep
Relaxation
Multiaxial relaxation
Uniaxial relaxation
Fatigue
High cycle fatigue
Low cycle fatigue (load control)
Low cycle fatigue (strain control)
Thermal fatigue
Thermo-mechanical fatigue
Irradiation
Irradiation creep
Swelling
In-pile relaxation
Tensile
Compression
Multiaxial tensile
Uniaxial tensile
Small punch tensile
Thermo-physical properties
Density
Electrical resistivity
Emissivity
Linear thermal expansion
Poisson's ratio
Specific heat
Shear modulus
Thermal conductivity
Thermal diffusivity
Young's modulus
Corrosion
High temperature corrosion

European R&D consortia. Just by opening their browsers any authorized partner can immediately access and evaluate data sets entered and validated by other partners.

The final goal of JRC is to provide the full cycle of data entry, retrieval and analysis over the Internet. Furthermore it is planned to network with partners in order to increase both, the amount of available data and the tools for analyzing the data.

The JAVA programmed user interfaces and evaluation routines are further developed and improved. On-line help assists in using the applications. Manuals for describing the databases and the analysis tools including e.g. descriptions of image and text thesauri, curve file structures, definitions of the test types are available for Mat-DB users from the ODIN portal.

3.1. Data entry and exchange

The JRC aim is direct web-enabled data entry from the machine into Mat-DB for all European projects and network partners by using XML (e*X*tensive *M*ark-up *L*anguage). 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: *N*ational *I*nstitute of *S*tandards and *T*echnology).

Tools within the Mat-DB allow users to convert their data into XML providing they are available electronically in a database or a spreadsheet. Once correctly formatted in XML the upload into Mat-DB is fast and easy because the data are correctly identified and transferred to Mat-DB. The same is valid for post processing tools of the machines, which are extended to export into the defined XML format. Source, material, specimen, test condition and joining metadata can then manually be completed within separate steps. The metadata can be linked to uploaded tests results. The completed data sets can be checked, updated and validated before they are uploaded into the relational database part and released after validation for clients. The XML based data entry procedure [11] for base material is meanwhile pilot tested within the running European R&D project 'TMF-Standard' [12]. The joining part will be implemented until end of 2007.

Fig. 1 shows the 'Specimen geometry and production' data entry screen. The yellow fields are mandatory. Alphanumeric expressions such as shown in the figure for the field 'Standard' are available from a thesaurus and can be selected from a text box. Unique specimen types can be selected from an image thesaurus. New expressions can be added to the thesauri. The data are automatically checked against constraints. Only after validation by the source responsible the data can be retrieved by other assigned users. Fig. 2 shows the XML code for the entered expressions shown in Fig. 1.

3.2. Data retrieval and analysis

The web-enabled data retrieval user interface follows the principles 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*,

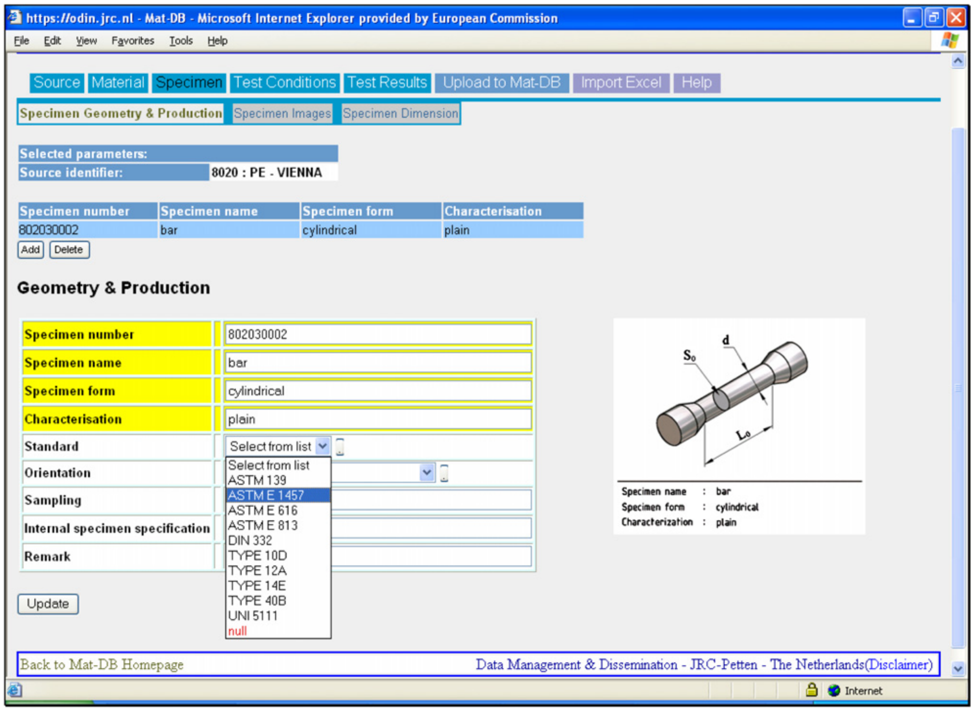

Fig. 1. Mat-DB screenshot showing specimen details for data entry.

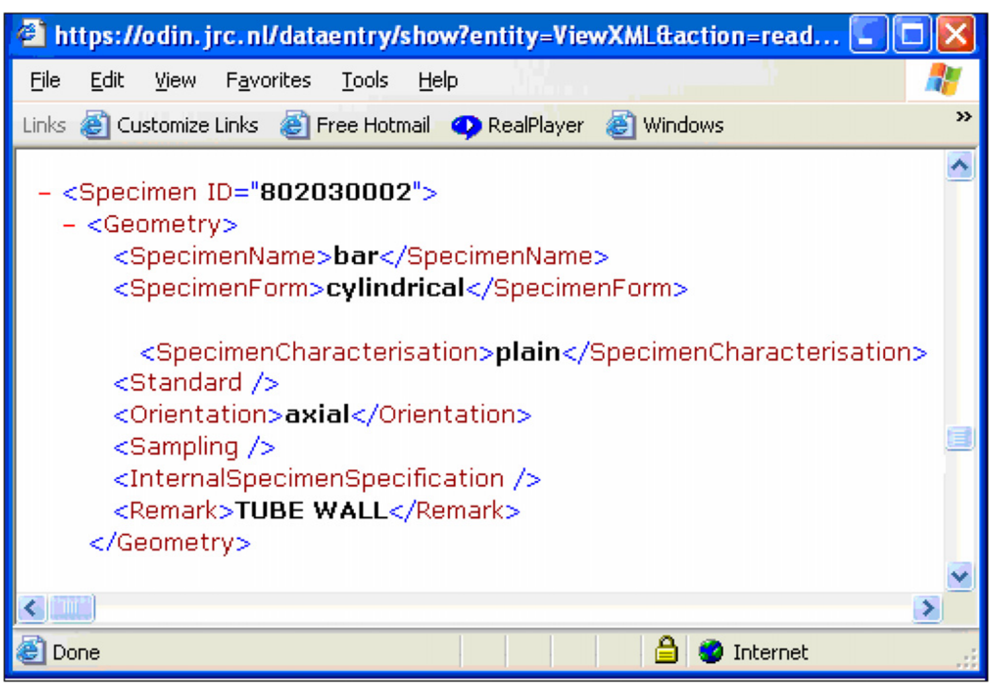

Fig. 2. Mat-DB screenshot showing XML text for entered specimen details.

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 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]. The analysis routines are re-programmed with Java and implemented into the Mat-DB web-application, but they can also be used independently of Mat-DB. The data can be uploaded directly from the clients PC following a simple XML related transfer procedure.

Currently, most of the creep programmes shown in Table 3 are implemented. The implementation of all other analysis routines should be finished by the end of 2007. The materials parameters calculated by the analysis routines are necessary for inelastic analysis calculations of high temperature exposed components. Fig. 3 shows Norton creep law results for 10 CrMo 9 10. The programme calculates numerically the temperature-dependent Norton parameters for the time at rupture and the laboratory as well as the calculated minimum creep rate. The laboratory minimum creep rate is the creep rate which has been entered by the data owner, the calculated minimum creep rate is automatically analysed by Mat-DB software by using a *seven point fitting method* as defined by ASTM E 647 while entering the creep curves. The evaluation programme library is shown in Table 3.

In addition to the existing database analysis routines, the JRC has integrated *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, which improves safety and reliability and saves costs.

Table 3
Mat-DB 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 and 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 Δm^2, parabolic $t_{1/2}$, $Kp(t)$, breakaway

4. Generation IV data management

As documented before Mat-DB and DoMa are very suitable for Generation IV data and document management and therefore part of the FP7 knowledge preservation strategy. Mat-DB provides access to public and confidential materials data. Confidential data sets are accessible by the related project participants only; they can be released into the public domain only after agreement by the data owners. The quality of validated data is the responsibility of the laboratory where they have been generated. JRC does not take any liability for the data.

Confidential Mat-DB data sets are for instance data of former German High Temperature and Fast Breeder Reactor programmes [15,16], which could be of interest for new reactor types as well as also the IAEA pressure vessel data. By managing these data pools Mat-DB has shown that it is a valuable platform with the right structure to handle nuclear related materials data which have to take into consideration irradiation and/or joining details. Taking that experience into consideration JRC as a supra-national institution is planning to create a Generation IV database for JRC owned experimental materials data and offer this data management to all European Generation IV R&D activities. The EURATOM FP7 Generation IV programme is related until now to the following six reactor types:

- Sodium fast reactor
- Lead fast reactor
- Gas fast reactor
- Very high temperature reactor
- Supercritical water reactor
- Molten salt reactor

Following a proposal of DG-RTD JRC will create separate entries to guarantee a straight user controlled access to these pools within Mat-DB. This procedure is similar to the IAEA policy. Nobody else but assigned IAEA members can see their data.

European FP7 R&D projects which refer to the six reactor types can use Mat-DB free of charge. By including JRC in their projects they have only to pay for the administrative Mat-DB work (user access control, creating individual data entry pools, data check, etc.) and for necessary project related updates and upgrades. They do not pay for server costs and maintenance. Additionally they can store all their documentation within DoMa. The access to data and

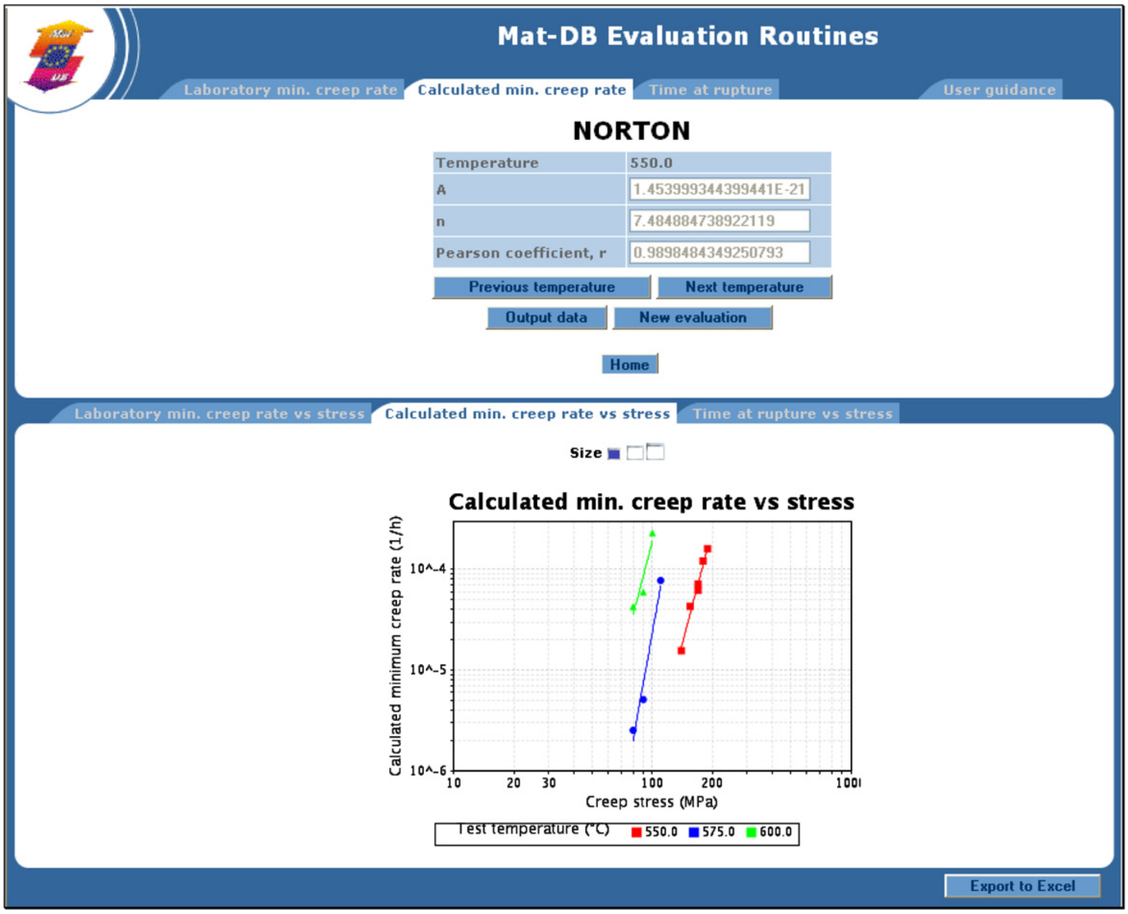

Fig. 3. Screenshot of Norton creep law results for 10 CrMo 9 10.

documentation can directly be controlled and administrated by the project responsible via Internet for project members who have registered at ODIN. The whole JRC policy is also for European (national or multi-national) R&D activities in general and it covers therefore also the *heavy liquid metals cooled reactor*.

5. Summary

The web-enabled Mat-DB is a state-of-the-art database for experimentally measured mechanical and thermo-physical properties and corrosion data of engineering alloys at low, elevated and high temperatures for base materials and joints. It is implemented within a powerful relational database management system and installed within a secure server portal which guarantees access control. Mat-DB offers the whole cycle from data entry via data retrieval to data evaluation. Additionally public and confidential project related data and documentation can be administrated in DoMa. Together Mat-DB and DoMa are very suitable for Generation IV reactor materials data and document management and therefore part of the FP7 knowledge preservation strategy.

European FP7 R&D projects which refer to the Generation IV reactor types or to the *heavy liquid metals cooled reactor* can use Mat-DB free of charge. By including JRC in their projects they have only to pay for the administrative Mat-DB work (user access control, creating individual data entry pools, data check, etc.) and for necessary project related updates and upgrades. They do not pay for server costs and maintenance. Additionally they can store all their documentation within DoMa. The access to data and documentation can directly be controlled and administrated by the project responsible via Internet for project members who have registered at ODIN.

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