Accelerate new green steel technologies by combined usage of knowledge bases and simulation

Dominik Zügner**, Sabine Zamberger**, Uwe Diekmann*, Alex Miron*, Petra Becker*

*Matplus GmbH, Hofaue 55, 42103 Wuppertal, Germany
**voestalpine Forschungsservicegesellschaft Donawitz GmbH, Leoben, Austria

Summary

The main future challenge for the steel industry and users is to manage the trade-off between the demands of agility and demographic change and technological renewal. A potential solution is the expansion of classic digitization, which has so far consisted of ERP (order processing), PLM (product development) and MES/BDE systems (production control). This extended digitalization integrates the topics of materials technology, manufacturing processes and energy together with the associated knowledge management into the IT infrastructure of the enterprise. In addition to the collection and processing of data, this includes the creation of knowledge that contributes to fact-based decision-making as a model library. A key aspect is to understand and to model the evolution of steel properties along the processing chain.
An overview of a new digitalization environment is given, which supports the holistic optimization of materials, processes, energy flows. It is practically in use at voestalpine to accelerate the development of new green technologies.

Key Words
Digitalization, materials databases, material modelling; processing chain, flow analysis, time series

Introduction

Agility is required to master the technological change to a decarbonized future in a competitive manner. Demographic change will further increase the shortage of skilled professionals. Brain drain becomes obvious when existing know-how simply evaporates into retirement, and it takes too long to train the next generation. Active knowledge management is a way to both conserve know-how and shorten the ramp-up time of new staff [1].

Decision support and streamlining of engineering processes require the availability of knowledge. Knowledge to be made available to the right users covers documents, reports, and data of past projects. It is a good practice to link such knowledge islands to materials master data, which are in turn linked to reference databases.

Even more important is the representation of scientific models, which represent materials and physical processes in a logical and objective way, so that they can be a substitute for measurements and experiments. Data-driven models are based on exploratory analysis of time series data supported by basic physics.

Such time series cover multiple scales, long periods to assess the entire production with regard to their ecological impact, processes and flows of specific production batches as well as very short periods of highspeed materials characterization.

The evolution of materials properties along the process chain can be optimized regarding cost functions for alloying elements and energy. This is the foundation of a holistic optimization of materials, processes, energy and can accelerate the implementation of green steel technology.

Matplus EDA® is an infrastructure that combines a scalable database, mathematical functions, and visualization capabilities in an extensible multi-user environment [2]. It is currently in use at several customers as a backbone for materials engineering and covers the use cases depicted in Fig. 1.

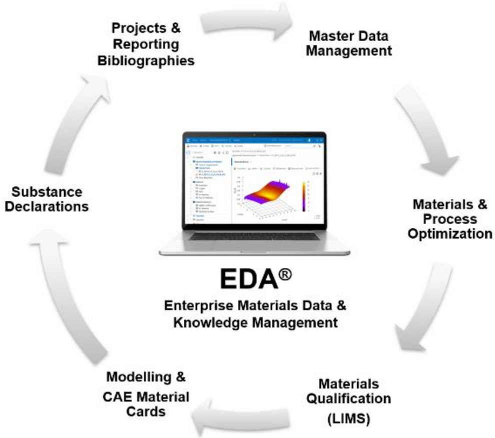

Figure 1: Digitalization environment Matplus EDA® for materials, processes, and energy

Voestalpine is an Austrian producer of high-quality steel and uses the EDA system with a focus on research and development. This includes the expansion of the master data system to include data from material simulation with JMatPro® and Matcalc®. Together with the evaluation of data from sophisticated material tests and process data, this infrastructure is used to accelerate the optimization of material technologies.

Master data management & reference databases

Material master data is an important core for practically usable knowledge management. Standard reference data, cross-references, classifications, models, and information from characterization projects are linked to them. Master data is formally released and used in production. All development activities aim to improve master data - the number of new revisions of master data released is a metric for the performance of research and development. Minimizing master data records can lead to a reduction in complexity - and thus improve resource efficiency, e.g. through more efficient casting sequences. Electronic workflows are used to control the release, revise, and withdrawal of master data.

The reference database Stahldat SX, which is maintained by the European Steel Registration Office within the framework of the VDEh, is an important component of the knowledge base of the material master data system. In addition to the official European material numbers and designations with their data, Stahldat contains an extensive knowledge base:

- A knowledge base consisting of all FOSTA research reports in full text
- All technical standards by VDEh, like SEP, SEW, SEB, etc.
- Textbooks, like the Atlas of Heat Treatment

Moreover, the system holds digitized test data and models which can be used in CAE applications:

- Thermo-physical data [3]
- Flow-curve models, created by IMF, TU Freiberg [4]
- CCT, TTT diagrams from [5] and other sources
- Hardenability models according SEP 1664 [6]
- Sheet steels data according SEP 1640 [7]

Figure 2 shows an exemplary materials data record of Stahldat SX in Matplus EDA®. Data is organized in a multi-tag structure, so that a single alloy can be present in multiple location of the knowledge tree (left side). The right side shows the table of content of the record. Multiple materials can be selected for comparison of data. This involves automated overlay of curves, which are graphical representations of underlaying data.

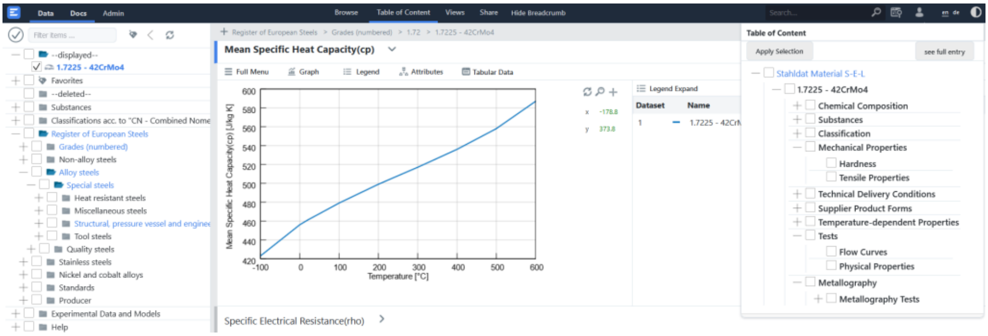

Figure 2: Exemplary record of 1.7225 – 42CrMo4 in Stahldat SX

Flow curves and Jominy curves are represented as mathematical models (equations) in Stahldat SX based on experimental work. Matplus EDA® allows the parametrization of such models in a user-friendly manner.

Figure 3 shows the exemplary variation of the hardenability of a CrMnB-alloy as function of C-content. A specific regression model is available for different steel groups. A

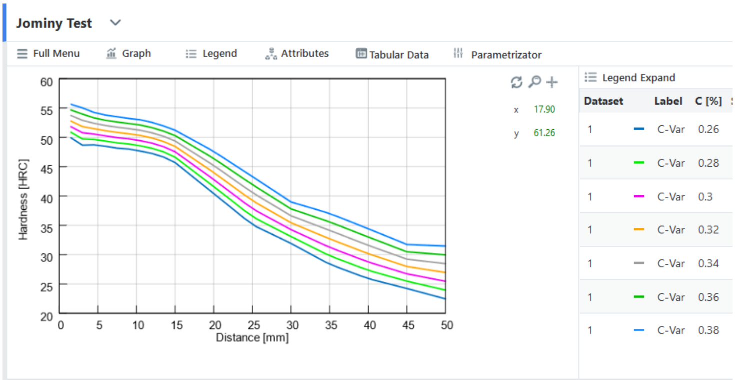

Figure 3: Exemplary parametrized hardenability model in Stahldat SX according SEP 1664 [6]

Stahldat SX is used as a solution template for the master data system, and, in addition, the content is linked to the company materials. The master data system at voestalpine is extended by data from materials simulation using JMatPro® and Matcalc®. All master records are enriched by calculated materials information for the target composition as well as lower and upper bound:

- TTT/TTA diagrams
- Thermo-physical properties
- Jominy curves.

The data can be accessed by users with the right permissions and can be used for comparisons to material tests and other practical work like processing of inquiries.

Lab information management and evaluations

In the past information from materials testing was evaluated on a project base and mainly focused on data needed for certificates. The new integrated approach of laboratory information management includes the storage and evaluation of raw test data from the testing devices using the database backed Matplus EDA®. Lab orders and associated test series are bundling the individual tests as shown in Figure 4.

By that even big material qualification projects can be stored and evaluated. The projects are linked to the central master data, so that results can easily be located. Tests are stored as parametrized arrays to represent time series data for force, displacement, stress, strain. The entire data format is JSON and is therefore suitable for a long-term readability by humans and machines.

Mathematical functions allow automated evaluations, e.g., to create true stress – true strain curves from the raw data. In a further integrated processing step the curve data can be fitted to plasticity models, like Johnson Cook and Zerilli Armstrong. Several such pre-defined equations can be used and modified as templates for own research work.

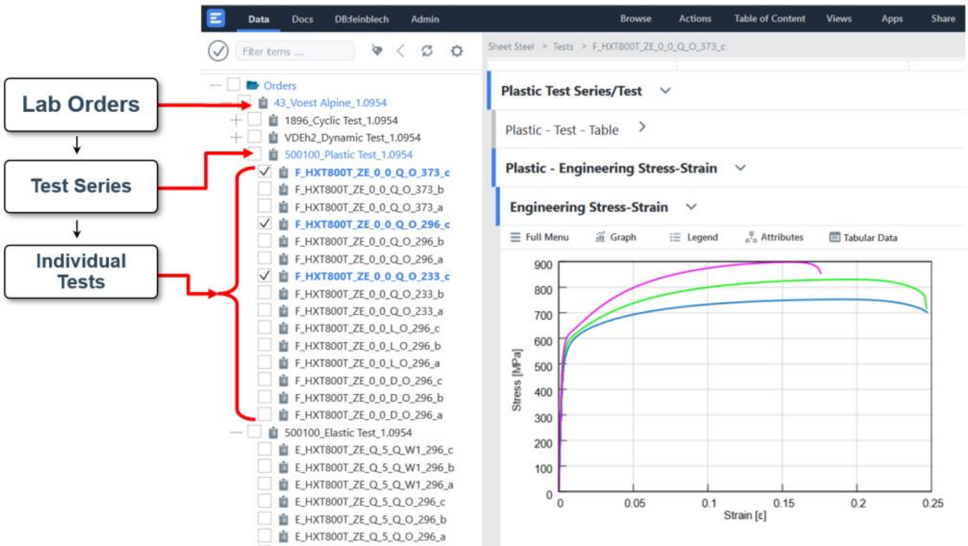

Figure 4: Laboratory information with raw test data are represented as time series with multiple views

A more complex example of the evaluation of the CMOD curve of a fracture toughness test according to ASTM E399 / EN13674-1 is shown in extracts in Figure 5. For the determination of the necessary parameters of the KIC value, in this special case various case distinctions are made by the system based on the course of the curve with "pop-ins" which are also determined automatically, but which can also be changed manually by the user in the evaluation process. The validity checks based on the criteria specified in the standard is made transparent; any non-compliance can be indicated immediately by means of a "mouse-over". In addition, a query is made for user-controlled entries that cannot be determined from the machine data.

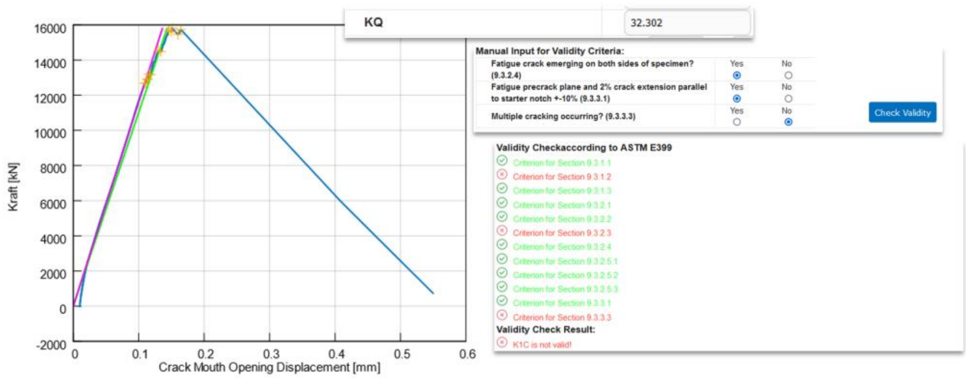

Figure 5: Automated evaluation of a CMOD curve including validity checks

Process data and time series

Knowledge of the development of material properties over the entire process history is a prerequisite for holistic optimization. Until now, the measurement of properties in material qualification projects has been carried out using attributive descriptions of the processes. this is limited to qualitative data combined with selected default values [8].

The new approach pursued here is the mapping of concrete and complete process histories as linked time series with all information on temperature, casting and forming history. Analogous to the material flow analysis, the systematic separation between processes and flows is carried out. Processes contain the respective time series for production orders - flows are used to map mass and energy balances and the optional link to material qualification projects, as shown in Figure 6. By that the materials testing is linked to all upstream data starting from the melt.

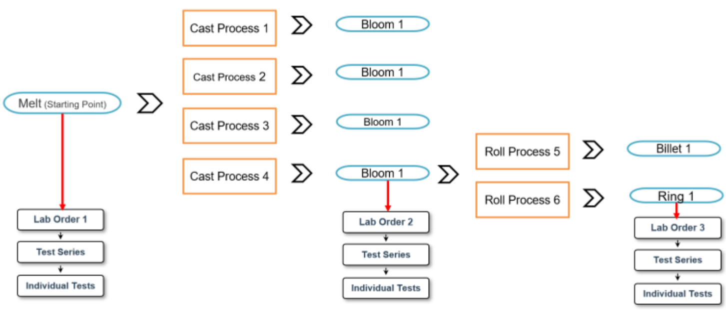

Figure 6: Exemplary process flow with linked lab orders

The underlying data model thus describes a graph or an ontology that puts the time series of the various objects into an evaluable semantic context. In the structure browser, this ontology can be visualized interactively in both directions - upstream and downstream, as shown in Figure 7.

Figure 7: Visualization of the process chain with flows and lab orders.

Based on the semantically linked structure, the data can be consolidated and evaluated at selectable stages of the process chain. As an example, figure 8 shows the temperature-time history from the final annealing to the walking beam furnace.

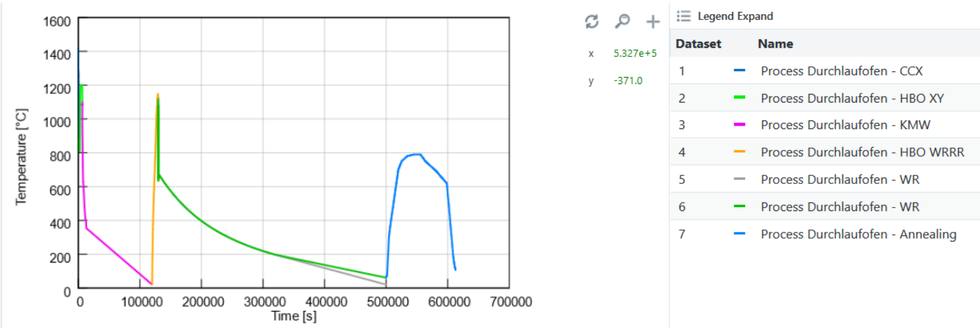

Figure 8: Exemplary consolidation of time series data after annealing

Such consolidated information can then be used for modelling, using different types of exploratory data analysis, ranging from statistical methods to AI methods, e.g., neural networks or random forest trees.

Conclusion

Materials knowledge management is more than maintaining catalogues. Integration of lab information, material simulation, material cards for CAE alone has business impact:

- Development processes can be accelerated because the correct versions of the relevant information can be found more quickly. Consistent material cards and material tests are easy to locate and related to master data.
- Costs for semi-finished products can be reduced. Reduction of complexity is possible, which leads to an aggregation of quantities, and the adaptation of delivery specifications.
- New employees become productive more quickly and can make better decisions using a corporate materials knowledge base.

Furthermore, the environment shown for the holistic optimization of materials and their properties, including process sequences, is a particularly suitable combination for accelerating new green steel technologies at voestalpine.

References

[1] G. D. Oreggioni *et.al.*., „Climate change in a changing world: Socio-economic and technological transitions, regulatory frameworks and trends on global greenhouse gas emissions from EDGAR v.5.0“, *Glob. Environ. Change*, Bd. 70, S. 102350, Sep. 2021, doi: 10.1016/j.gloenvcha.2021.102350.

[2] U. Diekmann, A. Miron, und A. Trasca, „Hybrid Modeling of Materials Properties for Improved CAE-Simulations“, in *Materials Science Forum*, Trans Tech Publ, 2016, S. 163–166.

[3] F. Richter, „Die physikalischen Eigenschaften der Stähle ‚Das 100 - Stähle - Programm'“. 2010.
[4] M. Spittel und T. Spittel, „2 Flow stress of steel“, in *Metal Forming Data of Ferrous Alloys - deformation behaviour*, H. Warlimont, Hrsg., in Landolt-Börnstein - Group VIII Advanced Materials and Technologies, Springer Berlin Heidelberg, 2009, S. 23–56.
[5] F. Wever, A. Rose, W. Peter, and W. Strassburg, *Atlas zur Wärmebehandlung der Stähle, Bd. 1*. Verlag Stahleisen, 1954.
[6] VDEh, *Supplement to SEP 1664: Determination of formulas by multiple regression for the calculation of hardenability in the face quench test from the chemical composition of steels (4th ed.)*. 2013.
[7] VDEh, *SEP 1240: Testing and Documentation Guideline for the Experimental Determination of Mechanical Properties of Steel Sheets for CAE-Calculations*. 2006.
[8] R. Schnitzer, D. Zügner, P. Haslberger, W. Ernst, and E. Kozeschnik, „Influence of alloying elements on the mechanical properties of high-strength weld metal“, *Sci. Technol. Weld. Join.*, Bd. 22, Nr. 6, S. 536–543, Aug. 2017, doi: 10.1080/13621718.2016.1274095.