ISSN 2070-0482, Mathematical Models and Computer Simulations, 2015, Vol. 7, No. 2, pp. 95–102. © Pleiades Publishing, Ltd., 2015.
Original Russian Text © V.V. Belikov, N.P. Vabishchevich, P.N. Vabishchevich, U.V. Katishkov, N.A. Mosunova, 2014, published in Matematicheskoe Modelirovanie, 2014, Vol. 26, No. 8, pp. 20–30.

Material Property Database

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Received June 19, 2013

Abstract—Based on the analysis of the existing software products, the experience and use of the computational codes on the nuclear power stations' (NPPs) safety analysis, the general requirements for the database on the properties of the materials used in nuclear power engineering are set forth. The architecture and the database on the properties of materials and the database management system with support of the user friendly graphic interface have been developed. The unified mechanism to use the database software products based on dynamically linked libraries is implemented. The paper presents an overview of the major functional opportunities and description of the key components of the developed database.

Keywords: database, material properties, user friendly graphic interface, functions library, nuclear engineering

DOI: 10.1134/S2070048215020027

INTRODUCTION

The modern systems of the engineering design and modeling (CAD/CAE systems) belong to the class of the general application software and include separate software modules to work with databases on the properties of materials. Within the user-friendly interface, the user has the possibility to choose the right material with certain properties for particular elements of design and to use these properties in the design-theoretical substantiation of his technical solutions.

The research calculation programs (codes) as a specialized applied software support are focused on solving a number of narrower tasks of numerical modeling, but also need to provide the properties of the materials. The task to create a unified modern database (DB) on the properties of the materials used in nuclear engineering is important and urgent, as the data on the thermophysical, physical-mechanical and chemical properties of materials are fundamental for the correct calculation and theoretical evaluation of the serviceability of nuclear power plants both under normal operating conditions and in case of accidents.

The task of finding and assessing data on the properties of materials is achieved by the creation of a new software system. It is particularly important to use the unified values of the properties of materials in software systems, which are ingredients of the integral computational codes that provide continuous automated calculation of the sequence of events and phenomena characterizing different operation modes of the object of simulation.

The analysis of the basic existing native and foreign databases, such as those of the Joint Institute for High Temperatures (JIHT), Russian Academy of Sciences (RAS) [1], THERPRO International Atomic Energy Agency (IAEA) [2], Material Property Database (MPDB), [3], Mat/PRO (Paulin Research Group, United States) [4], and WaterSteamPro (Moscow Energy Institute (MEI) (Thermodynamic Modeling (TM)), Russia) [5] makes it possible to conclude that to date there has been no unified native database which has the properties of the nuclear fuel, heat carriers, moderators, and other materials used in the field of nuclear engineering. The creation of a unified DB requires the development of a system of database control (SDBC), having a user-friendly graphic interface for editing, adding, search, mapping, and output of information in a convenient format. It is also necessary to provide a unified mechanism of the use of database in software products, including integral codes for analysis and substantiation of the safety of atomic power stations (APSs).

The purpose of this work is to collect, analyze and create a unified database on the properties of materials used in atomic power engineering, developing a system of DB control with the support of a user friendly graphic interface as an independent software product having all of the above-mentioned possibil-

ities and creating a joint mechanism of the DB application of software products as dynamically connected libraries of the calculation functions.

We consider here the basic principles in the database creation by the properties of materials, functional content and the user-friendly graphic interface in the DB management. We provide also a description of the libraries of calculation functions, whose data source is unified DB, as well as the basic principles in the use of libraries for calculation functions in the calculation codes. The first version of the unified database by the properties of the materials in the graphic-friendly interface was developed at the Institute of Nuclear Safety (INS), RAS, within the Creation of the Concept and Technology for the "Virtual APS with a Water-Moderated Power Reactor" project.

1. FILLING THE DATABASE

The properties of materials for the unified DB were selected after expert analysis and appraisal. In collecting the information on the properties of materials with account for DB specialization (materials used in the atomic engineering) the following principles were used:

—the properties are to include both the generally accepted (thermophysical, transport, physical-mechanical, dielectric) and specific ones used in simulating ongoing processes in the APS. For example, the yield of gas fission products, swelling speed, and emissivity;

—preference was given to the data from organizations working in the field of nuclear engineering;

—each property in the database shall contain a reference to the data source;

—the properties of water and steam must comply with the latest recommendations of the International Association on Water and Steam Properties (IAPWS).

The database was filled using the following key sources:

1. The data base of the Institute of Nuclear Safety, RAS created within project 3078p in affiliation with The French Alternative Energies and Atomic Energy Commission (CEA), France) [9, 10].

2. The data base of the calculation code, The System of Codes for Realistic Analysis of Severe Accidents (SOCRAT) [11].

3. THERPRO – the data base of the International Atomic Energy Agency (IAEA) [2].

4. INSC Material Properties Database—the database on the properties of materials of the International Atomic Safety Center, the United States [12].

5. IHTANTERMO—the database of thermodynamic properties of individual materials (JIHT RAS) [1].

6. Material Properties Database (MPDB), United States—the database of general purpose materials properties [3].

7. Standards of the International Association on Water and Steam Properties (IAWSP) of 1997 with supplements of 2007 [6] and tables created on their bases [7].

8. Other open literature, for example, [13–22].

At present the DB of the properties of materials used in the field of atomic engineering contains 180 materials and about 2500 properties. All the materials are divided into nine groups:

- incondensable gases;
- moderators;
- protective materials;
- construction materials;
- absorbing materials;
- oxidation products;
- heat carriers;
- fuel;
- elements of the Mendeleev periodic system.

The database is continuously updated according to the current queries of applied mathematic modeling. It is possible to create a user database that allows you to create a specialized database for a specific calculation code and to conduct experiments with a custom database without violating the unified database.

2. USER-FRIENDLY GRAPHICAL INTERFACE

The current database management system is executed in a modern graphic user interface, providing easy and convenient access to the database to look up, analyze, and select the desired information.

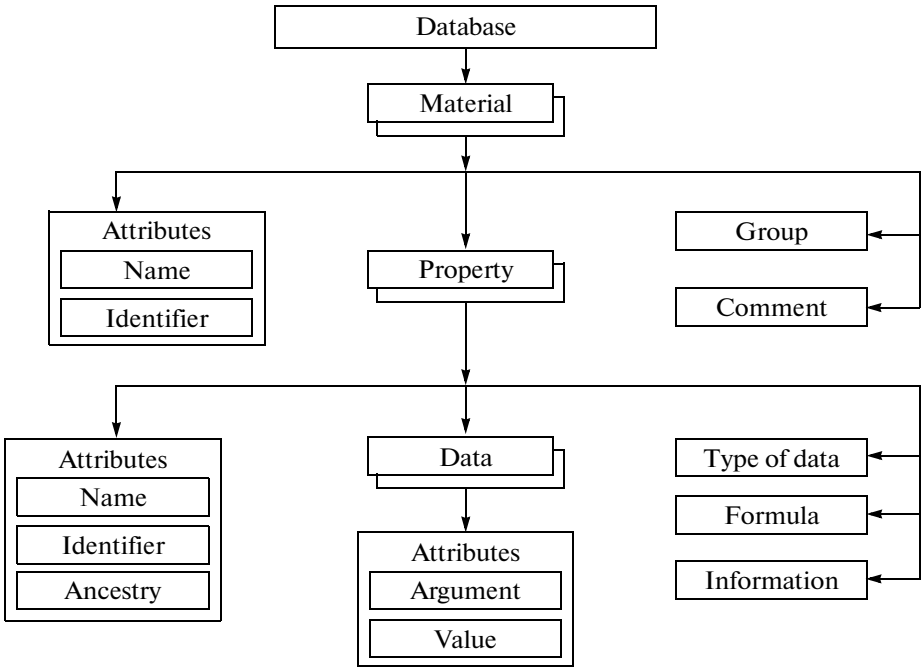

Fig. 1. The XML structure of the file.

The requirements for the graphical interface have been formulated based on the analysis of domestic and foreign databases [1–7] on the properties of materials used in the field of nuclear engineering and the experience in the development and use of computational codes for the safety analysis of nuclear power plants. The interface must provide the following possibilities:

- data editing (to add, delete, and modify the materials, properties, and the data presented in the form of formulas, tables, or constants);
- the graphical presentation of the dependence of the selected property on the argument;
- processing the formulas by the formula analyzer (parser);
- creating tables with the given parameters and saving them in various formats;
- the import of tables from the text documents to the database;
- the calculation of the current property by using the built-in calculators (rapid assessment of the correctness of the data entry);
- the graphical analysis of the properties taken from various sources;
- the printer outputs of the contents of the database with varying degrees of detail, and also of the created tables and graphs;
- the calculation of the properties of water in the formulation of the IAPWS.

In the overwhelming number of cases, using the formula analyzer eliminates the need for writing functions for each equation and describing the dependence of the property on the argument. As the parser, the freeware software product, muParser [8], was selected with its rather high data processing rate.

For DB storage and operation, the eXtensible Markup Language (XML) format was chosen. Taking into account that DB is hierarchical, the XML application allows easy extraction of the required data by means of the existing tools, for example, Document Object Model (DOM). Besides, XML has convenient tools for the input, output, export, and import of the data and is a universal format for the exchange of information between different, even incompatible, systems. The XML structure of the database file by material properties is shown in Fig. 1.

The scheme of the databse can be divided into three basic levels of hierarchy (Fig. 1). The first level is the level of the material having all of its required parameters: name, unique identifier within the total database, the group of the material, and the comments, as a rule, containing the basic properties under standard conditions.

The second level is the level of the property that is a sublevel of the material. It includes information of the property such as the name, a unique identifier within the table of the properties of the present material, type of data (table or formula), and the formula's dependence of the present property on the argument(s)

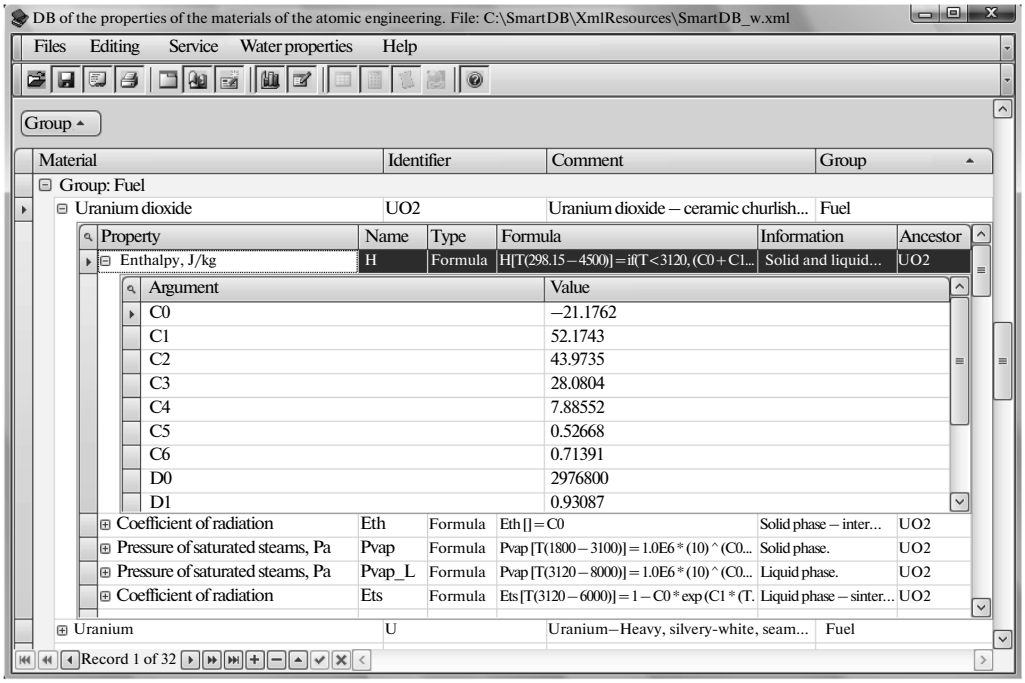

Fig. 2. The graphic interface of the database.

in the format of the analyzer of the formulas. In addition, the level of the property has a reference to the identifier of the material, which makes it possible to easily find the necessary node of the property in the XML file by means of the existing tools, for example, DOM, as well as brief information on the present property, necessarily including the data source.

The third level is the level of data, which is the sublevel of the property. It has no more than two parameters and is designed for storage of the data on the present property. For the tables, such data are the value of the argument and the value of the property, and for the formulas they are the formal presentation and the value of the coefficients in the equation.

The user-friendly graphic interface of the database is written in the C# language, with the use of specialized components that have a wide set of functions for working with the tables and DB. The main window of the program (Fig. 2) has the following components:

- the name with an indication of the loaded XML file with the database;
- main menu bar;
- tool palette;
- the workspace that displays the multilevel table of the unified database;
- navigator for managing the database records: movement, insertion/deletion of a line in the current table, entrance/exit from the editing mode.

The work area is a series of nested tables corresponding to the respective chosen scheme (Fig. 2)

- table of materials is the main table having the characteristic of the present material;
- the table of properties is built-in with respect to the main table of the present material and includes in itself the property's parameters;
- the data table is built-in with respect to the table of properties and serves as the input of both the data table and the data for the formulas.

The main menu of the program includes the following items:

- *Files* containg the standard operations in the work with files and the items on installation of the operating, print, and the database export modes.
- *Editing* has the full set of functions on filling and editing the unified database.
- *Service* is the derivation of the dependence graphic of the present property on the argument. Creation of tables with the given parameters for all the materials, except water.
- *Properties of water* is the creation of tables with the assigned parameters, determination of the basic properties of water and steam in the one-phase and two-phase domain by means of calculators.

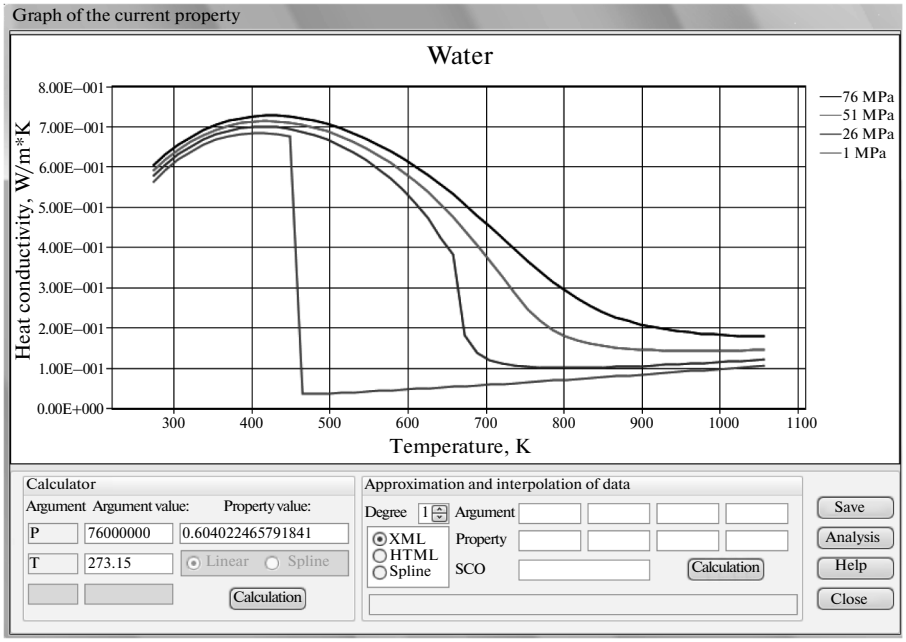

Fig. 3. The graph for the water heat conductivity.

• *Help* is the reference system of the database. Now we consider some items of the basic menu in more detail. *Editing* includes the following subitems:

To add a property is the addition of a new property to the present material. In the open dialog box, the user just has to select the desired property from the descending list and select the data type, table, or formula. If the desired property is absent from the list, it is necessary to select "Other", then to edit the name and the identifier of the new property. The constants are entered as formulas with one coefficient. If the desired material is not available, it is necessary to preliminarily add the material to the database using the navigator.

• *To insert data from the file* is the import of discrete values from a text file to the data table of the present property. This mode makes it possible to considerably reduce the time needed to import the data table.

Possibilities of editing the database such as the addition of new material and the addition or withdrawal of a line from any table are performed by use of the navigator. All the items of the Editing menu and the navigator control buttons are accessible only in the mode of database editing.

The menu item *Service* implements the basic service capabilities of the graphical interface and contains the following subitems*:*

• *The graph of the present* property is the derivation of the dependence of the of the chosen property on the argument. The opening dialog window has, besides the graph, a calculator for determining the value of the property at the given value of the argument, and makes it possible to graphically compare the data obtained from different sources. There is also a possibility to approximate the table data by a linear, square, or cubic polynomial and construct an interpolation spline. Figure 3 provides as an example the graph of the dependence of the water heat conductivity on pressure and temperature.

• *The table of the present property* is the creation of a table with the designated parameters for the present property that can be stored in various formats: binary, XML, PDF, HTML, TXT, CSV, Excel, and RTF.

The DB of the user is the creation by the user of his own data base for a specific calculation code. Such a database is far shorter than the unified DB and can faster process the required information. In this case the user acquires an opportunity for experimentation with his DB without changing the unified data base.

The calculation of the water and steam properties is implemented in a particular item of the basic menu and is based on the recommendations of the IAPWS of 1997 with supplements of 2007 [7, 8]. In the data base, the basic and auxiliary equations in the variables pressure–temperature, pressure–enthalpy, pressure–entropy, and enthalpy–entropy, as well as on the line of saturation and in the two-phase domain, are implemented.

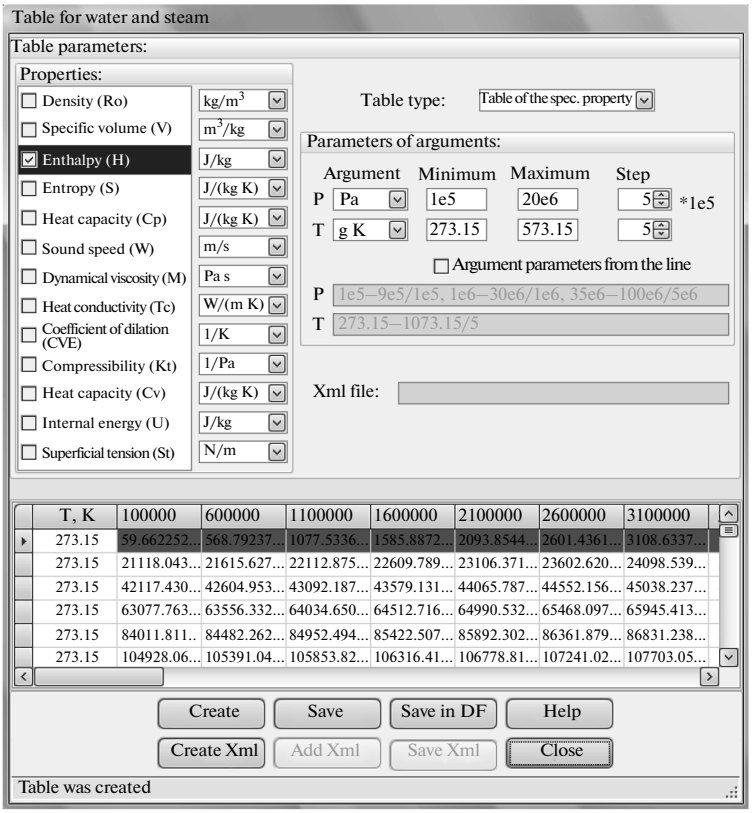

Fig. 4. Creation of the table with assigned parameters.

The *Water Properties* menu has the following subitems:

• *To create the table:* the creation of tables with the assigned parameters in the one-phase and high-temperature domain and on the line of saturation. Figure 4 supplies as an example a two-dimensional table for the enthalpy of water and steam within a temperature range from 298.15 K up to 573.15 K and pressure from 10^5 Pa to 20 MPa, with a step of 10^5 Pa and 1 K.

• The *calculator* is used for the calculation of the basic properties of water and steam at the given parameters in the variables pressure–temperature, pressure–enthalpy, pressure–entropy, enthalpy–entropy, and on the line of saturation.

The calculator of the two-phase domain is calculation of the basic properties of the water and steam mixture (enthalpy, entropy, internal energy, density, and content of the steam fraction) at the given values of pressure or temperature.

3. THE USE OF THE DATABASE IN SIDE PROGRAM PRODUCTS

In the program products (calculation codes) the database on the properties of materials can be used conventionally in the following way:

1. Tables of various format that can be inserted into the file of the source data or be used as particular files.

2. XML of the file containing all the necessary data on the materials' properties for a specific cost code. This XML file may have both the table data and formulas with the values of the coefficients and can be placed into the file of the source data of the program product as a block according to the materials' properties.

3. Formulas that, along with the coefficients, can be applied in the calculation code. In this case the user has to create the cost function himself.

All the above-mentioned ways have a significant shortcoming. It is necessary to perform a large volume of work by searching and exporting the required information from the DB, creating the file of the source data, organizing the reading, processing, and transporting of the data to the calculation code. In some

cases a special program unit should be created for each property. Moreover, this work has to be repeated actually for each program product.

As the only one and convenient mechanism of the application of the database, the libraries for the calculation functions were chosen based on dynamically linked libraries (DLLs). This direction of the database use is promising because of the following points:

• Libraries are a universal tool for calculation programs, written in different programming languages and in different operation systems.

• Libraries do not need the multiple creation of calculation functions in various codes for the same properties.

• Libraries reduce the time required to prepare operations on the database linking them to the calculation code. It is enough to include in the project the library files (*.dll and *.lib), as well as XML file with the unified database.

Within the works on the database of the material properties, two libraries for determining the material properties in cost codes have been created. The wpLibrary library is used to calculate the properties of water and water steam, and the mpUniLib library is used for all the remaining materials. This division is explained first of all by the fact that the formulas for determining the properties of water and steam are far more difficult than the formulas for the overwhelming number of other materials, which excludes the use of the formula analyzer.

A characteristic feature of the mpUniLib library is the use of special Handlers and the analyzer of the formulas for the calculation of the properties of the materials.

The handler is an indicator created at the stage of data initialization, which contains all the information required for the calculation of the desired properties of the material. This information is taken directly from the XML file, created by means of the graphic interface. The library is also able to deal with rather complicated formulas, when the use of a parser is inefficient. In this case, for a complicated formula, a special function is created, although the activation of the calculation functions remains unchanged. Thus, this library is related to the libraries with the universal interface.

The use of the mpUniLib library in program products includes three stages. At the first stage, it is the initialization of the DB and of all the necessary properties set by the user. At the second stage, the calculation of the properties in the calculation code is made. At the third stage, it is the liquidation of the indicators and exemption of the dynamic memory that is supposed to store the data.

In the mpUniLib library, the capabilities of automatically processing the meanings of arguments found outside the interval of measurements are implemented in the mode of data extrapolation. The library also has the possibility of automatically smoothing the thermophysical properties in the field of the phase transition. The library has the corresponding tools for implementation by the user of his algorithms for smoothing and extrapolating the data.

The wpLibrary contains calculation functions for determining the properties of water and steam in the variables pressure–temperature, pressure–enthalpy, ans pressure–entropy, as well as on the line of saturation and in the two-phase area. The calculation formulas for water and steam are rather difficult because of the large number of coefficients. This makes the use of the formula analyzer inefficient. Thus, for the basic and auxiliary formulas in the library, special calculation functions have been created. The library has two groups of functions: basic functions and table functions.

The basic functions implement the equations of the International Association on the properties of water and steam, so they are highly accurate, but have a low calculation rate. They do not require initialization and can be used immediately after the library files are connected to the project.

The use of the table functions presupposes also the presence of three stages, i.e., initialization of the user required properties, calculation, removal of arrears, and release from the dynamic memory. At the stage of initialization, the two-dimensional tables are created by use of the previously mentioned basic calculation functions that are used later for the calculation of properties. A good feature of this part of the library is also the calculation speed. Its shortcoming is the loss of accuracy due to bilinear interpolation. For comparison, the speed of the calculation of properties in the pressure–temperature variables in the use of the basic functions is 1000–4500 ns, whereas in the table functions, it is 14–16 ns.

CONCLUSIONS

Based on the analysis of the current databases on the properties of materials and of the experience in the development and use of calculation codes for the analysis of the safety of APSs, the requirements for the system of its management and the unified mechanism of the DB application to the cost codes have been determined. Taking into account the formulated requirement, an initial version of the data base has

been created, which has 180 materials and about 2500 properties. The data storage in the DB has been carried out based on the XML file.

The present graphic interface created for DB management offers the user many opportunities in editing and displaying graphic information, creating tables, as well as exporting and importing data.

A handy mechanism for the use of the data base for the external calculation codes has been created as dynamically connected libraries of calculation functions, considerably reducing the time for the development of codes in the part of operations required for implementing the properties of the materials and the mechanisms of their operation: it is sufficient to connect the files of the library (*.dll and *.lib) and the XML database file.

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Translated by D. Shtirmer