The application of service oriented architecture in calculation of thermochemical properties in web service form

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The paper is devoted to application of service oriented architecture in calculation of thermochemical properties. It describes for this purpose designed web service, its features and possibilities of utilization as well as basic principles of service oriented architecture that are used in web service design. As basic data sources were used NASA polynomials, CAS registry number and manually filled data. Web service has 23 particular functions, which is possible to use in various clients environments.

Key words: *SOA, thermochemical properties, web service, PHP*

Introduction

Service oriented architecture (SOA) is one of most frequented terms of present (more than 76 millions of hits). According the basic definition current SOA introduces architecture that supports service orientation by using web services [1]. Exact and detailed definitions states that "current SOA presents open, extendible, federative and composable architecture that supports service orientation and consists of services which are autonomous, meet the specific requirements of Quality of Service, support dealers variety, co-operation, discoverability and are implemented as web services" [1]. Applied definition says that SOA is form of technological architecture that is attached to services orientation principles. If it is realized through web services technological platform, SOA creates potential for support and improvement of these principles by means of control process and domains automation [1].

SOA is essentially a collection of services. These services communicate with each other. The communication can involve either simple data passing or it could involve two or more services coordinating some activity. Some means of connecting services to each other is needed [2].

SOA is the underlying structure supporting communications between services. SOA defines how two computing entities, such as programs, interact in such a way as to enable one entity to perform a unit of work on behalf of another entity. Service interactions are defined using a description language. Each interaction is self-contained and loosely coupled, so that each interaction is independent of any other interaction [3].

The SOA is based on components that work seamlessly with each other [4].

SOA establishes an architectural model that aims to enhance the efficiency, agility, and productivity of an enterprise by positioning services as the primary means through which solution logic is represented in support of the realization of the strategic goals associated with service-oriented computing [5].

Applying service-orientation to a meaningful extent results in solution logic that can be safely classified as "service-oriented" and units that qualify as "services". To understand exactly what that means requires an appreciation of the strategic goals of service-oriented computing [6] combined with knowledge of the following service-orientation design principles [7]:

- standardized Service Contract,
- service Loose Coupling,
- service Abstraction,
- service Reusability,
- service Autonomy,
- service Statelessness,
- service Discoverability,
- service Composability.

Fig. 1 illustrates mutual relations between individual service's attributes.

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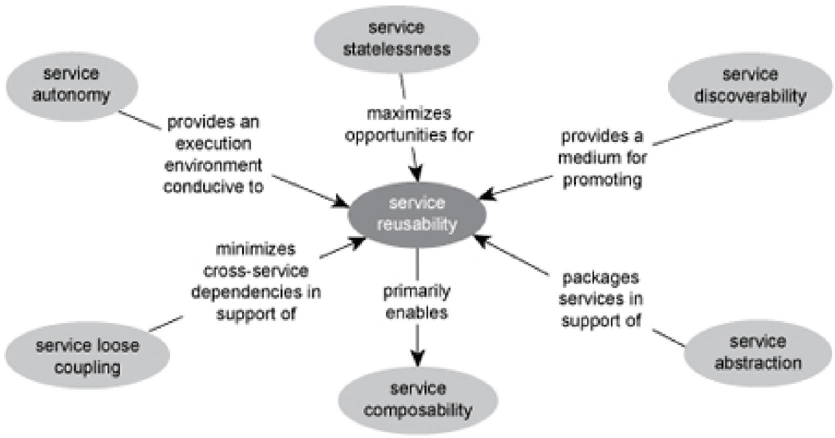

Fig. 1. Fundamental principle of service reusability [7] .

Actual state review

There are currently a considerable amount of web services (WS). Seekda GmbH [8] counts among the best-known intermediaries of web services, which specializes in the development and marketing of WS-oriented products. It allows to search, to provide and to use individual web services by its portal. It offers more than 28000 web services of different focus (from more than 7700 providers) but it does not provide any web service from the field of thermochemical data. Also other published analysis [9] note this state. CTserver [10] portal provides a little less web services from field of the thermodynamic calculations but based on older technology axis [11] and in considerably limited range of substances. The present article is a contribution in the field of providing thermochemical data by web service and options its use in different areas.

There are more sources of thermochemical data. In the first case there are book publications [12] where data is given in the form of tabulated values of individual properties (molar heat capacity, enthalpy, entropy, and so on) depending on temperature. The disadvantage of data published in this way is that values are given only for some temperatures, i.e. an interpolation is needed for calculation of values inside the temperature interval, and also in the case of automated calculations in the form of functions the data used in tabular form is inefficient and difficult. Thermochemical properties are better expressed in the form of functions dependent on temperature. In this case it is necessary to know the coefficients of the functions. Different shapes of the functions [13], [14], [15] and specific values of the coefficients for each substances respectively phases are published. Given the amount of substances and the shape of polynomials it appears as the most suitable source [13] known as NASA polynomials.

The work [13] documents the library of thermodynamic data which is used by the program CEA - NASA Glenn computer program CEA (Chemical Equilibrium with Applications). Library which contains data for over 2000 solid, liquid and gaseous phases for temperatures from 200 to 20000 K is also available for other programs. Data are expressed in the form by a method of least squares obtained coefficients for relationship of seven members for calculation $C°_p(T)/R$ and with the integration constant for $H°(T)/RT$ and $S°(T)/R$. NASA Glenn computer program PAC (Properties and Coefficients) was used for the calculation of thermodynamic functions and determining their coefficients. Input values for PAC were drawn from many sources. The work contains a complete extract database together with an overview of thermodynamic properties for 0 and 298,15 K.

Another source of thermochemical data are the different electronic sources from simple desktop applications (e.g. [16]) to network available applications [17, 18, 19, 20]. Among the networked available sources are for example ThermoBuild [19]' which presents an interactive tool based on the use of NASA thermochemical database. The tool allows to choose an element/elements (with the use Mendeleyev table of elements – Fig. 2) and to obtain tables of thermochemical properties of compounds containing the selected elements for a user defined range and dividing the interval of temperatures and also subsets of the thermochemical data with information on the coefficients which can be used in CEA or other programs [19]. A similar electronic source are also the NIST – JANAF Thermochemical Tables [20] where by entering a formula, a name or a CAS (Chemical Abstracts Service) parameter [21] and also by Mendeleyev table of elements it is possible to obtain in tabular form data about the thermochemical properties that can be saved to a file in text form. This source also provides coefficients for calculating the molar heat capacity, enthalpy and entropy depending on temperature. Other network resources are for example [10, 22, 23, 24, 25, 26, 27, 28]. The advantage of network-accessible resources is quickly obtaining the required data. Their disadvantage is a problematic incorporation to separated calculations respectively to simulation models implemented in a variety of applications.

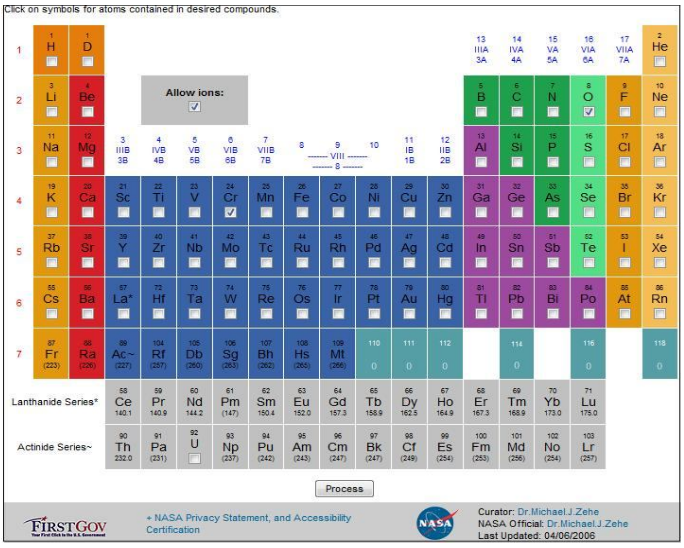

Fig. 2. Input form of ThermoBuild application (screenshot) [19].

Base and resources of web service

The data set on substance in the base database of web service arises from primary sources of NASA, which are complemented by data of parameter CAS and one possibly more of the names in two languages. The data set is therefore prepared in principle from three sources - sources of NASA, source CAS and manual source.

NASA sources: Different sources of the thermochemical properties are currently available namely in the form of tables or different polynomials [12, 13, 14, 29, 30, 31, 32, 33, 34, 35]. From a detailed analysis it is shown that the expression by NASA also includes other published shapes of polynomials and therefore it appears as a universal shape polynomial.

When calculating the basic thermochemical properties it is necessary to know their dependence on temperature. In the case of molar heat capacity it is dependent on temperature defined by the seven-member of polynomial

$$\frac{c_p^{\mathrm{o}}(T)}{R} = \sum_r a_i T^{q_i} \tag{1}$$

where r=7 and values q_i are temperature exponents (-2, -1, 0, 1, 2, 3, 4). This relation represents a new format NASA has used since 1994. Enthalpy and entropy will be obtained by integration of definition equation (1)

$$\frac{H_T^{\mathrm{o}}}{RT} = \frac{b_1}{T} + \frac{\int c_p^{\mathrm{o}}(T)\,\mathrm{d}T}{RT} \tag{2}$$

$$\frac{S_T^{\mathrm{o}}}{R} = b_2 + \int \left[\frac{c_p^{\mathrm{o}}(T)}{RT} \right] \mathrm{d}T \tag{3}$$

where b_1 and b_2 are obtained integration constants.

In the literature [33], [34], [35] a simplified record dependence of the molar heat capacity on temperature is mentioned in the form

$$\frac{c_p^{\mathrm{o}}(T)}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \tag{4}$$

where a_1, a_2, ... a_7 are constants obtained by experimental measurement of molar heat capacities at constant pressure. Enthalpy and entropy in a simplified form is given by

$$\frac{H_T^{\mathrm{o}}}{RT} = -a_1 T^{-2} + \frac{a_2 \ln T}{T} + a_3 + \frac{a_4 T}{2} + \frac{a_5 T^2}{3} + \frac{a_6 T^3}{4} + \frac{a_7 T^4}{5} + \frac{b_1}{T} \tag{5}$$

$$\frac{S_T^{\mathrm{o}}}{R} = -\frac{a_1 T^{-2}}{2} - a_2 T^{-1} + a_3 \ln T + a_4 T + \frac{a_5 T^2}{2} + \frac{a_6 T^3}{3} + \frac{a_7 T^4}{4} + b_2 \tag{6}$$

The above polynomials (4), (5) and (6) can be easily used in practical calculations. This data is transferred to the preparatory database using suitable algorithms [36].

CAS sources: In the current structure of the data are CAS registry number (a unique numeric identifier of a chemical compound, thus substance) and one or more names of substances in the English and Slovak language. There are several free resources available, for example [37, 38, 39, 40, 41]. Suitable algorithms are proposed for this data and realized for their transfer to the preparatory database.

Manual source: Presents a way of supplementing data, which is not possible to obtain by automated processing from the sources NASA and CAS, error correction of substance (from different reasons) or correction of some substance data. Manual source is presented as a form. The form is available for administrator of database infrastructure of web service.

Web service design and functions

Designing actual version of web service we consider only a few selected properties (as for example molecular mass, heat of formation and coefficients for calculation of molar heat capacity, enthalpy and entropy). The data model of web service's database infrastructure regards mentioned properties of substances, their phases and calculation parameters. Table tv_subst with substance's identifier Ids as primary key contains substance's chemical formula, another in chemical practice exerted identifier CAS [37], molecular mass and substance's group identifier Ig. Groups (as elements, oxides, etc.) enable substances sorting into smaller sections. Each substance is listed in corresponding group. Groups list contains the table tv_substgroup. Substance is created by one or more phases (species). Table tv_substspecies describes phase's list of particular substances. Table tv_substnames contains one or more substance's name in corresponding language. Table tv_species contains specific information about given phase (formula, comment, source of data, phase, heat of formation), table tv_interval specifies information about phases divided to appropriate number of temperatures intervals (coefficients for calculation molar heat capacity, enthalpy and entropy on given temperatures interval <tmin, tmax>). Table tv_atom specifies name and atomic weight of individual chemical elements and table tv_formula contains elements quantification in given substance – compound. The tv_substgroup and tv_substnames tables indicate groups and substances names in two languages. Each substance can have optional number of names – synonyms, but minimum one name. The first name is dominant and it figures in particular web service's functions. Number of names in various languages may not be the same. The tv_wsfunc and tv_wsfuncpar tables are holders of web service's functions names in various languages and corresponding parameters of particular web service's functions. Table tv_wserr contains meaning of individual codes of web service's error states in various languages. Complete graph of web service data model with relations between tables illustrates Fig. 3.

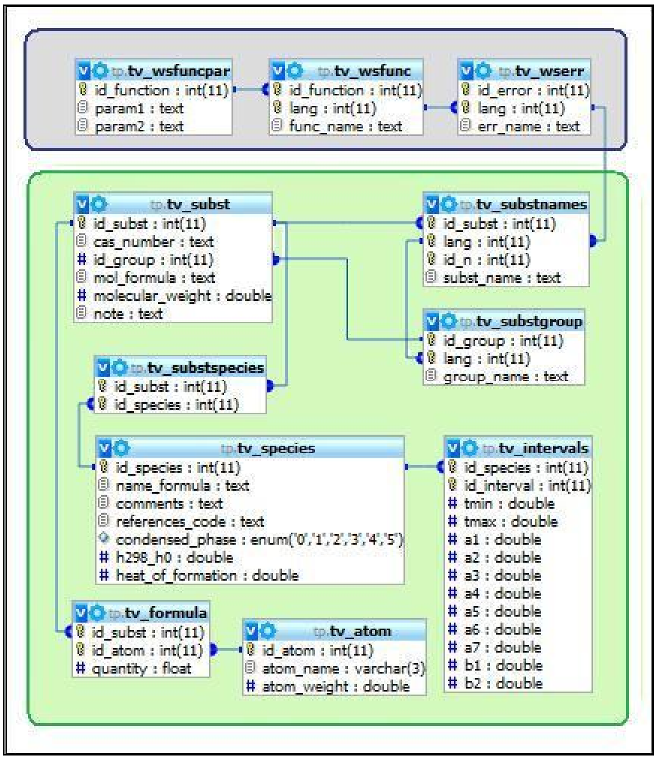

Fig. 3. Web service data model (screenshot).

Web service is realized in PHP5 development environment (required version PHP is 5 and more) and as database system is used MySQL also in version 5 (but it is not requirement). In actual web service version (with class name TermPropService, method name getTermProp() with three parameters, specified in TermPropService.wsdl file) there were up to now proposed 23 particular function that provide information about service itself, names and identification of all substances and phases, temperatures interval extent, molecular mass and heat of formation for given phase, values of molar heat capacity, enthalpy, entropy, coefficients for calculation of mentioned phases' properties for given temperature, all temperatures intervals and coefficients of given phase, summary of all values of given substance, list of web service's error codes as well as meaning of concrete error code.

WS Function	Regime	Param1	Param2
Info about WS	1	lang-1(sk)/2(en)	x
Ids, Id & phases' names	2	Ig	x
Temperatures interval of phase	3	Id	x
Molecular mass of phase	4	Id	x
Heat of formation of phase	5	Id	x
Specific heat of phase C	6	Id	T
Enthalpy of phase H	7	Id	T
Entropy of phase S	8	Id	T
Together C,H,S of phase	9	Id	T
Coefficients a(1-7), b(1-2) of phase	10	Id	T
All temperatures intervals of phase	11	Id	x
All coefficients a(1-7), b(1-2) of phase	12	Id	x
All phase's data	13	Id	x
Error meaning on WS call	14	lang	err
List of errors on WS call	15	lang	x
Substances' mol.formula, 1.name, Ids & CAS (Ig)	16	Ig	lang
Substances' mol.formula, 1.name, Ids & CAS (Fl)	17	Fl	lang
Substances' mol.formula, 1.name, Ids & CAS (CAS)	18	CAS	lang
Substance's molecular mass	19	Ids	x
Substance's phases list	20	Ids	x
Enthalpy & entropy of transition at substance's phase change	21	Ids	x
All substance's data	22	Ids	x
Gibbs energy of phase G	23	Id	T

Fig. 4. Web service functions (screenshot).

Summary of web service functions with their parameters illustrates Fig. 4. Parameter Regime defines concrete functions of web service. Parameter Param1 defines most frequently specification of given substance (Ids) or its phase (Id), but it can also specify substance group (Ig), CAS, first letter in substance's name or language of substance's name. Parameter Param2 defines usually temperature value (T) (in K) or error number (err) or output-required language. In functions where value of some parameter is unnecessary (in Fig. 4 indicated by x character) it enters arbitrary value on appropriate position (e.g. 0). Particular web service functions provide information about service itself, names and identification of all substances and phases, temperatures interval extent, molecular mass and heat of formation for given phase, values of molar heat capacity, enthalpy, entropy, coefficients for calculation of mentioned phases' properties for given temperature, all temperatures intervals and coefficients of given phase, summary of all values of given substance, list of web service's error codes as well as meaning of concrete error code.

Calling and outputs of web service

Web service communication (link) part is realized at omega.tuke.sk server in form of service's WSDL reference file (TermPropService.wsdl) that specifies all attributes of proposed web service needed for its calling on client side. Contemporaneously file contains also web service's URI (Unified Resource Locator) that is used for the creation of client's application direct connection to web service. Web service provides to client one method getTermProp(string Regime, string Param1, string Param2), which returns either standard XML structure in form depending on parameter Regime value or error structure that indicates error number and returns entered input parameters for service calling. Client's application creation with web service exploitation is supported in all actual development environments. First of all they are internet development environments (PHP, ASP, Java, and Ajax) but in like manner desktop development environments (MATLAB). We show example of web service calling in PHP and in MATLAB environment.

In PHP is realization of client application based on object instance creation that represents client's part of web service. The next step is calling of required function of web service with appropriate values of function's input parameters. Subsequently it is necessary to display output values of web service. Object instance creation is in form

```
$urlwsdl="http://omega.tuke.sk/wsdl/TermPropService.wsdl";
$service= new SoapClient ($urlwsdl);
```

whereby $urlwsdl specifies location of web service's WSDL file (its URI) and $service introduces object instance for communication with given web service. By reason that web service returns XML structure as output, the simplest way of its presentation is scan out of this structure that can be in form

```
$reg = '5'; $id = '8'; $t = '300';
print $service ->getTermProp($reg,$id,$t);
```

whereby $reg is function operation regime, $id means entered phase identification and $t is temperature.

View of results presentation on screen is desirable to ensure by means of CSS file in which is for every concrete element of output XML structure prescribed corresponding way of presentation (first of all by appropriate coloring of particular items). Items of XML structure that is necessary for any reason not reflect is possible to label by option display: none. For client creation is needed version PHP 5 or higher. In actual Linux distributions this version is already included.

In MATLAB is client application realization in the first step based on object instance creation accordingly as in the case of PHP

```
url = 'http://omega.tuke.sk/wsdl/TermPropService.wsdl';
createClassFromWsdl(url);
service = SluzbaTermProp ;
```

The second step is calling of needed function of web service with corresponding values of function's input parameters

```
$reg = '5'; $id = '8'; $t = '300';
result = getTermProp(service,reg,id,t);
```

By reason that web service returns XML structure as output value its scan out is simple way of its presentation in form disp(result);

For next application of numeric values is necessary to convert the XML structure saved in variable result into numeric values. In terms of this is needed into structure insert leading and ending tag container. Then is needed to rewrite character array into structure in variable xmlR using function xml_parse() and finally convert corresponding item to number according to following code

```
result=strcat('<container>',getTermProp(service,rez,id,t),'</container>');
xmlR = xml_parse(result);
A = {xmlR(1,1).response.data.heat_of_formation};
X = str2double(A);
```

For client creation is needed MATLAB from version 7.01 and for XML structure processing is needed free available function library „xml_toolbox“ [42].

The web service’s output is standard XML structure in form depending on parameter Regime value or error structure that indicates error number and returns entered input parameters of service calling. Each structure is delimited by format

<?xml version="1.0"?><response><data><err_state>E</err_state><xxx></data></response>,

whereby value E=0 stands for standard structure that contains one or more records in dependence on parameter Regime value. Value E=1 stands for error structure with nearer error specification that contains values of all three parameters of service calling and error number which arose. For values $reg = '6'; $id = '8'; $t = '500'; has output structure fraction <xxx> form

<regime>6</regime><idspecies>8</idspecies><temp>500</temp><c>63.528200797674</c>

Tab. 1. Formats of XML structures for particular web service regimes.

Structure for regime	**count**
_ <regime>1</regime><func_name>Info o WS</func_name> <id_function>1</id_function><param1>1(sk)/2(en)</param1><param2>x</param2>	23
<regime>2</regime><idspecies>11</idspecies><namespecies>CO</namespecies>	nl
<regime>3</regime><idspecies>8</idspecies><interval>1</interval> <temp_min>200</temp_min><temp_max>3220</temp_max>	1
<regime>4</regime><idspecies>8</idspecies> <molecular_weight>61.8867</molecular_weight>	1
<regime>5</regime><idspecies>8</idspecies> <heat_of_formation>-337649</heat_of_formation>	1
<regime>6</regime><idspecies>8</idspecies><temp>500</temp> <c>63.528200797674</c>	1
<regime>7</regime><idspecies>8</idspecies><temp>500</temp> <he>-337132.69527876</he>	1
<regime>8</regime><idspecies>8</idspecies><temp>500</temp> <sx>44.133645255659</sx>	1
<regime>9</regime><idspecies>8</idspecies><temp>500</temp> <c>63.528200797674</c><he>-337132.69527876</he><sx>44.133645255659</sx>	1
<regime>10</regime><temp>500</temp><idspecies>8</idspecies><interval>1</interval> <a1>-54791.2</a1><a2>9328.69</a2><a3>-63.8626</a3><a4>0.242993</a4> <a5>-0.00043042</a5><a6>3.79265e-007</a6><a7>-1.31741e-010</a7> <b1>-84242.6</b1><b2>339.299</b2>	1
<regime>11</regime><idspecies>8</idspecies><interval>1</interval> <temp_min>200</temp_min><temp_max>800</temp_max><idspecies>8</idspecies> <interval>2</interval><temp_min>800</temp_min><temp_max>3220</temp_max>	1
<regime>12</regime><idspecies>8</idspecies><interval>1</interval><a1>54791.2</a1> <a2>9328.69</a2><a3>-63.8626</a3><a4>0.242993</a4><a5>-0.000430423</a5> <a6>3.79265e-007</a6><a7>-1.31741e-010</a7><b1>-84242.6</b1><b2>339.299</b2>	ni
<regime>13</regime><idspecies>8</idspecies><interval>1</interval> <molecular_weight>61.8867</molecular_weight> <heat_of_formation>-337649</heat_of_formation><temp_min>200</temp_min> <temp_max>800</temp_max><h298_ho>5487</h298_ho><a1>54791.2</a1> <a2>9328.69</a2><a3>-63.8626</a3><a4>0.242993</a4><a5>-0.000430423</a5> <a6>3.79265e-007</a6><a7>-1.31741e-010</a7><b1>-84242.6</b1><b2>339.299</b2>	ni
<regime>14</regime><id_error>5</id_error> <err_name>Pripojenie na MySQL server zlyhalo</err_name>	1
<regime>15</regime><id_error>4</id_error> <err_name>Neexistujúca identifikácia jazyka</err_name>	13
<regime>16</regime><mol_formula>TiN</mol_formula> <substname>nitrid titánu</substname><idsubst>5</idsubst><cas>25583-20-4</cas>	ng
<regime>17</regime><mol_formula>O2</mol_formula><substname>kyslík</substname> <idsubst>2</idsubst><cas>7782-44-7</cas>	0-n
<regime>18</regime><mol_formula>CO</mol_formula> <substname>oxid uhoľnatý</substname><idsubst>7</idsubst><cas>630-08-0</cas>	1
<regime>19</regime><idsubst>1</idsubst> <molecular_weight>18.01528</molecular_weight>	1

<regime>20</regime><idsubst>1</idsubst><idspecies>1</idspecies> <namespecies>H2O</namespecies><regime>20</regime><idsubst>1</idsubst> <idspecies>2</idspecies><namespecies>H2O(cr)</namespecies><regime>20</regime> <idsubst>1</idsubst><idspecies>3</idspecies><namespecies>H2O(L)</namespecies>	n
<regime>21</regime><idsubst>2</idsubst><chng_count>0</chng_count> <regime>21</regime><idsubst>1</idsubst><chng_count>1</chng_count> _ <chng_num>1</chng_num><id_phase1>2</id_phase1><id_phase2>3</id_phase2> <temp_ph_chng>273.15</temp_ph_chng><namespecies>H2O(cr)</namespecies> <he_add>6009.9197720196</he_add><sx_add>22.004528892399</sx_add>	0-4
<regime>22</regime><idsubst>2</idsubst><mol_formula>O2</mol_formula> <molecular_weight>31.9988</molecular_weight><cas>7782-44-7</cas> _ <idspecies>4</idspecies><namespecies>O2</namespecies><interval>1</interval> <h298_h0>8680.104</h298_h0><heat_of_formation>0</heat_of_formation> <temp_min>200</temp_min><temp_max>1000</temp_max><a1>-34255.6342</a1> <a2>484.700097</a2><a3>1.119010961</a3><a4>0.00429388924</a4> <a5>-6.83630052e-007</a5><a6>-2.0233727e-009</a6><a7>1.039040018e-012</a7> <b1>-3391.45487</b1><b2>18.4969947</b2>	ni
<regime>23</regime><idspecies>11</idspecies><temp>500</temp> <gibbs_en>-211021.68849869</gibbs_en>	1
<id_error>3</id_error><regime>19</regime><param1>11</param1><param2>2</param2>	1

Error states are results of web service's input parameters check or can arise within realization of particular web service regimes. Centralized manner of web service's input parameters check requires suitable solution of error states handling on the server side and their forwarding to client side. Error state signalization to client is realized in form so-called error XML structure (in contrast to normal return structure with service results). List of realized and handled error states illustrates Fig. 5. Preponderance of these error states (codes 2, 3, 4, 5, 6, 7, 10, 11) rises directly abreast of service's input parameters check. Others error states (codes 0, 8, 12, 13) can rise within solution of particular web service regimes over its database infrastructure.

Error code	Error meaning
0	Connection to a MySQL server failed
2	Non existing regime of WS
3	Non existing substance identification (Ids)
4	Non existing phase identification (Id)
5	Non existing group identification (Ig)
6	Non existing language identification (lang)
7	Non existing error identification (err)
8	Temperature out of allowed interval
9	MySQL_query failed - error in SQL statement (;!)
10	Non existing error & language identification (err,lang)
11	Non existing group & language identification (Ig,lang)
12	Non existing first letter (Fl) of substance's first name
13	Non existing substance identification (CAS)
14	Empty result of selected group (Ig)

Fig. 5. List of web service error codes (screenshot).

Web service presentation and utilization

For web service presen-tation purposes is built-up web application with Ajax technology exploitation that enables regime selection and assignation of two input parameter for web service calling (in terms of service's functions in Fig. 4). The application is located at the address http://omega.tuke.sk/tp/ klienttermprop.php. On the present within the frame of service's database infrastructure there are disposable 106 substances and their 274 phases whereby currently they are completed. Demonstration of web application sheet in conjunction with result illustrates Fig. 6.

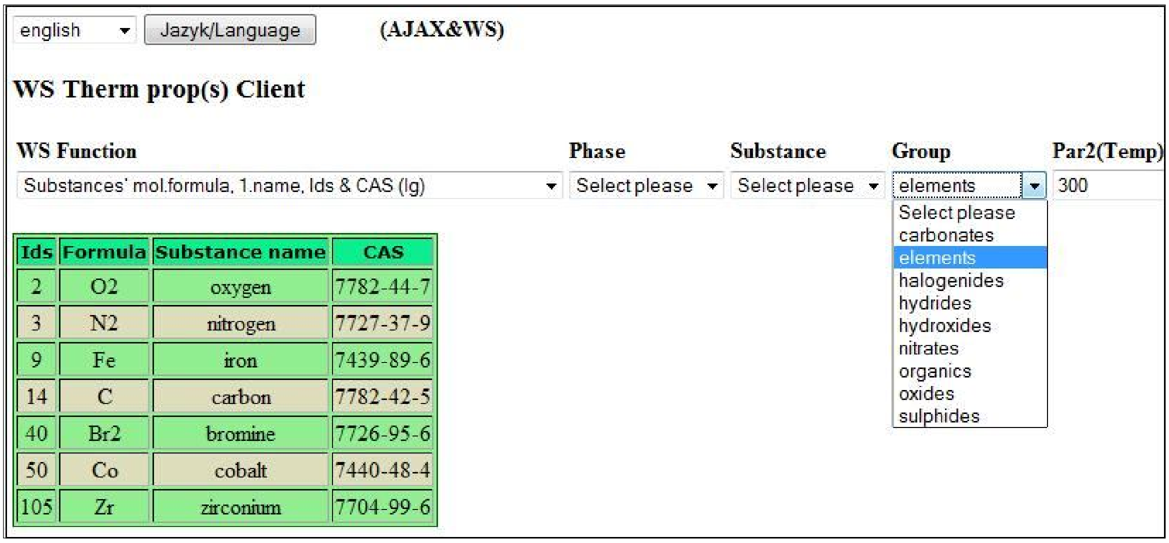

Fig. 6. Web application's illustration (screenshot).

The compiled web service provides a wide range of use within the meaning of those 23 partial functions. The service can continuously provide the necessary results of calculations, also it is preferable to obtain the necessary computed coefficients for the application (typically a desktop) by the service and then resolve the calculations in the given application. The service can be used directly as part of the client application in different network and desktop environments (e.g. PHP, Ajax, ASP, MATLAB, Java, Perl, Octave) but can also be used as part of another web service. The service provides the output in a range of one string (or number) to the complex structure of more sentences according to table 1 depending on the specified mode. To illustrate we will mention some possible areas of application - modeling processes where heating, cooling, phase transformation, chemical reaction, and other calculations in which the thermochemical properties of substances are necessary [43, 44, 45, 46, 47].

Conclusion

The web service provides a unified source of thermochemical properties and calculations for the needs of mathematical modeling (processes for obtaining and processing of raw materials and synthesis of their control). A significant benefit solution can be identified by the fact that the use of the web service (whether online or offline) eliminates the difference of heat physical data from different sources, which can lead to undesirable differences during calculations. Another advantage of the proposed solution is the central administration of individual data on one web server and component character of the service, allowing the direct incorporation into the final client application as in the area of direct control processes as well as in the area of modeling and simulation processes.

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References

[1] Erl, T.: Servisně orientovaná architektúra SOA, kompletní průvodce. Brno : *Computer Press, 2009. ISBN 978-80-251-1886-3.*

[2] Barry, D.K.: Service-oriented architecture (SOA) definition. *[online] : Barry & Associates, Inc., 2011. cited [10.6.2011]. available from* <http://www.service-architecture.com/web-services/articles/service-oriented_architecture_soa_definition.html>.

[3] SearchSOA.com. Definition service-oriented architecture (SOA). *[online] 2003. cited [10.6.2011]. available from* <http://searchsoa.techtarget.com/definition/service-oriented-architecture>.

[4] TechTerms.com The Tech Terms Computer Dictionary. *SOA. [online] 2011. cited [10.6.2011]. available from* <http://www.techterms.com/definition/soa>.

[5] Erl, T.: What is SOA? An Introduction to the Service-Oriented Computing. *[online] 2011. cited {10.6.2011]. available from* <http://www.whatissoa.com/>.

[6] What is SOA? An Introduction to the Service-Oriented Computing. Goals and Benefits of Service-Oriented Computing. *[online] 2011a. cited [10.6.2011]. availlable from* <http://www.whatissoa.com/p16.php>.

[7] Principles of Service-Orientation. *[online] 2006. cited [10.6.2011]. available from* <http://searchsoa.techtarget.com/tip/The-principles-of-service-orientation-part-6-of-6-Principle-interrelationships-and-service-layers>.

[8] Seekda! Web Services Search Engine @seekda.com. *[online] Innsbruck; Austria, 2009. cited [19.9.2011]. available from* <http://webservices.seekda.com/>.

[9] Bhattacharjee, S.: An Object Oriented Approach to Computational Thermodynamics. *MME Symposium Series. [online] 2. October 2008. [cited 9.9.2009]. available from* <http://www.mme.wsu.edu/symposia/symposia_08-09/bhattacharjee.pdf>.

[10] Ghiorso, M.S. and Kress, V.C.: CTserver Web Services. *[online] cited [19.9.2011]. available from* <http://ctserver.ofm-research.org/webservices.html>.

[11] Horovčák, P. and Dorčák, Ľ.: Creating Web Services with Axis. *Proceedings of 5th International Carpathian Control Conference. 2004, Zv. Volume I, ISBN 83-89772-00-0, p. 409 - 414.*

[12] Barin, I.: Thermochemical Data of Pure Substances. *Weinheim, New York : VCH, 1993. p. 1356. ISBN 3-527-28531-8.*

[13] McBride, B. J., Zehe, M. J. and Gordon, S.: NASA Glenn Coefficients for Calculating Thermodynamic Properties of Individual Species. *NASA TP–2002-211556. [online] 2002. cited [10.6.2011]. available from* <http://www.archive.org/details/nasa_techdoc_20020085330>.

[14] Komorová, Ľ. a Imriš, I.: Termodynamika v hutníctve. *Bratislava : Alfa, 1992. p. 296. ISBN 80-05-01077-X.*

[15] Chase, M.W., Curnutt, J.L., Hu, A.T., Prophet, H., Syverud, A.N. and Walker, L.C.: JANAF Thermochemical Tables, *1974 Supplement. [online] Midland, Michigan 48640 : Thermal Research, The Dow Chemical Company, 1974. cited [19.9.2011]. available from* <http://www.nist.gov/data/PDFfiles/jpcrd50.pdf>.

[16] Hlubuček, V.: FYDEX – fyzikální data látek do EXCELu. *Chemagazin. 2011, Zv. XXI, 3, p. 32 - 33. available from* <http://www.chemagazin.cz/userdata/chemagazin_2010/file/CHEMAGAZIN_XXI_3_cl12.pdf>.

[17] Bhattacharjee, S.: The Expert System for Thermodynamics. *[online] 2011. available from* <http://www.ulb.ac.be/sma/testcenter/, http://www.thermofluids.net/>.

[18] TEST, The Expert System for Thermodynamics. *[online] San Diego State University, 2003. cited [19.9.2011]. available from* <http://thermo.sdsu.edu/testhome/booksite/paperByBhattacharjee.pdf>.

[19] Zehe, M.J.: Chemical Equilibrium with Applications. *[online] : NASA Glenn research center, 2006. cited [10.6.2011]. available from* <http://www.grc.nasa.gov/WWW/CEAWeb/ceaThermoBuild.htm>.

[20] National Institute of Standards and Technology. NIST-JANAF Thermochemical Tables. *[online] 2000. cited [19.9.2011]. available from* <http://kinetics.nist.gov/janaf/>.

[21] The Physical and Theoretical Chemistry Laboratory Oxford University. *Chemical and Other Safety Information. [online] cited [5.2.2010]. available from* <http://msds.chem.ox.ac.uk/>.

[22] Roine, A.: HSC – Chemistry 7. *[online] : Outotec Research Oy. [cited 19.9.2011]. available from* <http://www.hsc-chemistry.com/>.

[23] Dinsdale, A.T.: SGTE – Scietntific Group Data Europe. *[online] cited [19.9.2011]. available from* <http://www.sgte.org/>.

[24] Bale, C.W.: FactSage – CRCT – ThermFact Inc. and GTT Technologies. *[online] cited [19.9.2011]. available from* <http://www.factsage.com/>.

[25] Davies, R.H., Dinsdale, A.T., Gisby, J.A., Robinson, J.A.J. and Martin, S.M..: The NPL Software tool for the calculation of phase equilibria and thermodynamic properties. *[online] cited [19.9.2011]. available from* <http://www.npl.co.uk/upload/pdf/mtdata_calphad_paper.pdf>.

[26] Ghiorso, M.S. and Kress, V.C.: CTserver Home Page. *[online] cited [19.9.2011]. available from* <http://ctserver.ofm-research.org/index.html>.
[27] Ghiorso, M.S. and Sack, R..O.: MELTS Home Page. *[online] cited [19.9.2011]. available from* <http://melts.ofm-research.org/>.
[28] Ghiorso, M.S. and Hirschmann, M.M.: LEPR - Library of Experimental Phase Relations. *[online] cited [19.9.2011]. available from* <http://lepr.ofm-research.org/YUI/index.php>.
[29] Liley, P. E.: 2000 Solved Problems in Mechanical Engineering Thermodynamics. *New York : McGraw-Hill, 1989. ISBN 0-07-037863-0.*
[30] Molnár, F., Rybárová, Ž., Slivová, J., Lavrin, A.: Príručka pre výpočty z chemickej termodynamiky. *Bratislava : Alfa, 1977. p 180.*
[31] Surový, J.: Chemickoinžinierska termodynamika. *Bratislava, 1991. ISBN 80-05-00823-6.*
[32] McBride, B. J., Gordon, S. and Reno, M. A.: Coefficients for Calculating Thermodynamic and Transport Properties of Individual Species. *1993. NASA TM–4513.*
[33] Thermodynamic Data for Fifty Reference Elements. *2001. NASA TP–3287-REV1.*
[34] Brizuela, E. A.: Computing Mixture Temperature from Enthalpy Using NASA Polynomials. *IFRF Combustion Journal. Communication No 200001, October 2000. ISSN 1562-479X.*
[35] Burcat, A.: Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for Combustion. *Technion-Israel Institute of Technology, 2001. TAE 867.*
[36] Sabo, M.: Návrh administrácie databázovej infraštruktúry webovej služby na podporu termodynamických výpočtov. *Košice : Bakalárska práca. Technická univerzita v Košiciach, Fakulta baníctva, ekológie, riadenia a geotechnológií, 2010. p. 44.*
[37] American Chemical Society. CAS REGISTRY and CAS Registry Numbers. *[online] 2010. cited [6.9.2010]. available from* <http://www.cas.org/expertise/cascontent/registry/regsys.html>.
[38] National Institute of Standards and Technology. NIST. *[online] 2009. cited [3.9.2010]. available from* <http://www.nist.gov/>.
[39] Matouš, J. and Šípek, M. NIST WebBook Chemie. *[online] 2008. cited [3.9.2010]. available from* <http://webbook.nist.gov/chemistry/>.
[40] Nicklaus, M.C.: CADD Group Chemoinformatics Tools and User Services. *[online] : e Computer-Aided Drug Design (CADD) Group of the Chemical Biology Laboratory (CBL), 16. 08 2010. cited [3.9.2010]. available from* <http://cactvs.cit.nih.gov/>.
[41] Cartwright, H.M.: Chemical and Other Safety Information from the Physical Chemistry Laboratory, *Oxford University. [online] 2010. cited [6.9.2010]. available from* <http://msds.chem.ox.ac.uk/#MSDS>.
[42] Molinari, M.: XML Toolbox. *[online] 2005. cited [5.2.2010]. available from* <http://www.mathworks.com/matlabcentral/fileexchange/4278-xml-toolbox>.
[43] Horovčák, P., Terpák, J. and Cirbes, P.: Process modelling supported by web services and client technologies. In: *Proceedings of 11th International Carpathian Control Conference. 26-28 May, 2010, Eger, Hungary. - Miskolc : Rekatel, 2010 p. 355-358. ISBN 978-963-06-9289-2.*
[44] Terpák, J., Horovčák, P., Dorčák, Ľ. and Kukurugya, J.: Modelling of phase transition by the heating. In: *Proceedings of the 12th International Carpatian Control Conference : 25-28 May 2011, Velké Karlovice, Czech Republic. IEEE, 2011 p. 398-401. ISBN 978-1-61284-359-9.*
[45] Laciak, M., Škvareková, E., Durdán, M., Kostúr, K. and Wittenberger, G.: Štúdium podzemného splyňovania uhlia v laboratórnych podmienkach. *Chemické listy. Vol. 106, no. 5(2012), p. 384 - 391. ISSN 0009-2770*
[46] Terpák, J., Kukurugya, J. and Pitoňák, M.: Simulation Model for Analisis of Thermal Processes in Thermo-Insulating Food Packaging. In: *Proceedings of the 13th International Carpatian Control Conference : 28-31 May 2012, Podbanské, Slovak Republic. IEEE, 2012 p. 403-407. ISBN 978-1-4577-1866-3.*
[47] Laciak, M., Durdan, M. and Kačur, J.: Utilization of indirect measurement in the annealing process of the steel coils. *Acta Metallurgica Slovaca. Vol. 18, no. 1(2012), p. 40 - 49. ISSN 1338-1156*