

## NEW GENERATION OF COMPUTER-AIDED TOOLS FOR THERMAL CALCULATIONS

**OCHKOV Valeriy**

*The work provides principle of application of new tendencies in computer-aided engineering for thermal calculations. Examples of different types of Internet resources with a wide range of on-line, interactive tools and algorithms, ready-made templates and worksheets are presented in the paper.*

**Keywords:** on-line, interactive tools, “cloud” technologies, thermal calculations

---

### Introduction

Computer-aided engineering is widely applied to aid in thermal analysis tasks. There are established and successfully operated powerful programs for this. Most of these softwares are usually considered as “black box input-output” ones in the sense that there is no possibility to manipulate analytical expressions of the objective function or to observe the way in which those expressions are internally treated. Some of them can be applied to a very narrow area. In order to solve non-standard tasks users combine several types of programs. In some cases such integration cannot be used directly and needs preprocessing. Moreover, such type of software can be used and reached by limited number of investigators. In addition, these “program-monsters” are very expensive and require complex and expensive servicing and that their study requires a lot of time and effort, which is never enough.

Computer simulation of heat and mass transfer or energy conversion needs special software which enables to calculate thermophysical properties of working fluids. Such software should be installed on a computer and needs to be updated periodically. It is mainly due to the fact that new working fluids and formulations emerge. In addition, errors and inaccuracies in existing computer programs take place, their application domains are extended, and their performance is improved. Such programs are also continuously updated due to changes made in the hardware and operating system software. Users of computer programs on properties of working fluids frequently fail to notice these changes and work with outdated versions. Also, users face additional difficulties if they change their computer and/or operating system: old computer programs cannot be installed and started any longer. Besides most such programs have quite narrow possibilities of their further application in computer simulation. Moreover, it is not possible and/or unreasonable to save in one program or one computer data about all existing working substances.

New paradigm within information technologies - cloud computing has become a great solution for providing a flexible, on-demand, and dynamically scalable computing infrastructure for many applications. Cloud computing presents a significant technology trend and many experts expect that it will substantially reshape information technology processes. Advantages of the cloud computing technology include cost savings, high availability, easy scalability, flexible accessibility, etc [1].

The work is devoted to development of new types of computation tools for thermal calculations based on open, interactive algorithms and „cloud“ technologies.

## 2. Methodology

Maple, Mathematica, Matlab, MathCad, SMath, etc. are among the most widely used interactive, general purpose softwares for doing mathematics and engineering. They all have “higher level” programming capability, high-quality graphics, extensive libraries of mathematical functions, and have substantial capacity for numerical computation. Most of them also have major “symbolic” capability, e.g., the ability to perform analytically complex algebraic manipulations and calculus operations (including differentiation, integration, power series expansions, etc.). These packages are designed for those wishing to have control over the details of setting up and solving their problems.

It is proposed to develop computational tools on the basis of Mathcad and Maple and their interactive web-based publishers Mathcad Application/Calculation Server, PTC Mathcad Gateway and MapleNet.

Mathcad and its newest version Mathcad Prime are among of the most suitable softwares for engineering purposes, because they have three advantages: universality, accessibility, and cheapness. This package was originally designed as a package of numerical mathematics, which later was extended with symbolic kernel of the Maple.

Maple was developed in Waterloo, Ontario, Canada. It has substantial symbolic capability and is available on a wide range of computing platforms. It is very useful in theoretical analysis. The latest version Maple 2016 provides data, computation and visualization tools for application with thermophysical properties of different working fluids which is especially valuable for a wide variety of thermal calculations.

Most today’s softwares’ developers propose web-based users’ communities where it is possible to discuss projects, create documentation, share applications, ready-made templates, connect with peers and help others get the most out of the products – all these encourage collaboration and facilitate participation and interaction. Such users’ communities exist within Mathcad and Maple softwares which was also used in the proposed tools.

One of the e-publishing house – Knovel – provides an online library focused on engineering topics. Its products can be operated within Mathcad and SMath (which is conceptually similar to Mathcad and freely distributed) environments. Online-tools with so called Interactive Equations are included into Knovel’s web-site. Interactive Equations of Knovel allow not only looking over those that formulas but interactively work with them almost the same way as in Mathcad Calculation Server. Mathcad users can also apply for ready-made solution at Knovel web-site without leaving Mathcad before they solve a new task. These features are going to be applied within the work.

A specific technology developed in [2] was used where a number of tools for the creation of the open and interactive algorithms were applied (Fig. 1). The algorithms 1 contain the following components: part 2 associated with the formulas for the calculation of parameters of a thermal unit (thermophysical properties, performance characteristics, etc.) and the corresponding Mathcad code 7; text part 3 that includes support information on formulas, notes to mathematical formulas and the description of the calculations, etc; part 4 related to computer and Internet technologies. The resource 1 provides a client with a number of options, including calculation of characteristics when manipulating data, reading of the text information and copying mathematical formulas or code in general. These options are executed on a remote server not on a personal computer of a user. The packages Mathcad Calculation Server 8 and Microsoft Expression Web 3 9 play an important role in the formation of the resource 1 (Fig. 1).

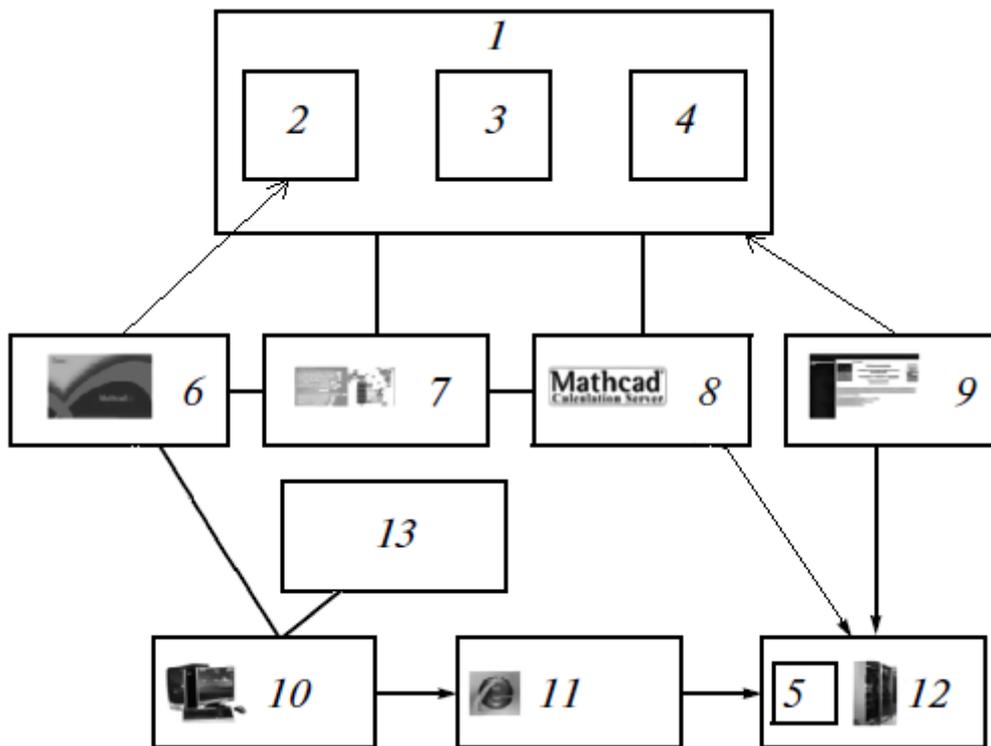


Figure 1. Sources of information and tools used to create an open interactive algorithm: the open interactive algorithm (1), Mathcad field of the algorithm (2), text (3), part associated with Computer Science and Internet technologies (4), the template (5), Mathcad-tools (6), Mathcad-program (7), Mathcad Calculation Server (8), package Microsoft Expression Web 3 (9), PC user (10), Internet (11), the remote server (12), the individual user program (13) [2]

### 3. Results

Figure 2 presents the Internet-resource [http://tw.t.mpei.ac.ru/OCHKOV/VPU\\_Book\\_New/mas/eng/index.html](http://tw.t.mpei.ac.ru/OCHKOV/VPU_Book_New/mas/eng/index.html) which has been developed using technology Mathcad Application/Calculation Server (MA/CS) in National Research University Moscow Power Engineering Institute. A block of input data for on-line, interactive thermodynamic computing of Brayton cycle is illustrated in Figure 3.

Interactive SMath-calculation of water pump power made within Knovel's web-site where a hidden area with a function calculating water density depending on pressure and temperature is shown in Figure 4.

Mathcad's user discussion forum of the author's book "Thermal Engineering studies with Excel, Mathcad and Internet" is presented in Figure 5.

Screenshot of the web-page of the Maple application center offering free downloading a Maple document for thermal calculation of nuclear power plant cycle with pressurized water reactor is shown in Figure 6.

Calculation Server of National Research University Moscow Power Engineering Institute (MPEI)

Search: [Search]

Contents

- Interactive reference books
  - Higher mathematics
  - Mathematical functions
  - Power & heat engineering
  - Water and Steam Properties
  - Properties and processes of working substances and materials of nuclear power engineering
  - Thermophysical properties of thermal power engineering working substances**
  - Hydraulic gas dynamics
  - Physical quantities
  - Pipelines of heat power plant
  - Thermodynamic cycles
  - Chemical kinetics
  - Chemical thermodynamics
  - Electrical materials
  - Theory of automatic control
  - Energy-saving
  - Power equipment noise dropping
  - Labour protection in Electric Engineering
  - Properties of Gas Hydrates
  - Properties of Ionic Liquids
- Online calculations
- Parts from books & articles of Valery Ochkov
- About MAS/MCS technology
- Other calculation servers

RUSSIAN VERSION

### Web-version of reference book

## Thermophysical properties of thermal power engineering working substances

Alexandrov A.A., Orlov K.A., [Ochkov V.F.](#)

About this reference book >>>

Last update : 16 August 2012

Some calculations are located on two or three servers: MAS11 - Mathcad Application Server 11, MCS14 - Mathcad Calculation Server 14 and sometimes WebMath. You can use anyone.

Show structure of reference book as its contents "Live" formulations from book

- region 1 IAPWS-IF97 (water)
- region 2 IAPWS-IF97 (steam)
- region 3 IAPWS-IF97 (near-critical region)
- region 4 IAPWS-IF97 (saturation line)
- region 5 IAPWS-IF97 (steam at high temperature)
- functions defined for all regions, described in IAPWS-IF97
- metastable region
- dynamic viscosity
- thermal conductivity
- surface tension
- static dielectric constant
- refractive index
- ionization constant
- thermodynamic properties of gases

Thermodynamic properties of water and steam  
 Thermodynamic properties of gases and seawater  
 Diagrams and graphical dependences  
 Properties of some refrigerants and working fluids for thermopumps

Figure 2. One of the web-pages of Mathcad Calculation Server developed in National Research University Moscow Power Engineering Institute

Calculation of Brayton Cycle with Two-Stage Compression and Regeneration

Mass flow of inlet air $G_{in}$ , kg/sec	1	Inlet air temperature $t_{in}$ , °C	15	Inlet air pressure $p_{in}$ , MPa	0.1013
Relative humidity of inlet air $\phi_{in}$ , %	60	Isentropic efficiency of compressor $\eta_{is_c}$ , %	38.2		
Isentropic efficiency of gas turbine $\eta_{is_t}$ , %	88.4	Cycle pressure ratio $\pi_c$	10.549		
Gas turbine inlet temperature $t_3$ , °C	1050	Lower heating value of fuel $Q_l$ , MJ/kg	50.056		
Temp. of determining lower heating value of fuel $t_{Ql}$ , °C	15	Fuel content $X_{CH_4}$ , %	100		
Pressure increase in the 1st compressor stage $\pi_{c_1st}$	3	Cooler outlet temperature $t_6$ , °C	100		
Temperature of inlet fuel $t_f$ , °C	15	Isentropic efficiency of fuel compressor $\eta_{is_{fc}}$ , %	90		
Pressure of inlet fuel $p_f$ , MPa	0.6	Fuel surplus pressure before fuel combustor $\Delta p_{f_{comb}}$ , MPa	0.5		
Pressure drops in fuel combustor $\delta p_{f_{comb}}$ , %	5	Effectiveness of fuel combustor $\eta_{f_{comb}}$ , %	99.8		
Pressure of air drops in regenerator $\delta p_{r_{air}}$ , %	5	Pressure of exhaust gases drops in regenerator $\delta p_{r_{ex_g}}$ , %	5		
Efficiency of electric generator $\eta_{e_{gen}}$ , %	99.8	Mechanical efficiency $\eta_{m}$ , %	99.8		
Regenerator outlet temperature of the air $t_8$ , °C	537	Pressure drops in cooler $\delta p_{cool}$ , %	3	Recalculate	

Figure 3. Input data block of the web-sheet prepared on technology of Mathcad Calculation Server for thermodynamic analysis of Bryaton cycle

**Power Requirement for a Water Pump**

An equation for calculating the power requirement of a water pump as a function of water density. Water density is calculated as a function of its temperature and pressure per IAPWS Formulation for Region 1. This equation can be used for pump selection in a variety of industries, including chemical process and power generation.

Contributed by: Valery Ochkov

References:

[http://app.knovel.com/web/view/swf/show.v?cid:kpASHRAEA2/cid:kt00AFVIV3/viewerType:pdf/root\\_slug:ashrae-handbook-heating-3?cid=kt00AFVIV3&page=7&b-toc-cid=kpASHRAEA2&b-toc-root-slug=ashrae-handbook-heating-3&b-toc-url-slug=centrifugal-pumps&b-toc-title=2012%20ASHRAE%20Handbook%20-%20Heating%2C%20Ventilating%2C%20and%20Air-Conditioning%20Systems%20and%20Equipment%20%28SI%20Edition%29](http://app.knovel.com/web/view/swf/show.v?cid:kpASHRAEA2/cid:kt00AFVIV3/viewerType:pdf/root_slug:ashrae-handbook-heating-3?cid=kt00AFVIV3&page=7&b-toc-cid=kpASHRAEA2&b-toc-root-slug=ashrae-handbook-heating-3&b-toc-url-slug=centrifugal-pumps&b-toc-title=2012%20ASHRAE%20Handbook%20-%20Heating%2C%20Ventilating%2C%20and%20Air-Conditioning%20Systems%20and%20Equipment%20%28SI%20Edition%29)

Citations: 1.) 2012 ASHRAE Handbook - Heating, Ventilating, and Air-Conditioning Systems and Equipment (SI Edition). Page 44.7. American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., 2012. 2.) International Association for the Properties of Water and Steam, "Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam", 2007, Lucerne, Switzerland, <http://www.iapws.org/relguide/I97-Rev.pdf>

Mass flow rate of water	$q_{\text{mass}} := 120 \frac{\text{M}^3}{\text{s}}$
Inlet pressure of water	$P_{\text{in}} := 2 \text{ ATM}$
Outlet pressure of water	$P_{\text{out}} := 7 \text{ ATM}$
Temperature of water	$T := 90 \text{ }^\circ\text{C}$
Pump efficiency	$\eta_{\text{pump}} := 0,85$

Density of water as a function of p and T

$$\rho := \rho_{\text{water}} \left( \frac{P_{\text{in}} + P_{\text{out}}}{2}; T \right) = 965,48 \frac{\text{kg}}{\text{M}^3}$$

Flow rate of water:

$$q_{\text{volume}} := \frac{q_{\text{mass}}}{\rho} = 124,2904 \frac{\text{M}^3}{\text{s}}$$

Power requirement for the water pump:

$$N_{\text{pump}} := \frac{q_{\text{mass}} (P_{\text{out}} - P_{\text{in}})}{\rho \cdot \eta_{\text{pump}}} = 20,578 \text{ kW}$$

Figure 4. Interactive calculation of pump power at Knovel's web-site

<https://www.ptcusercommunity.com/groups/thermal>

<https://www.ptcusercommunity.com/thread/128043?sr=stream&ru=32113>

Valery Ochkov 13.10.2015 4:21

### Study 1. Properties of working fluids, coolants and structural materials for thermal engineering calculations

You will learn how to create a function that returns thermophysical properties of working fluids, heat transfer and energy materials using interpolation and smoothing. You will also learn what a cloud function for the thermal calculations is.

Mathcad 15 and Mathcad Prime 3 sheets of the study in attach.

- 1-1-Ro-p-t.xmcd.zip 32.4 K
- 1-2-Ro-p-t.modx.zip 7.6 K
- 1-13-NaCl-Water-Solution-t-omega.xmcd.zip 51.4 K
- 1-17-T90-Ta8.xmcd.zip 58.0 K
- 1-2a-wspgAir-PT.xmcd.zip 10.1 K
- 1-8-Tab-5-5-0-2-Therm-Cond-Solids.xmcd.zip 68.4 K
- 1-2a-NaCl-Water-Solubility.modx.zip 11.1 K
- 1-27-HCl-Lurie-Tab-7-251.xmcd.zip 25.8 K
- 1-30-wspTCPT.xmcd.zip 140.1 K

Figure 5. A forum of the book "Thermal Engineering studies with Excel, Mathcad and Internet" located at PTC Community

The screenshot shows the Maple application center interface. At the top, the URL is [www.maplesoft.com/applications/view.aspx?SID=154033](http://www.maplesoft.com/applications/view.aspx?SID=154033). The navigation bar includes links for PRODUCTS, SOLUTIONS, ACHATS, SUPPORT, RESSOURCES, and ENTREPRISE, along with a search bar. The main content area features a schematic diagram of a steam turbine cycle with a Pressurized Water Reactor (PWR). The diagram shows a primary circuit with a nuclear reactor, a steam generator (SG), and a high-pressure cylinder (HPC). A secondary circuit includes a separator (S), a superheater (SH), a low-pressure cylinder (LPC), and a condenser (C). The cycle is driven by a pressurized water reactor (PWR) and includes a feed pump (FP), a condenser pump (CP1), and a reactor pump (CP2). The diagram is labeled with various components and flow paths, including  $\alpha_{SH}$  and  $1+\alpha_{SH}$ .

**Thermal Efficiency of Steam Turbine Cycle NPP with PWR**

This application calculates the thermal efficiency of a steam turbine cycle in a Nuclear Power Plant (NPP) with a Pressure Water reactor (PWR).

Pressurized water flows from the nuclear reactor (NPP primary circuit) to the steam generator (SG) and transfers heat to the boiling water of the second circuit. Saturated steam is supplied from the steam generator to the high pressure cylinder (HPC) of the steam turbine. Part of the live steam from the steam generator enters the superheater. Before being superheated, the exhaust steam from the HPC is partially dried in the separator (S), where some water is separated from the wet steam, and then returned to the circuit with bypass of the low pressure cylinder (LPC) of the steam turbine.

The thermal circuit of an NPP introduces a risk factor not found in fossil fuel power plant. In an NPP, if saturated steam is supplied to a turbine, whose outlet pressure is 5-4 kPa, moisture in the last stages of the turbine will be unacceptably high; this may lead to steam turbine failure.

**Maple Player** Don't have Maple? [Download the free Maple Player](#) to view and interact with Maple documents!

**Application Details**

Author: [Prof. Valeriy Ochkov](#)  
 Application Type: [Maple Document](#)  
 Publish Date: March 4, 2016  
 Created In: [Maple 2016](#)  
 Language: English  
 Category: [Engineering: Thermodynamics](#)

**Toolkit**

- [Download attached file](#)
- [Download PDF preview](#)
- [Preview this Application](#)
- [Contact the Author](#)
- [Evaluate Maple](#)

**Community Rating:**

**Your Rating:**

Move the slider to rate

**New Application**

Figure 6. Screenshot of the web-page of the Maple application center where a Maple document for thermal calculation of nuclear power plant cycle with pressurized water reactor is proposed for reviewing downloading

#### 4. Discussions

One of the web-page - web-version of reference book “Thermophysical properties of thermal power engineering working substances” which is demonstrated in Figure 2 deals with thermophysical properties of working fluids: reference to “cloud” functions, downloading and on-line interactive calculations. The data on properties of water and steam, the main working fluid in thermal engineering, are programmed according to the formulations of Association for the Properties of Water and Steam approved in 1997 and refined in 2007 [3]. The functions on properties of ideal gases and their mixtures are provided based on system of equations from [4]. In [5] a methodology was proposed for creation of forward and backward functions that return the values of the thermophysical properties of refrigerants on the basis of tabular values in different areas of the state: single-phase region, two phase region, the saturation line. The tabulated data were generated in the NIST program REFPROP (<http://www.nist.gov>). The reference book “Thermophysical properties of thermal power engineering working substances” is located in the list of interactive reference books (see Figure 2).

In general the developed Internet-resource [http://tw.t.mpei.ac.ru/OCHKOV/VPU\\_Book\\_New/mas/eng/index.html](http://tw.t.mpei.ac.ru/OCHKOV/VPU_Book_New/mas/eng/index.html) enables to solve a wide variety of thermal engineering tasks which is illustrated in [5] and other published works. Besides direct dealing with thermophysical properties of working fluids it is possible to do numerical interactive investigations of different thermal technologies. A user can manipulate input data, see not only final but also intermediate results within proposed methodology and have a possibility to download worksheets as ready-made templates for developing further investigations. Figure 3 demonstrates such options for case of interactive thermodynamic analysis of simple open Brayton cycle. Using an Internet browser an investigator, engineer etc.

fill in input data which are located in special “live” cells then press button “Recalculate” and receive both intermediate and final results of computing (numerical, analytical, graphical) similarly as in case of using Mathcad.

The similar options are proposed through cloud-based platform Knovel. As it can be seen from Figure 4 that visitors of the Knovel’s webpage are not only able to see and analyze “static” formulas when calculating power input for water pump but also can carry out computing by these formulas and transfer these formulas to their worksheets. The calculation shown in Figure 4 incorporates the function returning the density of water depending on its pressure and temperature. The website shown in Figure 4 contains a reference to the authoritative source published by ASHRAE (see [www.ashrae.org](http://www.ashrae.org)), in which the “static” formula itself for calculating the pump power capacity is presented and described in detail. A reader of this handbook (a visitor of the Elsevier website) can directly carry out calculation by these formulas and transfer there formulas into his/her application calculations. It should be noted that Knovel being a part of Elsevier has turned attention to SMath package as a tool for supplementing the technical handbooks and scientific technical articles published on the Elsevier website for free or paid access with interactive calculations.

As a result of development of on-line, interactive tools and algorithms for thermal calculations the author with his colleagues have published a book “Thermal Engineering Studies with Excel, Mathcad and Internet“ [5] The work provides the fundamentals of the application of mathematical methods, modern computational tools (Excel, Mathcad, SMath, etc.) and Internet to solve the a wide variety problems of heat and mass transfer, thermodynamics, fluid dynamics, energy conservation and energy efficiency. Technology for creating and “cloud” dealing with databases on various properties of working fluids, coolants and thermal materials is discussed within the book. All calculation methods are provided with links to online computational pages. The book is complemented with a forum on PTC community where it is possible to download Mathcad- files, comment and propose own solutions (see Figure 5).

Maple is another software which also provides cloud computing services. Including data about thermophysical properties of working fluids in the latest version Maple 2016 enables to perform thermal calculations in Maple without referring to external programmes. A set of Maple documents for thermal calculations are prepared by the author and uploaded to the Maplesoft user community for reviewing, discussing and sharing. Figure 6 presents one of such document for analysis of nuclear power plant cycle with pressurized water reactor. In this document functions on thermodynamic properties of water and steam were fruitfully used. Next phase of implementation of these Maple-based computing is online web-based applications using the technology of MapleNet.

## Conclusion

New tendencies in computer-aided engineering based on “cloud” technologies enable to develop web-based generation of computing tools in thermal engineering.

The mathematical package Mathcad with Mathcad Calculation Server (Mathcad Net Publisher) allowed to develop a “cloud” server [http://tw.t.mpei.ac.ru/ochkov/VPU\\_Book\\_New/mas/eng/index.html](http://tw.t.mpei.ac.ru/ochkov/VPU_Book_New/mas/eng/index.html) for engineers and scientists who perform computer simulations and modeling of thermal systems. The server considers online service that offers data processing over a web-interface using a software (in this case Mathcad) that runs remotely within the “cloud”.

Knovel’s platform also provides web-based open interactive tools for thermal calculations.

Another powerful mathematical tool for analyzing, exploring, visualizing, and solving thermal tasks is Maple software and its Internet publisher MapleNet. One of the outstanding features of its latest version, Maple 2016, is including a library for thermophysical properties of working fluids.

Internet forum is another type of “cyberspace” for solving thermal engineering tasks where it is possible to discuss tasks, download, add new or adjust old worksheets of thermal calculations.

### **Literature**

- [1] Furht B., Escalante A. eds.. “Handbook of Cloud Computing”. New York: Springer, 2010, 634 p. ISBN 978-1-4419-6523-3
- [2] Ochkov V., Ustyuzhanin E., Ko Ch. K., Shishakov V. Thermophysical Databases: From Tables to Interactive Internet Resources and Cloud Templates. High Temperature, 2015, Vol. 53, No. 4, pp. 515–520.
- [3] Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (The International Association for the Properties of Water and Steam, Lucerne, Switzerland, August 2007), [www.iapws.org](http://www.iapws.org).
- [4] Aleksandrov A., Ochkov V., Orlov K. Equations and Computer Program for Calculating the Properties of Gases and Combustion Products. Thermal Engineering, Vol. 52, No. 3, 2005, pp. 221–229.
- [5] Ochkov V., Orlov K., Voloshchuk V. Thermal Engineering Studies with Excel, Mathcad and Internet. Switzerland: Springer International Publishing, 2016. 307 p. ISBN 978-3-319-26673-2.

### **Acknowledgment**

This study was supported by a grant from the Russian Fund for Fundamental Research No. 16-08-01222.

---

Prof. Ochkov Valeriy, Moscow Power Engineering Institute National Research University, Department of Thermal Power Plants, Krasnokazarmennaya st. 14, 111250, Moscow, Russia, Phone: +7-495-362-71-71, Email: ochkov@twi.mpei.ac.ru