COMPLEXO DE SOFTWARE PARA RESOLVER AS DIFERENTES TAREFAS DA
DINÂMICA DE GÁS FÍSICOSOFTWARE COMPLEX FOR SOLVING THE DIFFERENT TASKS OF PHYSICAL GAS
DYNAMICSПРОГРАММНЫЙ КОМПЛЕКС ДЛЯ РЕШЕНИЯ РАЗЛИЧНЫХ ЗАДАЧ ФИЗИЧЕСКОЙ
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RESUMO

Este artigo é relevante devido ao fato de que a complexidade dos problemas científicos resolvidos pelos métodos de modelagem física e matemática, os requisitos crescentes para a precisão de sua solução levam a um aumento no volume de dados processados durante os experimentos computacionais. O objetivo do trabalho é reduzir os custos monetários e de tempo para o trabalho do pessoal científico que surgem ao usar o software fracamente estruturado que requer um grande número de atividades secundárias não relacionadas à atividade no desempenho de cálculos, bem como fornecer os meios de intercâmbio de dados entre as áreas de pesquisa relacionadas. Este artigo discute um algoritmo computacional e um conjunto de ferramentas de software para modelar a estrutura fina de fluxos de gás reativos multicomponentes não estacionários e fornece a estrutura do complexo, bem como a descrição de elementos individuais e exemplos. Um conjunto de ferramentas de software para fornecer a modelagem numérica de problemas na dinâmica de gases físicos, incluindo os componentes gráficos e de informação que suportam os estágios intensivos de recursos de experimentos computacionais é descrito. O complexo de ferramentas de software consiste em uma concha gráfica de elementos de controle do sistema; banco de dados de propriedades termodinâmicas de substâncias e mecanismos cinéticos, e a interface gráfica para controlá-lo; visualização de módulos dos resultados de resolução de problemas computacionais; componentes de software da preparação automatizada de dados de entrada para o problema de modelagem de fluxos instáveis do gás reagente. O conjunto desenvolvido de programas pode ser usado para resolver os problemas da dinâmica dos gases reagentes, que são de importância prática, bem como o ilustrador de cursos de treinamento na dinâmica física de gases.

Palavras-chave: *suporte de informação para os problemas de dinâmica de gás físico, tecnologias de informação, ferramentas de software, os experimentos computacionais, um algoritmo computacional.*

ABSTRACT

This article is relevant due to the fact that The complexity of scientific problems solved by the methods of physical and mathematical modeling, the increasing requirements for the accuracy of their solution leads to an increase in the volume of data processed during the computational experiments. The aim of the work is to reduce the monetary and time costs for the work of scientific personnel which arise when using the weakly structured software that requires a large number of secondary activities not related to the activity on the performance of calculations, as well as providing the means of data exchange between the related research areas. This article discusses a computational algorithm and a set of software tools for modeling the fine structure of non-stationary multicomponent reactive gas flows and provides the structure of the complex, as well as the description of individual elements, and examples. A set of software tools for providing the numerical modeling of problems in the physical gas dynamics, including the graphic and information components supporting the resource-intensive stages of computational experiments is described. The complex of software tools consists of a graphical shell of control elements of the system; database of thermodynamic properties of substances and kinetic mechanisms, and the graphical interface for controlling it; module visualization of the results of solving computational problems; software components of the automated preparation of input data for the problem of modeling unsteady flows of

the reacting gas. The developed set of programs can be used to solve the problems of the reacting gas dynamics, which are of practical importance, as well as the illustrator of training courses in the physical gas dynamics.

Keywords: *information support for the physical gas dynamics problems, information technologies, software tools, the computational experiments, computational algorithm.*

АННОТАЦИЯ

Данная статья актуальна в связи с тем, что из-за сложности научных задач, решаемых методами физико-математического моделирования, возрастающие требования к точности их решения приводят к увеличению объема данных, обрабатываемых в ходе вычислительных экспериментов. Целью работы является снижение денежных и временных затрат на работу научного персонала, возникающих при использовании слабоструктурированного программного обеспечения, для которого требуется большое количество дополнительных действий, не связанных с деятельностью по выполнению расчетов, а также обеспечение средства обмена данными между смежными областями исследований. В данной статье рассматриваются вычислительный алгоритм и набор программных средств для моделирования тонкой структуры нестационарных многокомпонентных потоков химически активного газа, а также приводится структура комплекса, а также описание отдельных элементов и примеры. Описывается комплекс программных средств обеспечения численного моделирования задач физической газовой динамики, включающий графические и информационные компоненты поддержки ресурсоемких этапов вычислительных экспериментов. Комплекс программных средств состоит из графической оболочки управления элементами системы; базы данных термодинамических свойств веществ и кинетических механизмов, и графического интерфейса управления ею; модуля визуализации результатов решения вычислительных задач; программной компоненты автоматизированной подготовки входных данных для задачи моделирования нестационарных течений реагирующего газа. Разработанный комплекс программ может использоваться для решения задач динамики реагирующего газа, имеющих прикладное значение, а также в качестве иллюстратора учебных курсов по физической газовой динамике.

Ключевые слова: *информационная поддержка задач физической газовой динамики, информационные технологии, комплекс программных средств, вычислительные эксперименты, вычислительный алгоритм.*

1. INTRODUCTION

The complexity of scientific problems solved by the methods of physical and mathematical modeling, the increasing requirements for the accuracy of their solution leads to an increase in the volume of data processed during the computational experiments. Performing mathematical calculations is an alternative and addition to the physical experiment, and it allows to identify the detailed structure of the process which is physically impossible to observe in experimental studies, saves considerable material resources and time when performing field experiments, anticipating and greatly facilitating, and sometimes replacing them completely (Kovshov et al., 2019).

The field of application of the created software product is mainly the physical gas dynamics, but the results obtained can be used in a wide range of calculation problems subject to the certain number of conditions (Gidaspov and Severina, 2015a; Gidaspov and Severina, 2017; Gidaspov et al., 2018). For example, (Gidaspov et

al., 2016) describes a similar complex that is focused only on solving the problems of modeling the quasi-one-dimensional non-stationary reacting flows (Korshunov et al, 2016a).

The aim of the work is to reduce the monetary and time costs for the work of scientific personnel which arise when using the weakly structured software that requires a large number of secondary activities not related to the activity on the performance of calculations, as well as providing the means of data exchange between the related research areas.

The reduction in the number of subtleties of operational nature corresponding to the introduction of the system during the performance of calculations will sufficiently reduce the threshold for young professionals with respect to the practical use of existing design programs which can also be called the goal of this work. Works (Gidaspov et al., 2016; Formalev and Kolesnik, 2019; Kolesnik, 2014; Formalev and Kolesnik, 2007; Formalev et al., 2009; Formalev and Kolesnik, 2013; Kurbatov et al., 2018; Bulychev et

al., 2018a; Bulychev *et al.*, 2018b; Krasovskii *et al.*, 2018; Rabinskiy and Tushavina, 2018; Bulychev *et al.*, 2018c; Lurie *et al.*, 2017; Kakhramanov *et al.*, 2017; Formalev *et al.*, 2018a; Formalev *et al.*, 2018b; Formalev *et al.*, 2017a; Formalev *et al.*, 2017b; Formalev and Kolesnik, 2017; Formalev *et al.*, 2018c; Formalev *et al.*, 2015; Astapov *et al.*, 2018; Bulychev *et al.*, 2018d; Lomakin *et al.*, 2018) present various physical problems for which such systems are necessary.

This article discusses a computational algorithm and a set of software tools for modeling the fine structure of non-stationary multicomponent reactive gas flows and provides the structure of the complex, as well as the description of individual elements, and examples.

2. METHODOLOGY

Despite the development of multidimensional modeling techniques, the one-dimensional models have retained their importance. In particular, they allow, by comparing numerical and experimental results, to verify the models describing the non-equilibrium chemical transformations in the gas phase, to prepare the initial data for multidimensional calculation, to carry out the full-scale engineering calculations when designing the real promising power plants.

A quasi-one-dimensional non-steady flow of a reacting gas in the flow continuity areas can be described by a system of partial differential equations, written in its characteristic form (Pirumova, 1988): Equations (1), (2).

Here ρ , u , p , e , h , a is the density, velocity, pressure, specific internal energy and enthalpy of gas, sound speed, respectively, γ_i are the molar -mass concentrations, N is the number of considered components, W_i is the formation rate of the i -th component in the unit volume as a result of chemical reactions, $F(x)$ is the dependence of the cross-sectional area on the longitudinal coordinate. The subscripts "T", "P", " γ_i " denote the private differentiation by the corresponding parameter. The effects of viscosity, thermal conductivity, and diffusion are neglected.

When passing through the shock wave and the contact discontinuity, the relations of Renquin – Hugoniot type are fulfilled which are a consequence of the integral conservation laws which can be written in the form (Pirumova, 1988): Equations (3), (4), (5).

The index "L" marks the parameters to the

left of the gap, "P" – to the right. In the case of shock wave: D – the velocity of the shock wave, the concentration during the transition through the shock wave does not change: $\gamma_{Li} = \gamma_{Pi}$. In case of contact break: $D = u_{Li} = u_{Pi}$, respectively: $p_{Li} = p_{Pi}$, the change of the remaining quantities is arbitrary.

The thermodynamic properties of the reacting gas are described using the model of multicomponent perfect gas within the assumption of the equilibrium population of energy levels corresponding to all internal degrees of the freedom of molecules and atoms (Gurvich *et al.*, 1982). In this case, the specific Gibbs thermodynamic potential is as follows Equation (6).

Here $p_0 = 101325 \text{ Pa}$ is the standard pressure, $G_i^0(T)$ is the temperature part of the standard Gibbs molar potentials of the individual components (Gurvich *et al.*, 1982). The reference literature specifies the polynomial approximation formulas for a reduced standard potential $\Phi_i^0(T)$ which is associated with $G_i^0(T)$ by the formula (Equation 7), where $h_i^0(0)$ – is the standard enthalpy $h(T)$ at the absolute zero, $h_i^0(T_0)$ – is the standard enthalpy $h(T)$ at $T_0 = 298.15 \text{ K}$. To set $\Phi_i^0(x)$ ($x = 10^{-4} T$), the work uses the polynomials similar to those specified in the reference book (Gurvich *et al.*, 1982) (Equation 8).

Here $\varphi_i, i = 1, 2, \dots, 3$ are the numerical factors that are individual for each substance. Other thermodynamic quantities used in the mathematical modeling are expressed in terms of the Gibbs potential and its partial derivatives. In the case of the arbitrary mechanism of N_r reversible chemical reactions of the form (Gidasov and Severina, 2014; Kondratyev, 1970) (Equation 9, 10).

Here M_i is the symbol of the i -th substance, $\bar{\nu}_i^{(r)}$ are the stoichiometric coefficients, the rate constants of direct $\bar{K}^{(r)}$ and reverse $\bar{\tilde{K}}^{(r)}$ reactions are connected through the equilibrium constant (Gardiner, 1988). To approximate the temperature dependence of the rate constants of direct reactions, the generalized Arrhenius formula (Gidasov and Severina, 2014) is used (Equation 11).

A , n , E are some constant values, individual for each reaction. The selection of reaction rate constant in the opposite direction depends on whether the reaction is reversible or not. In the case of a reversible reaction, the rate constant can be selected either through the equilibrium constant or through the Arrhenius formula.

3. RESULTS AND DISCUSSION:

3.1. Analysis of requirements for the construction of a mathematical model

The development of information support for the resource-intensive gas dynamics tasks implies the active use of database technologies for the storage, manipulation, analysis, and graphical processing of the large-scale numerical content (Marasanov and Rotanina, 1993).

The considered mathematical model determines a set of requirements for the developed set of programs. The used model of thermodynamics and chemical kinetics (Gidaspov *et al.*, 2008; Gidaspov and Severina, 2015b; Mustafaev *et al.*, 2000) determines the structure of the database for the thermodynamic properties of substances and chemical reactions. In particular, each substance is determined by a set of individual data: molecular weight, composition matrix, formation enthalpy, as well as the coefficients of polynomials of the reduced Gibbs potential for the corresponding temperature range (in real calculations, as a rule, not more than two), etc. To describe a chemical reaction, it is necessary to know the patterns of its occurrence in time. To approximate the temperature dependence of the rate constants of direct reactions, the generalized Arrhenius formula is used. The reactions of a maximum of the third order are considered in this model; the speed of each reaction can be described from various literary sources. The speed of the reverse reaction, depending on the mechanism, can be calculated from both the equilibrium condition (Gardiner, 1988; Skvortsov and Karizin, 2012) and the Arrhenius form.

After analyzing the above requirements for the information support, a database was designed with the following scheme (Figure 1). Figures 2-3 show the database management interfaces formed in accordance with the layout shown in Figure 1. The resulting software product completely covers the information needs of the computing module.

It should be noted that the method used in the computational module on which the testing was carried out while modeling all the gaps (Gidaspov *et al.*, 2008) entails a non-standard output data format and, as a result, the non-standard ways of their processing and displaying. All the intersections of grid lines are processed by the special algorithms and go to the exact coordinate when visualization is required to produce it correctly. The visualization system shall have the full range of capabilities of standard graphics systems for preparing the high-quality graphics for the color and black-and-white publications: line styles, axis labels, axis markings, etc (Korshunov *et al.*, 2016b).

Solving the problems of information support is concentrated within single centralized management of data and computing modules, providing the communication between the user and the package as a whole (interface component), as well as between the individual subsystems inside the package (streaming component). The description of the selected data classes allows to specify their semantic content, establish the necessary links, and form the sub-models.

3.2. The architecture of the complex

Based on the analysis of the features of domain, a structure has been developed for the information support system for the tasks of physical gas dynamics (Figure 4).

Let us list the main features of the system:

1. The user is provided with the opportunity to edit autonomously the database of the thermodynamic properties and chemical reactions, both with a view to modifying the stored information, and to create the consistent "mixtures" and "kinetic mechanisms" that can later be used in the calculations.

2. The interface for editing the configurations and launching a calculation module provides the setting of initial data for numerical simulation which include: geometry of the computational domain and boundary conditions; splitting the computational domain into subdomains with different initial values of gas-dynamic quantities, thermodynamic properties, and physical processes; adjustment parameters for the calculation module; characteristics of the numerical simulation technique used. The ability to store the typical tasks and configurations is provided. The interface provides access to the database of numerical simulation results, provides

a view of the results and, if necessary, the restart of the calculation module.

3. The results of the calculation module operation are presented in the form of two tabular files with an explicit relational component; therefore, they can be called the surrogate of the database for the storage of calculation results which have a dynamic structure that ensures the storage of the results of calculations of problems having the significantly different output data structures. Like regular files, the "database" provides the storage, import, and export of the graphics and textual material of the user related to the calculation. Algorithms of work with the "base" are implemented in the corresponding subsystems.

4. The calculation visualization subsystem takes into account the specifics of the problem being solved. Namely: the hyperbolicity of the problem – the number of steps in the march variable, as a rule, significantly (by many orders of magnitude) exceeds the number of cells of the difference grid; there are various types of grid lines, the number of grid lines is variable – they can disappear and appear; the number of parameters visualized is variable. The following types of graphs are implemented: distribution of parameters (functions of parameters) for arbitrary (available in the results file) value of the march variable; change of arbitrary parameter (set of parameters) along the arbitrary grid line and the fixed value of non-marching variable; process time-based sweep, 3D visualization of the computational domain. The function of the grid lines thinning is implemented for the results presentation clarity. The visualization subsystem allows both the color and black-and-white forms for the representation of graphic material and provides the data export.

The goal of the common interface is to combine all the modules of software package in one application in order to provide the user with quick access to any of them. The transition to one of four specific interfaces is carried out as part of the single user interface: interface for editing the gas mixtures and kinetic mechanisms, the interface of calculation module, an interface for visualizing the results, and editing the text data.

Figure 5 shows the complex control module. Standard screen forms of popular text editors and integrated development environments, as well as the existing mathematical design packages adapted to the existing realities and needs, were taken as the basis for the development of the graphical interface.

During its creation, the following entities were introduced. A set of executable files consisting of the following will be called as a task:

1. Calculation program.
2. Interface for editing the configurations of the calculation program of item 1.
3. Help file.

As follows from the universality of the developed software, there can be many tasks. At the expense of this, it is possible to use the control module with a variety of calculation modules. The calculation will mean a directory on the hard drive of the computer in which the initial data for a task will be formed later, and after the calculation is done, the output data will also be generated.

For carrying out several similar but not identical computational experiments, an additional abstraction is introduced – the project. This is the directory on the hard drive of the computer containing a set, possibly empty, of the calculations and the file with their description.

To set the initial data, a specialized interface was developed (Figure 4). The type of problems to be solved assumes the piecewise-continuous nature of the distribution of flow parameters in the computational domain at the initial moment of time which allows to define the computational domain in the form of singular points and subdomains the borders of which are the given points, and then determine the flow parameters in each of the subdomains. The user creates a list of special points. He sets the type of each singular point, the coordinate and speed of its movement. Then he describes the parameters of the subdomains. The following types of special points are provided: "input boundary", "output boundary", "combustion chamber", "exit to the atmosphere", "left wall", "right wall", "disintegration of gap", "extreme characteristic of the fan of waves", "fixed point", "shock wave". The subdomain description includes the following:

1. flow parameters (pressure, speed, temperature);
2. type of field point (characteristic (C_+ , C_- , C_0), wall, contact discontinuity, shock wave, gas trajectory, discontinuous characteristic, field fixed point)
3. the number of split points in the domain;
4. the strategy of filling the subdomain with nodes of the difference grid (moving or fixed nodes);

5. type of gas (inert, reactive, equilibrium-reactive);

6. composition of mixture (for each subdomain a different composition is allowed. The program connects to the database and gets a list of all the specified chemical mixtures. The user selects the type of mixture and sets the molar fraction of each substance contained in the mixture).

In addition to the setting of the computational domain, it is possible to set the control parameters for the calculation:

1. startup type (from the start or from control point);

2. interpolation type (linear or quadratic);

3. frequency of discharge to the file of the control layer;

4. frequency of the discharge of layers to graphics files;

5. type of problem (about the piston, the breakup of discontinuity in the closed region, about detonation wave, etc.).

Figure 6 shows the interface for setting the initial data and starting the calculations for one of the typical tasks. For clarity, the right side of the interface contains a diagram that displays all the current subdomains, types, and coordinates of points. The current editable point and subdomain are highlighted in red.

The visualization interface allows processing the data of unlimited size that is achieved by preprocessing the calculation results, which is the creation of data structure in the file system of the machine. The data obtained as a result of the work are organized in a tree structure. The directory with the name specified by the user is located at the root of the structure. This directory contains, as subdirectories, the results of parsing. Also, the subdirectory saves the service information that displays the structure of *f_grg* file at the time of parsing.

Const *t* parsing. The file name used inside the system is formed as “point of time” – “*x*” – “physical value that changes over time”. Time file that contains all points at the time of calculation is generated for the service needs.

When parsing, the *d_grg* file is sorted. For each of its completely discarded layers, a dictionary of file descriptors is formed in accordance with the structure of the *f_grg* file. Next, the range of nodes of this layer in the *f_grg* file is sorted. Information from the node is recorded

in the corresponding descriptor. In the case of incompletely discharged layer, the sorting is idle. The time complexity of the algorithm operation is $O(n + m)$, where *n* is the length of the *d_grg* file, *m* is the *f_grg*, respectively. Spatial complexity is $O(1)$. Parsing leads to the duplication of information.

AlongID and XT parsing. The file name used inside the system is generated as “node ID” – “node type”. ID file containing all the IDs of the settlement points with their types is generated for the service needs. When parsing, a dictionary of file descriptors with a key — the file name — is formed. The *d_grg* file parsing is carried out. For each layer, it reads the specified range of lines *f_grg*. If the dictionary has a descriptor that needs to be recorded, then the data is written; if not, a file is pre-created and added to the dictionary. The time complexity of the algorithm is $O(n + m + \log(k))$, where *n* is the length of the *d_grg* file, *m* is the *f_grg*, respectively, *k* is the number of different id values in the calculation. Spatial complexity is $O(k)$. Parsing leads to the duplication of information. This stage was introduced to accelerate the work. Because parsing into smaller parts requires a large amount of memory, if you store the descriptors, or a lot of time if you do not.

3D parsing. The file name used inside the system is generated in the form of “Renewable parameter”. A dictionary of file descriptors with a key — physical parameter — is formed. Further reading of the *d_grg* file and the corresponding *f_grg* ranges with the recording of information on the created descriptors is performed. For greater clarity, double nodes are spread along the coordinate at the small distance. The time complexity of the algorithm operation is $O(n + m)$, where *n* is the length of the *d_grg* file, *m* is the *f_grg*, respectively. Spatial complexity is $O(1)$. Parsing leads to the duplication of information.

The visualization interface allows the user to set the graphics rendering settings or select the already rebuilt one. When you start the interface, a series of queries to the database are performed to get general information about its contents – a list with point types for the first type of chart, a list with layer times for the second chart and a list with point coordinates for the third one.

The graph visualization module is a specially developed application that implements the basic capabilities for displaying the two-dimensional graphs. The application was developed in C, and the Gnuplot implementation was selected as the graphics library. Figure 7 shows the user interface of the calculation results

visualization module. The use of additional features is implemented as the application menu.

4. CONCLUSIONS:

The paper describes a set of programs for the numerical simulation of the physical gas dynamics problems, including the subsystems of information support and visualization. The feature of the developed complex is its versatility, the possibility of applying for a different class of tasks from different application areas, a pronounced modular structure: it contains four weakly dependent components: base of thermodynamic and kinetic data, calculation module with user interface, database for storing the results of numerical simulation, and system for visualizing the results. All components of the complex can function autonomously and be used by various software products. The development of a software product is seen in the final testing and commissioning. As a result of the implementation, the money and time costs of the work of the scientific staff which arise when using the weakly structured software that requires a large number of secondary activities not related to the calculation activity will be reduced. Means of data exchange between the adjacent research areas are also provided, the number of operational intricacies during calculations is reduced.

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$$\frac{dx}{dt} = u \pm a: \quad du \pm \frac{1}{\rho a} dp \pm \left(ua \frac{d \ln F}{dx} + \sum_{i=1}^N \frac{\rho_{\gamma_i} e_T - e_{\gamma_i} \rho_T}{\rho^2 a (e_T \rho_p - e_p \rho_T)} W_i \right) dt = 0, \quad (\text{Eq. 1})$$

$$\frac{dx}{dt} = u: \quad dh - \frac{1}{\rho} dp = 0, \quad d\gamma_i - \frac{1}{\rho} W_i dt = 0, \quad i = 1, \dots, N. \quad (\text{Eq. 2})$$

$$\rho_{\text{л}}(D - u_{\text{л}}) = \rho_{\text{п}}(D - u_{\text{п}}), \quad (\text{Eq. 3})$$

$$p_{\text{л}} + \rho_{\text{л}}(D - u_{\text{л}})^2 = p_{\text{п}} + \rho_{\text{п}}(D - u_{\text{п}})^2, \quad (\text{Eq. 4})$$

$$\rho_{\text{л}}(D - u_{\text{л}}) \left(h_{\text{л}} + \frac{(D - u_{\text{л}})^2}{2} \right) = \rho_{\text{п}}(D - u_{\text{п}}) \left(h_{\text{п}} + \frac{(D - u_{\text{п}})^2}{2} \right). \quad (\text{Eq. 5})$$

$$G(p, T, \bar{\gamma}) = \sum_{(i)} \gamma_i [RT \ln(p \gamma_i / p_0 \sum_{(j)} \gamma_j) + G_i^0(T)]. \quad (\text{Eq. 6})$$

$$G_i^0(T) = \Delta_f H_i^0(T_0) - [h_i^0(T_0) - h_i^0(0)] - T \Phi_i^0(T), \quad (\text{Eq. 7})$$

$$\Phi_i^0(x) = \varphi_0 + \varphi_{\ln} \ln(x) + \varphi_{-2} x^{-2} + \varphi_{-1} x^{-1} + \varphi_1 x + \varphi_2 x^2 + \varphi_3 x^3. \quad (\text{Eq. 8})$$

$$\sum_{i=1}^N \tilde{v}_i^{(r)} M_i \Leftrightarrow \sum_{i=1}^N \tilde{v}_i^{(r)} M_i, \quad r = 1, 2, \dots, N_r, \quad (\text{Eq. 9})$$

$$W_i = \sum_{r=1}^{N_r} (\tilde{v}_i^{(r)} - \bar{v}_i^{(r)}) (\vec{K}^{(r)} \prod_{j=1}^N (\rho \gamma_j)^{\tilde{v}_j^{(r)}} - \bar{K}^{(r)} \prod_{j=1}^N (\rho \gamma_j)^{\bar{v}_j^{(r)}}). \quad (\text{Eq. 10})$$

$$\vec{K}(T) = AT^n \exp\left(-\frac{E}{T}\right). \quad (\text{Eq. 11})$$

Figure 1. Database layout

Figure 2. Blend editing interface

Figure 3. The kinetic mechanism editing interface

Figure 4. The architecture of the complex

Figure 5. Control module

Figure 6. Interface for setting the initial data and running the calculations

Figure 7. Visualization module interface