

# High Technology Software Web-Tools to Solve Environmental Problems of Coal Region

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**Abstract.** The paper is dedicated to the pilot system of the computer information portal, that is being designed in Kemerovo State University in order to enable engineers, students, postgraduate students and other users to get an expanded access to solutions of environmental applied problems in Kuzbass. The following elements are considered to be pilot system elements: solution of the grit motion in a flooded shaft problem, virtual laboratory of parallel programming, distributed computer resources access system. The present research is based on the task 2014/64 of state research Scientific research organization.

**Keywords:** computer information portal, mathematical modeling, high performance computing.

## 1 Introduction

Coal companies are known for their huge negative effect on Kuzbass environment and the adverse changes they cause. High cost of environmental facilities, lack of investment, unavailability of scientifically proven recommendations on how to reduce mine work adverse impact on environment and to eliminate that impact make the environmental situation even worse.

Coal companies development requires water consumption increase needed for coal production and further coal preparation. Coal companies are major environment contaminators with increasing waste water discharge. Various industrial methods of waste water treatment require great costs.

Waste water treatment by using flooded waste mining workings requires less costs compared to other methods. Kolchuginskaya coal mine was the first in the world to apply this method to purify Komsomolec (coal preparation plant) slurry water. Liquid wastes are pumped into worked-out area of a flooded mine. Natural purification of wastewater is supposed to take place in mine workings due to the water precipitation and mixture with influent underground water. Although the

method requires low costs it is essential to be researched to forecast possible effects of treatment processes in the flooded mine. Flooded mine working can be defined to be a black box with only input and output data possible to be estimated. Numerical simulation of the treatment process is almost the only possible way to estimate this method impact on the environment.

Taking into consideration current ecological situation the Russian government approved the state long term coal industry development program for the period until 2030, that includes measures aimed at coal consumption increasing by domestic power industry and scientific and technology capability development via the adoption of innovation technologies of coal processing and utilization such as underground coal gasification. This technology is considered to be the most ecologically friendly. Numerical simulation of underground coal gasification enables to identify qualitative composition of combustion gas in the coal mine under consideration.

Kemerovo State University develops the project targeted at high technology software complex development in order to solve environmental problems of the coal region that can be available for research community, managers, engineers, students and post graduates.

Software tools are often used by either developers or limited group of experts in the form of problem-oriented software. It happens because software is mostly aimed at single-discipline problem solving, sophisticated to use, and it requires upgrading in case the problem formulation changes. Such kind of software is considered to be unique and requires pricy operating license (\$2500 for a processor or \$900 - \$1500 for a user). Modern information technologies enable to cut simulation experiment costs and make it available for more users by creating cloud computing and special purpose web-services.

The following tasks are solved:

- mathematical modeling to solve applied ecological problems,
- carrying out simulation experiments based on the multiple access computing center of high performance computing,
- development of applied software based on web-services (information-computer portal),
- creating virtual laboratory courses for educational process based on information-computer portal,
- leasing the developed software out.

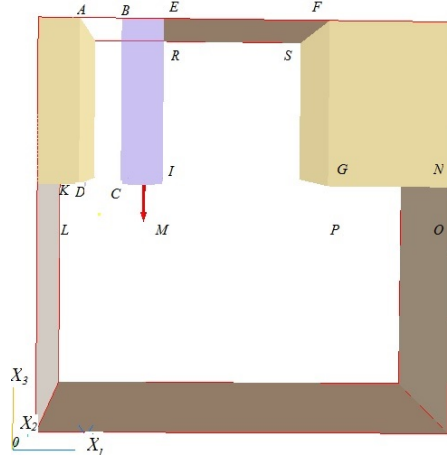
Here are the main project streams:

- development of mathematical and software components to solve the problems of waste water treatment in flooded mines and underground coal gasification,
- development of software technology platform with set of services to perform functions of information-computer portal,
- KemSU computing resource (multiple access computing center of high performance computing) and other computing resources access arrangement, which are provided for users and based on external platforms or cloud.

## 2 The problem of waste water treatment in a flooded mine

Water body pollution by mining and quarry waters is a typical problem for Kuzbass and many other mining regions [3]. Mining waters usually contain particles of coal dust, clay, calcium compounds, magnesium, oil products, etc. Light substances (which density is less than water density) such as oil products accumulate on water surface while other particles remain suspended or sediment gradually. The problem of mining water treatment by pumping into abandoned mines and further use of it after precipitation of impurities (for heavy particles) or impurity floating up (for light particles) is of great interest.

The paper considers fluid flow containing impurity particles in a flooded mine. To analyze float impurities distribution a square form mine is under consideration. It has a ledge at the top (shown in Fig. 1).



**Fig. 1.** Computational domain scheme

Underground water inflows into the domain thorough the boundaries KD, CI and GN. Fluid leaves the domain though the boundary AB. Impurity layer stays inside the domain at the initial time. Influenced by a flow some impurities leave the domain while the remaining part stays in the domain. To describe this transfer process differential equation system is used. The equations express the laws of conservation of mass, momentum and elements concentration in the domain. Mathematically the following differential equation system for turbulent flow should be solved in the following way:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}(-\overline{\rho u'_i u'_j}) - \rho S C_d u_i |\vec{u}| - \rho g_i, \quad (2)$$

$$\rho\left(\frac{\partial Y_k}{\partial t} + u_1 \frac{\partial Y_k}{\partial x_1} + (u_3 - u_{3k}) \frac{\partial Y_k}{\partial x_3}\right) = \frac{\partial}{\partial x_j}(-\overline{\rho Y'_k u'_j}), \quad (3)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(u_i \rho k) = \frac{\partial}{\partial x_i} \left[ \left( \frac{\mu_t}{\sigma_k} + \mu \right) \frac{\partial k}{\partial x_i} \right] - \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} \\ - \beta \rho g_i \frac{\mu_t}{Pr} \frac{\partial T}{\partial x_i} - \rho \varepsilon, \end{aligned} \quad (4)$$

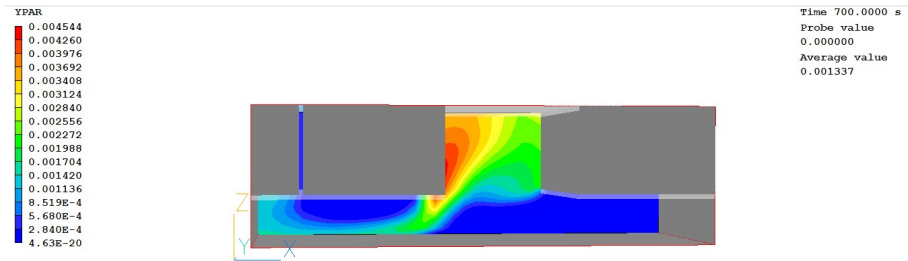
$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(u_i \rho \varepsilon) = \frac{\partial}{\partial x_i} \left[ \left( \frac{\mu_t}{\sigma_\varepsilon} + \mu \right) \frac{\partial \varepsilon}{\partial x_i} \right] + C_1 \frac{\varepsilon}{k} (G_k + G_B) - C_2 \rho \frac{\varepsilon^2}{k}, \quad (5)$$

$$p = \rho R_0 T \sum_k \frac{Y_k}{M_k}, \quad \vec{g} = (0, g), \quad u_{3k} = \frac{g d_k^2}{18\nu} \left( \frac{\rho_k}{\rho} - 1 \right). \quad (6)$$

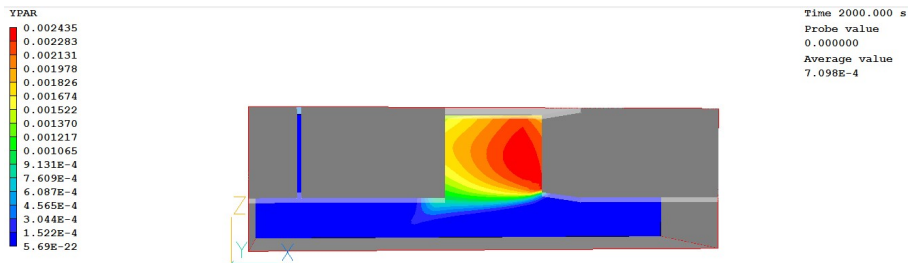
Here,  $t, x_i$  - time and spatial coordinates ( $i = 1, 3$ );  $u_i$  - velocity vector projection on the corresponding axis of cartesian reference system,  $p$  - pressure;  $g$  - gravitational acceleration,  $R_0$  - absolute gas constant,  $M_k$  - molecular weight of  $k$  - component,  $\rho$  - density of fluid and particles mixture,  $\nu$  - kinematic viscosity coefficient,  $D_t$  - diffusion coefficient,  $d_k, \rho_k, u_{3k}$  - diameter, density and velocity of particle settling,  $Y_k$  - mass concentrations of  $k$  - component ( $k = 1$  - water, 2 - solid particles);  $\mu_t = \rho C_\mu k^2 / \varepsilon$  - coefficient of turbulent viscosity,  $k = \overline{u'_i u'_j} / 2$  - turbulent kinetic energy;  $\varepsilon$  - its dissipation,  $C, \sigma_k, \sigma_\varepsilon, C_1, C_2$  - empirical constants, and  $G_k, G_B$  - turbulence caused by forced convection and natural convection.

Based on mathematical formulation of the problems (1)-(6) numerical calculations were made to determine the pattern of float impurity distribution process in a flooded mine [4].

Vector fields of velocity and impurity distribution at different time moments were obtained as the result of numerical integration of equation system (1)-(5). Side walls are considered not to influence the impurity distribution process and fluid flow. Thus the problem is solved in the two-dimensional domain  $X_1 O X_3$ . A mine (length – 10 meters horizontally, height – 3 meters) is under consideration (Fig. 1.). Underground water without any impurity enters the domain. Impurity concentration equals 1 inside the domain. Particles size is  $d_k = 5 * 10^{-5}$  m. Impurity particles density is  $500 \text{ kg/m}^3$ . The velocity of groundwater inflow from the upper layers is  $0.1 \text{ m/s}$ . The distributions of impurity are numerically calculated at different time moments (Fig. 2- 3). These figures show that the flow becomes stable and impurities accumulate in the upper part of the domain as time goes. It happens faster compared with the previous case because the particles density is two times less.



**Fig. 2.** Distribution of impurity which density is  $250\text{kg}/\text{m}^3$ ; ( $t=700$  sec)



**Fig. 3.** Distribution of impurity which density is  $250\text{kg}/\text{m}^3$  ( $t=2000$  sec)

The mathematical model presented in this paper can be used to analyze mining water treatment process due to environment and evaluate its further possible improvements.

### 3 Problem of ignition and combustion of combustible gas and coal particles gas-dispersion mixture

Flame front distribution in gas-dispersion medium is under consideration, when exothermic chemical reactions take place in the gas phase and on the surface of disperse phase particles with one of gas phase components. Those processes accompany combustion process of methane-air mixture with coal particles in mixture of gases (oxidant, combustible gas and inert gas), where small coal particles that can be heterogeneously reactive with gas mixture oxygen are evenly distributed. The oxidant is supposed to be involved into the particle surface reaction. Gas-dispersion mixture has specified velocity. The particles have equal sizes and spherical shape. Heat exchange between particles and gas follows the Newtons law. The rate of gas chemical reactions and particle surface chemical reactions depends on the temperature according to the Arrhenius law. Gases are the resultants of heterogeneous reaction on particles. Thermal expansion of gas mixture can be ignored. The ignition source is situated at the boundary of  $x = 0$  (combustion temperature is specified). Mathematical model of this mixture combustion takes into consideration the complexity of gas phase and

two-temperature medium [8, 9]. Taking into account the conditions above, the equation system appears to be as follows:

$$\frac{\partial}{\partial t}(\rho + mN) = 0 \quad (7)$$

$$\rho \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} \right) = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial x} \right), \quad (8)$$

$$\begin{aligned} \rho c_p \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} \right) = \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) + q \rho^2 c_1 c_2 k_0 \exp(-E/RT) - \\ - S \alpha N (T - T_S) - (c_p T - c_S T_S) N \frac{\partial m}{\partial t}, \end{aligned} \quad (9)$$

$$m c_S \frac{\partial T_S}{\partial t} = S \alpha (T - T_S) - q_S \frac{\partial m}{\partial t}, \quad (10)$$

$$\rho \left( \frac{\partial c_1}{\partial t} + u \frac{\partial c_1}{\partial x} \right) = \frac{\partial}{\partial x} \left( \rho D \frac{\partial c_1}{\partial x} \right) - \rho^2 c_1 c_2 k_0 \exp(-E/RT), \quad (11)$$

$$\rho \left( \frac{\partial c_2}{\partial t} + u \frac{\partial c_2}{\partial x} \right) = \frac{\partial}{\partial x} \left( \rho D \frac{\partial c_2}{\partial x} \right) - \alpha_S \rho^2 c_1 c_2 k_0 \exp(-E/RT) + N \frac{\partial m}{\partial t}, \quad (12)$$

$$\frac{\partial m}{\partial t} = -\frac{S \rho c_2 R_S \beta_m}{R_S + \beta_m}, \quad R_S = k_S \exp(-E_S/RT_S), \quad \beta_m = \frac{Nu_D D}{d} \quad (13)$$

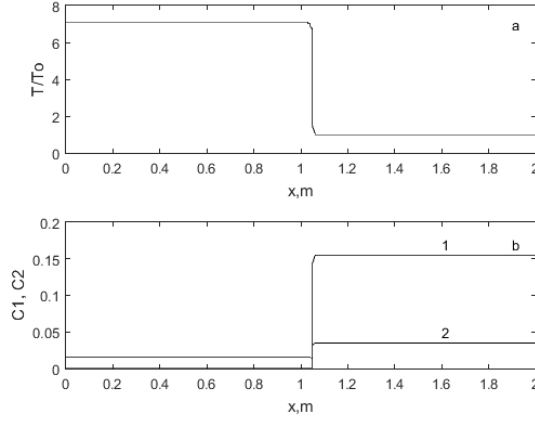
where  $t$  - time,  $x$  - coordinate,  $u$  - velocity,  $T$  - temperature,  $\rho$  - density,  $p$  - pressure,  $q$  - heat of gas chemical reaction,  $q_S$  - heat of particle surface chemical reaction,  $E, E_S, k, k_S$  - activation energies and pre-exponential factors of gas and particle surface chemical reactions,  $d, S$  - diameter and particle surface area;  $N$  - number of particles per unit volume;  $\lambda, \alpha, \beta_m, D$  - coefficients of heat conduction, heat mass exchange and diffusion;  $R$  - absolute gas constant,  $c_1, c_2$  concentrations of combustion gas and oxidant,  $Nu_D$  - Nusselt diffusion number,  $\alpha_S$  - stoichiometric coefficient,  $l$  - size of computational domain.

$$t = 0 : \rho = \rho_0, T = T_0, c_1 = c_{10}, c_2 = c_{20}, m = m_0, \quad (14)$$

$$x = 0 : u = u_0, \frac{\partial T}{\partial x} = 0, \frac{\partial c_1}{\partial x} = 0, \frac{\partial c_2}{\partial x} = 0, \quad (15)$$

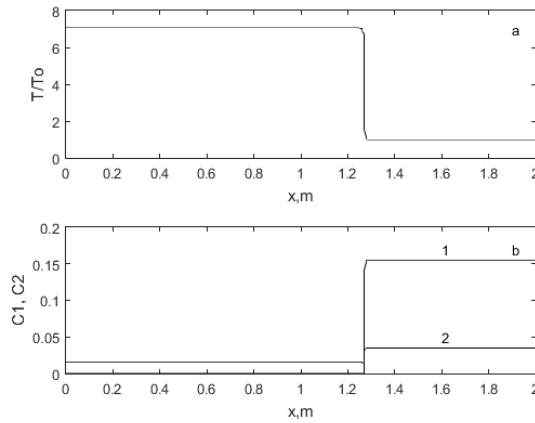
$$x = l : \frac{\partial u}{\partial x} = 0, \frac{\partial T}{\partial x} = 0, \frac{\partial c_1}{\partial x} = 0, \frac{\partial c_2}{\partial x} = 0. \quad (16)$$

The indexes refer to: 1 - combustible gas, 2 - oxidizing agent (oxygen),  $s$  - disperse phase, 0 - initial conditions. Basic data are found in [8–10].



**Fig. 4.** Distribution of temperature (graph a), combustible gas concentration (graph b, curve 2), oxygen (graph b curve 1) and combustible gas (graph b line 1);  $t=15$  s

Equation system (7)-(13) with initial and boundary conditions (14)-(16) was numerically solved. Control volume approach [4] was used to achieve discrete analog. Distributions of temperatures and components in the domain under consideration are identified by using numerical integration. The mixture of three gases is studied: overoxidized ( $c_{10} = 0.0349, c_{20} = 0.15504$ ), stoichiometric mixture ( $c_{10} = 0.0402, c_{20} = 0.15504$ ) and underoxidized ( $c_{10} = 0.0405, c_{20} = 0.15504$ ).



**Fig. 5.** Distribution of temperature (graph ), combustible gas concentration (graph b, curve 2), oxygen (graph b curve 1) and combustible gas (graph b line 1);  $t=18$  s

For example, on Fig. 4- 5 show gas phase temperature distribution and distribution of combustibles and oxidizing agent due to different time moments. It is obvious that flame front develops because maximum temperature area moves. According to that, the concentration of the combustible  $C_1$  is reduced and the concentration of the oxidant  $C_2$  decreases to almost zero point.

## 4 Information-computer portal

Software (in the form of web-services intergated into engineer and computing portal) based on the problems mentioned in sections 2-3 was developed.

Fig. 6 shows the architecture of portal prototype as a deployment diagram.

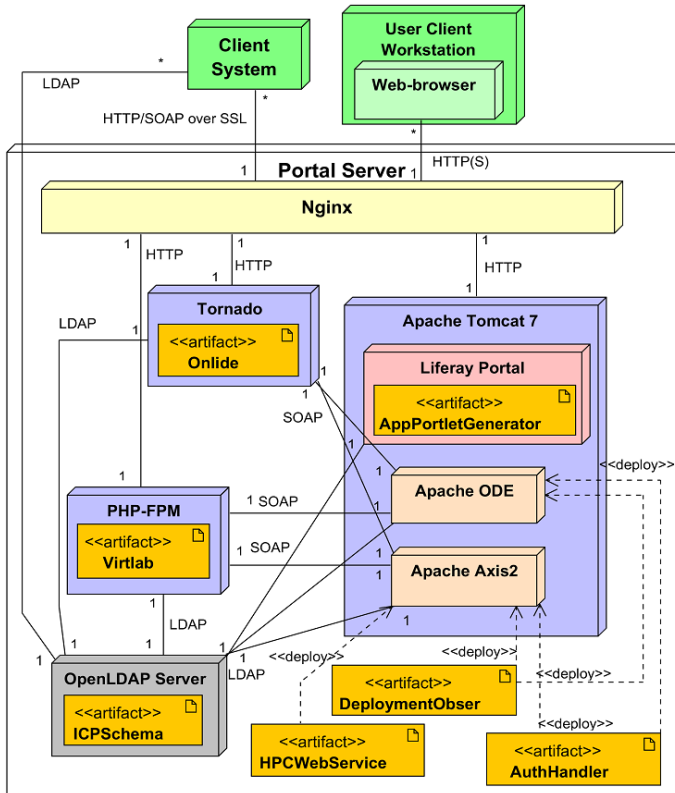


Fig. 6. The architecture of portal prototype as a deployment diagram

OpenLDAP Server is a server of LDAP-catalogue used to create single user base, web-service registry, business processes, high-end computing resources and some other data.



Client system is any external client system that interacts with web-services / business processes of the portal and/or with LDAP-catalogue.

User Client Workstation is a user personal computer, for example, a personal computer with web-browser.

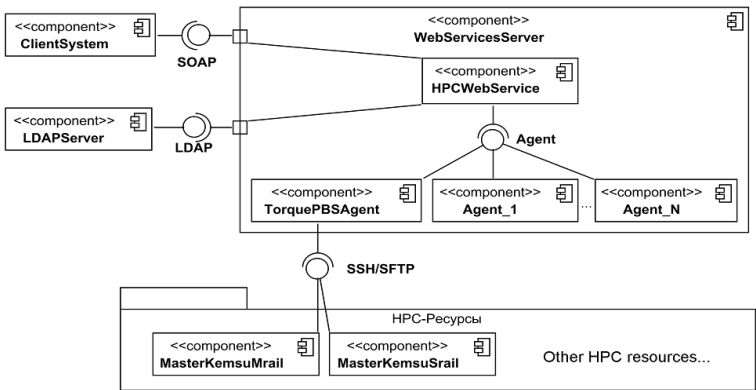
Liferay Portal (<https://www.liferay.com>) is a configurable complex solution to develop web-portals. Portlet technology is used to create portal pages. Portlet is a web-application designed in accordance with JSR-168 or JSR-286 specification [5]. They generate portions of some content (usually fragments of HTML- or XML layout) embedded into a web-page. Such kind of a web page can include many portlets. Liferay enables each user to create personal pages. That opportunity is used to create personal user work space that aggregates services to meet his personal needs.

Apache Axis2 is an integration and web-service life-cycle management system (<http://axis.apache.org/axis2/java/core/>).

Apache ODE is an integration system of web-service orchestration (<http://ode.apache.org>) that is a mixture of web-service capabilities to compose new higher level web-service called business process. BPEL based on XML is a standard descriptive language for business processes.

Nginx is a high-end HTTP-server and reverse proxy, e-mail proxy server as well as general purpose TCP/UDP proxy server (<http://nginx.org/ru/>). In this context it is used as a proxy server to forward requests to other components (Apache Tomcat 7, Tornado PHP-FPM). Though, there are some exceptions (requests for static files): images, JavaScript-files, etc. the reason is that Nginx is optimized for such kind of requests.

Tornado is a web-server that hosts online development environment system Onlide [7].



**Fig. 7.** Web-service model providing access to the HPC resources (components and internal structure diagram)

PHP-FPM is a process manager FastCGI used to generate PHP dynamic content of the Virtual laboratory course system [6]. It is used due to the fact that Nginx has no native support for such content generation.

Apache Tomcat 7 is an application web-server with servlet specification support. It hosts Liferay, Axis2 and ODE.

Web-service HPCWebService is created to interact with high-end computing resource (HPC resources). Fig. 7 shows the service model.

Web service has the functions targeted at compute cluster- based sequential and parallel program compiling and running, program outputs, task monitoring, clearing up space for a user.

Depending on operating system and task management system (if there is any) the interaction with computing resources may vary. Therefore web-service interacts with HPC-resources via proxy agents.

Agents can be targeted at each individual resource in order to create multi-purpose agents interacting with many computing resources. For example, to interact with Linux-system and task management system Torque PBS clusters TorquePBSAgent is created. This agent is currently used to interact with main KemSU cluster (master.kemsu.ru).

Algorithms to solve applied problems, to access high performance resources and etc. are developed as web services. User interface used to interact with web services of the portal (solvers) is created either as portlets or with the help of purpose built format based on XML- SolverXML. The format is developed in the way that enables to use component kit to create solvers. This kind of approach enables to create reusable component-solvers which can be used to create fully-featured tools. It also makes it easy for a solver to meet users needs compared with its portlet-based implementation.

The screenshot displays a web-based interface for configuring a solver task. On the left, a 'Project Tree' shows a hierarchy: 'my-project-1' containing 'job-1', which in turn contains 'configuration' and 'visualization'. The 'configuration' node is selected. On the right, a configuration form contains several input fields for parameters. The parameters are organized into two columns:

The height of mine channel: 1,0	The length of the inclined part: 3,0
The length of the main horizontal part: 12,0	The length of the horizontal small portion: 0,2
The length of the horizontal small part: 0,05	Grid time step: 0,01
Input flow rate: 0,01	Reynolds number: 200
The number of time steps: 10	The number of fraction: 1

At the bottom of the form, there are two buttons: 'param\_emp' and 'param', with 'param' being highlighted in blue.

**Fig. 8.** An example of the solver interface to launch tasks on cluster, which is described with the help of SolverXML-format

SolverXML-description consists of not more than seven blocks: *< imports >*, *< js >*, *< gui >*, *< vars >*, *< externals >*, *< handlers >*, *< actions >*.

The `< imports >` block lists imported JavaScript-files, user interface elements for data input/output (widgets) and SolverXML-descriptions of other solvers stored in the LDAP-catalogue.

The `< js >` block is used to add some JavaScript - based algorithms.

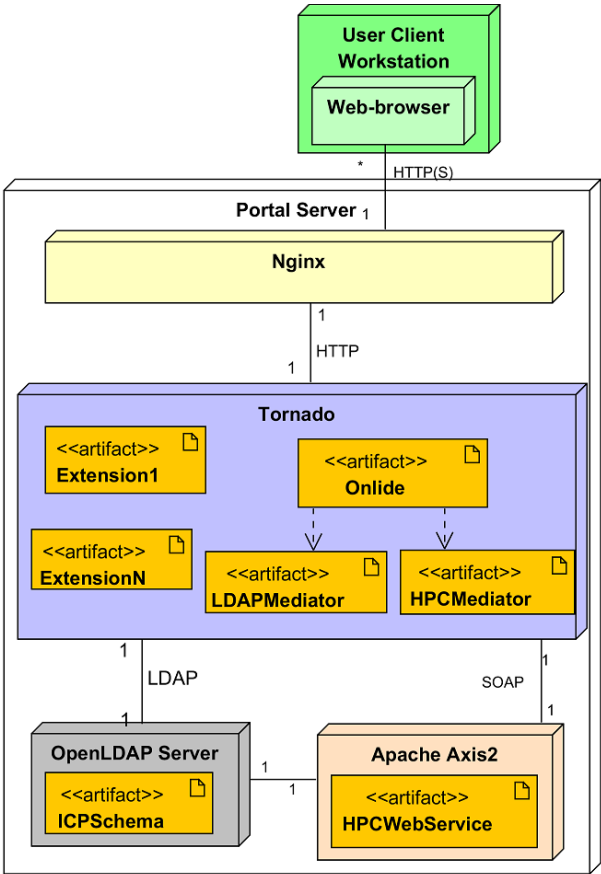
The `< gui >` block has user interface description.

The `< vars >` block has variable list which store or provide some value.

To make components interact with each other the `< externals >` block is used. It lists widgets and variables to address widgets and variables of other component.

The `< handlers >` block is used to specify handlers of widget and solver events.

The `< actions >` block describes the interaction with web services / business processes.



**Fig. 9.** Architecture of the Onlide system as a deployment diagram

Fig. 8 shows an example of solver interface based on the format under consideration.

The Onlide system is developed for remote development and launching of sequential and parallel programs at high-performance computing resources. It has the following functions: 1) development of software projects, consisting of many software texts based on different programming languages; 2) project editing; 3) project compilation and launching; 4) usage of extensions to increase capability options of development environment.

Fig. 9 shows the system architecture as a deployment diagram. LDAPMediator and HPCMediator (proxy agents) are developed in order to interact with LDAP-catalogue and HPCWebService. Onlide module is responsible for HTTP- and Ajax-requests processing and HTML-layout generation.

## 5 Conclusion

Multi-parameter model of incompressible fluid hydrodynamics is developed as a result of the project. Mathematical model of combustion of gas disperse phase with particles is presented. Numerical study of disperse phase and combustible gas and oxygen impact on the flame front rate in gas-disperse medium is carried out. According to calculation data the flame front rate depends on the gas and disperse phase parameters.

The algorithms are created and tested. Principles of information and computer portal based on service-oriented architecture are presented. The developed prototype of web-oriented technology software complex includes the following modules: software component of impurity motion in a flooded mine problem computation; virtual laboratory of parallel computing; component kit for interaction with distributed computing resources.

Practical relevance of the research enables to use prototype of technology software complex in order to conduct simulation experiments and teach high performance computing technologies to students and postgraduates.

The developed high technology product is supposed to attract additional investments in order to study new regional ecological problems.

The research is based on the state task № 2014/64, the state project Scientific researches organization. The results of the numerical calculations and problem formulation will be used by the educational resources information portal that offers students, postgraduate student and academic researches different educational services.

## References

1. A.M.Goudov, S.Y.Zavozkin, I.V.Grigorieva, L.V.Bondareva, N.N.Okulov. High technology software WEB-tools to solve environmental problems of coal region//Vestnik of Kemerovo State University, 2015, Vol. 1, N 2 (62), pp.22-29.

2. V.A. Perminov, A.M. Goudov Mathematical modeling of contaminant flow in closed reservoir / Proceedings of fifth international conference GEOMATE 2015 Geotechnique, construction materials and environment, Osaka, Japan, 16-18 November, 2015, pp. 844-846.
3. Zakharov, Y.N., Potapov, V.P., Schastlivcev, E.L., Chiruykina, A.V. Modelirovanie rasprostraneniya zagryaznyayuchikh veshstv v zatoplennykh gornykh vyrabotkakh [Simulation of impurities distribution in flooded mine workings] (2009) Vestnik NGU (Seriya Informacionnye tekhnologii), 7(4), pp.66-72.
4. Patankar, S.V. Numerical Heat Transfer and Fluid Flow New York: Hemisphere Publishing Corporation (1981), 214 p.
5. Introduction to the Java Portlet Specification, <http://www.developer.com/open/article.phppr/3547186/Introduction-to-the-Java-Portlet-Specification.htm>.
6. Grigorieva I.V., Savitskiy Y.V. The system of virtual laboratory course // Vestnik of Kemerovo State University. 2013. N 4 (56).
7. Sotnikov I. Y. Web-system Paralarea for e-learning and development of high-performance computing programs // Proceedings of XVI all Russian mathematical modeling conference of young scientists. Krasnoyarsk city, Russia. October 28-30, 2015 - Novosibirsk: ICTSB RAS, 2015. - pp. 91-92.
8. Mathematical theory of combustion and explosion / Y. B. Zeldovich, G. I. Barenblatt, V. B. Librovich, G. M. Makhviladze. .: Nauka, 1980.
9. Fundamental theory of combustion: Manual for higher education institutions / edited by V. V. Pomerntsev. L.: Energoatomizdat, 1986.
10. Heat exchange units guide. .2. M.: Energoatomizdat, 1987.