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THE DEVELOPMENT OF FREE ENGINEERING SOFTWARE PACKAGE FOR NUMERICAL SIMULATION OF HYDRODYNAMICS, HEAT TRANSFER, AND CHEMICAL REACTION PROCESSES

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Krasnoyarsk Subsidiary of Kutateladze Institute of Thermophysics SB RAS and the Department of Thermophysics of the Siberian Federal University are developing a freely distributable "SigmaFW" software package for numerical simulation of the hydrodynamics, heat and mass transfer problems. It is assumed that the software package will be used in scientific and educational institutions as well as industrial enterprises in Russian Federation. Mathematical models realized in the software package describe steady and unsteady laminar and turbulent single- and multicomponent flow taking into account the dispersed phase, the conjugate and radiative heat transfer, and homogeneous gas-phase chemical reactions. The "SigmaFW" contains the necessary tools for building numerical domains, carrying out multi-threaded calculation, and visual analysis of the results. The article describes the three main blocks of software package: the grid generator, calculation module and analysis of the results. In addititionn, a number of test and application tasks are presented to demonstrate the capabilities of the software.

Keywords: numerical simulation; computational fluid dynamics; software package.

Introduction

Numerical simulation of hydrodynamics and heat and mass transfer processes is used successfully throughout the world as one of the important tools for conducting scientific fundamental and applied research, process flow analysis, optimization and modernization of technological systems and installations. At that, the level of use of this tool in Russia is still quite low. This is due to several reasons, the most notable of which are the financial costs associated with the purchase and support of appropriate software, and the lack of a sufficient number of qualified specialists dealing with numerical simulation of hydrodynamics, heat and mass transfer processes. The use of the most advanced foreign software systems CFD ANSYS or STAR-CCM+ requires investments of tens to hundreds of thousands of dollars. The only Russian commercial CFD software package "FlowVision" has less functional capabilities. Just like in the world, the Russian Federation is involved in the development of industry-specific and university programs. The most famous industry-specific software system is "LOGOS", which is task-oriented to military industrial establishment and the nuclear energy problems. At the moment, "LOGOS" is not available for general use. SaintPetersburg software "VP-2/3" and "SINF" can serve an example of university developed codes. There is a number of free access software (for example, "OpenFOAM") abroad, which are also used by Russian researchers, though their learning requires much more time and high qualification of the user. Thus, the development of free software package for simulation of the hydrodynamics and heat and mass transfer problems, available to scientific and educational organizations, as well as industrial enterprises in Russia, is an acute issue. Such software package is developed in the Krasnoyarsk Subsidiary of the Institute of Thermophysics SB RAS on the basis of the "SigmaFlow" original designers code [1].

1. Brief Description of the Software Package

The SigmaFW software package consists of three main blocks: preparation of the calculation, calculation module, and analysis of the results. Calculation preparation block includes the grid generator and the module to define the boundary and initial conditions, thermophysical properties, and the parameters of the mathematical model. In the grid generator, the discretization of the computational domain is based on a third-party (imported) geometry, pre-prepared in an external CAD system. The grid generation process is based on the octal partition of the geometry space. First, on the basis of a geometrical size of an object the program builds a single spatial element (cube), which contains studied object (Fig. 1). This element, in turn, is divided into eight elements (cubes) and the process is repeated for each element. The time point corresponding to the creation of the first element will comply with the first level of partitioning. Choosing parts for further partitioning and the time moment corresponding to termination of splitting the element, we achieve the desired fineness of the future grid in the desired areas of a geometric object. Thus, the octree is built for computational domain with the necessary blocking factor within and on the boundary of concerned geometry. The obtained octree leaf cells determine the nodes of the future grid. In the course of partitioning, the elements are divided into three groups: the elements, which are outside the object's boundary, the elements inside the object, and the elements, which cross the boundary of the object. The user interface allows specifying a desired level of partitioning within the object, at its boundaries, at a certain distance from the selected boundary, or in a closed rectangular area, specified by the user. Next, the finite grid is constructed based on the resulting spatial distribution of elements. As a result, we obtain unstructured hybrid grid (Fig. 1), which includes a hexahedral elements (cubes) that are mostly inside the object area, and polyhedral elements (pyramids, prisms, and tetrahedrons), located in the transition areas (where the neighboring elements of the preliminary partition have a different segmentation depth) and on the boundaries of the object.

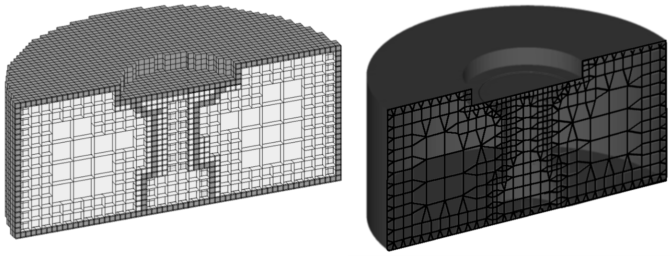

Fig. 1. The transition from the pre-partitioning of the computational domain to construction of the final grid

The calculation module includes implemented mathematical models describing steady and unsteady laminar and turbulent single- and multicomponent flow taking into account the dispersed phase, the conjugate and radiative heat transfer, and homogeneous gas-phase chemical reactions. Discretization of the hydrodynamic equations is carried out based on the control volume approach. To simulate turbulence of gaseous phase in stationary and non-stationary flows we use Reynolds-averaged Navier – Stokes equations (RANS). For closing the Reynolds equations we apply models, using both eddy viscosity hypothesis, and the supposition based on transport equations for Reynolds tensions. The program implements two models of the eddy viscosity, which allow resolving turbulent boundary layers. These are two-parameter k-ω SST model [2] and the four-parameter k-ϵ f-ζ model [3]. Simulation of solid particles transfer is based on diffusion-inertia model of the low-inertia particles motion, which is a simplification of two-fluid model of disperse flows [4]. In this case, assuming that the deviations of the particle velocities in comparison with the velocity of the carrier phase are too small, the transport equations of the dispersed phase are reduced to single equation of the diffusion type for the impurity concentration. A mathematical model of the radiation transport is based on the finite volume method (FVM) [5]. The optical properties of the medium are described by WSGG (weighted sum of gray gas) models that provide reasonable accuracy for a large class of applied problems associated with the burning of carbon fuels. The calculation of chemical kinetics of gaseous fuel combustion is based on the use of a combination of global irreversible reactions between reactants to form reaction products, and turbulent combustion model (Eddy brake up model). In addition, calculation module supports multi-threaded computing. Parallelization of algorithms of computational fluid dynamics is based on the decomposition of the computational domain and the use of the MPI standard. The SigmaFW code allows performing parallel calculations using both personal computers, and modern cluster systems with Windows and Linux operating systems. The analysis of the calculation results is carried out based on the software package, which includes a 3D-visualization module that allows displaying scalar values of physical quantities in arbitrary cross-sections in the form of isosurfaces and diagrams, as well as along the selected intervals. The module allows also displaying vector physical quantities in arbitrary cross-sections, and in the form of vector fields, as well as displaying the geometry of the computational domain and grid discretization. The program documentation contains training examples of some flow and heat transfer problems. As an example we consider the flow in an asymmetric diffuser [6]. A fully developed turbulent flow is set at the inlet section. The Reynolds number is defined by the velocity in the center of the inlet section and its height Re=20000. Due to the positive pressure gradient in this channel flow separation takes place at the non-fixed separation point. Fig. 2 presents the geometric formulation of the problem and the designed grid. The comparison of calculation results with experiment [6] is represented in terms of the longitudinal velocity component reduced to the volumetric average velocity at the inlet, along the vertical lines located at a distance of 13,5H and 27H from the inlet of the diffuser. Fig. 3 shows a comparison between calculated and experimental longitudinal velocity component.

The second problem represents the comparison of the calculation results of the radiation field with the data from the work of J.M. Yu [7], obtained using the discrete ordinates method. The problem represents a closed cylinder filled with a gas mixture (H_2O – 20%, CO_2 – 10%, N_2 – 70%.) with a homogeneous temperature. The calculation

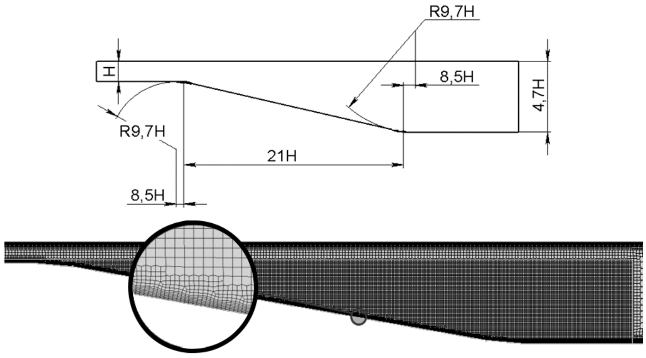

Fig. 2. Computational geometry with inlet and outlet section and the grid

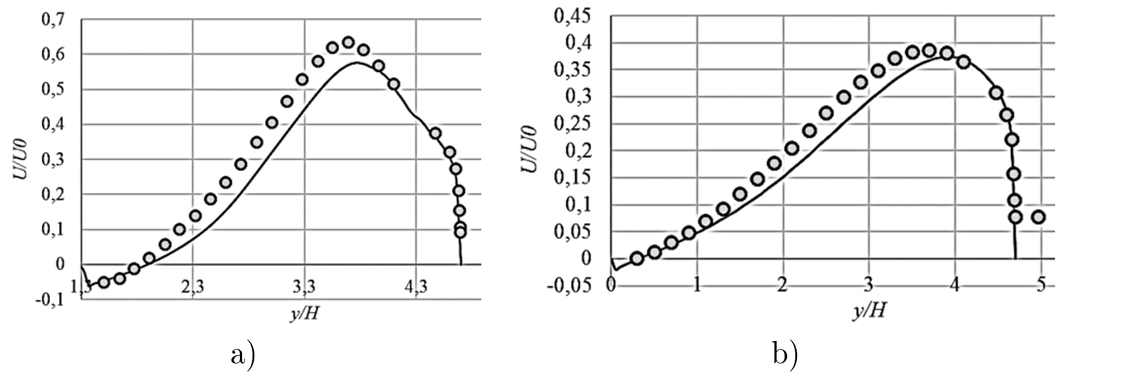

Fig. 3. The distribution of the longitudinal velocity component along the vertical lines at a certain distance. Points correspond to experimental data, while solid line shows calculation by SigmaFW: a) 13,5H; b) 27H from the inlet of the diffuser

of radiative heat transfer was performed based on finite volume method with 96 discrete directions, using the WSGG model to calculate the absorption coefficient [8] (as in [7]) and the "gray gas" model built on its basis. Comparison of the results was carried out in terms of the thermal radiation to the side wall of the cylinder. When using the WSGG model, the distribution of the radiation flux at the wall is almost the same, while the use of "gray gas" approximation essentially overstates the radiation flux (Fig. 4 b).

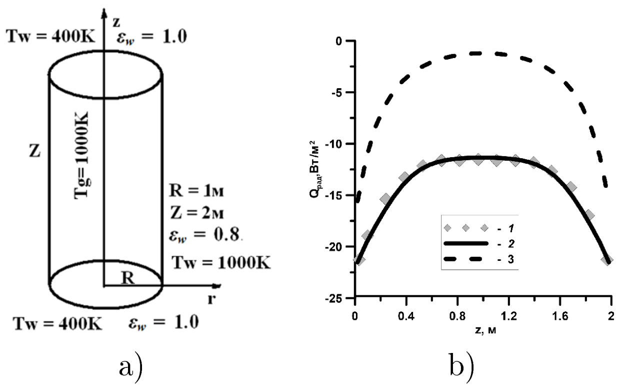

Fig. 4. A closed cylinder filled with a mixture of radiating gases: a) problem formulation; b) distribution of the radiation flux at the side wall of the cylinder: 1 – Yu et al., 2000; 2 – SigmaFW (FVM with WSGG); 3 – SigmaFW (FVM with then "grey gas" approach)

In the framework of the numerical simulation of operating process inside graphite vacuum furnace we carried out comparative calculation of heat transfer based on the authorial software package "SigmaFW" and commercial software "ANSYS Fluent". The technological process is carried out inside the retort (less than 1m in height), which is located in the furnace and is at the same time the heater. The characteristic operation cycle time of the furnace is one or two days. The dominant heat transfer mechanism in the furnace is radiation. The flow of gases inside the furnace is laminar due to the low density and small velocities (Re 10). Grids for "SigmaFW" (630000 cells) and ANSYS (850000 cells) were built based on geometry imported from CAD system (Fig. 5 a, b). For numerical simulation of radiation heat transfer, ANSYS used a discrete-ordinate method, while "SigmaFW" used FVM. The maximum discrepancy for the temperature is less than 15 K (Fig. 5 c, d).

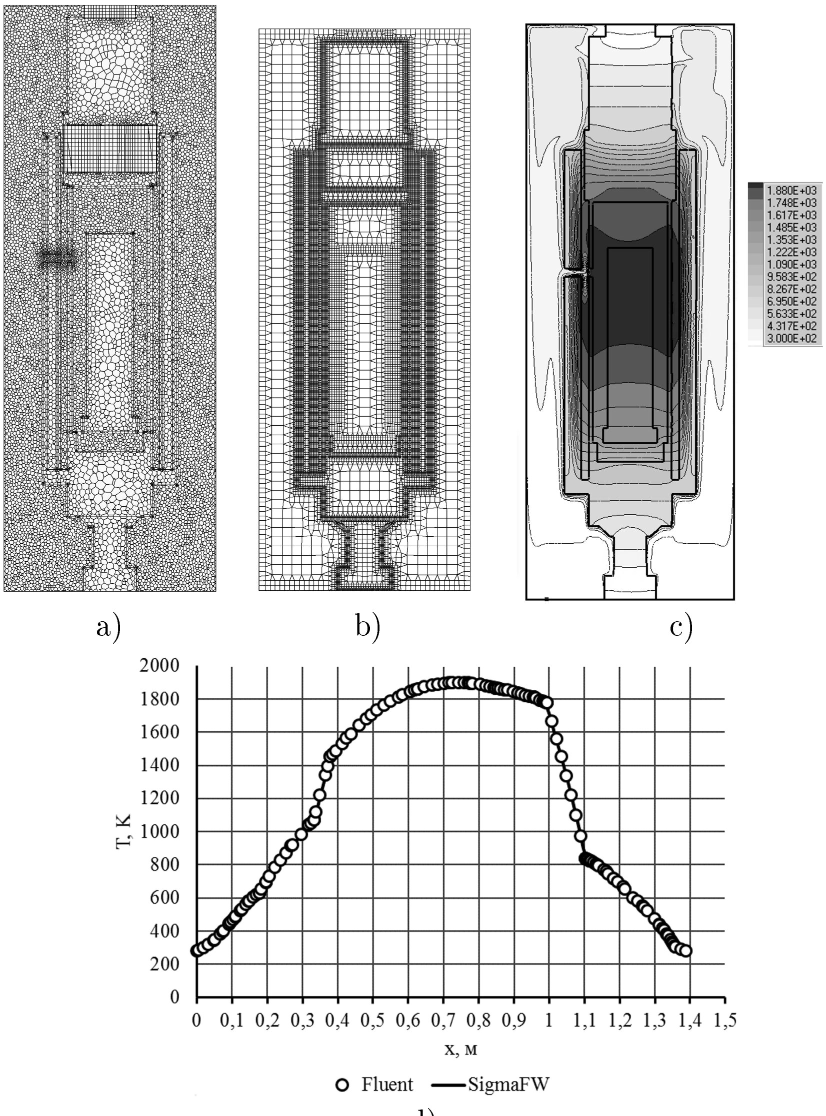

Fig. 5. Comparison of simulation results of a chemical reactor in terms of temperature fields. The calculation is performed using programs a) grid for "ANSYS"; b) grid for "SigmaFW"; c) temperature field, "SigmaFW"; d) distribution of temperature along the horizontal line passing through the hole

To demonstrate the capabilities of the "SigmaFW" software we present here the numerical simulation of flow around a KAMAZ truck, whose solid model is presented in Fig. 7. For the computational domain we constructed polyhedral grid with a size of 1 200 000 cells, whose fragment is presented in Fig. 6.

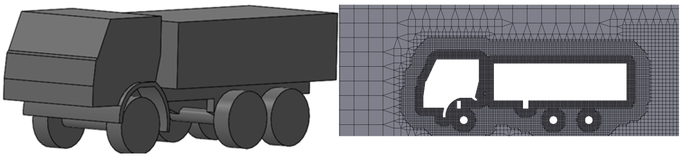

Fig. 6. Geometry and computational grid of the truck presented by the "SigmaFW" software package

The free-stream velocity was taken equal to 60 km/h. Obtained velocity field is presented in Fig. 7, which shows the formation of separation areas on the upper front edge of the driver's cabin and behind the vehicle's axes, as well as the formation of a rarefaction zone behind the truck.

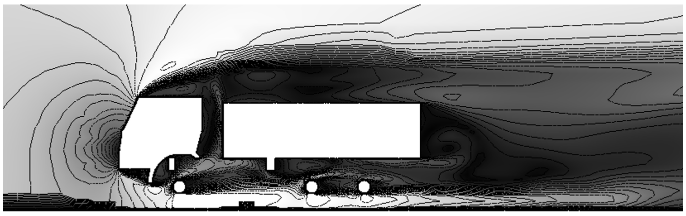

Fig. 7. Velocity field at flow around the vehicle by ram air

Conclusion

Thus, we have developed freely distributable software for Russian users which enables solving fundamental and applied problems of hydrodynamics and heat transfer based on simulation of interrelated physical and chemical processes, and contains all the necessary tools to create computational grids, carrying out multi-threaded calculations, and presenting whole analysis of the calculation results.

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РАЗРАБОТКА ИНЖЕНЕРНОГО СВОБОДНО РАСПРОСТРАНЯЕМОГО ПРОГРАММНОГО КОМПЛЕКСА ДЛЯ МОДЕЛИРОВАНИЯ ПРОЦЕССОВ ГИДРОГАЗОДИНАМИКИ, ТЕПЛООБМЕНА И ХИМИЧЕСКОГО РЕАГИРОВАНИЯ

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В Красноярском филиале ИТ СО РАН и на кафедре теплофизики СФУ разрабатывается свободно распространяемый программный комплекс «SigmaFW» для численного моделирования задач гидрогазодинамики и тепломассообмена, который предполагается использовать в научных и образовательных организациях и промышленных предприятиях в РФ. Математические модели, реализованные в программном комплексе, позволяют описывать стационарные и нестационарные ламинарные и турбулентные одно- и многокомпонентные течения с учетом дисперсной фазы, сопряженного теплообмена, переноса излучения и гомогенных газофазных химических реакций. Программный комплекс «SigmaFW» содержит необходимые инструменты для построения вычислительной области, проведения многопоточных вычислений и визуального анализа результатов. В статье описывается три основных блока программного комплекса: генератор сетки, расчетный модуль и модуль анализа расчетов. Кроме этого, в статье представлен ряд тестовых и прикладных задач для демонстрации возможностей программы.

Ключевые слова: численное моделирование; вычислительная гидродинамика; программный комплекс.

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