Applications of the DNS CONV-3D Code for Simulations of Liquid Metal Flows

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Abstract. To simulate the thermal hydraulics processes in fast reactors with a liquid metal coolant DNS CFD code CONV-3D has been developed. The paper presents the results of the application of CONV-3D code for simulation of sodium natural convection in the upper plenum of the MONJU (Japan) and BN-600 (Russia) reactor vessel, the calculation results of the experiment conducted on the Phenix facility (France) with sodium coolant. The results of simulation of heavy-liquid metal (LBE) flow and heat transfer along a hexagonal 19-rod bundle with wire spacers (KALLA, Germany) are presented also. A satisfactory agreement of the numerical predictions with experiments is demonstrated, in particular for the temperature distribution vs the coordinates. The results obtained allow to conclude that using of CONV-3D code with high predictive power can be recommended for reactor applications.
Key Words: CFD, CONV-3D, LBE, liquid metal coolant.

1. Introduction

One of the practical examples of the use of CFD in the nuclear industry may be modeling the thermal stratification of the coolant. The operating experience of the BN-600, experimental study and numerical simulation of BN-800 showed that in the upper reactor chamber and at the inlet of the heat exchanger there is a temperature stratification of the heat carrier (stratification) [1]. This issue is relevant for reactors of the fourth generation. Thermal stratification of the coolant leads to the formation of stagnant and recirculation zones with large gradients and temperature surges at the boundaries of isothermal zones, which cause additional thermal Cycling loads on the equipment and can have a significant influence on the service life of load-bearing structures.

The investigation of thermal hydraulic characteristics of stratified flow in the elements of the circuit of a fast reactor in different modes of operation, development of recommendations for reducing the temperature non-uniformity, as well as confirmation of the adopted design decisions on the effectiveness of a passive emergency heat removal with submersible heat exchanger in the upper chamber of the reactor are basic objectives of the numerical simulation. These tasks require a significant computational cost at the supercomputers under use of RANS CFD codes.

For the simulation of the thermalhydraulic processes in fast reactors with liquid metal coolant DNS CFD code CONV-3D has been developed [2—4]. This code has ideal scalability and is very effective for calculations on high performance cluster computers. The code has been validated on the set of analytical tests and experiments in a wide range of Rayleigh and Reynolds numbers, in particular, at extremely small Prandtl numbers [5—7]. The paper presents the results of the application of CONV-3D code for simulation of sodium natural convection in the upper plenum of the MONJU (Japan) and BN-600 (Russia) reactor vessel. A satisfactory agreement of the numerical predictions with experiments is demonstrated. The calculation results of the experiment conducted on the Phenix facility (France) with sodium

coolant are demonstrated. The experiment focuses on the mixing of two fluxes at different temperatures in the secondary circuit of reactor facility with liquid metal coolant in the presence of a bending tube. A small pipe is connected via T-connection to the main pipe and unloads of sodium in the main pipe at a temperature which is higher than in the main pipe. A satisfactory agreement of the numerical predictions with experiments is demonstrated, in particular for the temperature distribution vs the coordinates. The results of simulation of heavy-liquid metal (LBE) flow and heat transfer along a hexagonal 19-rod bundle with wire spacers (KALLA, Germany) are presented.

The results obtained allow to conclude that using of CONV-3D code with high predictive power can be recommended for reactor applications.

2. Mixing of fluxes in the upper chamber of the reactor BN-600

Half of the flowing portion of the upper mixing chamber of the reactor BN-600 is seen. Geometric model for calculations was transmitted electronically in the format “x_t”. As boundary conditions at the ends of the fuel assembly was specified by mass flow rate and the temperature. The same conditions are specified on the boundaries corresponding to the overflow windows of the rotary tube, the annular gap around the support, the cut-out in the backup and exit from the bypass flowmeter (*see FIG. 1*).

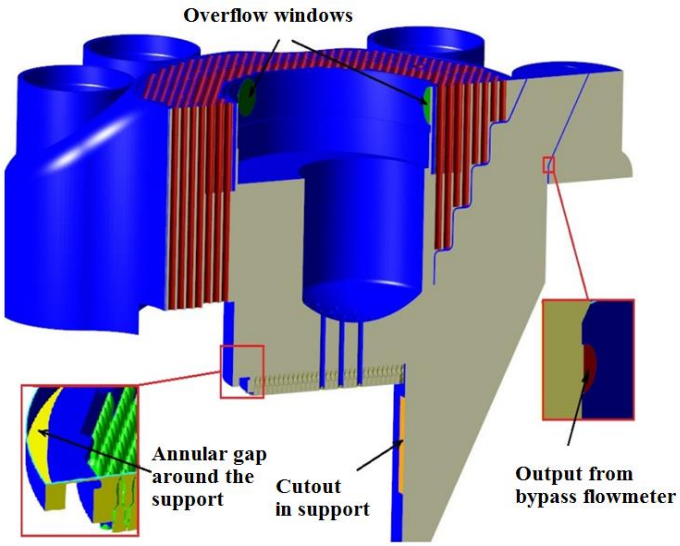


FIG. 1. Input areas

The resistance of PTO (i.e. intermediate heat exchanger) for the first circuit is 7220 Pa, at a flow rate of sodium coolant in the annular space 1111 kg/s. At the outlet of the heat exchangers is set to a condition of zero perturbations in the static pressure. In the plane dividing the chamber into two halves, the condition of symmetry is set. On all the walls no-slip and no-permeability conditions are defined. When modeling the flow of sodium in the flowing part of the construction of the zero hydrostatic level is defined on the upper boundary of the computational domain. Thermophysical properties of sodium (density, viscosity, heat capacity and thermal conductivity) are a function of temperature and is defined in accordance with [8].

The characteristic plane intersecting PTO shown in *FIG. 2*. The program CONV-3D to perform the calculations of the upper chamber of the reactor BN-600 used a quasi-DNS approach and a uniform grid dimension 2049x1025x257 (539 757 825 nodes).

The grid generation was carried out in the package GeometryEditor. As a scheme the transfer scheme was used with directional differences. The Courant number is 10. The time step is 0.01 seconds. The calculations were performed on a cluster of IBRAE using 256 cores. The results are shown at the exit of the solution to quasistationary. *FIG. 3* shows the temperature fields of the upper chamber sodium reactor BN-600 in the plane of symmetry and in transverse direction (section 3), respectively.

For the CONV-3D numerical simulation observed inclined flow when you exit the active zone in the direction of protection rods without explicit vertical or horizontal nature. The calculation results of temperature change at the location of the tank thermocouples show oscillatory character. The maximum amplitude of the oscillation is ~ 30 °C. The difference in the oscillation frequency may be associated with different time-step reporting the results.

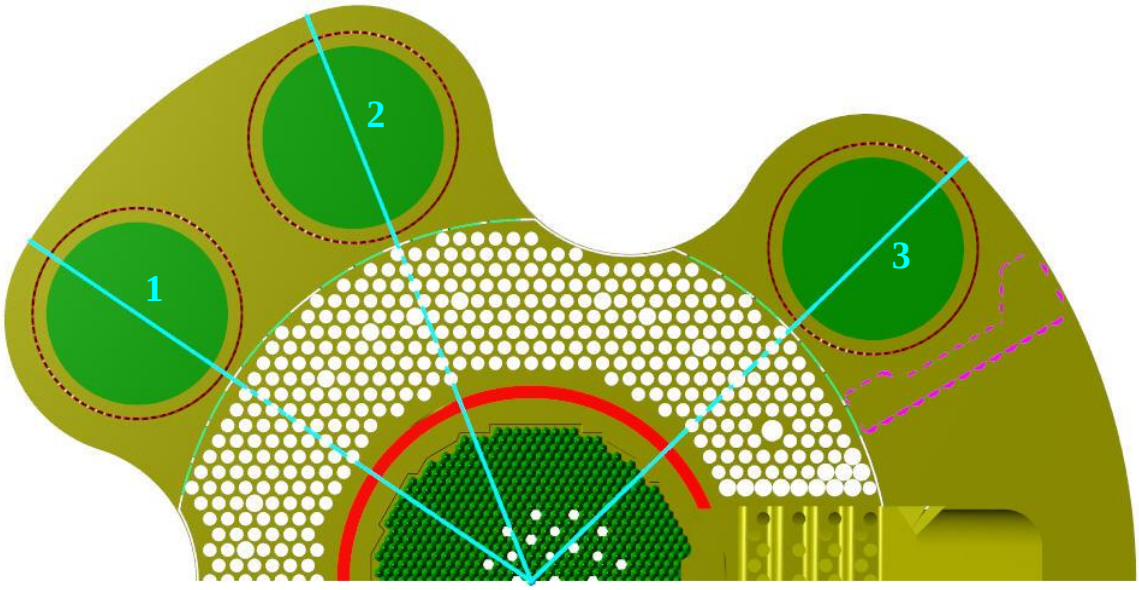


FIG. 2. Typical plane cutting the PTO in the longitudinal direction

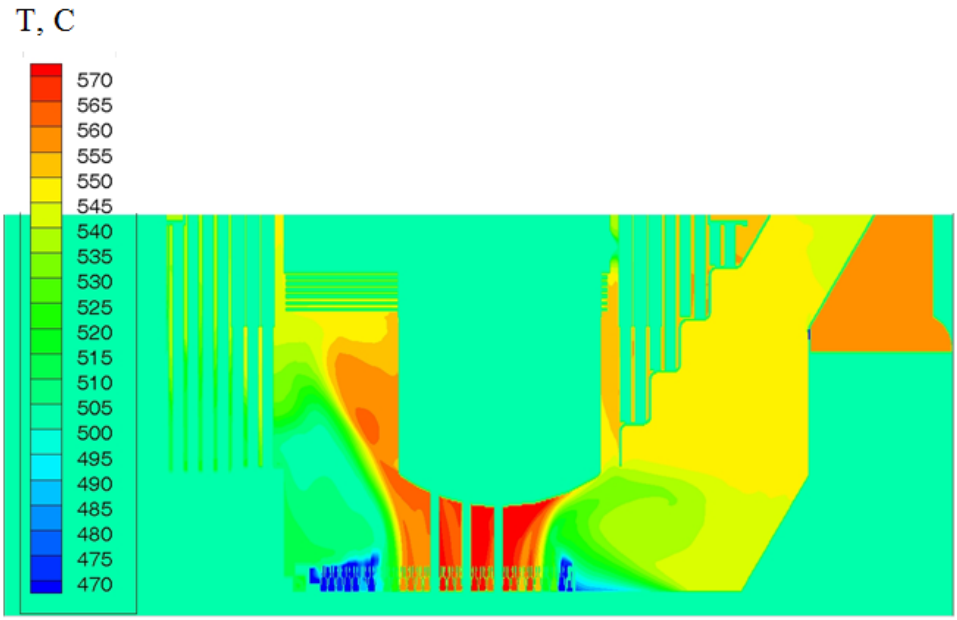
Profiles of temperature, obtained in the result of the calculation at the entrance to PTO are in satisfactory agreement with the operational data; the relative deviation does not exceed 11 %.

$$\delta_T = \frac{T_{calc} - T_{\exp}}{T_{\max} - T_{\min}} \cdot 100\%,$$

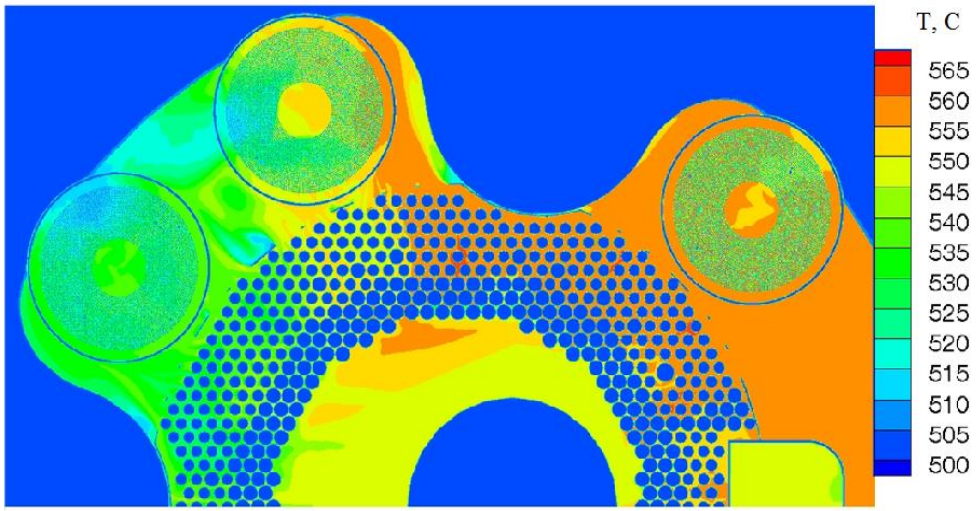
where T_{calc} – the result of the calculation of the sodium temperature at the program, ^{o}C; T_{exp} – performance data, ^{o}C; T_{max} – the maximum temperature of the sodium in the computational domain, ^{o}C; T_{min} – minimum temperature of sodium in the computational domain, ^{o}C .

For a comparison of the numerical predictions with the data of the BN-600 reactor was performed averaging of temperature values at the control points and calculation of the relative deviation according to the upper formula. When comparing the results for CONV-3D software with operational data for 5 PTO - A then was received the maximum deviation of ~ 4

% , for the 4 PTO–B a maximum deviation of no more than 9 %. The difference results from operational data according to the testimony of the tank thermocouple amount to 6.5-7.5 percent. Comparison of calculation results and operation data are given in table 1, where $T_{max} - T_{min}$ =218.



a)



b)

FIG. 3. Temperature fields: a) in the plane of symmetry and b) in transverse direction (section 3)

It should be noted that the results in the program CONV-3D, based on the requirements of the DNS approach were obtained on a grid of ~ 540 million cells.

TABLE I. COMPARISON OF CALCULATION RESULTS WITH OPERATIONAL DATA

№ thermocouples	**Experiment**	**CONV-3D**	
		T, °C	**δ_T, %**
Input 5 PTO–A			
T1	529	536	2,21
T2	533	534	0,46
T3	534	535	0,46
T4	538	534	1,83
T5	542	534	3,67
T6	539	535	1,83
T7	543	534	4,12
Input 4 PTO–Б			
T8	540	545	2,29
T9	523	536	5,96
T10	530	549	8,72
T11	535	546	5,04
T12	537	541	1,83
Input 4 PTO–A			
T15	539	559	9,17
Tank thermocouple			
Tank	512	526	6,42

3. Modeling of reactor MONJU

MONJU — reactor facility of loop type with fast reactor with sodium coolant. The geometry of the upper chamber of the reactor MONJU has a complicated structure. System of tubes located above the exits from the active zone, creating a very complex flow in the region under the column. The size of these tubes is significantly less than the size of the camera. However, their influence on the course should be taken into account for the successful modeling of physical processes in the upper reactor chamber.

In 1995, tests were conducted on the crash of the MONJU reactor during its operation at a power level of 40 %. The transition of the reactor emergency cooling were simulated by applying a signal AZ "the Failure of the main condenser" and shutdown of the turbine. Experimentally investigated the stationary flow of the coolant in the MONJU reactor chamber in the cooling mode. The starting point corresponds to the mode of operation of the reactor at 40 % power.

To study the convection of sodium in the upper chamber of the reactor MONJU as the estimated area of the selected sector of the reactor 60º [9]. The outlets of fuel assembly

presented hexagonal. Because of the complexity of the design all of the elements in above zonal region are not explicitly taken into account.

As boundary conditions at the ends of the fuel assemblies are defined flow rate and temperature. The output from model is given by the condition of zero perturbations on the static pressure. On the planes clipping of sector as well as at the upper boundary of the computational domain, simulating the "sodium-argon" interface, the slip condition at the wall was defined. On all the walls the condition of no permeability set with a turbulent boundary layer, characterized by a logarithmic law of variation of the tangential component of the velocity.

The numerical simulations were performed for two modes of operation of the reactor MONJU: stationary regime at a power of 40% and in the cooling mode. The results of calculations were obtained by code CONV-3D using the quasi-DNS approach and the computational grid with size 321x257x513 (number of elements ~ 42 million), which was built using three-dimensional Geometry Editor [10]. *FIG. 4* shows the temperature profiles in the altitude chamber of the reactor MONJU in the location of the probe for 1) stationary and 2) mode of cooling at the time of time of 120 seconds, obtained in the experiment and by means of the CFD code CONV-3D. In both cases, a satisfactory coincidence of results of numerical predictions with experiment is observed. Mode cooling results are also satisfactory, with the standard deviation in time is 120 seconds received code-CONV-3D is 7.1 °C (~3,4 %).

FIG. 5 shows graphs of changes with time of the temperature of sodium at the points of location of the thermocouples of the probe, namely for thermocouple TE3 [9], obtained for cooling mode in the experiment and calculation codes CONV-3D. The temperature change in both cases is similar. Thus, for both modes were obtained satisfactory results. The root mean square deviation of the calculated average values of temperature in comparison with the readings of the thermocouples in the experiment for the top of the mixing chamber does not exceed 9%.

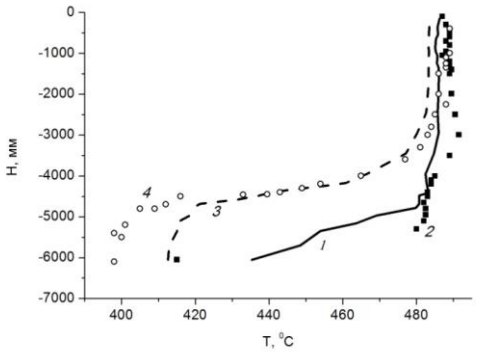


FIG. 4. Profile of temperature along the height of reactor chamber: stationary (1) and experiment (2); in the mode cooling at the 120 s (3) and experiment (4)

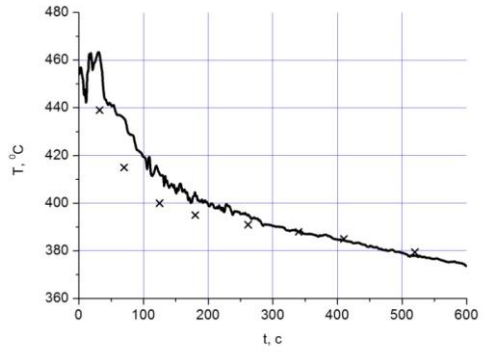


FIG. 5. Profile of temperature change in the position of the sensor TE3 (—) and experimental (×)

For stable mode there is observed a decrease of the temperature distribution on the interval from -5000 to -6000 mm that can be caused by the simulating in 1/6 part of the total

geometry. But even in this case the discrepancy in the values does not exceed 10 degrees, which corresponds to a 10% error.

Mean absolute temperature deviation Δ_T °C is of 5.6 °C, mean relative deviation in temperature, δ_T % – 2,7 %.

The following formula is used for variance calculation:

$$\Delta_T = /T_{exp} - T_{CFD}/ \quad \text{and} \quad \delta_T = \frac{/T_{exp} - T_{CFD}/}{T_{max} - T_{min}} \cdot 100\%$$

where T_{exp}, T_{CFD} – the experimental and calculated temperature at the selected by height point, correspondingly; T_{max}, T_{min} – maximum and minimum temperature in the experiment, correspondingly.

4. Simulation experiment "Phenix" with sodium cooled

This experiment is designed to study the mixing of two flows at different temperatures in the secondary circuit. During normal operation, sodium at a low temperature flows into the main pipe of the second circuit. A small pipe connected via T-connection with the main pipe, carries the sodium in the main pipe at a temperature higher than in the main pipe [11]. The agreement between calculated and experimental temperature is satisfactory. A difference numerical predictions and experimental results does not exceed 5 % (*see FIG. 6*).

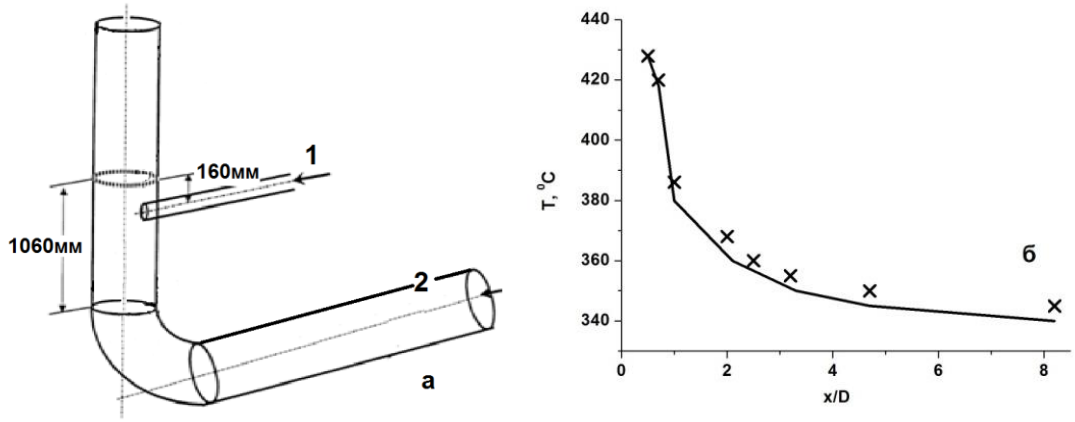


FIG. 6. Geometry of the experimental setup "Phenix" (a), calculated using the code CONV-3D temperature on the distance x/D from the tee (—) and experimental (×) (b): 1 — small pipe, the temperature of the coolant 430 ℃ with a consumption of 7 kg/s, d=68 mm; 2 — big pipe, the temperature of the coolant 340 ℃ with a flow rate of 800 kg/s, D=494 mm

5. Heavy-liquid metal (LBE) flow along a 19-rod bundle with wire spacers

Description of the experiment is given in [12]. For a better understanding of heat transfer and pressure drop in rod bundles with liquid metal cooling in typical conditions of the reactor, was running an experimental campaign in the Laboratory liquid metals Karlsruhe (KALLA) of the Karlsruhe Institute of Technology (KIT).

The campaign focuses on two goals: to justify existing empirical correlation for the operating conditions of fuel assemblies for the reactor MYRRHA [13] and obtain reliable experimental

data for validation of modern CFD simulations and analysis tools of subchannels. Only stationary, adiabatic and forced-convection conditions are considered in [12]. After the experiment, 2014, an experiment was conducted in 2016: for eutectic bismuth+lead in the 19-rod bundle with wire spacers.

A test domain, installed vertically with upward flow, consists of a bundle of nineteen electrically heated rods embedded in a hexagonal channel. For practical research, the concept of double-casing was chosen. The inner casing forms a hexagonal channel for the flow, while the exterior it acts as a case of high external pressure. The staging domain is filled with a fluid – static eutectic lead-bismuth (LBE). FIG. 7 shows a schematic view of fuel assembly (top view).

In the experiment [12] evaluated the coefficient of friction. In the calculations used properties from [12]. The calculation of the coefficient of friction for the task with winding is carried out according to the formula: $\frac{d_г^{снав.}}{\Delta z} = \frac{7,5}{870} = 0,00862\frac{u_b^2}{2} = 0,63^2*0,5 = 0,198 f_1 = \frac{\Delta p}{\rho}\frac{d_г}{\Delta z u^2/2}$. The dimensions of the computational domain are 66x60x1230 mm. $\frac{d_г^{снав.}}{\Delta z} = \frac{7.5}{870} = 0.00862\frac{u_b^2}{2} = 0.63^2*0.5 = 0.198 f_1 = \frac{\Delta p}{\rho}\frac{d_г}{\Delta z u_b^2/2} = \frac{\Delta p}{\rho}\frac{0.00862}{0.198}*10^{-6} = \frac{\Delta p}{\rho}*0.0435*10^{-6}$

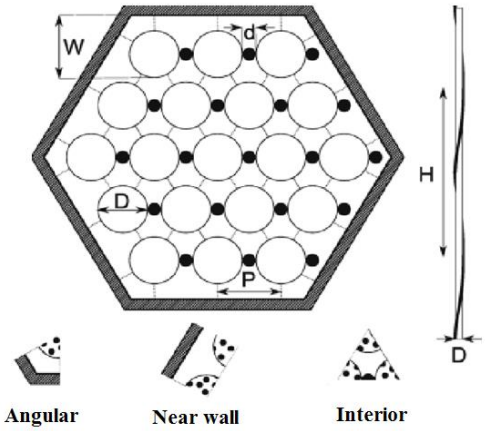


FIG. 7. A schematic view of fuel assembly (top view)

Formula Novenstern (the accuracy of the equation – 30%)

$$f_2 = \frac{0,3164}{Re^{0,25}}\left[\frac{1,034}{(P/d)^{0,124}} + \frac{29,7(P/d)^{6,94}Re^{0,086}}{(H/d)^{2,239}}\right]^{0,885},$$

where $1,06 \le s/d \le 1,42;\ 2,6*10^3 \le Re \le 2*10^5; 8,0 \le h/d \le 96.$

The formula is (accuracy of equation – 15%) [14]

$$f_3 = \frac{0,210}{Re^{0,25}}\left\{1 + \frac{124*Re^{0,06}}{(H/d)^{1,65}}\left[1,78 + 1,485\left((S/d) - 1\right)\right]\left((S/d) - 1\right)\right\},$$

where $1,0 \le s/d \le 1,5;\ 10^4 \le Re \le 2*10^5; 8,0 \le h/d \le 50.$

Evaluation of friction coefficient on the basis of numerical experiment for the geometry "as is" in the experiment, with turbulence at the inlet and outlet are summarized in table II. Test 1 performed on the grid 129x129x513 with skew symmetrical scheme with upwind differences The following characteristics for calculations are used: average velocity $\bar{w} = 549\ mm/s$; a

hydraulic diameter $d_г^{с\ нав.} = 7{,}5mm$; this correspond to the Reynolds number $Re = 1{,}8 * 10^4$. Test 2 performed on the grid 129x129x513. The following characteristics for calculations are used: average velocity $\bar{w} = 1637$ *мм/с* ; a hydraulic diameter $d_г^{с\ нав.} =$ 7,5*мм*; this correspond to the Reynolds number $Re = 5{,}3 * 10^4$.

TABLE II. FRICTION COEFFICIENT FOR THE GEOMETRY "AS IS" IN THE EXPERIMENT WITH TURBULENCE AT THE ENTRANCE AND THE EXIT

№	$experiment$	f_1 **(results of numerical modelling)**	f_2 **(Formula Novenstern)**	f_3 **(normative document)**
1	0,028	0,022	0,029 $f_2^{-30\%} = 0{,}020$	0,023 $f_3^{-15\%} = 0{,}020$
2	0,025	0,018	0,022 $f_2^{-30\%} = 0{,}016$	0,018 $f_3^{-15\%} = 0{,}015$

Conclusions

Developed DNS CFD code CONV-3D for the simulation of thermal hydraulic processes in fast reactors with liquid metal coolant allows to simulate flows in the structural components of nuclear power plants in a wide range of parameters Ra < 10^{16} and Re=10^3—10^5. This is evidenced by the results of the qualitative and quantitative coincidence with the experiment.

1) According to the results of numerical simulation of mixing flows of different temperatures of sodium in half of a flowing part of the upper mixing chamber of the reactor BN-600 temperature profiles obtained with the help of CONV-3D code, the calculation at the entrance to the PTO, in good agreement with operational data, the relative deviation does not exceed 11 %. The difference CONV-3D results and the operational data for 5 of the PTO-A does not exceed ~ 4% and for 4 PTO–B the difference does not exceed 9 %. The difference results from operational data according to the testimony of the tank thermocouple amount to 6.5-7.5 percent.
2) According to the results of numerical simulation of MONJU reactor root mean square deviation of the calculated average values of temperature in comparison with the readings of the thermocouples in the experiment for the top of the mixing chamber does not exceed 9%.
3) Demonstrated satisfactory agreement of numerical predictions with experiment on the setting of the Phenix (France) with sodium coolant. A difference numerical predictions and experimental results does not exceed 5%.
4) For numerical modeling the flow of the LBE in the 19th rods assemblies in the range of the Reynolds number ≤10^4 the results obtained by means CONV-3D code are in good agreement with the correlations.

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