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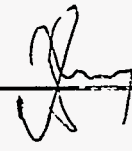
COMPARISON BETWEEN VNIIEF COMPUTER
PROGRAMS USED TO STUDY NPP SAFETY
AND SIMILAR WESTERN CODES.

Report on the third stage of Subject Order 007 under
University of California - VNIIEF subcontract N0002P00004-95.

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ABSTRACT

The report gives schematic comparison between VNIIEF computer programs used to study NPP safety and similar western codes. This comparison is schematic and in no way pretends to be complete.

The work is performed within Subject Order 007 under University of California - VNIIEF subcontract N0002P00004-95.

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1. COMPARISON BETWEEN VNIIEF COMPUTER PROGRAMS USED TO STUDY NPP NEUTRON-NUCLEOUS PROCESSES WITH SIMILAR WESTERN CODES.

1.1. COMPARISON AMONG CODES DESIGNED FOR CELL PARAMETER COMPUTATION.

The LOMA-2K program is designed for computation of various types of reactor power facility cell parameters in the multi-group 2D kinetic approximation [3]. The LOMA-2K program is used both independently and in combination with the BEND program complex to compute few-group constants.

Schematic comparison among the LOMA, TWODANT, WIMS-D [4] programs is given below.

Program	LOMA	TWODANT THREEDANT	WIMS-D
Classes of solved problems	Kinetic multi-group equation is solved.	Kinetic multi-group equation is solved.	Kinetic multi-group equation is solved.
Constant support	At group constant preparation nuclei thermal motion, chemical bonds of atoms are accounted. There is a possibility to account all types of resonance self-shielding (in homogeneous mixture of fuel nuclei from heterogeneous fuel location and mutual		69-group library of microconstants with augmentation capability (without (n,2n) reaction cross section and without account of resonances at scattering in a resonance region).

	self-shielding of fuel blocks).		
Computation geometry	Infinite cylinder, (X,Y); (r,z); (x,y,z)	(X,Y); (r,z); (x,y,z)	Spherical, cylindrical, (r,θ); (v,z)
Leakage computation	Trough boundary conditions.		Leakage is computed either by Bi method or in the diffusion approximation.
Boundary conditions	Vacuum and reflection conditions.	Vacuum and reflection conditions.	"White" reflection, free boundary.
Burnup model	The system of equations describing kinetics, burnup of actinides, debris and burning-up absorbers is solved.		Like LOMA, but (n,2n) reactions are not accounted in burnup kinetics.
Spatial grids	In two dimensions regular quadrangular, irregular grids composed of convex polygons, including triangular and hexagonal, are used. In three dimensions regular grids composed of hexahegra are used.	In two dimensions regular quadrangular grids are used, in three dimensions regular grids composed of parallelepipeds are used.	
Grid approximation	Dsn-method type schemes constructed on the above grid types are	Dsn-method type schemes constructed on the above grid types are	

	used. Various quadrature types are used to approximate the equation by angular variables.	used. Various quadrature types are used to approximate the equation by angular variables.	
Methods of grid equation solution	For computation of critical parameters and the spectrum. the use of various iterative method types is possible: the Kellog method, the direct method, the combined method, the method of source iteration. Special methods of iteration convergence acceleration [1] are used.	Problems are computed with the DSA methods in combination with the multi-grid method [2] used for the sake of acceleration.	DSn and Collision Probability method.
Programming language	Fortran-77		Fortran
Types of problems being solved	Computation of critical parameters, neutron spectrum, reactivity lifetime. Computation of polycells is possible.	Computation of critical parameters, neutron spectrum, reactor protection.	Neutron-physical computation of reactor type cells. K_{eff} , K_{in} neutron spectra both over regions and over a system as a whole with and without account

			of leakage, reaction numbers, group cell constants are computed. Computation of polycells is possible.
Program testing	The program was verified on test multi-group problems for WWER, RBMK and SNR type reactors.	It was tested on a wide range of reactor problems.	It was tested on a wide range of reactor problems.

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1.2. COMPARISON BETWEEN S-90 MONTE CARLO PROGRAM COMPLEX (VNIIEF) AND MCNP CODE.

The program S-90 is designed for computing the problems of consistent neutron and gamma-quanta transport using the Monte Carlo method and is a multi-purpose program, i.e. solves both the problems for a given source and the problems for computing the effective neutron multiplication factor, k_{eff} [1].

The program provides wide capabilities both on initial data setting and tools for computation efficiency improvement. For many years the program was being used at VNIIEF to analyze physical experiments.

Schematic comparison of the S-90 program with the well-known MNCP program [2] which is most close to it in its capabilities and intention is given below.

S-90	MNCP
<p>Programming language. EL-76. The FORTRAN-77 program version is currently being completed.</p>	<p>FORTRAN-77</p>
<p>System geometry. The program allows to describe 3D geometry systems. System geometry description employs the block principle with setting the nesting system. A block is described by a set of surfaces which can be the second - order surfaces of revolution and planes (use of arbitrary second - order surfaces is permitted, however, in this case the program does not control consistency of the preset data). The nesting system determines consistent block allocation relative to each other. In doing so several nesting levels are allowed. Nestings of each next level indicate allocation in the block which is the basic system. If at</p>	<p>Arbitrary 3D geometry with bodies confined by second-order surfaces (some fourth-order surfaces may be used).</p>

some nesting level a block is allocated which contains next level nestings, then they are allocated together with it at each its nesting of this level.

Neutron-nuclear constants. Neutron transport computations, as a rule, make use of the neutron-nuclear constant library BAS-78 [8] developed under the leadership of A.P.Vasilyev, a member of VNIITF staff. In addition, there are cold constants for a number of elements from various versions of the ENDL and ENDF/B libraries. (*The algorithm used in the program allows to take into account thermal Maxwellian motion of medium nuclei in modeling on cold cross sections*). For some elements there are cross sections of interaction with account of chemical bonds. (Model $S(\alpha, \beta)$). Prompt augmentation of the constants library is possible on the base of the estimated neutron data library using the BEND program complex.

There is a constant library large in the number elements. The constants can be used both in the pointwise and group approximation. There is a capability of prompt augmentation of the library on the base of ENDL, ENDF/B and others using the NJOY complex.

Sources. Both the programs exhibit wide capabilities on setting spatial and spectral - angular distribution of independent sources. Arbitrary surfaces and domain systems, as well as off - geometry entities can serve as particle sources.

Results. In both programs the functionals being computed are subdivided into volume and surface ones. Distribution of each result over various states of phase coordinates of the particle from which it is taken is permitted. The surface results are flows and particle flows through system surfaces, as well as their convolutions with arbitrary energy functions. (They are computed at intersection of a given surface). The volume results are flows and the numbers of reactions. Their computations, as a

rule, use the path estimate. A computation of the number of reactions may also use the collision estimate. *For reactor computations the capability is implemented to obtain group cell neutron constants.*

Tools for computation efficiency improvement. Both the program have an essential stock of such tools. These involve: value by domains, splitting and a tape - line, exponential transformations, the sample particle method (an analog of DXTRAN), local estimations, as well as various methods of trajectory cut - off.

In addition, the program has a large set of boundary conditions which allow to solve problems on grid systems, both unlimited and with finite number of cells.

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[2] MCNP-A General Monte Carlo Code for Neutron and Photon Transport.
LA-7396-M.

1.3. COPMARISON AMONG PROGRAMS DESIGNED FOR NPF DYNAMICS NEUTRON COMPUTATIONS.

The KORAT 3D [1,2] code is designed for numerical solution of stationary and non-stationary problems of neutron transport in the group diffusion approximation.

The KORAT 3D code is based on the following propositions:

- 3D diffusion equation presentation in the Cartesian coordinate system is used;
- with respect to the time variable the diffusion equation is approximated by an implicit scheme with weights;
- at spatial variable approximation two types of non-orthogonal spatial grids are used: regular grids and grids essentially irregular in horizontal cross sections.

An important element of the technique used in the code is a new method for acceleration of iteration convergence by the right-hand side of the system of non-stationary group diffusion equations.

The NEU [3] code for 3D few-group equation of neutron diffusion is intended to be used within program complex of nuclear power facility (NPF) dynamics with 3D modeling of core processes.

Schematic comparison among KORAT, NESTLE [4] and NEU codes is given below.

Code	KORAT 3D	NESTLE	NEU
Classes of problems being solved.	Computation of critical parameter K_{eff} , fixed source problems, neutron spectra computations in the multi-group approximation, dynamic computations of reactivity lifetime.	Computation of critical parameter K_{eff} , fixed source problems, neutron spectra computations in the multi-group approximation, dynamic computations of reactivity lifetime.	Computation of critical parameter K_{eff} fixed source problems, dynamic computation of reactivity lifetime.
Constant support.	Neutron constants are prepared using a	Neutrons constants can be	Neutrons constant can be

	special program package accounting thermal motion of nuclei, chemical bonds of atoms, resonance self-shielding.	prepared using standard cell software.	prepared using standard cell software.
Computation geometry.	(X,Y,Z)	(X,Y,Z)	(X,Y,Z)
Boundary conditions.	It is possible to set any of three boundary condition types for the diffusion equation. At various boundary points various boundary condition types can be set.	----- // -----	----- // -----
Outburn model.	Like in LOMA.	The equation system for recovery and burnup of actinides and debris with cell mean concentrations is solved.	None.
Spatial grids.	Both regular (i.e. of matrix structure) and irregular grids composed of convex quadrangles are used. Hexagonal grids are described by fragmentation to quadrangles.	Rectangular and hexagonal.	Trangular, rectangular.
Grid appro- ximation.	With respect to time: implicit with weight selected by special formulas with respect to	With respect to time: implicit with respect to spatial variables: the finite-	With respect to time: implicit with exponential approximation. With

	spatial variables: the scheme of the finite-difference and finite-element methods.	difference method scheme (the nodal scheme).	respect to space: finite-difference.
Solution techniques for grid equations.	Critical parameter computations: the iterative method with spectrum offset in combination with special methods of internal iteration acceleration. Dynamic computations: the method of external and internal iterations in combination with special methods of iteration convergence acceleration.	A non-linear iterative strategy is used. On external and internal iterations methods of iteration convergence acceleration are used.	Critical parameter computations: external iterations the method of backward iteration with eigenvalue specification using the Rayleigh ratio in combination with the Rayleigh iteration method internal iterations- the Lantsish method. Dynamic and source computations the Lantsish method.
Programming language.	Fortran-77		RATFOR-IV (FORTRAN-77)
Code testing.	The code was verified on two- and four-group stationary problems for WWER and RBMK type reactors.		The code was tested on a set of both static and dynamic problems (including Benchmarks) in the two- and four-group approximations.

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2. THERMOHYDRAULIC CODES

2.1. COMPARISON OF RATEG CODE WITH TRAC AND RELAP CODES

The RATEG code [1] is intended for numerical simulation of transient thermohydraulics of pipe network of water cooled nuclear power plants (NPP). The code has been being developed since 1990 by small collective body (2-4 investigators). Currently the code lags behind codes representing the state-of-the-art in computational thermohydraulics of NPP such as TRAC and RELAP that already have been already developed about twenty years by relatively large group of specialists.

A brief description of the last RATEG code version as compared to the TRAC-PF1/MOD2 [2] and RELAP5/MOD3¹ codes is given below. The main differences of the RATEG code from the TRAC and RELAP codes are summarized in Table 1.

Flow model. The RATEG, as well as TRAC and RELAP codes, uses a two-velocity, two-temperature (2V1T) model of two-phase coolant flow. However, in the RATEG model there are no equations to describe non-condensable gas and liquid contaminant transport present in the TRAC and RELAP models.

Geometry. In contrast to TRAC where there is a 3D 2V2T thermohydrodynamics module, RATEG uses only 1D thermohydraulics approximation.

¹ Authors have not the complete description of the last versions of the RELAP . Their opinion on the code is based on the separate publications and can be not in all exact.

Closing relations. In RATEG as well as in TRAC and RELAP flow structure dependent closing relations are used. However, the system of closing relations is developed only for vertical channels.

Critical flows. Currently in RATEG there are no critical flow models similar to choking models in the TRAC and RELAP codes. Therefore, to describe such flows a fine computational grid has to be used which makes the computations considerably more expensive

Heat transfer in thermal elements. Unlike TRAC and RELAP using 2D models of heat transfer in thermal elements, in RATEG heat transfer is computed in the 1D (radial) approximation.

Reactor-core power model. In the code there is no module for the reactor-core power computation. Core power can be specified as temporal and spatial dependencies obtained from various sources, for example, computed by special codes.

Network component models. In this RATEG version the network component models set is not complete. For example, there are no quite acceptable models of pumps, a vapor generator, etc.

Method of solution. To approximate laws of conservation RATEG uses a semi-implicit one-step difference scheme basically coinciding with the scheme [3]. This scheme, as the predictor-corrector schemes used in TRAC-PF1/MOD2 [4] and RELAP5/MOD3 [5], does not limit the timestep by the Courant stability conditions.

Validity of models and solution methods. To validate models and methods only analytical and separate-effect tests were used. The modeling of the integral tests has not yet been performed.

Table 1

Basic differences of the RATEG code from the TRAC and RELAP codes

	RATEG	TRAC	RELAP
1. Geometry	1D	1D+3D	1D
2. Flow model	2V2T	2V2T	2V2T
3. Number of equations	6	8	8
4. Closing relations	vertical channels	arbitrary channels	arbitrary channels
5. Critical flows	fine grid	choking model	choking model
6. Heat transfer in solid elements	1D	2D	2D
7. Reactor-core power	defined table	point-kinetics	point-kinetics
8. Network component model set	not complete	complete	complete
9. Method of solution	semi-implicit, one-step [3]	SETS[4], predictor-corrector type	nearly-implicit[5], predictor-corrector type
10. Verification	separate-effect tests	separate-effect tests, integral tests	separate-effect tests, integral tests

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2.2 COMPARISON AMONG TECHNIQUES FOR FUEL ELEMENT BEHAVIOR COMPUTATION.

Item 2.2 compares the TVEL[7] technique used at VNIIEF with Gapcon-Thermal, NSR-77 and TRAC codes.

The TVEL code was originally developed for computational support of experiments with reactor fuel at the BGR pulsed reactor (VNIIEF). It determined principal features of the first technique version:

- detailed description of state of fuel element itself;
- the form of the boiling curve used for small coolant flow velocities.

Thermomechanical model.

To describe fuel elements behavior a routine set of continuum mechanics equations is used. Like in other codes for fuel element computations (Gapcon-Thermal [1], NSR-77 [2,3] TRAC [4] and others) a quasi-static approximation is used. It is assumed that inertial effects are small and corresponding term in the equation of motion can be neglected. One can also use the dynamic approximation if needed allowing to describe propagation of compression unloading waves.

The principle difference of the TVEL code from other codes is that the equation system is complemented with the thermodynamical equations of state $P = P(\rho, T)$, $E = E(\rho, T)$ and the Prandtl-Reiss relations for the stress deviator.

For numerical solution of the equations the method of splitting by physical processes is used. At each time step two simpler problems are solved successively:

1. Solution of the heat conduction equation;

2. Estimation of the displacement and stress fields by the computed temperature field. At this stage the equation of equilibrium (the equation of motion for the quasi-static approximation) are solved complemented with the equations of continuity, energy and relations for computing the stress deviator.

This method of computing fuel element behavior can be reduced to solution of a simpler problem of temperature stress estimation. used in the TRAC code should the following simplifying propositions be applied:

- a) Deformations are elastic.
- b) Shear deformations are small. In this case the Hooke law is written not in the terms of deformation increment but in the terms of full deformations.
- c) Temperature changes and volume deformations are small and, therefore, the Duhamel-Neumann hypothesis can be used.
- d) The changes in internal energy through action of pressure forces at shear and volume deformations may be neglected.

Application of conditions a) through d) allows to write the equations of equilibrium relative to medium displacement and obtain solution in quadratures at a known temperature field like it is realized in the TRAC code.

In the Gapcon-Thermal and NSR-77 codes the fuel deforming model is close to that used in the TRAC code. In that codes models are introduced to describe the change in mass of the layer that cracked in the process of fuel thermal expansion. In the TVEL technique it is suggested to introduce a model of fuel cracking close to that used in NSR-77:

- In the process of thermal expansion thermal stresses are estimated and when fracturing stresses are achieved fuel is considered as cracked. At

further deformation strength (fluidity) limit is made to be zero for this fuel portion.

To describe fuel element shell behavior, the Gapcon-Thermal and NSR-77 codes use the thin-wall shell approximation.

The use of a more general approach in the TVEL technique when describing fuel element behavior allows to describe the fuel element dynamics at loading more exactly. Thermal expansion of materials (including porous) can be computed with account of shear strength, plasticity, phase transitions (the change in density at melting).

In connection with the use of various thermomechanical models behavior of the gap between fuel and fuel element shell is also described variously.

At the gap dynamics computation the TRAC code does not account presence of gas in the gap. (At least, this follows from the materials put at our disposal.). The gap width is estimated from fuel and fuel element shell thermal expansion. The minimum width is estimated through setting a characteristic value of surface roughness.

The Gapcon-Thermal and NSR-77 codes account gas presence in a gap, gas impact on internal pressure, gas flow from a gap to a pressurizer and among various fuel element sections. Similar models are also used in the TVEL code.

In all the codes material properties (heat capacities, heat conduction factors, strength parameters, etc.) are usually set in the form of analytical functions of temperature and pressure.

Heat transfer in a gap

To describe heat transfer in a gap, the following mechanisms are taken into consideration:

- Molecular heat conduction of gas - a_g .

To account it, gap gas parameters need not be necessarily computed since gas heat conduction does not depend on pressure till the gas size is greater than several tens of gas molecule free paths. At pressures $\sim 1-10$ atm. and temperature $\sim 1000^{\circ}\text{K}$ this value makes $\sim 10^{-2} - 10^{-3}$ mm. At computations of heat transfer in narrow gaps to account this effect and incompleteness of energy exchange among gas molecules and surfaces (the accommodation factor is less than 1), the notion of temperature jump distance (TJD), (g_1+g_2) , is introduced. When computing heat transfer, (g_1+g_2) is added to the gap width. The notion (g_1+g_2) is the function of gas temperature, pressure, composition and viscosity [1].

- Contact heat conduction factor, a_{cont} .

It is used to compute heat conduction at gap shut-off.

$$\dot{a}_{cont} = \frac{a_m(P)}{b_0 R^{0.5} H} + \frac{a_g}{c(R_1 + R_2) + (g_1 + g_2)} + a_r$$

where $a_m = \frac{2a_1 a_2}{a_1 + a_2}$; $R = (\sqrt{0.5(R_1^2 + R_2^2)})$; $b_0 = 0.5 \text{ cm}^{-0.5}$;

a - heat conduction factors;

R - surface roughness values.

Indices 1 and 2 pertain to fuel and shell, respectively.

c - the value of contact pressure;

a_r - radiation factor of heat conduction. It is practically the same for all techniques. The only difference is in description of material blackness

degree. Thus, the TVEL code merely uses constants, while the TRAC code both constants and temperature functions.

When the gap is not shut off then the gap heat conduction factor (a_{gap}) is:

$$a_{gap} = \frac{a_g}{\Delta_{gap} + (g_1 + g_2)} + a_r$$

Δ_{gap} - fuel-shell gap width.

a_{cont} - is used in the above form in the Gapcon-Thermal and NSR-77 codes. In the TRAC code the formula for a_{cont} is only used. The notion ($g_1 + g_2$) is replaced with a certain constant value of the order of the sum of surface roughness values and TJD.

In the first TVEL code version when gap is shut-off, heat transfer through fuel-shell interface was merely computed. Now a_{cont} is introduced similar to those used in the Gapcon-Thermal and NSR-77 codes.

Fuel element shell oxidation.

In all the codes other than Gapcon-Thermal one and the same parabolic law base model of external shell boundary oxidation through vapor-zirconium reaction is used.

Heat exchange with coolant

The simplest dependence is used in the Gapcon-Thermal code, that is the formula applied for force convection of single-phase coolant.

In the TVEL and NSR-77 codes close boiling curves are introduced. Thus, in the TVEL code it involves the following modes: convection, convection-nucleate boiling transition region, nucleate boiling, transition

boiling, film boiling, overheated vapor convection, and radiation heat exchange.

In the NSR-77 code there is a block for computing thermal hydraulics of single-phase coolant. The first TVEL code version was intended for computational maintenance of ampoule experiments with fuel elements. Therefore, in it initial coolant parameters are set while the change in coolant state is determined by heat withdrawal from fuel element. Currently activities are commenced to develop a code where behavior of fuel element (or a group of fuel elements) is described with a series of sections in which the TVEL technique is used. While to describe coolant the RATEG technique is used (see item 2.1). I.e. a thermal hydraulics block will be developed similar to those used in the TRAC and RELAP codes.

Release of gaseous fission products from fuel

It is not accounted in the TVEL and RATEG codes. In Gapcon-Thermal and NSR-77 the dependencies of release rate on temperature are introduced. In the future it is suggested to introduce them to the TVEL technique as well. Account of this effect is especially necessary for description of irradiated fuel element emergencies.

Program testing

The TVEL code was tested in nuclear fuel experiments on pulsed reactors, primarily NSRR (Japan) [2,3,...] and IGR (now Kazakhstan) [5,...].

Other techniques were tested on various reactors and device experiments and analytical models. Detailed description of the tests can be found in respective references: [1] for Gapcon-Thermal, [6] for TRAC, [2,3] for NSR-77.

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2.3. 3D CODE CONVECT AND PROSPECTS OF ITS DEVELOPMENT.

The CONVECT code was developed to predict effects of accident processes in closed rooms (for example, with some nuclear reactor accident types) and to predict transport of hazardous contaminants at venting under conditions of complex terrain.

Problems of computing effects of accidents in closed rooms and predicting industrial plant venting product propagation are complex and need preliminary solution of a number of particular problems.

Some of them are of individual interest and their solutions can be applied for local predictions. Such types of problems may involve, for example, the problem of contaminants transport at a priori given velocity field and turbulent diffusion coefficient distribution.

Numerical techniques basis for solving such problems are hydrodynamic equations, heat transfer equations, and contaminant transport equations.

Since in many cases flow has a relatively low velocity (much less than sound speed), one may neglect variations in flow density which occurs from such motion and assume it to be incompressible fluid.

Equation describing fluid dynamics (Navier-Stokes equation) used in incompressible approximation seems more preferable as compared to the complete system of compressible gasdynamic equations to solve problems with relatively low flow velocities. It seems so from the viewpoint of numerical computation cost and accuracy as for similar problems one do not have to describe acoustic and shock waves generation and propagation.

In the first approximation atmospheric turbulence can be accounted in terms of the Navier-Stokes equations by choice of appropriate viscosity coefficients. To describe convection, force of buoyancy directed opposite to force of gravity and proportional to actual decrease in density of air from its thermal (isobaric) expansion must be introduced to the equation of fluid motion, while the equation system must be extended through addition of the heat transfer equation where the temperature conduction coefficient is turbulent in its character.

Contaminants transport is also described by diffusion type equations which account the effect of particle (aerosol) precipitation in the field of gravity. The diffusion coefficients are also turbulent in their character.

In the simplest approximation turbulent coefficients are set phenomenologically in the form of characteristic constants or functions.

Since development and debugging of 3D codes is a complex and time-consuming procedure, it was split into several stages:

- development and debugging of the autonomous code THERMOS for computing 3D equations of heat transfer where velocity field is set a priori in the form of three 3D arrays of velocity components; this technique is also intended for computation of contaminant transport in the atmosphere with a preset velocity field;
- development and debugging of the autonomous 3D code HYDROS for computing dynamics of constant density incompressible fluid without account of buoyancy forces and heat transfer effects; this code can compute velocity field generation when there are no convection processes;
- development of the complex 3D code HYDROTHERM which combines equations describing the above-listed processes;

- development of the 3D code CONVECT 1.0 and CONVECT 1.1 adapted to some environment problems in nuclear reactors (for example, convective flows in vapor-gas mixture at core drying and core temperature computation);
- development of methods for laboratory modeling allowing to test computational techniques.

The basic approximations and equations used in the CONVECT code are given in the report on the first stage under this contract.

Below the basic characteristics of the CONVECT technique are given in comparison with some characteristics of the GASFLOW technique.

The symbol *) denotes the code blocks under development. A dash in the tables means that we do not have appropriate data available.

1. Flow model.

CONVECT	GASFLOW
Constant density incompressible flow.	Compressible gaseous
Variable density incompressible flow *).	flow with real
Variable density adiabatically compressible flow *).	equation of state.

2. Equation of motion.

CONVECT	GASFLOW
3D time-dependent Navier-Stokes equation for incompressible flow.	Gasdynamic equations (3D time-dependent Navier-Stokes equation

for compressible flow).

3. Heat transfer.

CONVECT

Equation of heat conduction with account of volume sources of energy release and absorption.

Heat transfer in structure elements^{*)}.

GASFLOW

Equation of heat conduction with account of volume sources of energy release and absorption.

Heat transfer in structure elements.

Radiation heat transfer.

4. Contaminant transport.

CONVECT

Diffusion equation with account of gas flow.

System of diffusion equations with account of gas flow and sedimentation processes intended for aerosol transport description^{*)}.

GASFLOW

Equation of multi-component contaminant transport.

5. Buoyancy.

CONVECT

Buoyancy force in the Navier-Stokes equation is described in the approximation of weak flow compressibility.

GASFLOW

Is accounted automatically by introduction of gravity

force to the equation of motion.

6. Description of turbulent characteristics and processes.

CONVECT

Coefficients of turbulent viscosity and turbulent diffusion are set a priori in the form of constants or functions corresponding to flows being described. Turbulent processes are described using k- ϵ approximation*).

GASFLOW

Algebraic model.
Model of mixing-length turbulence.
k- ϵ model.
Account of buoyancy production terms.

7. Local kinetic processes.

CONVECT

Processes of evaporation and condensation in volume*).

Chemical reactions*).

Processes of aerosol formation*).

GASFLOW

Chemical kinetics and combustion of gases, fluids and solids.
Aerosol generation, transport and precipitation.

8. Geometry of computations.

CONVECT

The computational domain is a parallelepiped. Complex geometry is described by eliminating unnecessary cells; division of a domain into individual blocks

GASFLOW

Complex geometry of facilities: multiblock for separate structures or eliminating unnecessary

interrelated by intermediate boundary conditions.

cells; 1D network connects blocks with ventilation system models.

9. Mesh.

CONVECT

3D Cartesian orthogonal non-uniform grid.

GASFLOW

3D Cartesian orthogonal non-uniform grid, Body-fitted coordinates*).

10. Account of design features.

CONVECT

In regions filled with a great number of small-scale objects (rods, pipes, hanger bars, etc.) resistance forces and heat exchange are accounted in terms of phenomenological models by introduction of volume forces and heat sources to the equations of motion and heat transfer, respectively.

GASFLOW

Description of complex geometry using multi-block structure.

11. Boundary conditions for hydrodynamics.

CONVECT

On external boundaries either velocity components or their normal derivatives are

GASFLOW

preset; on the eliminated cells surfaces adhesion conditions are preset (all the velocity components are set zero)

12. Boundary conditions for heat transfer.

CONVECT

GASFLOW

Third kind combined boundary conditions.

Boundary conditions describing evaporation and condensation on structure surfaces.

Non-linear boundary conditions accounting energy losses for radiative cooling^{*}).

—

13. Boundary conditions for contaminants transfer.

CONVECT

GASFLOW

Third kind combined boundary conditions.

—

14. Numerical algorithms for hydrodynamic equations.

CONVECT

GASFLOW

Fluid dynamics equations are solved by the splitting method with divergence recovery using implicit schemes.

Modified ICEd-ALE method.

15. Numerical algorithms for heat conduction equation.

CONVECT

GASFLOW

The heat conduction equation are solved by the method of two-cycle splitting using implicit schemes.

Modified ICEd-ALE method.

16. Numerical algorithms for contaminant transport equations.

CONVECT

GASFLOW

The contaminant diffusion equations are solved by the method two-cycle splitting using implicit schemes.

Modified ICEd-ALE method.

17. Programming Language.

CONVECT

GASFLOW

FORTRAN

FORTRAN

18. Code testing.

CONVECT

GASFLOW

Using analytical solutions of 1D and 2D test problems and using the results of small-scale laboratory experiments.

Small-scale laboratory experiments.
Full-scale experiments.

19. Efficiency features.

CONVECT

GASFLOW

Computations of incompressible flow dynamics in combination with 3D heat transfer with the number of cells being about 85000 require ≈ 8 Mbytes of main memory.

Computation time per one step takes 3...12 minutes (for PC Pentium-60) and depends

—

on features of a specific problem.

20. Types of problems which have been solved.

CONVECT

Convective flows in vapor-gas mixture at nuclear reactor accidents with core dryout.

Corium cooling.

Contaminant transport in complex-shaped closed rooms.

Contaminant transport in the atmosphere on complex terrain.

GASFLOW

A wide range of problems of gaseous flow dynamics, hydrogen transport, combustion.

21. Display.

CONVECT

Tables; 1D and 2D sections (velocity fields, temperature and contaminant concentration isolines); plane projections of 3D geometry and spatial distributions of values.

GASFLOW

flexible 2-D, 3-D graphics, color mapping of scalar variables as spatial profiles and contours, overlay of velocity vectors, movies of behavior.

3. COMPUTATION OF GASDYNAMICAL FLOWS AND TIME DEPENDENT PROCESSES IN DEFORMABLE SOLIDS

Paper [1] gives a brief description of MIMOZA, B-71 and DRAKON program complexes intended for solving non-stationary gas dynamics and continuum mechanics problems, namely:

- problems with gas detonation or condensed explosive detonation;
- shock wave propagation in air and soils;
- heavy accidents at nuclear power facilities (reactor coolant release, hydrogen safety of nuclear reactors, thermal detonation, etc.);
- cumulative jet generation and propagation;
- problems of high-speed acceleration, impact and penetration;
- swaging;
- determination of complex spatial structure response to various effect types, etc.

In this paper we make comparison with the DYNA code [2] similar in its capabilities. Unfortunately, the information about this code accessible to us is extremely limited and, therefore, the comparison can not be complete. For the MIMOZA code which is discussed first in the paper appropriate information about the DYNA code is given by each comparison item. For further codes (B-71 and DRAKON) the information about the DYNA code is not presented to avoid repetition.

MIMOZA

DYNA2D,DYNA3D

Medium model

Compressible gaseous medium and isotropic elastoplastic medium. There is a capability to compute shells in the shell approximation (in two dimensions only). The code was mainly developed for gaseous medium computations.

Compressible gaseous medium and a model set for elastoplastic medium computation, more suited for computation of low-velocity problems.

Mathematical model

Gas dynamics, elastoplasticity, diffusion equations.

The equations are the same.

Equation approximation method

The finite difference method. (Integrointerpolation method and variational methods of difference equation derivation)

The finite element method.

Computation geometry

Computational domains are of 2D or 3D matrix regular structure. A more complex geometry is implemented by integration of computational domains and their interaction through internal boundary conditions.

There is no regular structure and for each cell there is a list of pointers to its nodes.

Computational grid

Each computational domain is composed of quadrangles (2D) or hexahedra (3D).

Cells can have up to 4 nodes, in 3D up to 8 nodes.

Boundary conditions

In the 3D code sliding surfaces are only possible between domains, in the 2D, in addition, domain paste and Eulerian boundaries are possible.

In the 3D code sliding surfaces are only possible between domains, in the 2D, in addition, domain paste and Eulerian boundaries are possible.

Grid reconstruction in the process of problem solution

There is a capability to maintain an acceptable computational grid in the course of computation. Grid and value updating is at every computation step. In addition, there is a capability of global grid reconstruction.

Material separation by concentrations

There is a capability to separate various materials by concentrations and track their interfaces for computations in Lagrangian-Eulerian coordinates without interface separation by Lagrangian lines. This technique is more developed for two dimensions.

There is a imilar capability in the PAGOSA code [3].

MIMOZA

DYNA2D,DYNA3D

Pre-processor

Initial computation data are set using special language constructs which allows to describe a broad class of problems in two dimensions. Capability to compute initial data in 3D is limited.

Post-processor

Both in 2D and 3D there is a wide set of procedures allowing graphic output of computed data.

B-71 Code

Medium model

- compressible gas dynamics with real equations of state of materials;
- continuum with the Mi-Grueneisen equation of state.

Mathematical model

2D gas dynamics equations in plane or cylindrical geometry.

Heat transport

Phenomenological medium-grid heat exchange.

Detonation

FOREST-FIRE type model of wave detonation excitation. Separation of detonation and shock waves in discontinuity.

Equation approximation method

The gas dynamics equations written in the form of laws of conservation of mass, momentum and energy are solved either by the Godunov scheme or by the modified Godunov scheme with higher approximation order.

Computation geometry and grid

Complex domain geometry with splitting into subdomains. Arbitrary curvilinear coordinates. The grid is adapted to the initial geometry and the flow implemented in the computation process.

B-71 Code

Design feature account

In domains filled with a great number of small-scale objects (pipes, grids, etc.) the medium flow resistance force and heat exchange are computed by empirical dependences in the equation of motion and the equation of energy conservation.

Boundary conditions

On external domain boundaries normal velocity or pressure can be set. Shock and detonation waves can also be external boundary conditions. Internal boundaries can be: contact discontinuities, Eulerian movable shock waves, rarefaction waves.

Result representation

Results are represented in the form of tables, graphs, velocity fields, isolines.

Program testing

Programs were tested on a number of known exact solutions of gas dynamics equations, self-similar solutions and by comparison with computed results by other codes.

DRAKON program complex

Medium model

- viscous-elastoplastic isotropic medium with real equations of state with account of porosity and model parameter dependence on current state;
- branching shells supported with rigidity edges with attached masses;
- thin-wall elements made of composite materials with account of mechanical property anisotropy (for two dimensions);
- thin-wall elements made of reinforced concrete with elastoplastic reinforcement deformation and anisotropy of concrete strength properties;
- contact interaction among structure elements is taken into account.

Mathematical model

- variational dynamics equation;
- continuum mechanics equations;
- geometrically non-linear theory of Timoshenko type shells;
- theory of composite orthotropic shells;
- theory of flow with combined strengthening;
- at discontinuous solution computations artificial viscosity is used.

Equation approximation method

- variational-difference method of solution by explicit scheme "Krest" in Lagrangian coordinates using "natural" approximation of derivatives by spatial variables;
- for thin-wall structure computations an efficient regularization technique is implemented allowing to increase an integration step up to Courant number equal to unity without loss of scheme approximation accuracy irrespective of element thickness;
- a method is developed to remove distortions of a quadrangle difference grid through account of triangular cell contribution.

DRAKON program complex

Computation geometry and grid

- computational domains are of regular structure for two dimensions;
- arbitrary structure for three dimensions (for each computational cell there is a list of pointers to its vertices);
- the computational domain is composed of quadrangular cells.

Boundary conditions

On external domain boundaries kinematic, force (concentrated or distributed loadings) and contact interaction conditions are set:

- contact surface conditions provide separation, sliding (with account of friction) or adhesion;
- an algorithm of contact on consistent and inconsistent difference grids is implemented which is based on estimation of contact pressure and friction forces in currently contacting zones.

Grid reconstruction in the process of problem solution

There is a capability of global difference grid reconstruction.

Pre-processor

- for 2D modules initial data for a computation are set using special language constructs;
- for 3D modules domain geometry and topology are derived using available geometric pre-processors. The pre-processor of the DRAKON complex allows to set boundary and initial parameters with full visualization of a structure computational scheme.

Post-processor

Provides computational domain visualization with color representation of obtained stress, strain, velocity, etc. fields, as well as allows to map computation results in the form of temporal dependencies.

DRAKON program complex

Program testing

The complex was tested through comparison with exact solutions and results obtained by other codes as well as through comparison with experimental data.

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