SINARA code: Simulation of turbulent mixing on gas interfaces

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INTRODUCTION

The SINARA code was created to simulate some emergency processes in fast nuclear reactors [1]. The code solved boundary-value problems for 2D non-stationary equations in cylindrical coordinate system (the R, Z geometry). The code was applied to simulate destruction of reactor core casing, and assess an emergency situation at destruction of atomic power station structures, etc. [2].

The SINARA code was adapted to simulate problems of heat and mass transfer [3, 4]. Accuracy of the Eulerian stage of the calculations was improved. Implicit algorithm was enhanced for fluid simulations, in which material velocity was significantly smaller than the speed of sound and therefore, Mach number is much smaller than unity. The method was modified to incorporate capabilities of simulating both compressible and incompressible flows in one code. Physical viscosity and a number of models of turbulent flows were developed in the SINARA code. A geometry-based model was implemented to include heat radiation. Boundary conditions of mass inflow and outflow at the arbitrary boundary parts were implemented for the Eulerian stage of the simulations. A difference scheme for the equations with the periodic coefficients was developed.

The method of decomposition into the physical processes was used. To solve a specific problem, it is possible to use an arbitrary set of package modules. In this case different physical processes and their interaction with each other are simulated, and the appropriate equations are solved simultaneously. In particular, the package solves the problems of heat and mass transfer using jointly non-stationary hydrodynamics and heat conduction modules.

1. BRIEF CHARACTERISTIC OF THE SINARA CODE

The SINARA code solves boundary-value problem for 2D non-stationary equations in cylindrical system of coordinates (R-Z geometry).

Processes that can be simulated:

- motion of multi-component one-velocity viscous medium,
- account for elastic-plastic and strength features of materials,
- turbulence,
- linear heat conduction
- radiation.

The codes are implemented as individual modules. The SINARA code includes the following modules.

1) Module for non-stationary hydrodynamics.
2) Module for turbulent mixing.
3) Module for non-stationary hydrodynamics including elastic-plastic and strength features of medium.
4) Module for solving heat conduction equations.
5) Module for radiation.

Medium models:

- Model of ideal fluid including multi-component medium.
- Model of elastic body including plasticity, compressibility, failure, melting and evaporation.
- Model of viscous fluid including multi-component medium.
- Model of turbulence.
- Geometry-based model of radiation.

Construction of a computational model was based on decomposition into physical processes. At a time step the system under consideration is decomposed into several subsystems soled sequentially. This approach allows description of problems in different approximations with the help of an arbitrary set of the equations.

1.1. EXPLICIT-IMPLICIT ALE-METHOD

An approach of the ALE-method [5] was used to solve equations describing a multi-component single-velocity flow. At the first phase the equations are solved in Lagrangian coordinates. The phase consists of explicit and implicit steps. The explicit step uses a staggered mesh. Velocities and coordinates are stored in mesh nodes and the rest variables are in cell centers. At the implicit step we add the determination of pressure at an advanced time. For this purpose we linearize equations in which time derivatives are replaced by finite differences and equations of state to obtain the following system of first-order equations for viscous pressure and velocity functions:

$$\begin{cases} P^{n+1} + \psi \cdot div\, \vec{U}^{n+\frac{1}{2}} = \varphi. \\ \vec{U}^{n+\frac{1}{2}} + \dfrac{\tau}{\rho^{n+1}} \cdot grad\, P^{n+1} = 0 \end{cases} \tag{1}$$

Two options are possible.

The first involves the solution of the system (1) to obtain velocity vectors in cell centers and then interpolate velocities in nodes and obtain the other sought functions.

The second option implies the use of acceleration $\vec{W}^{n+\frac{1}{2}} = \frac{1}{\tau}(\vec{U}^{n+1} - \vec{U}^{n})$ instead of $\vec{U}^{n+\frac{1}{2}}$. Then the system (1) is solved using only the found viscous pressure which is then used to determine node velocities on the staggered mesh.

The system (1) is solved using approximations of the diamond type [6]. The equations are approximated within one cell of quadrilateral mesh. The resulted equations contain unknown functions in the center and on four edges of each cell. With a stabilizing corrections method, the system is reduced to two systems of one-dimensional difference equations. For each of them, the functions in cell centers are replaced by the expressions

$$U_{i+\frac{1}{2}} = \frac{1}{2}\left(U_{i+1} + U_i\right) + \theta_{i+\frac{1}{2}}\left(P_{i+1} - P_i\right), \quad P_{i+\frac{1}{2}} = \frac{1}{2}\left(P_{i+1} + P_i\right) + \delta_{i+\frac{1}{2}}\left(U_{i+1} - U_i\right), \tag{2}$$

Where δ and θ are parameters defining the scheme properties. With the equations (2), the one-dimensional difference equations are reduced to linear equations for unknown functions on cell edges. These equations are solved by sweeping.

It is not necessary to apply splitting in solving (1). We can modify (2) so as to obtain a system of difference equations for unknowns on all cell edges. This system of linear algebraic equations can be treated with any solver available.

In all cases, the solution of the system (1) obtained with a diamond approach is more accurate than that obtained with traditional schemes which use approximations over several cells (9 in the 2D case).

1.2. IMPROVEMENT OF SIMULATION EFFECTIVENESS FOR ALMOST INCOMPRESSIBLE FLOW

A peculiar feature of such flows is that medium velocity is much less than the speed of sound; therefore, Mach number is much less than a unity. Any compression or rarefaction occurs at practically constant pressure. The objective of the work was to modify the technique so that to make it suitable for simulation of both incompressible and compressible flows. To simulate such flows in the SINARA code, an iteration parameter was introduced in the equation of momentum conservation, which increased Mach number beyond the limits of a subsonic flow.

The iteration parameter scaling the pressure gradient was introduced in order to change pressure perturbation in the subsonic flows and improve computational efficiency without any changes to other flow features. Conservation equation of momentum now includes parameter α. The modified equation is as follows:

$$\frac{\partial \rho \vec{u}}{\partial t} + \vec{\nabla}\left(\rho \vec{u}\vec{u}\right) = -\frac{1}{\alpha^2}\vec{\nabla}P + \vec{\nabla}\vec{G} + \rho\vec{g}$$

For efficient computations, parameter α should be as large as possible keeping value of $\delta P_\alpha / \overline{P}$ small compared to one. The SINARA code selects α so that $\delta P_\alpha / \overline{P}$ <0.04, provided the selected α is larger than one.

1.3. MODELS OF TURBULENT MIXING IN THE SINARA CODE

To include turbulent mixing, two models were implemented in SINARA code: *Lν*-model and *kε*-model of turbulence.

1.3.1. Kε-model of turbulence

Model $k\varepsilon$ is a model of the first-order closure, which means that a sequence to correlate turbulent components of different values ceases at the first-order correlation equations.

Transition from layer n to $n+1$ is iterative. An iteration loop has three stages**:** A, B, C and D. Stages A, B and C together constitute the computations where computational cells move together with gas and fluid.

- stage A solves gas dynamic equations with the generation part of $k\varepsilon$-model equations;
- stage B accounts for turbulent diffusion and turbulent pressure and solves energy equation;
- stage C accounts for heat flow and turbulent heat transfer.

During stage D, flow field is "frozen" and recalculated into a new mesh.

1.3.2. Lv –model

Model lv is a model of the first-order closure, it is based on the similarity to molecular transport processes and introduction of turbulent viscosity coefficient. This model is reduced to the system of Navier-Stokes equations.

Turbulent viscosity coefficient is determined with Prandtl formula, which is $\mu = \rho L^2 \left(\vec{G} : \vec{\nabla}\vec{u}\right)^{1/2}$, where L is turbulence length. Physical sense says that L is a characteristic size of the main eddies in the flow. If the flow is limited with rigid walls L could be estimated as $L=\alpha R$, where $\alpha\approx 0.1$ is an empiric constant, R is the characteristic size of the flow.

1.4. IMPROVING THE ADVECTION ACCURACY

The SINARA code exploits ALE-method [5] for numerical simulation of flows. The step calculation is split into two stages. At the first one the equations are solved in the Lagrangian variables, in this case the computational mesh deforms together with the material. During the second stage a new mesh is constructed. And then the recalculation of all values from the first mesh onto the second one is carried out.

Flow computation can be done in two steps: first, construct an interpolation function and second, directly compute the flows.

Linear density distribution with a cell is used. After gradient field is calculated, the monotonicity-ensuring technique [7] is applied, which smoothes the gradients wherever their monotony is disturbed.

When calculating velocities, the cell momentum is used as a function to be recalculated. An additional mesh is constructed to calculate the momentum: each cell is decomposed into four smaller cells.

1.5. TESTING OF THE SINARA CODE

The modified technique was tested with the following problems [3, 4].

- Tests for hydrodynamics and heat conduction equations [8, 9]
- Viscous incompressible flows.
    - Simulation of air convection in a square area under gravity. Temperatures, velocities and densities computed with the CFX code [10] and SINARA codes coincided at the moment of transition to the steady state.
    - The Pouasel flow is a flow of incompressible fluid in a cylindrical tube. Boundary conditions of material inflow and outflow were used. Maximum discrepancy between the numerical and analytical solutions is no more than 0.1%.
- Turbulence tests.
    - Mixing in 2D stationary plane layer. The Kε-model was used. The obtained results are in good agreement with the experimental data and simulations done with other codes.
    - The problem of flow through a rough pipe. Simulations employed the Lv –model of turbulence. Simulations were done until solution reached the steady state. The results were compared to the analytical solution.
- Testing of the advection scheme.
    - The Sod problem. The results obtained with different schemes were compared to the analytical solution.

- Gas expansion into vacuum from initial triangular prism configuration. This 2D problem has an exact solution.

To test the radiation module we considered a problem about emissivity of two parallel plates of finite size. The obtained result was compared to the solution derived from the analytical solution in assumption that the plate length is much larger than the distance between them.

2. SINARA APPLICATION TO THE DIRECT SIMULATION OF FAS INTERFACE INSTABILITIES

Many physical applications require studying fluid interface dynamics. These include, for example, high energy density physics, astrophysics, or physics of atmosphere and ocean. Flows of such kind are often unsteady and any initial perturbations present on the interface grow beyond all bounds. Rayleigh-Taylor instability results from the orthogonal acceleration acting on the interface of fluids of different densities. It occurs if density and pressure gradients are directed oppositely from the interface. In case of pulsed acceleration, or shock wave, the interface is always unstable (Richtmyer-Meshkov instability).

Numerical simulations play a great role in hydrodynamic instability research. One of the problems that inevitably arise in the computation of physical systems is the necessity of establishing the credibility of such simulations. In order to accomplish this task, it is necessary to carefully examine both idealized numerical simulations and experimental data.

A number of experiments were done with the electromagnetic shock tube developed at RFNC-VNIITF [11]. They aimed to study the evolution of initial sinusoidal perturbations on the boundary of noble gases under the action of a decelerating shock wave. Experimental data on instability evolution and turbulent mixing on artificially perturbed interfaces of gases of different density are available.

The evolution of perturbations was recorded using the IAB-451 schlieren-system optically aligned with two high-speed photography cameras of SFR-2m or VFU types implementing simultaneous shooting. The measurement error depended on the resolution of the cameras: 0.5mm for the photochronograph and 0.8mm for the SFR camera. The perturbation amplitude or the width of the perturbation zone was determined by measuring the distance between the left and right edges on the image of the perturbed interface of two gases.

The following two cases are considered:

- The shock wave moves from the light gas to the heavy one and generates Richtmyer-Meshkov instability; the rarefaction wave makes the interface gravitationally stable;
- The shock wave moves from the heavy gas to the light one, generating Richtmyer-Meshkov and Rayleigh-Taylor instabilities.

2.1. PROBLEM STATEMENT

2.1.1. Configuration 1

The decelerating shock wave moves from the heavy gas to the light one. Region I: krypton (Kr) of initial density $\rho_0 = 3.36 \cdot 10^{-3}$ g/cm^3, adiabatic exponent γ =1.689. Region II: helium (He) with $\rho_0 = 3.36 \cdot 10^{-3}$ g/cm^3 and γ =1.63.

Fig.1. Computational setup for configuration 1

The initial pressure in the entire system is p_0=0.984 bar. Initially the gases are at rest.

Boundary conditions: on the left boundary (y=0), $u=U_0\exp(-t/\tau)$ where U_0=0.948 mm/μs, τ =153.56 μs (the values are taken from the 1D simulation of the experiment).

y=1500 mm, x=0 mm, and x =100 mm are rigid walls.

The boundary between regions I and II is defined as $y=y_0 + a_0 \cos(2\pi x/\lambda)$, where y_0=240mm, λ=50mm, $x \in [0;100]$ mm. The calculations were done for a_0 = 1 and 2.5 mm.

2.1.2. Configuration 2

The shock wave moves from the light gas to the heavy one. The computational configuration is shown in Fig.2.

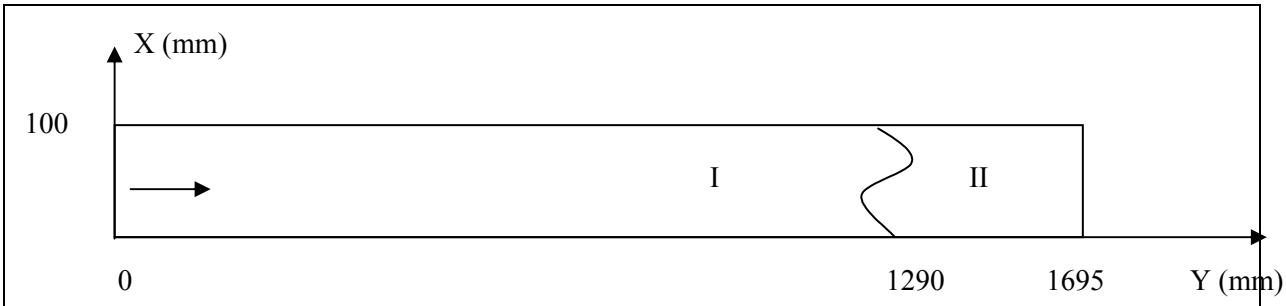

Fig.2. Computational setup for configuration 2

Region I: helium (He) of initial density $\rho_0 = 1.63 \cdot 10^{-4}$ g/cm^3, γ =1.665

Region II: xenon (Xe), $\rho_0 = 5.383 \cdot 10^{-3}$ g/cm^3, γ =1.667

The initial pressure in the entire system is p_0=0.976 bar. The initial velocity is u=0.

Boundary conditions: on the left boundary (y=0), the pulsed pressure was

$$P(t) = \begin{cases} P_n, & 0 \le t \le t^* \\ P^* \exp(-2t/\tau)\sin^2(2\pi t/T), & t^* \le t \le T/2, \\ 0, & t \ge T/2 \end{cases}$$

where P_n=1.217 bar, P^*=123.3 bar, t^*=1.2 μs, τ =97.4μs, T=75μs, and y=1695mm, x=0, x=100mm are rigid walls.

The boundary between regions I and II was $y=y_0 + a_0 \cos(2\pi x/\lambda)$,where y_0=1290mm, λ=50mm , $x \in [0;100]$ mm. The calculations were made for a_0=1, 2.5, and 7.5 mm.

All calculations were focused on the time history of the mixing zone $|y_{\max} - y_{\min}|$. It was assumed that the shock wave crossed the interface at t=0.

2.2. MIXTURE MODELS

SINARA implements several mixture models. Each of them shows its advantages and disadvantages, and their applicability is limited. All the models treat single-velocity flows.

The simplest homogeneous model assumes that all materials in a mixed cell have equal densities and pressures. Each material has its mass fraction. All thermodynamic functions (TDF) in a cell are calculated by averaging appropriate functions for each material with respect to its mass fraction.

In heterogeneous models, each material in a mixed cell has its own density and temperature. The mean values of TDFs in a cell are calculated with some weight functions which depend on volume fractions. The construction of these models requires special assumptions, such as

- Equal compressibility of materials in mixed cells, i.e., equal velocity divergences;
- Equal pressure increments and ability to equalize material pressures in a cell;
- Dynamic equilibrium, i.e., equal pressures of material in the mixed cell.

The first two do not require solving non-linear equations.

In addition to these models of mixed cell treatment, we use particle markers to ensure high accuracy of interface reconstruction. The approach is similar to that one used for the ALE-method [12].

2.3. PERTURBATION EVOLUTION CALCULATIONS: CONFIGURATION 1

The calculation was made for two amplitudes of the initial perturbation: a_0=1 and 2.5 mm. The number of intervals differed (see Fig.3 and Table 1).

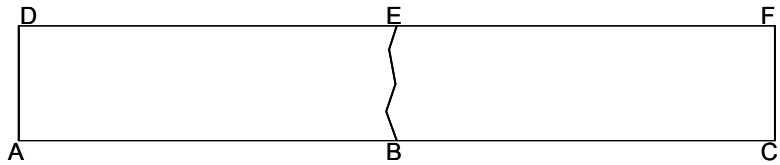

Fig.3. Computational geometry

Table 1. Number of intervals.

Segment / Variant #	AD	AB	BC
1	**80**	**120**	**230**
2	**200**	**205**	**300**
3	**300**	**315**	**450**

Figures 4a and 4b show the width of the mixing zone versus time obtained in experiment and calculation (a_0=1 mm and a_0=2.5 mm, respectively). Figures 5 show interface configurations at the terminal time.

2.4. PERTURBATION EVOLUTION CALCULATIONS: CONFIGURATION 2

The calculation was made for three amplitudes of the initial perturbation: a_0=1, 2.5 and 7.5 mm. The number of intervals differed (see Fig.3 and Table 1).

Figure 6 shows the relative amplitude a/a_0^+ of the interface versus time for a_0=1, 2.5 and 7.7 mm (the time when the shock wave reaches the perturbed interface is subtracted). Figure 7 shows interface configurations at the start and end (*t=448* μs) of calculation. Figures 8 and 9 present the same data for a_0=2.5mm (termination time 346 μs) and a_0=7.5mm (termination time 356 μs), respectively.

2.5. DISCUSSION OF RESULTS FOR CONFIGURATION 1

Calculated results presented in Fig. 4 (λ=50mm, $_0$=1 and 2.5 mm) are seen to agree rather well with experimental data. We may conclude that for λ=50 mm, the evolution is linear till *t*=130 μs; and here experimental results, calculations and the linear theory agree rather well.

Now consider the mixing constant α estimated from experimental data.

The transition to the turbulent phase depends on particular experimental conditions but the ultimate stage of turbulent mixing must not depend on initial conditions. It is almost impossible to implement the asymptotic stage of mixing in experiment because of the finite size of the tube and the short time of acceleration. We assume that in the described experiments the transition to the turbulent phase has occurred, and experimental results are interpreted following from the relationship for the real size of the mixing zone $\tilde{L}$ [13]

$$\sqrt{\tilde{L}} = \sqrt{L_0} + \sqrt{L} \, .$$

Here L_0 is the width of the initial turbulence zone and L is the self-similar width of the mixing zone (independent of initial conditions) written as $L = \alpha A 2 S$. Here $A = (\rho_1 - \rho_2)/(\rho_1 + \rho_2)$ is Atwood number (ρ_1 and ρ_2 are gas densities) and S is deceleration length defined as $S = \Delta U t - \Delta\tilde{L}$ where ΔU – is the increment of the interface velocity due to the shock wave, t is time relatively to that when the shock wave reaches the interface, and $\Delta\tilde{L}$ is the distance between the current and initial positions of the interface.

It should be noted that the above formulas apply only to the asymptotic stage of gravity driven mixing where the flow is chaotic. However, even at terminal times both experiment and calculation show sharp, non-destroying mushrooms of the heavy gas, and their number does not change, i.e. the initial configuration is not yet forgotten.

To describe the gravity driven turbulent mixing, we calculate $d\sqrt{E}/d(\sqrt{2S}) = \sqrt{\alpha A}$. Assuming a linear relationship between $\sqrt{E}$ and $\sqrt{2S}$, and using the least square method for S>10mm (t>150 μs), for all experiments we obtain $\alpha = 0.32$ independent on the initial amplitude.

If take into account experimental data for t>380 μs (S>63 mm) and formally recalculate this value, we obtain $\alpha \approx 0.26$. So, not accounting for the experimental data within (150μs, 380μs) representing the non-linear stage reduces the mean value of α which is constant for only the turbulent phase.

Our calculations show (see Fig. 10 presenting experimental and calculated results in ($\sqrt{E}$, $\sqrt{2S}$) coordinates for λ=50 mm, a_0=1 mm) that α seems to continue its slow decrease, i.e. the parameter is not yet constant.

Calculated and experimental data agree rather well.

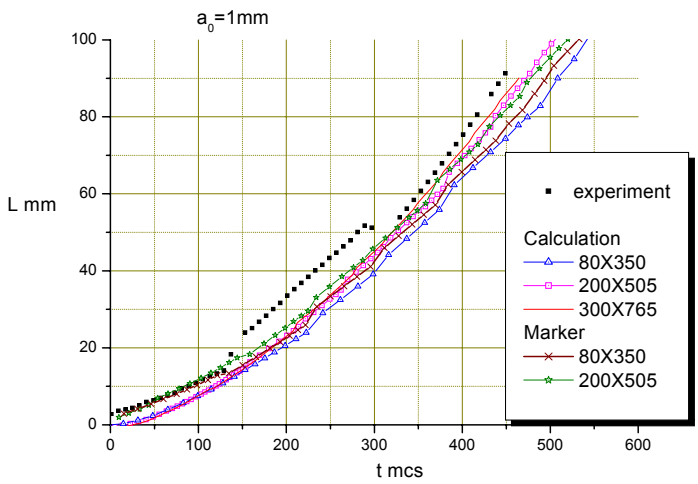

Fig.4a. Configuration 1: Turbulent mixing width versus time (a_0=1 mm)

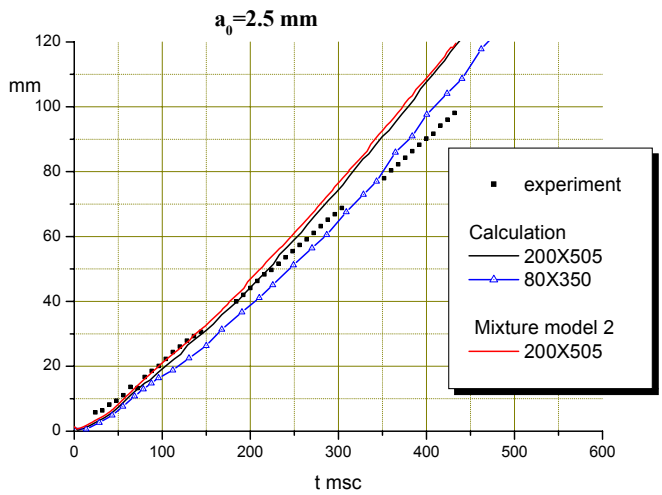

Fig.4b. Configuration 1: Turbulent mixing width versus time (a_0=2.5 mm)

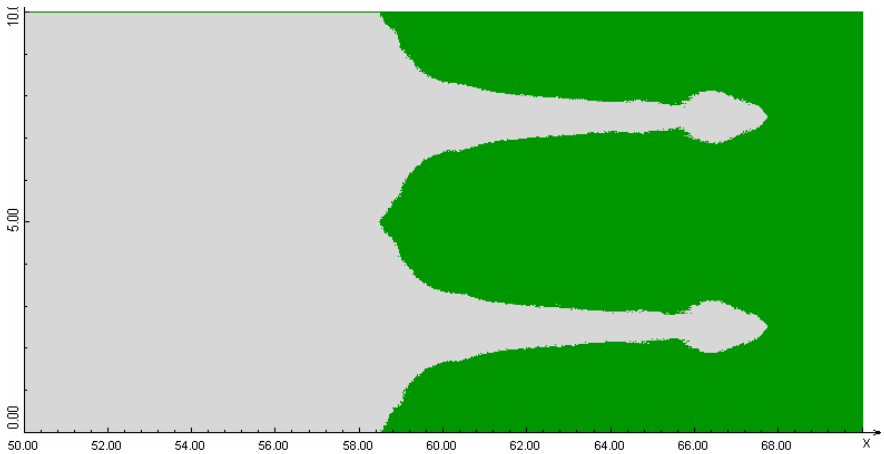

Fig.5a. Configuration 1: Gas interface at time t = 694 μs; a_0=1 mm

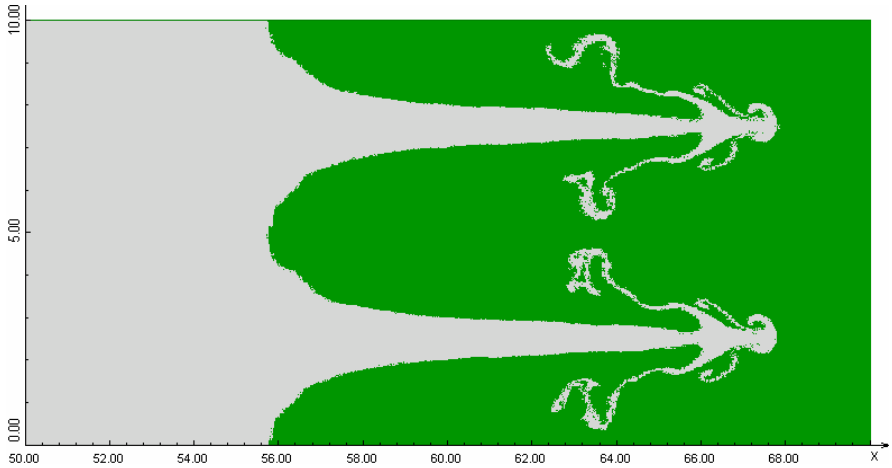

Fig.5b. Configuration 1: Gas interface at time t = 663 μs; a_0=2.5 mm

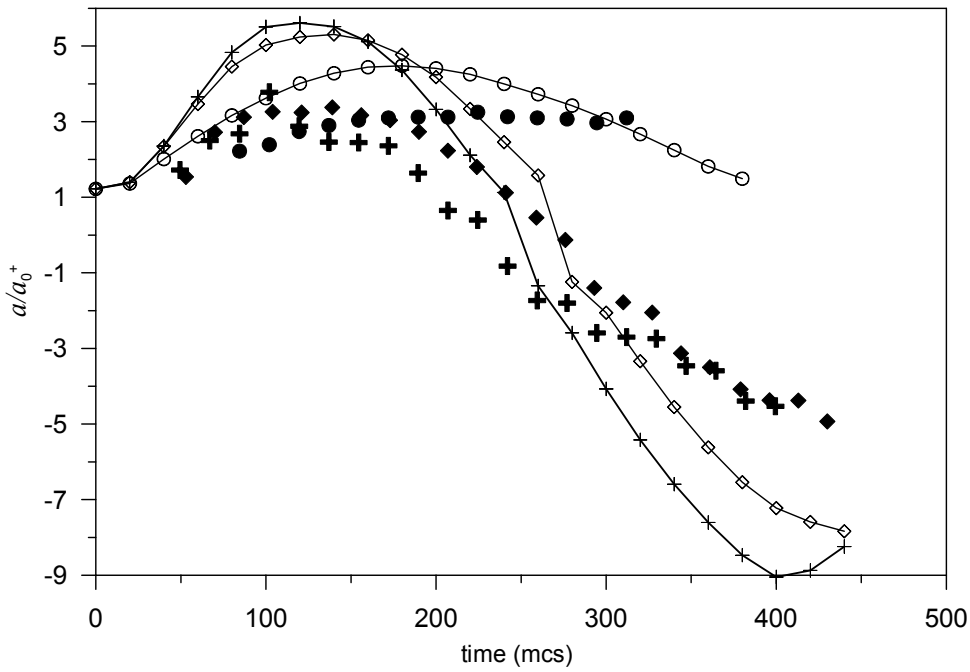

Fig.6. Relative perturbation amplitude $a(t)/a_0$ versus time; a_0 = 1mm: ✚- experiment, + - calculation; a_0=2.5mm: ◆- experiment, ◇ - calculation; a_0= 7.5mm: ●– experiment, ○– calcluation

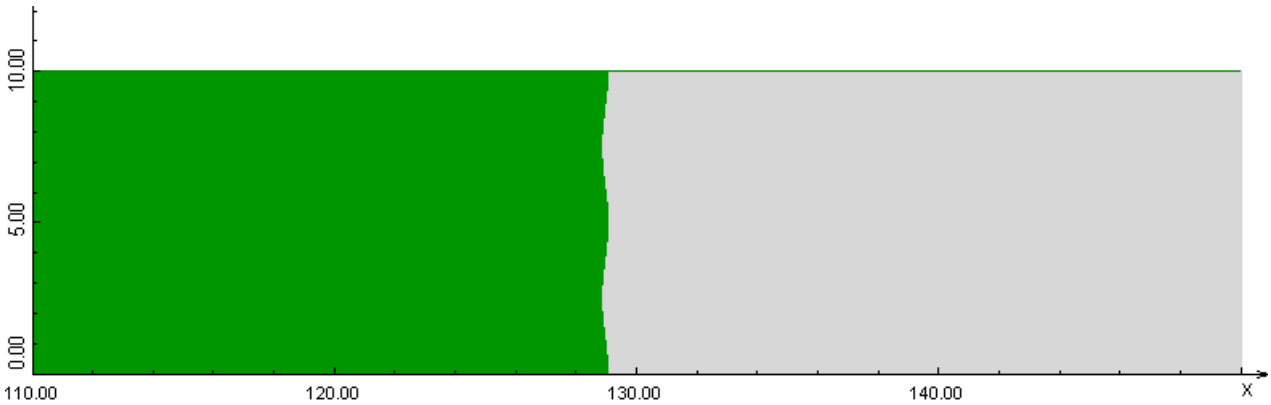

Fig. 7a. Configuration 2: Gas interface zero time; a_0=1mm

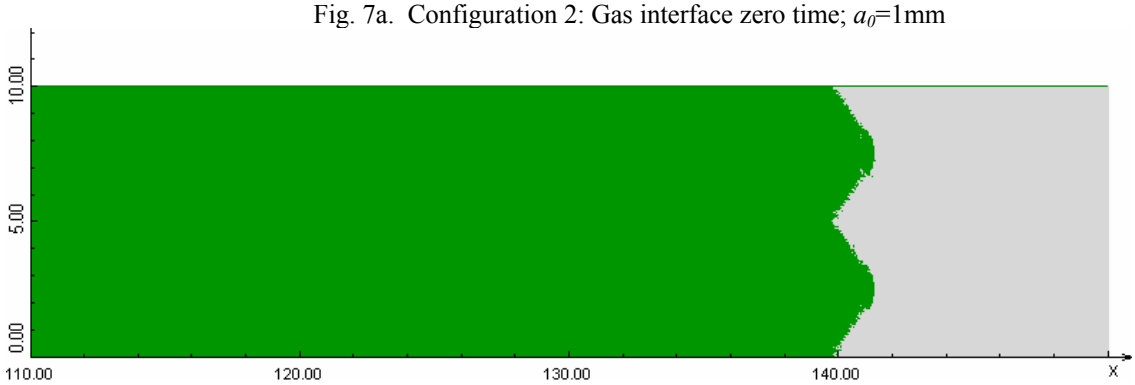

Fig. 7b. Gas interface at time t = 448 µs

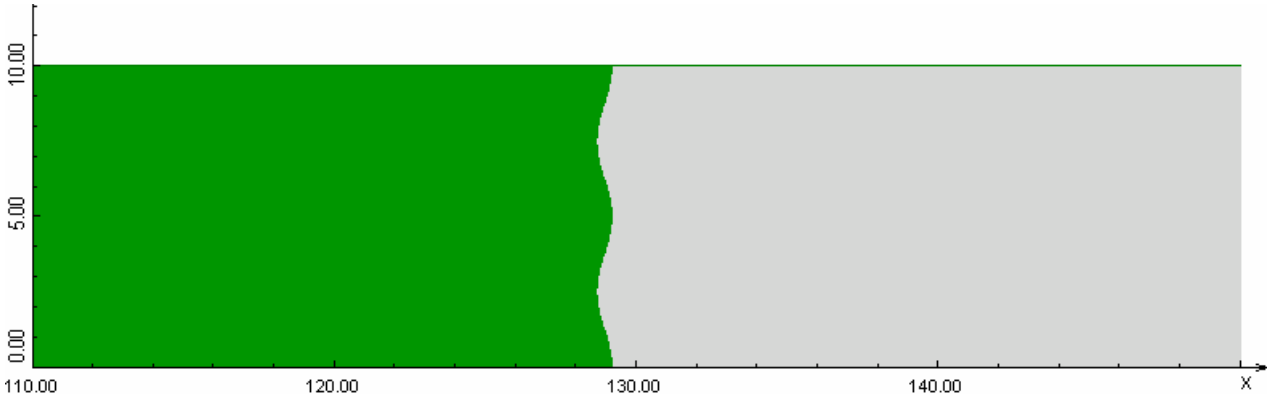

Fig.8a. Configuration 2: gas interface at zero time; a_0=2.5 mm

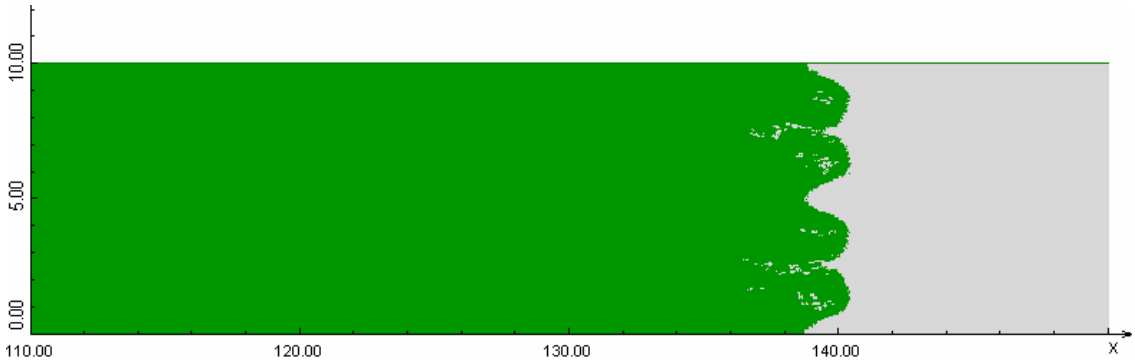

Fig.8b. Gas interface at time t = 346 µs

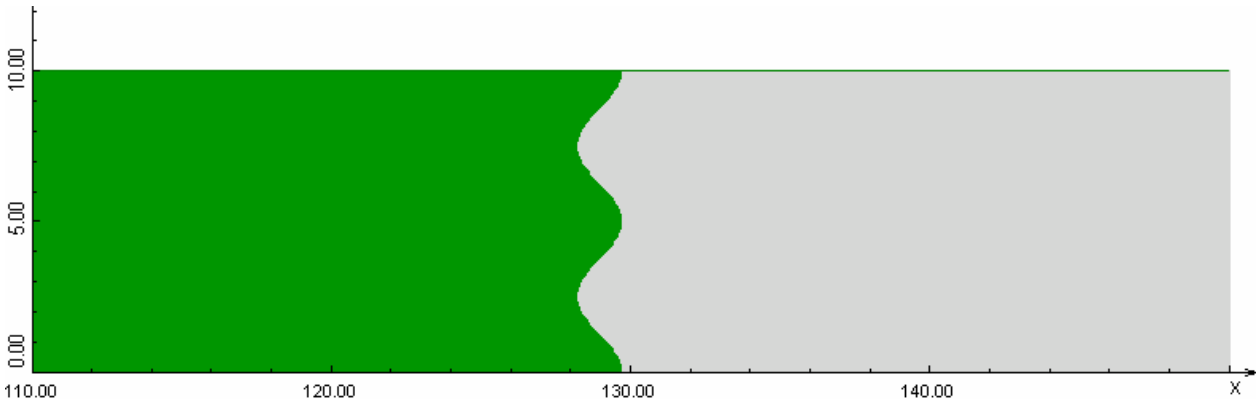

Fig.9a. Configuration 2: gas interface at zero time; a_0=7.5 mm

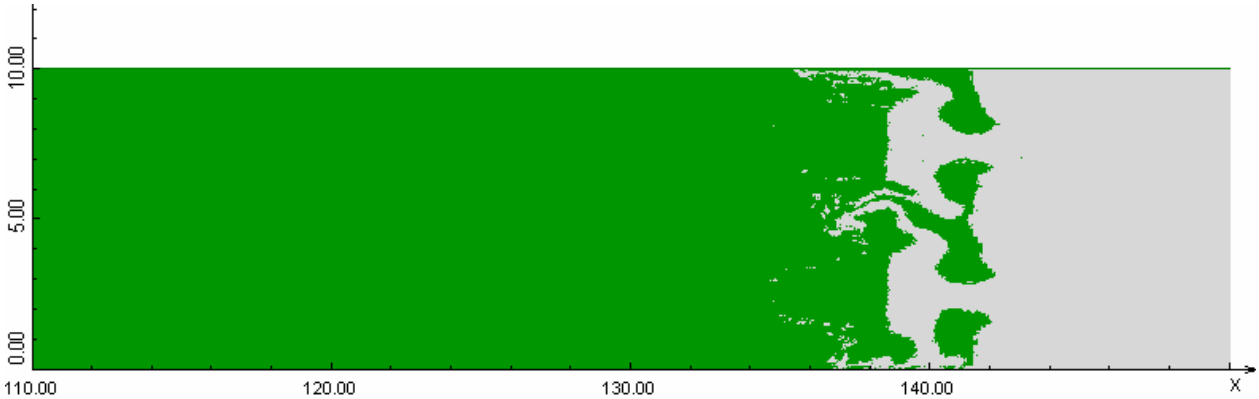

Fig.9b. Gas interface at time t = 356μs

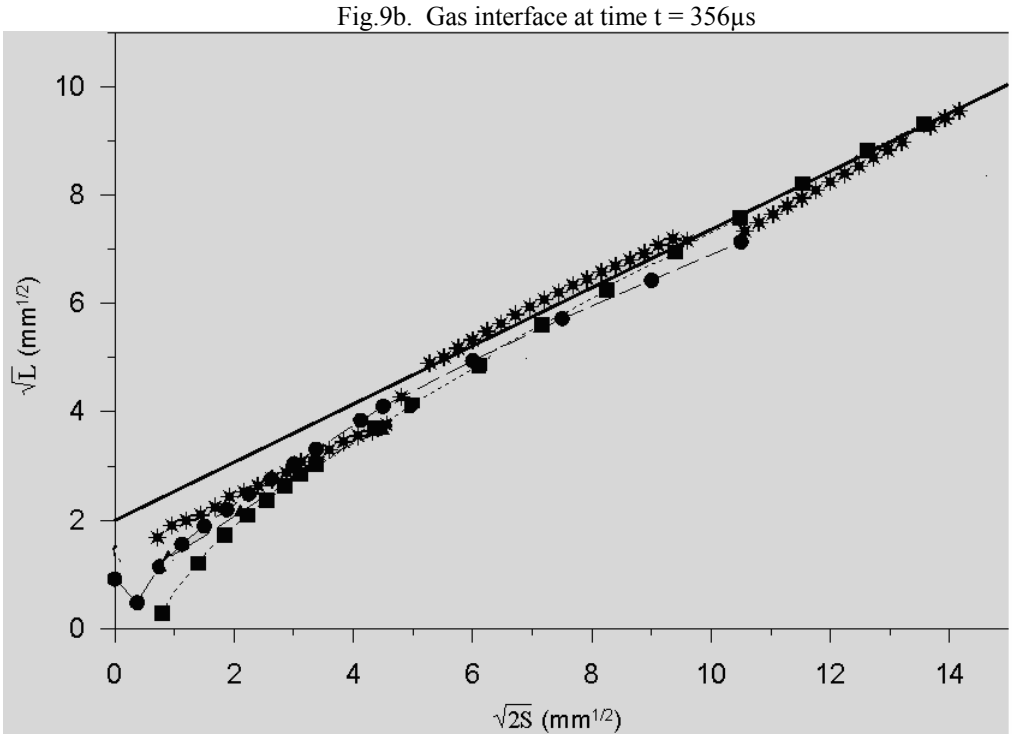

Fig. 10. $\sqrt{\mathcal{L}}$ versus $\sqrt{2S}$ for a_0=1mm and λ=50mm: * - experiment, ▬ averaged experimental results, • - calculation by the vortex method, ■ - SINARA calculation

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