Some Aspects and Applications of Implicit Stabilization Method for Solving Fluid Dynamics Problems

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Abstract: - This paper is concerned with implicit numerical method for solving fluid dynamics equations. Some important integral properties of differential operators and its discrete analogues, stability of numerical procedure are considered. Applications to numerical modeling of two-phase flows (subcooled boiling), thermal convection are presented. Results of numerical predictions and comparison with experimental data are described.

Key-Words: - Implicit numerical method, integral properties, thermal convection, two-phase flow

1 Introduction
Numerical methods for fluid dynamics are successfully applied in solving a wide variety of problems. They are the core of computational fluid dynamics (CFD) codes. The greatest progress has been made in numerical simulation of single-phase incompressible flows. Further development of numerical methods is connected with solving complex problems of fluid dynamics. Still an urgent task is the creating of novel, efficient and accurate numerical techniques.

Two-phase flows are widely spread in nature and technology. For instance, modern projects of nuclear reactors PWR-type require a thorough understanding of the local features of two-phase flows in variable conditions. Numerical simulation of two-phase flows results in the increasing of unknown variables, a strong non-linear system of equations, complex state equations, etc. In this paper implicit numerical method [1], [2] is developed and generalized to solve similar complicated systems of equations.

2 Implicit numerical method
Implicit numerical method [1], [2] has been developed on the base of monotonous balance neutral (MBN) difference schemes which allow to keep some important integral properties of differential operators. Monotonous schemes simulate important property of a fluid flow as a downstream transfer of some disturbance due to a convection motion. A balance (conservation) property is a discrete analogue of the Ostrogradski-Gauss theorem. These properties allow the method to avoid the accumulation of errors due to additional approximation sources and to obtain physically realistic solutions.

Consider the following system in a bounded domain Ω
\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u^1}{\partial q^1} + \frac{\partial \rho u^2}{\partial q^2} + \frac{\partial \rho u^3}{\partial q^3} = 0 \] (1)
\[ \rho \frac{\partial \phi}{\partial t} + \Lambda(\phi) = f, \] (2)
where \( \Lambda(\phi) = \rho u^j \frac{\partial \phi}{\partial q^j} - \frac{\partial}{\partial q^j} \eta^{ij} \frac{\partial \phi}{\partial q^i} \). Here substance \( \phi \) may be a velocity component, an enthalpy, a concentration, etc. A balance (conservation) property can be written as (Ostrogradski-Gauss theorem):
\[ \frac{\partial}{\partial t} \int_{\Omega} \rho \phi \, d\Omega = \int_{\Omega} f \, d\Omega - \int_{\partial \Omega} \rho \phi u^i n_i \, d\Omega \] (3)
Neutral property of \( \Lambda \) operator can be formulated in the form of the integral relationship
\[ \int_{\Omega} \frac{\partial \rho \phi^2}{\partial q^j} \, d\Omega \left|_{t=0}^{t} \right. + \int_{0}^{t} dt \int_{\partial \Omega} \frac{\partial \rho \phi}{\partial q^j} \, d\partial \Omega = \int_{0}^{t} dt \int_{\partial \Omega} f \, d\Omega \] (4)
Integral relationship (4) shows null contribution of the terms describing convection transfer,
derivation of pressure difference equation. Its implicit iterative procedure is the base for solving non-linear system of difference equations (6), (7). Index “L” denotes a number of iteration, $\gamma_{L}$ is a step of stabilization. Linearizing procedure is carried out in such way that operator $A$ becomes linear relatively to $u_{k+1/2}$, when $u_{k+1/2}$ is known. Implicit numerical procedure is written as follows (1)$\leq i$ $\leq n$

$$\frac{n}{n} \Delta q_{k}^{\beta} + \delta^{i + 1/2} \rho_{m}^{k + i/2} \phi_{k + i/2} - \phi_{k + i/2} \Delta t_{m}$$
$$+ A(\phi_{k + i/2}) = \frac{n}{n} \Delta q_{k}^{\beta} + \delta^{i + 1/2} \rho_{m}^{k + i/2} f_{k + i/2}$$

The equation (5) is not directly included in the implicit iterative procedure but is the base for derivation of pressure difference equation. Its general form can be presented as:

$$\left( \sum_{\beta=1}^{n} \Delta q_{k}^{\beta} \right) \frac{\rho_{m}^{k+1/L} - \rho_{m}^{k}}{\Delta t_{m}} + P_{k}(\rho_{k}) = f_{k}$$

Pressure, concentration, temperature are computed in the centers of grid cells, components of velocity vector - in the centers of faces. Both the MBN-schema and a displacement of coordinates of a grid functions enable to obtain physically realistic fields of computed values.

Implicit numerical procedure is developed for solving non-linear system of difference equations (6), (7). Index “L” denotes a number of iteration, $\gamma_{L}$
3 Numerical modelling of subcooled boiling

In general case, two-phase fluid dynamics processes in drift-flux approach can be described by a system of partial differential equations, which involves continuity, momentum, heat transfer equations, state equations and others [4]. In a vector form continuity and momentum equations can be written as follows:

\[
\begin{align*}
\frac{\partial \rho_u}{\partial t} + \text{div} \rho U &= 0, \\
U &= (u^1, u^2, u^3), \quad (9)
\end{align*}
\]

\[
\begin{align*}
\rho &= \alpha \rho_g + (1 - \alpha) \rho_f, \quad (10)
\end{align*}
\]

\[
\begin{align*}
\left( \frac{\partial \bar{U}}{\partial t} + (\bar{U} \text{grad}) U \right) &= \rho \bar{F} - \text{grad} p, \\
+ \text{div}(\tau + \tau^d) &= \frac{2}{3} \text{grad}(\mu \text{div} \bar{U} + \rho K), \quad (11)
\end{align*}
\]

where \( \rho \) is a mixture density, \( \alpha \) - a void fraction, \( \rho_g \) - a gas (vapour) density, \( \rho_f \) - a fluid density, \( p \) is a pressure, \( \rho_m \) - a coefficient of molecular viscosity, \( \mu_t \) - turbulence viscosity, \( \mu = \mu_m + \mu_t \), \( K \) - a turbulent kinetic energy, \( \bar{U} = (u^1, u^2, u^3) \) is the mixture center mass velocity vector, \( \tau \) - a tensor of velocity deformation; \( \tau^1 \) - a turbulent stress tensor, \( \tau^d \) - a drift stress tensor. Drift stress tensor can be approximated as in [4]

\[
\tau^d = c(1 - \alpha)^{-1} \rho_f \bar{u}_{gi} \bar{u}_{gi}, \quad (12)
\]

\( \bar{u}_{gi} \) is a drift velocity, \( c = \alpha \rho_g / \rho \) - a vapour concentration. Zuber-type correlation is employed as a closure relationship

\[
u_{gi} = \text{const} (1 - \alpha)^k \quad (13)
\]

We suppose that turbulent viscosity \( \mu_t \) is subdivided into two components \( \mu_t = \mu_1 + \mu_2 \), one \( \mu_1 \) due to inherent liquid wall-generated turbulence independent of relative motion of gas phase and the other \( \mu_2 \) due to the additional turbulence caused by bubble agitation. For \( \mu_1 \) we employ algebraic relationships and (K-ε)-turbulent models. The additional turbulent viscosity \( \mu_2 \) is modeled using Sato [5] correlation with Van Driest type factor.

Mixture enthalpy is defined as

\[
h = (\alpha \rho_g h_g + (1 - \alpha) \rho_f h_f) / \rho = \chi h_g + (1 - \chi) h_f, \quad (14)
\]

where \( h_g \) - vapour enthalpy, \( h_f \) - a fluid enthalpy. Energy equation can be written in the following form

\[
\rho(\frac{\partial h}{\partial t} + \bar{U} \text{grad} h) = -\text{div} \bar{q} + \frac{\partial p}{\partial t}, \quad (15)
\]

\[
-\text{div}(\rho_f \bar{u}_{gi}(h_g - h_f)) + Q_v
\]

where \( Q_v \) - volumetric heat generation, \( \bar{q} \) - heat flux.

Mass transfer equation is formulated for concentration \( c \) as follows:

\[
\rho(\frac{\partial c}{\partial t} + \bar{U} \text{grad} c) = \Gamma_{gen} - \Gamma_{cond} - \text{div} \bar{q}_{m}, \quad (16)
\]

\[
-\text{div}(\rho_f \bar{u}_{gi})
\]

where \( \Gamma_{gen}, \Gamma_{cond} \) - functions of vapour generation and vapour condensation, \( \bar{q}_{m} \) - a mass flux. After calculating of vapour concentration void fraction can be found as

\[
\alpha = c \rho_f / (c \rho_f + (1 - c) \rho_g) \quad (17)
\]

Mass fluxes are implemented as the boundary conditions in the inlet and in the outlet of a channel. On the wall no-slip conditions for velocity components are employed. Non-zero value of normal velocity can be putted when vapour concentration is determined on the wall.

In case of a single-phase flow heat flux condition or wall temperature are employed as the wall boundary conditions for the energy equation (15). When the wall temperature \( T_w \) exceeds saturation temperature \( T_{sat} \) and subcooled boiling is observed then heat flux should be partitioned: one part is used for vapour generation, another is transfered by liquid phase. Following [6] the wall heat flux can be presented as follows

\[
q = q_f + q_q + q_e, \quad (18)
\]

where \( q_f \) is the heat flux transferring by turbulent liquid flow, \( q_q \) - the so called quenching heat flux, connected with detaching processes of bubbles, \( q_e \) - heat flux used for evaporation.

The heat flux \( q_f \) transferring by turbulent liquid flow can be obtained solving conjugate energy problem and calculating wall temperature \( T_w \). For some channels \( q_f \) can be estimated using known single-phase heat transfer coefficients. Quenching heat flux \( q_q \) is proportional to the fraction of the wall surface, influenced by the detaching bubbles, a bubble detachment frequency, wall temperature [6], [7]. The heat flux spent on the generation of vapour is proportional to the number of nuclear sites, to the bubble detachment frequency \( f \), the energy to form a single bubble.
Boundary condition for concentration transfer equation (16) can be defined as a wall vapour generation. In subcooled liquid flow vapour bubbles, which are at saturation temperature, transfer across interface stored energy and condense. Condensation source term $\Gamma_{\text{cond}}$ in equation (16) can be calculated as in [7].

Mathematical model and developed implicit numerical method have been realized in the range of FLUID2D code. The experimental data [8] have been used for examination of model and numerical method in various regimes of two-phase flow. The article [8] presents the results of simultaneous measurement of void fraction and coolant temperature in 19 points on the diameter of a smooth vertical heated tube inside diameter 10 mm. The study was conducted in subcooled boiling regime, using a micro-thermocouple and realizing method of the active acoustic sensing. Profile distributions of void fraction and temperature along diameter were obtained with different parameter values: pressure ($P$), inlet mass flux ($G$), heat flux ($q$), various levels of subcooling (inlet coolant temperature $T_{\text{inlet}}$).

Numerical results presented in fig.1-fig.6 have been obtained for parameters, close to nuclear reactors conditions, $P = 14\,\text{MPa}$, $T_{\text{inlet}} = 290^{\circ}\text{C}$, $G=900\,\text{kg/(m}^2\text{s)}$, $q= 0.5\,\text{MW/m}^2$, $R_t$ - tube radius. Code FLUID2D computes velocity, pressure, enthalpy, liquid temperature, vapour concentration and void fraction fields, thermohydraulic characteristics: friction, heat transfer coefficient and other values. Heat flux partitioning is shown in fig.1. Comparison of the local distributions of liquid temperature, void fraction shows a satisfactory agreement.

The discrepancy between the experimental and numerical results for liquid temperature in the center is $4-12^{\circ}\text{C}$, relative error forms $2-4\%$. However, the description of some characteristics (void fraction first of all) near the wall should be improved.

Calculations of mean values of mixture enthalpy, void fraction for $P = 10\,\text{MPa}$, $T_{\text{inlet}} = 275^{\circ}\text{C}$, $q= 0.35\,\text{MW/m}^2$ are presented in fig.4-fig.5.
Two-dimensional fields of relative enthalpy, void fraction (fig. 6) demonstrate physical process of the gradual heating of the coolant, boiling on the wall and void fraction transfer to the center of flow.

4 Numerical Results for 3-D Thermal Convection

Thermal convection is of great importance in various fields of science and technology. For example, thermal convection has a strong influence on the distribution of impurities during crystal growth from the melt, which significantly affects the quality of the crystals. Therefore, the important task is the task of precise calculating of heat convection processes.

Thermal convection Benchmark computations play an important role in testing numerical methods and codes. Benchmark problems[9], [10] is suggested as a mechanism of validation of physical and computational models, codes, and solutions [11]. Benchmark exercise deals with heat convection problem in a cubical air-filled enclosure. A sketch of the experiments is shown in Fig. 7, width of the cubic $L=0.1272\text{m}$, the inclination angle $\varphi$ is set to $0^\circ$, $45^\circ$, and $90^\circ$, the cube sidewall temperature varies linearly from cold face to hot face, $T_c=300\text{ K}$, $T_h=307\text{ K}$. Gas properties are evaluated at the mean temperature $T_m=303.5\text{ K}$, $Pr=0.71$, the pressure is equal to the pressure that gives the desired Rayleigh number.

Three-dimensional case of implicit numerical method is realized as FLUID3D code. As a test of the numerical method and the code benchmark computations have been performed.

Nondimensional criteria are defined in the following way: $Ra=GrPr$ - Rayleigh number, $Gr=g\beta_tL^3\Delta T/\eta^2$ - Grashoff number, $Pr=\eta/\chi$ - Prandtl number, $Nu=qL/(k\Delta T)$- Nusselt number, where $\eta$ (m$^2$/s) - kinematical viscosity, $k$ (W/(m·K)) - thermal conductivity, $\chi$(m$^2$/s) - thermal diffusivity, $\beta_t$ (1/K) - thermal expansion coefficient, $g$(m/s$^2$) - gravitational acceleration, $q$(W/m$^2$) - heat flux.

Fig. 7. Schematics of the cubical cavity benchmark.
Calculations have been conducted using uniform and non-uniform grids and different number of grid nodes: 40, 60, 100. Thermal convection have been analyzed for different parameters, such as Rayleigh number. Some results are presented in fig. 8-12.

Good agreement with experimental numbers $\text{Nu}_{\text{exp}}$ is obtained for the calculated average Nusselt numbers $\text{Nu}_{\text{cal}}$. So for $Ra = 10^7$, $\text{Nu}_{\text{exp}} = 12.98 \pm 0.16$, $\text{Nu}_{\text{cal}} = 13.13$. Local distributions of Nusselt numbers are shown in fig.10, fig.11.

Fig. 8. Flow patterns in the plane $z=0.5$, $\varphi = 90^\circ, Ra = 10^7$.

Fig. 9. Temperature contours in the plane $z=0.5$, $\varphi = 90^\circ, Ra = 10^7$.

Fig. 10. Distribution of the local Nusselt number on the cold wall, $\varphi = 90^\circ, Ra = 10^7$.

Fig. 11. Distribution of the local Nusselt number on the hot wall, $\varphi = 90^\circ, Ra = 10^7$.

Fig. 12. Temperature contours in the plane $z=0.5$, $\varphi = 45^\circ, Ra = 10^7$.
5 Conclusion
Capabilities of implicit stabilization method are demonstrated. Subcooled boiling is simulated using drift flux model. Performed calculations show the need to further development of the wall boiling physical model and numerical model near wall, lateral drift, empirical correlations of bubble diameter, turbulent bubble influence.

Acknowledgments. This work was supported in part by the Russian Foundation for Fundamental Studies under Grant № 09-01-97529, 09-02-97516.

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