WAHA Code
Numerical Method of WAHA Code

I. Tiselj, G. Černe, I. Parzer, A. Horvat

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Institute "Jožef Stefan", Ljubljana, Slovenia
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1 Introduction

Goal of the Workpackage 2 (WP2) of the WAHALoads project (ref. [1]) is development of the new computer code named WAHA specialised for the simulations of the two-phase flow water hammer phenomena. This documents describes the numerical scheme, which is planned to be used in the WAHA code. Work within the WP2 is currently divided into three main tasks:

1) development of the physical model for the WAHA code,
2) testing of different numerical schemes for fast transients in two-phase flow with separate "test codes",
3) development of the first version of the WAHA code.

The first task is being performed mainly by Universite catholique de Louvain (UCL) and CEA Grenoble, while the second and third tasks are mainly performed by Institute "Jožef Stefan" (IJS). A separate deliverable D60 (see description of work in [1]) is planned after the first year of the project for the first task, deliverable D63 [15] describing the current status of the code development is planned after the first year for the third task. The present document, i.e. deliverable D62 describes the numerical scheme, which is used in the first version of the WAHA code [15] and is planned to be used in the future versions of the WAHA code.

IJS experience with numerical schemes for two-phase flow modelling are based on simple and user-unfriendly test codes, which were developed for simulations of different two-phase flow transients in the past years [2,3]. These test programs are not useful for potential users of WAHA code, however, they are very suitable for testing of different numerical approaches. The main goal of the research in the first year of the WAHALoads project was accurate and efficient treatment of the stiff source terms, i.e. algebraic terms that describe the inter-phase exchange of mass, momentum and energy.

The numerical scheme described in this document is according to our knowledge and expertise the optimal scheme for the simulation of the fast transients in two-phase flow, however we will try to remain open for possible improvements of the scheme.

2 Numerical scheme

Previous IJS experience with numerical schemes for two-phase flows are summarised in references [2] and [3]. The test programs from [2] and [3] were developed for solving RELAP5 6-equation single-pressure two-fluid model [4]. In the first year of the project we tested also a 7-equation two-fluid model proposed by Saurel and Abgrall [5]. Saurel and Abgrall proposed a two-pressure instead of a single-pressure two-fluid model. Because of the different phasic pressures their model contains 7 partial differential equations. Some tests were performed also with the simplest two-phase flow model: 3-equation homogeneous-equilibrium model (HEM).

The same numerical scheme was applied for all two-phase flow models. It is based on the Godunov methods, i.e. high-resolution shock-capturing methods, which are widely used in aerodynamics. No matter whether we are talking about RELAP5 6-equation model, 7-equation...
model of Saurel and Abgrall or 3-equation HEM model, the system of equations can always be written in the following form:

\[
A \frac{\partial \tilde{\psi}}{\partial t} + B \frac{\partial \tilde{\psi}}{\partial x} = \tilde{S},
\]

where \( \tilde{\psi} \) represents the vector of independent variables (for example, in RELAP5 6-eq. model one can choose \( \tilde{\psi} = (p, \alpha, v_f, v_g, u_f, u_g) \)), \( A \) and \( B \) are system matrices and \( \tilde{S} \) is a vector with nondifferential terms in the equations. Dimension of the vectors \( \tilde{\psi} \) and \( \tilde{S} \) as well as matrices \( A \) and \( B \) is equal to the number of partial differential equations used, i.e: 6 - for 6-eq. model, 7 - for 7-eq. model. In order to use the numerical schemes described in this report, the system of equations (1) must be hyperbolic. This is not always the case for two-fluid models; however, the hyperbolicity can usually be ensured with appropriate form of the additional differential terms for virtual mass and/or interfacial pressure (6-eq. model of RELAP5 code is such example, see [2] for details). It should be noted that the Saurel-Abgrall's 7-eq. model and HEM 3-eq. model are unconditionally hyperbolic.

The proposed numerical scheme is a two-step scheme with operator splitting; i.e. convection and sources in Eq. (1) are treated separately:

\[
A \frac{\partial \tilde{\psi}}{\partial t} + B \frac{\partial \tilde{\psi}}{\partial x} = 0, \quad (2)
\]

\[
A \frac{d \tilde{\psi}}{dt} = \tilde{S}. \quad (3)
\]

Second-order accuracy can be achieved with Strang splitting [6]. One time step includes the following three substeps (superscripts \( n, n+1 \) denote time levels - *, ** denote intermediate time levels):

1) - integration of the sources - Eq. (3) - over half of the time step:

\[
\tilde{\psi}^*_{j} = \tilde{\psi}_{j}^{n} + \int_{i^n}^{i^{n+\Delta t/2}} A^{-1}(i \tilde{\psi}_{j}) \tilde{S}(\tilde{\psi}_{j}(t)) \, dt \quad (4)
\]

2) - convection - Eq. (2):

\[
\tilde{\psi}^{**}_{j} = \tilde{\psi}^{*}_{j} - \Delta t \left( (A^{-1}B)^* \frac{\partial \tilde{\psi}^{*}}{\partial x} \right)_{j} \quad (5)
\]

3) - integration of the sources - second half of the time step:

\[
\tilde{\psi}^{**}_{j} = \tilde{\psi}^{*}_{j} + \int_{i^{**}}^{i^{**+\Delta t/2}} A^{-1}(i \tilde{\psi}_{j}) \tilde{S}(\tilde{\psi}_{j}(t)) \, dt \quad (6)
\]

Each of the substeps is solved with the second-order accurate method described below.
2.1 Convection terms

Equation (2) multiplied by $A^{-1}$ from the left gives

$$\frac{\partial \tilde{\psi}}{\partial t} + C \frac{\partial \tilde{\psi}}{\partial x} = 0 .$$

(7)

$C = A^{-1} B$ is the Jacobian matrix, which can be diagonalised as

$$C = L \Lambda L^{-1}$$

(8)

where diagonal matrix $\Lambda$ is matrix of eigenvalues and $L$ is matrix of eigenvectors of the matrix $C$. The diagonalization (8) of the matrix $C$ is not always straightforward, as the eigenvalues and eigenvectors may contain very long algebraic expressions (for example eigenvalues of RELAP5 6-eq. model described in [2] contain very long and complicated expressions). Decomposition of the Jacobian matrix (8) in [2] has been performed with analytical approximations for moderate interphase relative velocities ($v_r < 20m/s$), and numerically for larger $v_r$. The test codes and the proposed numerical scheme work only for problems with real eigenvalues of the Jacobian matrix. The calculation is interrupted if complex eigenvalues are found and equations become non-hyperbolic. An advantage of the Saurel-Abgrall's 7-eq. two-fluid model [5] over the RELAP5 6-eq. model [2-4] is much simpler structure of eigenvalues and eigenvectors and uncoditionally hyperbolicity of the equations.

Characteristic variables are introduced as

$$\delta \xi = L^{-1} \delta \tilde{\psi} ,$$

(9)

where $\delta \xi$ represents an arbitrary variation: $\partial \xi/\partial t$ or $\partial \xi/\partial x$. The characteristic form of the Eq. (2)

$$\frac{\partial \xi}{\partial t} + \Lambda \frac{\partial \xi}{\partial x} = 0 .$$

(10)

presents a basis for the second-order accurate numerical schemes.

Problems of the pure second-order accurate discretization - Lax-Wendroff for example - are oscillations, which appear in the vicinity of the nonsmooth solutions. The problem is solved (Leveque, [6]) if a combination of the first and second-order accurate discretizations is used. Part of the second-order discretization is determined by the limiters, which "measure" the smoothness of the solutions. If the solutions are smooth, larger part of the second-order discretization is used, otherwise larger part of the first-order discretization is used. An improved characteristic upwind discretization of the Eq. (10) was used as a first-order discretization (Hirsch, [7]).
Combination of the first and second-order accurate discretizations of the Eq. (10) is [2,3]:

\[
\frac{\xi_j^{n+1} - \xi_j^n}{\Delta t} + (\Delta^{++})_{j-1/2}^{n} \frac{\xi_j^n - \xi_{j-1}^n}{\Delta x} + (\Delta^{--})_{j+1/2}^{n} \frac{\xi_{j+1}^n - \xi_j^n}{\Delta x} = 0 .
\] (11)

Elements of the diagonal matrices \(\Delta^{++}\), \(\Delta^{--}\) are calculated as:

\[
\lambda^{++}_k = \max(0, \lambda_k) + \frac{\phi_k \lambda_k}{2} \left( \frac{\lambda_k}{\Delta t} \Delta x \right), \quad k = 1, K ,
\]

\[
\lambda^{--}_k = \min(0, \lambda_k) - \frac{\phi_k \lambda_k}{2} \left( \frac{\lambda_k}{\Delta t} \Delta x \right), \quad k = 1, K .
\] (12) (13)

with \(K\) equal to the number of the partial differential equations, i.e. \(K=3\) (HEM), \(K=6\) (RELAP5 model), \(K=7\) (Saurel-Abgrall's model).

The flux limiter \(\phi_k\) is calculated using one of the following limiters [6]:

**MINMOD:** \(\phi_k = \max(0, \min(1, \theta_k)), \quad k = 1, K ,\)

**Van Leer:** \(\phi_k = (|\theta_k| + \theta_k) / (|\theta_k| + 1) ,\)

**Superbee:** \(\phi_k = \max(0, \min(2\theta_k,1), \min(\theta_k,2))\)

where \(\theta_k\) measures the ratio of the left and the right gradients in the grid point \(j + 1/2:\)

\[
\theta_{k,j+1/2} = \frac{\xi_{k,j+1} - \xi_{k,j}}{\xi_{k,j+1}^{m} - \xi_{k,j}^{m}}, \quad m = \left( \frac{\lambda_{k,j+1/2}}{\lambda_{k,j+1/2}} \right), \quad k = 1, K , \quad j = 1, N - 1 .
\] (15)

The steepest waves are obtained with Superbee limiter, while the most smeared waves (but still second-order accurate) are obtained with MINMOD limiter. Solutions obtained with Van Leer limiter lie between the solutions obtained with MINMOD and Superbee limiters (see LeVeque, [6] for details on limiters). First-order accurate characteristic upwind scheme is obtained if the values of the limiters (14) are set to zero.

If Eq. (11) is transformed back into the basic variables, we obtain a difference scheme that is used in the test codes for the convective part of the Eq. (1):

\[
\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} + C_{j-1/2}^{++} \frac{\psi_j^n - \psi_{j-1}^n}{\Delta x} + C_{j+1/2}^{--} \frac{\psi_{j+1}^n - \psi_j^n}{\Delta x} = 0 ,
\] (16)

with

\[
C_{j-1/2}^{++} = L_{j-1/2}^{2} A_{j-1/2}^{2} L_{j-1/2}^{i} , \quad C_{j+1/2}^{--} = L_{j+1/2}^{2} A_{j+1/2}^{2} L_{j+1/2}^{i} .
\] (17)
The stability domain for the integration of the convective terms is limited by the CFL (Courant-Friedrichs-Levy) condition:
\[ \Delta t \leq \Delta x / \max(\lambda_j), \ j = 1, K. \] (19)

A specific problem of the application of the second-order accurate schemes in two-phase flow is degeneration of the eigenvectors as relative interphase velocity approaches zero. Only five linearly independent eigenvectors exist in that case. The problem remains solvable, if a small artificial \( |v_r| = 10^{-9} \text{ m/s} \) is maintained [2].

### 2.2 Averaging of the Jacobian matrix \( C_{j+1/2} \) between the grid points

In the test codes a simple average of the non-conservative variables was used for the evaluation of the Jacobian matrix at the point \( j + 1/2 \):

\[ C_{j+1/2} = C[(\hat{\psi}_j + \hat{\psi}_{j+1})/2] \] (18)

A similar approach has been taken by Gallouet and Masella [8], who showed that this type of averaging had given surprisingly good results for Euler equations. They emphasized that the averaging (18) must be performed with primitive variables (pressures, velocities, densities). Another more complicated and possibly more accurate alternative proposed by Toumi and Kumbaro in [9] was not adopted in the present work. They attempted to evaluate the Roe approximate Riemann solver [10] for the six-equation Jacobian matrix \( C_{j+1/2} \) and proposed a complicated procedure for the evaluation of the Jacobian matrix between the grid points from the left and right states \( j \) and \( j + 1 \).

### 2.3 Choice of variables - components of vector \( \hat{\psi} \)

Section 2.3 gives a brief discussion on the choice of the basic variables, i.e. components of the vector \( \hat{\psi} \) in Eq. (1). Numerous tests were performed with 6-eq. model (described in [2]) with different basic variables and the most successful set of variables turned out to be \( \hat{\psi} = (p, \alpha, v_f, v_g, u_f, u_g) \). This set of variables is very close to the so-called primitive variables, where the phasic internal energies \( u_f, u_g \) should be replaced with phasic densities \( \rho_f, \rho_g \), however internal energies were retained due to the applied water property subroutines.

The preferred set of variables were conservative variables:
\[ \hat{\psi} = [(1 - \alpha) \rho_f, \alpha \rho_g, (1 - \alpha) \rho_f v_f, \alpha \rho_g v_g, (1 - \alpha) \rho_f w_f, \alpha \rho_g w_g] \] with specific total energies \( w = u + v^2 / 2 \). Conservative form of equations usually means also numerical conservation of mass, momentum and energy, however there are some specific problems with conservative formulation of multi-fluid two-phase flows:

1) The continuity and energy equations can be written in the conservative form, while the fluxes for the momentum equations do not exist due to the pressure gradient terms and virtual mass terms. The momentum equations thus cannot be written in the conservative (flux) form.
2) Oscillations appear in the vicinity of particular discontinuities, if complex systems of equations are solved with conservative variables (Tiselj, Petelin, [2]). Abgrall [11] explained such oscillations for the four-equation model (two continuity, one momentum and one energy equation). Oscillations do not depend on the numerical scheme accuracy and can be observed in the results of first and second-order schemes.

3) New water properties subroutines are required that calculate two-phase properties \( (p, \alpha, \rho_f, \rho_g) \) from the conservative variables \( ((1-\alpha)p_f, \alpha \rho_f, (1-\alpha)p_g, \alpha \rho_g u_g) \).

Equations of the Saurel-Abgrall's 7-eq. model were solved only with non-conservative - primitive variables: \( \psi = (\alpha, p_f, \rho_g, v_f, v_g, \rho_f, \rho_g) \), whereas 3-eq. HEM model equations were solved with conservative and with primitive variables. Only in the case of the 3-eq. HEM model the results of the conservative test code were better than results of the code with primitive variables (the arguments 1) and 2) against conservative variables do not hold for the 3-eq. HEM model).

According to the our experience, non-conservative variables present an acceptable approximation for fast transients while for the long transients, where conservation of mass and energy is very important, this might be a serious drawback. In the test calculations presented in [2] and [3] negligible fluctuations of the overall mass and energy have been observed despite the non-conservative scheme.

An advantage of the conservative variables, which is not completely clear yet, is simpler and more accurate treatment of the source terms due to the variable pipe cross-section. Mainly due to that reason, our WAHA code ([15] - D63) is currently still open for both types of variables.

2.4 Integration of the source terms

The form of the source term is very important for the behaviour of the equations. Sources for the inter-phase exchange of mass, momentum and energy in the system of equations for steam-water mixture are stiff, i.e. their characteristic time scale can be much lower that the time step from the CFL condition (19). Integration of the sources in Eqs. (4) and (6) is thus performed with the explicit second-order accurate Euler method, which allows variations of the time step:

\[
\begin{align*}
\psi_{m+1} &= \psi_m + A^{-1}(\psi^*) S(\psi^*) \Delta t_s / 2 \\
\psi^* &= \psi^m + A^{-1}(\psi^*) S(\psi^*) \Delta t_s
\end{align*}
\] (20)

The time step \( \Delta t_s \) for the integration of the source terms is not constant and is controlled by the relative change of the basic variables. The maximal relative change of the basic variables in one step of the integration is currently set to 0.001. Source terms describing inter-phase exchange are weak when the two-phase mixture is close to the thermal and mechanical equilibrium. In that case the time step for their integration \( \Delta t_s \) is equal to the convection time step \( \Delta t \). When the mixture is far from equilibrium, the source term integration time steps \( \Delta t_s \) can be a few orders of magnitude shorter than \( \Delta t \). As a consequence a few hundred sub-steps can be required to integrate the sources over a single convection time step \( \Delta t \). Numerical scheme described by Eqs. (4), (5), (6) produces a specific error, which appears as a result of the operator splitting.
scheme applied for the equations with stiff source terms. This type of error is described and discussed in the next section.

3 Accuracy of the operator splitting for stiff source terms

Operator splitting as shown in Eqs. (4)-(6) is a very simple and "easy-to-use" tool, however, it can also be a source of a specific non-accuracy, which is analysed in this section. It can be easily analysed with the test case, which simulates the Simpson's water hammer experiment [12], where liquid water flows from the large tank through the horizontal pipe. At time zero the valve, which is located 36 meters away from the tank, is instantaneously closed. A pressure wave is created. If the initial conditions are appropriate, the cavitation starts near the valve approximately at time 0.05 seconds, when the wave, reflected from the tank, hits the valve (see results of the simulation in [3]).

The results of Saurel-Abgrall's 7-eq. model [5] are compared with 3-eq. Homogeneous-Equilibrium model (HEM) and the single-pressure 6-eq. two-fluid model used in our previous works [2, 3]. Results of the 6-eq. and 7-eq. models are obtained with instantaneous relaxation of velocities, pressures (only for 7-eq.), and temperatures. In other words: infinitely fast heat, mass, and momentum transfer is assumed - inter-phase exchange sources are thus infinitely stiff. Of course, there is no infinitely stiff source terms in the real world, however such test presents a very useful limiting and demanding test of the numerical schemes.

Our assumption is that due to the instantaneous relaxation the results of 6-eq. and 7-eq. models should be equal to the 3-eq. HEM model.

The Figures 1-3 show the results of the Simpson's water-hammer transient calculated with the Saurel-Abgrall's 7-eq. two-fluid model [5], the 6-eq. two-fluid model (RELAP5, [2-4]) and the 3-eq. HEM model. Fig. 1 gives the vapor volume fraction in the point, where the cavitation occurs, i.e. near the valve and Fig. 2 gives the pressure in the same point. Figure 3 shows the total volume of vapor in the pipe during the transient, which is very similar in all three models. It should be stressed that all three calculations were done on 100 grid points with the same time step and with the same numerical scheme described in this report (i.e.: Van Leer limiters, Strang operator splitting, no wall-friction ...).

The conclusion of the Figs. 1-3 is that the spatial vapor profile in the pipe is more smeared for the 6-eq. model than for the 3-eq. model and is even more smeared in the 7-eq. model, despite the same amount of the numerical diffusion in all three models. This seems to be against assumption that the results of all models should be equal.

The 6-eq. and 7-eq. simulations were then repeated, but this time with decreased time step:

1) HEM-3-eq. model (on 100 cells with dt =0.9 CFL)
2) 6-eq. two-fluid model (on 100 cells with dt=0.9CFL/10 - **10 times shorter time step**)
3) 7-eq. two-fluid model (on 100 cells with dt=0.9CFL/20 - **20 times shorter time step**)

Results with the reduced time step are shown in Figs. 4 and 5. These results are very similar and show that the HEM model is really a limit of the 6-eq. and 7-eq. models. The differences seen in Figs. 1 and 2 stem from Strang operator splitting, which is not sufficiently accurate for simulations with infinitely fast inter-phase exchange of mass, momentum, and energy. Therefore, shorter time steps mean more accurate time integration - especially the operator...
splitting. The 7-Eq. model is more sensitive to that non-accuracy than the 6-Eqs. model because there is one more pair of variables to relax: pressures.

Later, search of the existing literature showed two papers that are dealing with the inaccuracy of the Strang operator splitting when stiff source terms are present [13, 14] from 1995 and 1996. Both works are from the area of particle-gas two-phase flow during the rocket fuel combustion. References [13] and [14] discuss the problem of solving the system of hyperbolic equations of the same form as Eq. (1), where some of the equations can be written as:

$$\frac{\partial \varphi}{\partial t} + C \frac{\partial \varphi}{\partial x} = \frac{\varphi - \varphi^*}{\varepsilon}$$

(21)

where superscript * denotes the equilibrium (thermal or mechanical) value of the parameter $\varphi$ and $\varepsilon$ denotes the characteristic time of relaxation. A relaxation time is a time period in which the relaxation quantity approaches to its equilibrium value. Numerical solution of the Eq. (21) obtained with operator splitting method converges toward the solution of the differential equation (21) as $\Delta x \to 0, \Delta t \to 0$ and when condition $\Delta t / \varepsilon \to 0$ (which is often not respected in two-fluid codes) is fulfilled. It is clear that the problems appear for small values of relaxation time $\varepsilon$.

Up to 4 non-equilibrium (relaxation variables) can be present in the two-phase water system, each of them has its own characteristic relaxation time:

1) Different phasic pressures: exact relaxation time unknown - known to be very short.
2) Vapor temperature not in saturation - relaxation times very short in most of the flow regimes.
3) Liquid temperature not in equilibrium - relaxation time not negligible.
4) Mechanical non-equilibrium: different phasic velocities - relaxation time not negligible.

The Saurel-Abgrall's 7-eq. model [5] can describe all four types of non-equilibrium, whereas the 6-eq. model. (RELAP5, [2-4]) model describes non-equilibrium no 2, 3, 4. The 5-eq. model is sufficient to describe non-equilibrium no. 3 and 4, whereas the simplest 3-eq. HEM model cannot describe any kind of non-equilibrium.

From the physical point of view more equations describe the system more accurately. However, as shown in Figs. 1-5, each type of non-equilibrium causes a numerical error, which behaves like numerical diffusion when the relaxation time is very short.

Because of the numerical non-accuracy of the operator splitting method, it is better to use two-fluid model with less equations for very short relaxation times (i.e. if all relaxation times are very short 3-eq. HEM model will be the optimal one). On the other side, relaxation times must be estimated from existing physical models for different types of non-equilibrium. First estimates show that extremely short relaxation times are seldom encountered.

Deficiency of the operator splitting method described in the section 3 of the present paper is seen as an additional numerical diffusion when extremely short relaxation times appear in the equations. With special transformation of the equations and with appropriate numerical schemes described in [13] and [14] this deficiency of the operator splitting method can be avoided. However, due to their complexity, the approaches from [13] and [14] will not be applied in the WAHA code.
Note: the results of Figs 1-5 are not grid independent (this does not change the conclusions above): In Figs. 6 it can be seen that the void fraction is very sensitive to the number of grid points. It is because the two-phase area appears only near the valve (if all vapor would be in a single bubble, this bubble would be 5 cm long - much less than a single cell length). At least 1000 grid points are required for grid independent results.
4 Conclusions

This document gives an overview of the numerical method, which is used in the current version of the WAHA code [15] and is planned to be used in the final version of the WAHA code. The described numerical scheme can be used with conservative, primitive, or with some other sets of basic variables. The final choice of the basic variables depends on the simulations of the smooth-area change flows that are currently tested.

Another undetermined choice is a number of the basic equations, which depends on the chosen physical model. The most likely choice is the 6-eq. two-fluid model, however, if the assumption of the thermal equilibrium of the vapor phase is adopted, the 5-eq. two-fluid model will be used.

Some minor details that are not clarified in the present version of the document (for example: treatment of very small vapor or liquid volume fractions) will be addressed in the next versions of the document.
Fig. 1: Comparison of the 3-eq.-HEM, 6-eq. and 7-eq. models: temporal development of the vapor volume fraction at the point where the cavitation starts.

Fig. 2: Comparison of the 3-eq.-HEM, 6-eq. and 7-eq. models: pressure history.
Fig. 3: Total volume of vapor created in the pipe predicted by the 3-eq., 6-eq. and 7-eq. models.

Fig. 4: Comparison of the 3-eq.-HEM, 6-eq. and 7-eq. models: temporal development of the vapor volume fraction in the point where the cavitation starts - the same grid but different time steps.
Fig. 5: Comparison of the 3-eq.-HEM, 6-eq. and 7-eq. models: pressure history.

Fig 6: Grid refinement study performed with the 3-eq.-HEM model.
5 References


