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ACCURACY OF THE OPERATOR SPLITTING TECHNIQUE FOR TWO-PHASE FLOW WITH STIFF SOURCE TERMS

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ABSTRACT

Code for analysis of the water hammer in thermal-hydraulic systems is being developed within the WAHALoads project founded by the European Commission [1]. Code will be specialized for the simulations of the two-phase water hammer phenomena with the two-fluid model of two-phase flow. The proposed numerical scheme is a two-step second-order accurate scheme with operator splitting; i.e. convection and sources are treated separately. Operator splitting technique is a very simple and "easy-to-use" tool, however, when the source terms are stiff, operator splitting method becomes a source of a specific non-accuracy, which behaves as a numerical diffusion. This type of error is analyzed in the present paper.

NOMENCLATURE

A,B	coefficient matrices	***Subscripts/Superscripts***	
C	Jacobian matrix	f	luid
L	transformation matrix	g	as
M	transformation matrix		
p	pressure	***Greek letters***	
S	source term	α	void fraction
t	time	ρ	density
u	specific internal energy	φ	conservative variables
v	velocity	ψ	rimitive variables
x	spatial coordinate	ξ	haracteristic variables
w	total energy	Λ	igenvalue matrix
		ϕ	imiter function
		θ	lope detector

INTRODUCTION

Appearance of water hammer in thermal-hydraulic systems was widely studied in the past. Nevertheless, the modeling of the water hammer transients, which include the two-phase flows phenomena, remains a challenge. One of the codes that are used today for simulations of two-phase water hammer phenomena is RELAP5 [4] (similar codes are CATHARE and TRAC), which was developed for simulations of the transients in the nuclear power plant systems. However, these codes are verified for certain spectra of transients, which do not include water-hammer transients. Some attempts to examine the RELAP5 and CATHARE behavior for one of the water hammer scenarios are described in [3] and [5]. Beside the deficiencies of the physical models, results of both codes suffer due to the obsolete first-order accurate numerical schemes.

As a consequence, one of major goals of ongoing WAHA Loads project (founded by the European Commission [1]) is development of a new computer code, which would be specialized for the simulations of the two-phase flow water hammer phenomena. The basic mathematical model is similar to the mathematical model of the computer codes RELAP and CATHARE, i.e. one-dimensional, 6-equation two-fluid model. These two-fluid models assume the same pressure for both phases and separate continuity, momentum and energy balances for vapor and liquid phase.

Beside the 6-equation two-fluid model of RELAP5 code, we tested also a 7-equation two-fluid model proposed by Saurel and Abgrall [6]. 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. Furthermore, we performed some tests also with the simplest two-phase flow model: 3-equation Homogeneous-Equilibrium Model (HEM).

In all cases mentioned above the equations of the two-fluid models and equations of the HEM model can be written in vector form as

$$\underline{A}\,\frac{\partial \vec{\psi}}{\partial t} + \underline{B}\,\frac{\partial \vec{\psi}}{\partial x} = \vec{S} \qquad (1)$$

where vector $\vec{\psi}$ stands for:

- $\vec{\psi} = (\alpha, p, v_f, v_g, \rho_f, \rho_g)$ for 6-eq. model taken from RELAP5of Saurel and Abgrall [6],
- $\vec{\psi} = (\alpha, p_f, p_g, v_f, v_g, \rho_f, \rho_g)$ for 7-eq. model of Saurel and Abgrall [6],
- $\vec{\psi} = (p, v, \rho)$ for 3-eq. HEM model.

Detailed form of the equations with all the differential terms that contribute to the matrices *A* and *B*, and with the non-differential source terms that contribute to the source term *S* can be found in [2] and [6].

In the present work the most important part of the source term vectors comes from the inter-phase friction and inter-phase exchange of mass and energy. We will not go into the details of the physical models for the inter-phase exchange, but it should be stressed that these models contribute a significant amount of uncertainty into the two-fluid models. Inter-phase exchange terms are actually based on empirical correlations, which depend on the regime of the two-phase flow. An overview of such a set of correlations is given in [2], while a detailed discussion is given in [4].

The numerical scheme applied in the test codes, described in this paper, is based on the Godunov methods, i.e. high-resolution shock-capturing methods. In order to use such numerical schemes the system equation (1) must be hyperbolic. This is not always the case for two-fluid models; for example, the hyperbolicity of the RELAP5 6-equation models must be ensured with appropriate form of the additional differential terms for virtual mass and/or interfacial pressure (see [2] for details on RELAP5 6-eq. model). Other two models, 7-equation model of Saurel and Abgrall and 3-equation HEM, are unconditionally hyperbolic.

NUMERICAL SCHEME

Further described numerical scheme was applied for all two-phase flow models. The proposed numerical scheme is a two-step scheme with operator splitting; i.e. convection and sources in Eq. (1) are treated separately:

$$\underline{A}\,\frac{\partial\vec{\psi}}{\partial t} + \underline{B}\,\frac{\partial\vec{\psi}}{\partial x} = 0 \ , \tag{2}$$

$$\underline{A}\,\frac{d\vec{\psi}}{dt} = \vec{S} \, . \tag{3}$$

Second-order accuracy can be achieved with Strang splitting [7]. One time step includes the following three substeps (superscripts n, $n+1$ denote time levels and *,** denote intermediate time levels):

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

$$\vec{\psi}_j^{\,*} = \vec{\psi}_j^{\,n} + \int_{t^n}^{t^n+0.5\Delta t} \underline{A}^{-1}\vec{S}\,dt \tag{4}$$

2.) convection - Eq. (2):

$$\vec{\psi}_j^{\,**} = \vec{\psi}_j^{\,*} - \Delta t \left((\underline{A}^{-1}\underline{B})^{*} \frac{\partial\vec{\psi}^{\,*}}{\partial x} \right)_j \tag{5}$$

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

$$\vec{\psi}_j^{\,n+1} = \vec{\psi}_j^{\,**} + \int_{t^{n*}}^{t^{**}+0.5\Delta t} \underline{A}^{-1}\vec{S}\,dt \tag{6}$$

Each of the substeps is solved with the second-order accurate methods described below.

Convection terms

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

$$\frac{\partial\vec{\psi}}{\partial t} + \underline{C}\frac{\partial\vec{\psi}}{\partial x} = 0 \ . \tag{7}$$

where $C = A^{-1}B$ is the Jacobian matrix. The matrix C can be diagonalised as

$$\underline{C} = \underline{L}\ \underline{\Lambda}\ \underline{L}^{-1} \tag{8}$$

where Λ is a diagonal matrix of eigenvalues and L is a 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 and complicated algebraic expressions (e.g. in [2]). An advantage of the Saurel-Abgrall's 7-eq. two-fluid model [6] over the RELAP5 6-eq. model [2-4] is much simpler structure of eigenvalues and eigenvectors, and unconditional hyperbolicity of the equations. For 6-equation RELAP5 model the decomposition of the Jacobian matrix (8) has been performed with analytical approximations for moderate interphase relative velocities ($v_r < 20 m/s$), 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.

Characteristic variables are introduced as

$$\delta\vec{\xi} = \underline{L}^{-1}\,\delta\vec{\psi} \ , \tag{9}$$

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

$$\frac{\partial \vec{\xi}}{\partial t} + \underline{\Lambda}\frac{\partial \vec{\xi}}{\partial x} = 0 \ . \tag{10}$$

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

Problems of the pure second-order accurate discretization (e.g. Lax-Wendroff) are oscillations, which appear in the vicinity of the nonsmooth solutions. The problem is solved (LeVeque, [7]), 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. In the developed code an improved characteristic upwind discretization of the Eq. (10) was used as a first-order discretization (Hirsch, [8]) and the Lax-Wendroff scheme as a second-order discretization.

Combination of the first and the second-order accurate discretizations of the Eq. (10) is

$$\frac{\vec{\xi}_j^{\,n+1} - \vec{\xi}_j^{\,n}}{\Delta t} + (\underline{\Lambda}^{++})_{j-1/2}^{n}\frac{\vec{\xi}_j^{\,n} - \vec{\xi}_{j-1}^{\,n}}{\Delta x} + (\underline{\Lambda}^{--})_{j+1/2}^{n}\frac{\vec{\xi}_{j+1}^{\,n} - \vec{\xi}_j^{\,n}}{\Delta x} = 0 \ . \tag{11}$$

Elements of the diagonal matrices $\underline{\Lambda}^{++}$, $\underline{\Lambda}^{--}$ are calculated as:

$$\lambda_k^{++} = \max(0,\lambda_k) + \frac{\phi_k\,\lambda_k}{2}\left(\lambda_k\frac{\Delta t}{\Delta x} - \frac{\lambda_k}{|\lambda_k|}\right), \quad k = 1,K \ , \tag{12}$$

$$\lambda_k^{--} = \min(0,\lambda_k) - \frac{\phi_k\,\lambda_k}{2}\left(\lambda_k\frac{\Delta t}{\Delta x} - \frac{\lambda_k}{|\lambda_k|}\right), \quad k = 1,K \ . \tag{13}$$

with K equal to the number of the partial differential equations, i.e. K = 3 (HEM), K = 6 (RELAP5 model) and K = 7 (Saurel-Abgrall's model). The flux limiter ϕ_k is calculated using one of the following limiters [7]:

$$\begin{aligned}
&\text{MINMOD:} && \phi_k = \max(0, m\text{in}(1,\theta_k)), \\
&\text{Van Leer:} && \phi_k = (|\theta_k| + \theta_k)/(|\theta_k| + 1) \ , \\
&\text{Superbee:} && \phi_k = \max(0, \min(2\theta_k, 1), \min(\theta_k, 2))
\end{aligned} \tag{14}$$

where θ_k measures the ratio of the left and the right gradients in the grid point j+1/2:

$$\theta_{k,j+1/2} = \frac{\xi_{k,j+1-m} - \xi_{k,j-m}}{\xi_{k,j+1} - \xi_{k,j}}, \ m = \frac{\lambda_{k,j+1/2}}{|\lambda_{k,j+1/2}|}, \ k = 1,K \ , \ j = 1,N-1. \tag{15}$$

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, which was used in the present paper, lie between the solutions obtained with MINMOD and Superbee limiters (see LeVeque, [7] for details on limiters).

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

$$\frac{\vec{\psi}_j^{\,n+1} - \vec{\psi}_j^{\,n}}{\Delta t} + \underline{C}_{j-1/2}^{++}\frac{\vec{\psi}_j^{\,n} - \vec{\psi}_{j-1}^{\,n}}{\Delta x} + \underline{C}_{j+1/2}^{--}\frac{\vec{\psi}_{j+1}^{\,n} - \vec{\psi}_j^{\,n}}{\Delta x} = 0 \ , \tag{16}$$

with

$$\underline{C}_{j-1/2}^{++} = \underline{L}_{j-1/2}\underline{\Lambda}_{j-1/2}^{++}\underline{L}_{j-1/2}^{-1}, \ \underline{C}_{j+1/2}^{--} = \underline{L}_{j+1/2}\underline{\Lambda}_{j+1/2}^{--}\underline{L}_{j+1/2}^{-1} \ . \tag{17}$$

The stability domain for the integration of the convective terms is limited by the CFL (Courant-Friedrichs-Levy) condition:

$$\Delta t \le \Delta x/\max(|\lambda_k|), \ j = 1,K \ . \tag{18}$$

A specific problem 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 relative velocity $|v_r| = 10^{-9}$m/s is maintained [2].

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:

$$\underline{C}_{j+1/2} = \underline{C}[(\vec{\psi}_j + \vec{\psi}_{j+1})/2] \tag{19}$$

A similar approach has been taken by Gallouet and Masella [9], who showed that this type of averaging had given surprisingly good results for Euler equations. They emphasized that the averaging (19) must be performed with primitive variables (pressures, velocities, and densities). Toumi and Kumbaro proposed in [10] another, more complicated and possibly more accurate alternative, which was not adopted in the present work. They attempted to evaluate the Roe approximate Riemann solver [11] 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, respectively.

The following paragraph gives a brief discussion on the choice of the basic variables, i.e. components of the vector ψ 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 $\psi = (p, \alpha, v_f, v_g, u_f, u_g)$. 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 ρ_f, ρ_g. However, internal energies were retained due to the applied water property subroutines. The preferred set of variables would be conservative variables:

$$\vec{\psi} = [(1-\alpha)\rho_f, \alpha\rho_g, (1-\alpha)\rho_f v_f, \alpha\rho_g v_g, (1-\alpha)\rho_f w_f, \alpha\rho_g w_g]. \quad (20)$$

Due to the specific problems of the conservative variables, which are described in [2] and [12], they were not applied in the present case. 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.

Integration of the source terms

The form of the source term is very important for the behavior 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 (18). 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:

$$\vec{\psi}^{*} = \vec{\psi}^{m} + (\underline{A}^{m})^{-1}\vec{S}^{m}\Delta t_S / 2 \quad (21)$$
$$\vec{\psi}^{m+1} = \vec{\psi}^{m} + (\underline{A}^{*})^{-1}\vec{S}^{*}\Delta t_S$$

The time step Δt_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 Δt_s is equal to the convection time step Δt. When the mixture is far from equilibrium, the source term integration time steps Δt_s can be a few orders of magnitude shorter that Δt. As a consequence a few hundred sub-steps can be required to integrate the sources over a single convection time step Δt. Numerical scheme described by Eqs. (4-6) 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.

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 analyzed in this section. It can be easily analyzed with the test case, which simulates the Simpson's water hammer experiment [13], where liquid water flows from the large tank through the horizontal pipe (Fig. 1). 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 (also see results of the simulation in [3]).

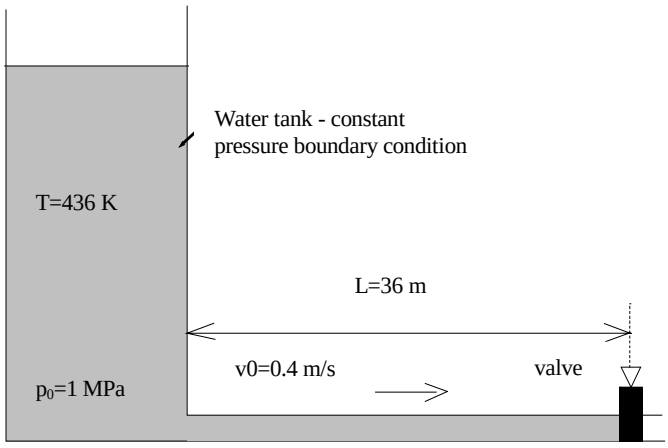

Figure 1: Scheme of the Simpson's water-hammer experiment with initial and boundary conditions. The transient is initiated by a rapid closure of the valve.

The results of the Saurel-Abgrall's 7-eq. model [5] are compared with 3-eq. 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. model) and temperatures. In other words, infinitely fast heat, mass, and momentum transfer was assumed - inter-phase exchange sources are thus infinitely stiff. For the Saurel-Abgrall's two-pressure 7-Eq. models infinitely fast relaxation of pressures is assumed too. We are aware that there are no infinitely stiff sources in the real world, however, such test presents a very useful limiting and demanding test for 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. The Figs. 2-4 show the results of the Simpson's water-hammer transient calculated with the Saurel-Abgrall's 7-eq. two-fluid model [6], the 6-eq. two-fluid model (RELAP5, [2-4]) and the 3-eq. HEM. Fig. 2 gives the vapor volume fraction in the point, where the cavitation occurs, i.e. near the valve and Fig. 3 gives the pressure in the same point. Figure 4 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, which is described in this report (i.e. Van Leer limiters, Strang operator splitting, no wall-friction).

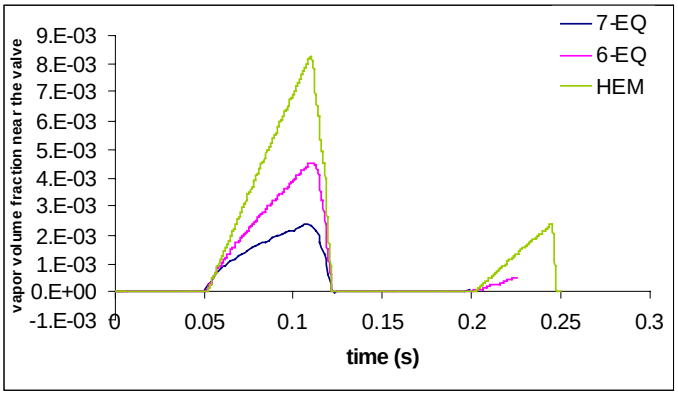

Figure 2: Comparison of the 3-eq.-HEM, 6-eq. and 7-eq. models: temporal development of the vapor volume fraction at the point where the cavitation starts - i.e. near the valve.

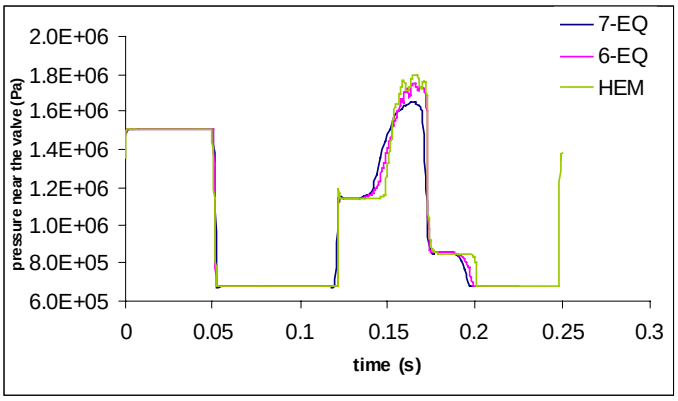

Figure 3: Comparison of the 3-eq. HEM, 6-eq. and 7-eq. models: pressure history near the valve.

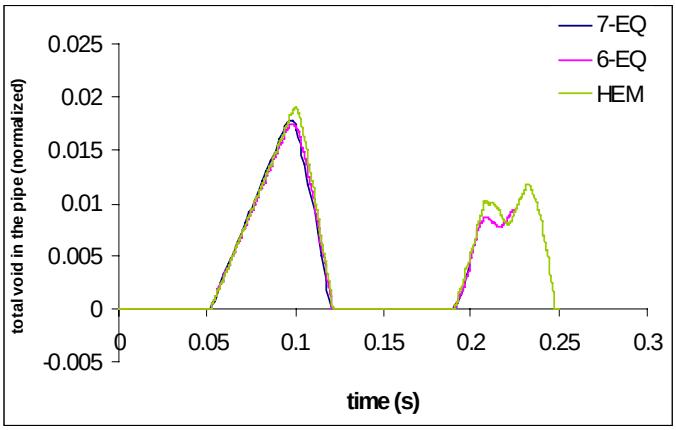

Figure 4: Total volume of vapor created in the pipe predicted by the 3-eq. HEM, 6-eq. and 7-eq. models.

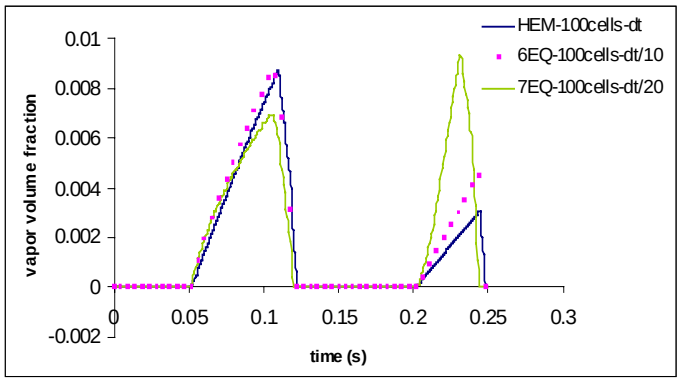

Figure 5: Comparison of the 3-eq. HEM, 6-eq. and 7-eq. models: temporal development of the vapor volume fraction in the point where the cavitation starts - the same grid but different time steps.

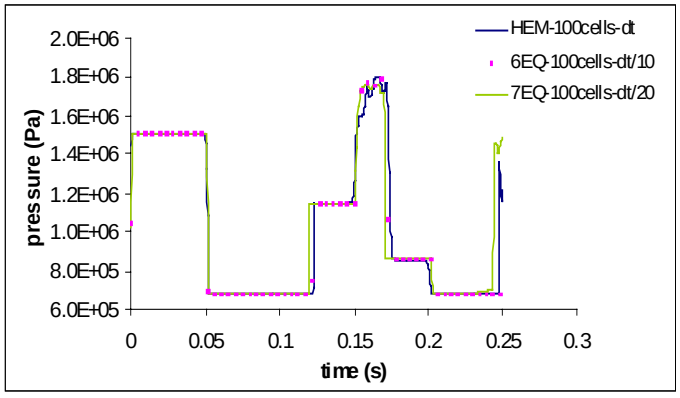

Figure 6: Comparison of the 3-eq. HEM, 6-eq. and 7-eq. models: pressure history near the valve.

The conclusion of the Figs. 2-4 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:

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

Results with the reduced time step are shown in Figs. 5 and 6. These results are very similar and show that the 3-eq. HEM is really a limit of the 6-eq. and 7-eq. models.

The differences seen in Figs. 2 and 3 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-eq. model because there is one more pair of variables to relax: pressures.

Search of the existing literature shows two papers that are dealing with the inaccuracy of the Strang operator splitting when stiff source terms are present [14, 15]. Both works are from the area of particle-gas two-phase flow during the rocket fuel combustion. References [14] and [15] 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:

$$\frac{\partial \varphi}{\partial t} + C\frac{\partial \varphi}{\partial x} = \frac{\varphi - \varphi^*}{\varepsilon} \qquad (22)$$

where superscript * denotes the equilibrium (thermal or mechanical) value of the parameter φ and ε 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. (22) 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 ε.

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 [6] 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 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. 2-6, 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. 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 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 [14] and [15] this deficiency of the operator splitting method can be avoided. However, due to their complexity, the approaches from [14] and [15] will not be applied in the code that is being developed within the WAHALoads project.

Note: The results in Figs 2-6 are not grid independent (this does not change the conclusions above): In Fig. 7 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 shorter than a single cell length). At least 1000 grid points are required for grid independent results.

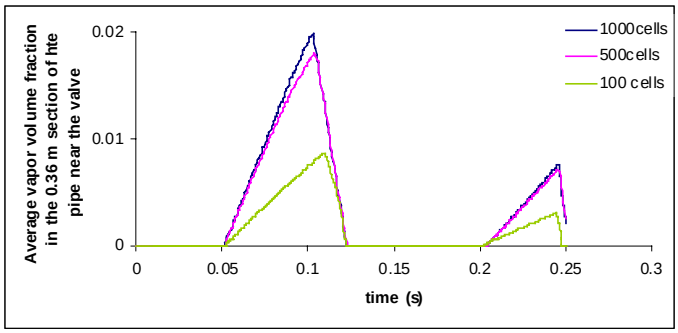

Figure 7: Grid refinement study performed with the 3-eq. HEM model: vapor volume fraction near the valve.

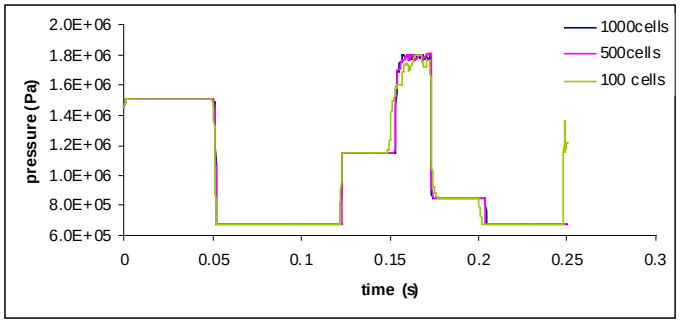

Figure 8: Grid refinement study performed with the 3-eq.-HEM model: pressure history near the valve.

CONCLUSIONS

This document paper gives an overview of the numerical method, which is used in the numerical code, which is being developed for the simulations of the two-phase water hammer transients. The proposed numerical scheme is a two-step scheme with operator splitting; i.e. convection and sources are treated separately with second-order accurate schemes. Operator splitting technique is successful for source terms of the moderate strength, while it becomes a source of a specific non-accuracy, when the relaxation times are decreased and the source terms become stiff. As shown in the present work, this non-accuracy of the operator splitting method is manifested as a numerical diffusion and can be partially avoided with shorter time step.

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