International Conference
Nuclear Energy for New Europe 2004
Portorož • Slovenia • September 6-9

port2004@ijs.si
www.drustvo-js.si/port2004
+386 1 588 5247, fax +386 1 561 2276
PORT2004, Nuclear Society of Slovenia, Jamova 39, SI-1000 Ljubljana, Slovenia

Development of Compressible Density-Based Steam Explosion Simulation Code ESE-2

Matjaž Leskovar
Jožef Stefan Institute
Jamova 39, SI-1000 Ljubljana, Slovenia
Matjaz.Leskovar@ijs.si

ABSTRACT

A steam explosion is a fuel coolant interaction process by which the energy of the corium is transferred to water in a time-scale smaller than the time-scale for system pressure relief and induces dynamic loading of surrounding structures. A strong enough steam explosion in a nuclear power plant could jeopardize the containment integrity and so lead to a direct release of radioactive material to the environment.

To help finding answers on open questions regarding steam explosion understanding and modelling, the steam explosion simulation code ESE-2 is being developed. In contrast to the developed simulation code ESE-1, where the multiphase flow equations are solved with pressure-based numerical methods (best suited for incompressible flow), in ESE-2 density-based numerical methods (best suited for compressible flow) are used. Therefore ESE-2 will enable an accurate treatment of the whole steam explosion process, which consists of the premixing, triggering, propagation and expansion phase.

In the paper the basic characteristics of the mathematical model and the numerical solution procedure in ESE-2 are described. The essence of the numerical treatment is that the convective terms in the multiphase flow equations are calculated with the AUSM+ scheme, which is very time efficient since no field-by-field wave decomposition is needed, using second order accurate discretization.

1 INTRODUCTION

Since the TMI-2 accident intensive research on severe accidents in nuclear power plants has been carried out to prevent and mitigate such accidents. One of the most important remaining issues in core melt progression during a severe accident are the likelihood and the consequences of a steam explosion, which may occur when the hot core melt comes into contact with the coolant water. A steam explosion is a fuel coolant interaction process by which the energy of the corium is transferred to water in a time-scale smaller than the time-scale for system pressure relief and induces dynamic loading of surrounding structures. A strong enough steam explosion in a nuclear power plant could jeopardize the containment integrity and so lead to a direct release of radioactive material to the environment.

Details of processes taking place prior and during a steam explosion have been experimentally studied for a number of years with adjunct efforts in modelling these processes to address the scaling of the experiments [1]. Despite great efforts in steam explosion research, confidence in prediction of reactor situations is not such that an unambiguous position can be taken whether the early failure of the containment due to a steam explosion is possible or not. There are still a number of unresolved issues - the

triggerability and the efficiency of reactor scale corium melt steam explosions are the most important ones.

To help finding answers on open questions regarding steam explosion understanding and modelling, the steam explosion simulation code ESE-2 is being developed. In contrast to the developed simulation code ESE-1 [2,3,4], where the multiphase flow equations are solved with pressure-based numerical methods (best suited for incompressible flow), in ESE-2 density-based numerical methods (best suited for compressible flow) are used. Therefore ESE-2 will enable an accurate treatment of the whole steam explosion process, which consists of the premixing, triggering, propagation and expansion phase.

2 MATHEMATICAL MODEL

A steam explosion is a complex coupled multi-component, multi-phase, multi-space-scale and multi-time-scale phenomenon. This has to be taken into account in the mathematical description of the steam explosion and the numerical solution procedure of the applied system of partial differential multiphase flow equations. ESE-2 is intended to be an accurate, robust and flexible steam explosion simulation code, where different steam explosion models and steam explosion treatments will be easily incorporated. Therefore the mathematical model and the numerical treatment are set up as systematically as possible, starting from the general 3-D multiphase model form

$$\frac{\partial \vec{U}}{\partial t}+\frac{\partial \vec{F}}{\partial x}+\frac{\partial \vec{G}}{\partial y}+\frac{\partial \vec{H}}{\partial z}=\vec{S}^{ns}+\vec{S}^{s}\ , \tag{1}$$

where $\vec{U}$ is the vector of conserved variables, $\vec{F}\,,\vec{G}\,,\vec{H}$ are the corresponding flux vectors, and $\vec{S}^{ns}\,,\vec{S}^{s}$ are the non-stiff and the stiff source terms, which are written separately due to their different numerical treatment.

Each phase p (the term “phase” is used in its widest meaning: it denotes the different components and the different phases of the same component) in the multiphase flow during a steam explosion is described using the averaged continuity

$$\frac{\partial\left(\alpha_p\rho_p\right)}{\partial t}+\frac{\partial\left(\alpha_p\rho_p v_{xp}\right)}{\partial x}+\frac{\partial\left(\alpha_p\rho_p v_{yp}\right)}{\partial y}=\Gamma_p\ , \tag{2}$$

momentum

$$\frac{\partial\left(\alpha_p\rho_p v_{xp}\right)}{\partial t}+\frac{\partial\left(\alpha_p\rho_p v_{xp}v_{xp}+\alpha_p p\right)}{\partial x}+\frac{\partial\left(\alpha_p\rho_p v_{xp}v_{yp}\right)}{\partial y}=p\frac{\partial\alpha_p}{\partial x}+\alpha_p M_{xp}+v_{ixp}\Gamma_p\ , \tag{3}$$

$$\frac{\partial\left(\alpha_p\rho_p v_{yp}\right)}{\partial t}+\frac{\partial\left(\alpha_p\rho_p v_{yp}v_{xp}\right)}{\partial x}+\frac{\partial\left(\alpha_p\rho_p v_{yp}v_{yp}+\alpha_p p\right)}{\partial y}=p\frac{\partial\alpha_p}{\partial y}+\alpha_p\rho_p g_y+\alpha_p M_{yp}+v_{iyp}\Gamma_p \tag{4}$$

and internal energy

$$\frac{\partial\left(\alpha_p\rho_p u_p\right)}{\partial t}+\frac{\partial\left(\alpha_p\rho_p u_p v_{xp}\right)}{\partial x}+\frac{\partial\left(\alpha_p\rho_p u_p v_{yp}\right)}{\partial y}=-p\left(\frac{\partial\alpha_p}{\partial t}+\frac{\partial\left(\alpha_p v_{xp}\right)}{\partial x}+\frac{\partial\left(\alpha_p v_{yp}\right)}{\partial y}\right)+\alpha_p E_p+h_{ip}\Gamma_p \tag{5}$$

equations, which are due to their extensiveness presented here only in their 2-D form. In these averaged multiphase equations (2) to (5) beside basic terms, which appear also in not averaged single phase equations (but without the volume fraction α), a number of additional terms appear during the averaging procedure, which have to be adequately modelled. For the sake of clarity all these terms were lumped together in the interphase mass, momentum and energy transfer variables Γ, M and E.

Transforming the 2-D transport equations (2) to (5) in the general multiphase model form (1) one obtains the following expressions for $\vec{U}$, $\vec{F}$, $\vec{G}$, $\vec{S}^{ns}$ and $\vec{S}^{s}$ for each phase

$$\vec{U}_p = \begin{pmatrix} \alpha_p\rho_p \\ \alpha_p\rho_p v_{xp} \\ \alpha_p\rho_p v_{yp} \\ \alpha_p\rho_p u_p \end{pmatrix}, \quad \vec{F}_p = \begin{pmatrix} \alpha_p\rho_p v_{xp} \\ \alpha_p\rho_p v_{xp}v_{xp} + \alpha_p p \\ \alpha_p\rho_p v_{yp}v_{xp} \\ \alpha_p\rho_p u_p v_{xp} \end{pmatrix}, \quad \vec{G}_p = \begin{pmatrix} \alpha_p\rho_p v_{yp} \\ \alpha_p\rho_p v_{xp}v_{yp} \\ \alpha_p\rho_p v_{yp}v_{yp} + \alpha_p p \\ \alpha_p\rho_p u_p v_{yp} \end{pmatrix},$$

$$\vec{S}_p^{ns} = \begin{pmatrix} 0 \\ p\dfrac{\partial\alpha_p}{\partial x} \\ p\dfrac{\partial\alpha_p}{\partial y} + \alpha_p\rho_p g_y \\ -p\left(\dfrac{\partial\alpha_p}{\partial t} + \dfrac{\partial(\alpha_p v_{xp})}{\partial x} + \dfrac{\partial(\alpha_p v_{yp})}{\partial y}\right) \end{pmatrix}, \quad \vec{S}_p^{s} = \begin{pmatrix} \Gamma_p \\ \alpha_p M_{xp} + v_{ixp}\Gamma_p \\ \alpha_p M_{yp} + v_{iyp}\Gamma_p \\ \alpha_p E_p + h_{ip}\Gamma_p \end{pmatrix}. \tag{6}$$

The relaxation source terms, which tend to establish mechanical and thermal equilibrium between the phases, are all located in the stiff source term part $\vec{S}^{s}$ since their characteristic times are much shorter than the characteristic times of other phenomena in multiphase flow - they are even shorter than the characteristic times of acoustic waves.

The choice of the number of dimensions and the number of phases in the mathematical model depends on the complexity of the steam explosion phenomena treated and the complexity of the steam explosion model used. A simple mathematical model of a steam explosion could be a 1-D 3-phase (liquid water, steam, fuel melt) description, whereas for a serious reactor application at least a 3-D 6-phase (liquid water, steam, continuous fuel melt, fuel melt drops, fine fuel fragments, non condensable gas) model is needed.

3 NUMERICAL TREATMENT

3.1 Solution Operator Splitting

The system of partial differential multiphase flow equations (2) to (5) transformed in form (1) is solved with the numerical finite volume method on a collocated grid. Due to its simplicity and straightforward implementation for different number of space dimensions the solution operator splitting method [5] is used in the numerical scheme of the ESE-2 code. In this approach multidimensional problems are solved with the use of fully discrete 1-D numerical methods, which are applied alternatively on 1-D problems in different space directions of the multidimensional geometry. In 2-D the solution operator splitting method has the form

$$\vec{U}^{n+1} = N^{\Delta t}\vec{U}^{n} = N_y^{\Delta t} N_x^{\Delta t}\vec{U}^{n}\ , \tag{7}$$

where $\vec{U}^{n+1}, \vec{U}^{n}$ are the solutions at the new $n+1$ and old n time steps, $N^{\Delta t}$ is the numerical solution operator for the time step of length Δt, and $N_x^{\Delta t}, N_y^{\Delta t}$ are the splitted numerical solution operators in the directions x and y. Due to the stiffness of some source terms and consequently the need of a smaller integration time step than for the convective terms to assure convergence, the solution operator splitting technique is used also for the source terms. The time integration of the system of transport equations (1) in 2-D is so performed on the following way

$$\begin{aligned}
\vec{U}_{j,l}^{\,n+1/4} &= \vec{U}_{j,l}^{\,n} - \frac{\Delta t}{\Delta x}\left[\vec{F}_{j+1/2,l}^{\,n} - \vec{F}_{j-1/2,l}^{\,n}\right], \\
\vec{U}_{j,l}^{\,n+2/4} &= \vec{U}_{j,l}^{\,n+1/4} - \frac{\Delta t}{\Delta y}\left[\vec{G}_{j,l+1/2}^{\,n+1/4} - \vec{G}_{j,l-1/2}^{\,n+1/4}\right], \\
\vec{U}_{j,l}^{\,n+3/4} &= \vec{U}_{j,l}^{\,n+2/4} + \left(\vec{S}^{ns}\right)_{j,l}^{n+2/4}\Delta t\,, \\
\vec{U}_{j,l}^{\,n+3/4+1/(4k)} &= \vec{U}_{j,l}^{\,n+3/4} + \left(\vec{S}^{s}\right)_{j,l}^{n+3/4}\left(\Delta t/k\right), \\
&\vdots \\
\vec{U}_{j,l}^{\,n+1} &= \vec{U}_{j,l}^{\,n+3/4+(k-1)/(4k)} + \left(\vec{S}^{s}\right)_{j,l}^{n+3/4+(k-1)/(4k)}\left(\Delta t/k\right),
\end{aligned} \tag{8}$$

where the subscripts j,l denote the mesh points, the superscripts $(n+...)$ the intermediate values of the solution and the variables, and $(\Delta t/k)$ is the length of the integration time step for the stiff source terms $\vec{S}^{s}$.

3.2 AUSM+ Scheme

The fluxes at the mesh cell interfaces $\vec{F}$ and $\vec{G}$ in equation (8) are determined by the AUSM+ (Advection Upwind Splitting Method) scheme [6], which was extended for the treatment of compressible multiphase models. The AUSM+ flux splitting scheme has the efficiency of flux-vector splitting methods and the accuracy of flux-difference splitting methods without the cost of field-by-field wave decomposition, and it is easy to generalize it to arbitrary equations of state. The essence of the AUSM+ scheme is that the convection and the acoustic waves, which are two physically distinct processes, are treated separately and in an adequate way. To be able to do that the fluxes in (6) have to be written as the sum of convective and pressure terms, what is here presented only for the flux in x direction

$$\vec{F}_p = \begin{pmatrix} \alpha_p\rho_p v_{xp} \\ \alpha_p\rho_p v_{xp}v_{xp} + \alpha_p p \\ \alpha_p\rho_p v_{yp}v_{xp} \\ \alpha_p\rho_p u_p v_{xp} \end{pmatrix} = v_{xp}\begin{pmatrix} \alpha_p\rho_p \\ \alpha_p\rho_p v_{xp} \\ \alpha_p\rho_p v_{yp} \\ \alpha_p\rho_p u_p \end{pmatrix} + \left(\alpha_p p\right)\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = v_{xp}\vec{U}_p + \left(\alpha_p p\right)\vec{I}_x\,. \tag{9}$$

The corresponding numerical flux at the mesh cell interface is

$$\left(\vec{F}_p\right)_{j+1/2,l}^{n} = \left(v_{xp}^{AUSM}\right)_{j+1/2,l}^{n}\left(\vec{U}_p\right)_{j+1/2,l}^{n} + \left(\left(\alpha_p p\right)^{AUSM}\right)_{j+1/2,l}^{n}\vec{I}_x\,. \tag{10}$$

The most important part of AUSM+ is the calculation of the velocity and pressure scalars for each phase, which are denoted in (10) with the superscript $AUSM$, what is done using the following polynomial functions

$$\begin{aligned}
&\mathcal{M}_1^{\pm} = \tfrac{1}{2}\left(M \pm |M|\right), \\
&\mathcal{M}_2^{\pm} = \begin{cases} \mathcal{M}_1^{\pm} & \text{if } |M| \geq 1 \\ \pm\tfrac{1}{4}\left(M \pm 1\right)^2 & \text{else} \end{cases}, \\
&\mathcal{M}^{\pm} = \begin{cases} \mathcal{M}_1^{\pm} & \text{if } |M| \geq 1 \\ \mathcal{M}_2^{\pm}\left(1 \mp 16B\mathcal{M}_2^{\mp}\right) & \text{else} \end{cases}, \\
&\mathcal{P}^{\pm} = \begin{cases} \mathcal{M}_1^{\pm}/M & \text{if } |M| \geq 1 \\ \pm\mathcal{M}_2^{\pm}\left(2 \mp M - 16AM\mathcal{M}_2^{\mp}\right) & \text{else} \end{cases}, \\
&A = 3/16, \quad B = 1/8.
\end{aligned} \tag{11}$$

The pressure scalar, which presents the pressure part of the splitted flux (10), is calculated as

$$\left(\left(\alpha_p p\right)^{AUSM}\right)_{j+1/2,l}^{n} = \mathcal{P}^{+}\left(\left(M_p^{L}\right)_{j+1/2,l}^{n}\right)\left(\alpha_p\right)_{j,l}^{n} p_{j,l}^{n} + \mathcal{P}^{-}\left(\left(M_p^{R}\right)_{j+1/2,l}^{n}\right)\left(\alpha_p\right)_{j+1,l}^{n} p_{j+1,l}^{n}, \tag{12}$$

where M^L and M^R are the Mach numbers at the left and the right side of the mesh cell interface based on the numerical speed of sound c

$$\left(c_p\right)_{j+1/2,l}^{n} = \sqrt{\left(c_p\right)_{j,l}^{n}\left(c_p\right)_{j+1,l}^{n}}, \quad \left(M_p^{L}\right)_{j+1/2,l}^{n} = \frac{\left(v_{xp}\right)_{j,l}^{n}}{\left(c_p\right)_{j+1/2,l}^{n}}, \quad \left(M_p^{R}\right)_{j+1/2,l}^{n} = \frac{\left(v_{xp}\right)_{j+1,l}^{n}}{\left(c_p\right)_{j+1/2,l}^{n}}. \tag{13}$$

The velocity scalar in the convective part of the splitted flux (10) is calculated as

$$\left(v_{xp}^{AUSM}\right)_{j+1/2,l}^{n} = \left(c_p\right)_{j+1/2,l}^{n}\left(M_p^{AUSM}\right)_{j+1/2,l}^{n}, \tag{14}$$

where the numerical Mach number at the interface, denoted with the superscript $AUSM$, is calculated as

$$\left(M_p^{AUSM}\right)_{j+1/2,l}^{n} = \mathcal{M}^{+}\left(\left(M_p^{L}\right)_{j+1/2,l}^{n}\right) + \mathcal{M}^{-}\left(\left(M_p^{R}\right)_{j+1/2,l}^{n}\right). \tag{15}$$

The convective part of the splitted flux (10) is calculated as

$$\begin{aligned}
&\left(v_{xp}^{AUSM}\right)_{j+1/2,l}^{n}\left(\vec{U}_p\right)_{j+1/2,l}^{n} = \\
&= \frac{1}{2}\left(v_{xp}^{AUSM}\right)_{j+1/2,l}^{n}\left(\left(\vec{U}_p^{L}\right)_{j+1/2,l}^{n} + \left(\vec{U}_p^{R}\right)_{j+1/2,l}^{n}\right) + \frac{1}{2}\left|\left(v_{xp}^{AUSM}\right)_{j+1/2,l}^{n}\right|\left(\left(\vec{U}_p^{L}\right)_{j+1/2,l}^{n} - \left(\vec{U}_p^{R}\right)_{j+1/2,l}^{n}\right),
\end{aligned} \tag{16}$$

where the vectors of conserved variables at both sides of the mesh cell interface $\vec{U}^L$ and $\vec{U}^R$ are calculated with second order accurate flux-limiter extrapolation, here shown only for $\vec{U}^L$

$$\left(\vec{U}_p^{\,L}\right)_{j+1/2,l}^{n} = \left(\vec{U}_p\right)_{j,l}^{n} + \frac{1}{2}\phi\left(\left(\theta^L\right)_{j+1/2,l}^{n}\right)\left(\left(\vec{U}_p\right)_{j,l}^{n} - \left(\vec{U}_p\right)_{j-1,l}^{n}\right),$$
$$\left(\theta^L\right)_{j+1/2,l}^{n} = \frac{\left(\vec{U}_p\right)_{j,l}^{n} - \left(\vec{U}_p\right)_{j-1,l}^{n}}{\left(\vec{U}_p\right)_{j+1,l}^{n} - \left(\vec{U}_p\right)_{j,l}^{n}}, \quad \phi(\theta) = \max(0, \min(1, \theta)). \tag{17}$$

To be able to treat also low Mach number flow, what is especially important for the modelling of the steam explosion premixing phase, the pressure and the velocity field have to be coupled at low speeds, since at low Mach numbers the AUSM+ scheme behaves more like a central difference discretization, which raises the possibility of odd-even mesh points decoupling. Therefore a pressure diffusion term has to be added in the convective part of the splitted flux (10) to ensure sufficient dissipation when the Mach number tends to zero [7].

3.3 Conservative and Primitive Variables

To assure conservation of mass, momentum and energy, the multiphase flow equations (2)-(5) are solved in their conservative form with conservative variables $\vec{U}$. From a physical point of view conservative variables are not convenient to work with, since initial and boundary conditions and above all the multiphase flow models are mostly specified in terms of primitive variables $\vec{V}$. Furthermore, from a numerical point of view, and especially in the AUSM+ scheme, primitive variables play a major role in the splitting and discretization of the fluxes. Therefore the values of primitive variables have to be known. For a 2-D 3-phase model as a simple example the conservative and primitive variables are

$$\vec{U} = \begin{pmatrix} (1-\alpha_2-\alpha_3)\rho_1 \\ \alpha_2\rho_2 \\ \alpha_3\rho_3 \\ (1-\alpha_2-\alpha_3)\rho_1 v_{x1} \\ \alpha_2\rho_2 v_{x2} \\ \alpha_3\rho_3 v_{x3} \\ (1-\alpha_2-\alpha_3)\rho_1 v_{y1} \\ \alpha_2\rho_2 v_{y2} \\ \alpha_3\rho_3 v_{y3} \\ (1-\alpha_2-\alpha_3)\rho_1 u_1 \\ \alpha_2\rho_2 u_2 \\ \alpha_3\rho_3 u_3 \end{pmatrix} = \begin{pmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \\ U_5 \\ U_6 \\ U_7 \\ U_8 \\ U_9 \\ U_{10} \\ U_{11} \\ U_{12} \end{pmatrix}, \quad \vec{V} = \begin{pmatrix} \alpha_2 \\ \alpha_3 \\ p \\ v_{x1} \\ v_{x2} \\ v_{x3} \\ v_{y1} \\ v_{y2} \\ v_{y3} \\ T_1 \\ T_2 \\ T_3 \end{pmatrix} = \begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \\ V_5 \\ V_6 \\ V_7 \\ V_8 \\ V_9 \\ V_{10} \\ V_{11} \\ V_{12} \end{pmatrix}. \tag{18}$$

Some of the primitive variables $\vec{V}$ and the specific internal energy u_p can be determined from the conservative variables $\vec{U}$ directly

$$v_{x1} = V_4 = \frac{(1-\alpha_2-\alpha_3)\rho_1 v_{x1}}{(1-\alpha_2-\alpha_3)\rho_1} = \frac{U_4}{U_1}, \; v_{x2} = V_5 = \frac{\alpha_2\rho_2 v_{x2}}{\alpha_2\rho_2} = \frac{U_5}{U_2}, \; v_{x3} = V_6 = \frac{\alpha_3\rho_3 v_{x3}}{\alpha_3\rho_3} = \frac{U_6}{U_3}, \tag{19}$$

$$v_{y1} = V_7 = \frac{(1-\alpha_2-\alpha_3)\rho_1 v_{y1}}{(1-\alpha_2-\alpha_3)\rho_1} = \frac{U_7}{U_1}, v_{y2} = V_8 = \frac{\alpha_2\rho_2 v_{y2}}{\alpha_2\rho_2} = \frac{U_8}{U_2}, v_{y3} = V_9 = \frac{\alpha_3\rho_3 v_{y3}}{\alpha_3\rho_3} = \frac{U_9}{U_3},$$
$$u_1 = \frac{(1-\alpha_2-\alpha_3)\rho_1 u_1}{(1-\alpha_2-\alpha_3)\rho_1} = \frac{U_{10}}{U_1}, u_2 = \frac{\alpha_2\rho_2 u_2}{\alpha_2\rho_2} = \frac{U_{11}}{U_2}, u_3 = \frac{\alpha_3\rho_3 u_3}{\alpha_3\rho_3} = \frac{U_{12}}{U_3}.$$

The remaining primitive variables $\vec{V}^{rem}$ are calculated numerically from the known variables $\vec{U}^{rem}$ with the Newton-Raphson method for nonlinear systems of equations [8]

$$\vec{V}^{rem} = \begin{pmatrix} \alpha_2 \\ \alpha_3 \\ p \\ T_1 \\ T_2 \\ T_3 \end{pmatrix} = \begin{pmatrix} V_1^{rem} \\ V_2^{rem} \\ V_3^{rem} \\ V_4^{rem} \\ V_5^{rem} \\ V_6^{rem} \end{pmatrix}, \quad \vec{U}^{rem} = \begin{pmatrix} (1-\alpha_2-\alpha_3)\rho_1 \\ \alpha_2\rho_2 \\ \alpha_3\rho_3 \\ u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} U_1^{rem} \\ U_2^{rem} \\ U_3^{rem} \\ U_4^{rem} \\ U_5^{rem} \\ U_6^{rem} \end{pmatrix},$$
$$\vec{F}^{NR}\left(\vec{V}^{rem}\right) = \vec{U}^{rem}\left(\vec{V}^{rem}\right) - \vec{U}_0^{rem}, \quad \underline{J}^{NR}\left(\vec{V}^{rem}\right) = \frac{\partial \vec{F}^{NR}\left(\vec{V}^{rem}\right)}{\partial \vec{V}^{rem}},$$
$$\vec{F}^{NR}\left(\vec{V}^{rem} + \delta\vec{V}^{rem}\right) = \vec{F}^{NR}\left(\vec{V}^{rem}\right) + \underline{J}^{NR}\left(\vec{V}^{rem}\right)\delta\vec{V}^{rem} + O\left(\delta\vec{V}^{rem\,2}\right) = 0 \Rightarrow$$
$$\Rightarrow \underline{J}^{NR}\left(\vec{V}^{rem}\right)\delta\vec{V}^{rem} = -\vec{F}^{NR}\left(\vec{V}^{rem}\right), \tag{20}$$

where the calculated corrections $\delta\vec{V}^{rem}$ move the initial guess for the remaining primitive variables $\vec{V}_{new}^{rem} = \vec{V}_{old}^{rem} + \delta\vec{V}^{rem}$ iteratively to the solution of $\vec{U}^{rem}\left(\vec{V}^{rem}\right) = \vec{U}_0^{rem}$, where $\vec{U}_0^{rem}$ are the values of the known variables. The Newton-Raphson Jacobian matrix in (20) has the form

$$\underline{J}^{NR}\left(\vec{V}^{rem}\right) = \begin{vmatrix} -\rho_1 & -\rho_1 & (1-\alpha_2-\alpha_3)\frac{\partial\rho_1}{\partial p} & (1-\alpha_2-\alpha_3)\frac{\partial\rho_1}{\partial T_1} & 0 & 0 \\ \rho_2 & 0 & \alpha_2\frac{\partial\rho_2}{\partial p} & 0 & \alpha_2\frac{\partial\rho_2}{\partial T_2} & 0 \\ 0 & \rho_3 & \alpha_3\frac{\partial\rho_3}{\partial p} & 0 & 0 & \alpha_3\frac{\partial\rho_3}{\partial T_3} \\ 0 & 0 & \frac{\partial u_1}{\partial p} & \frac{\partial u_1}{\partial T_1} & 0 & 0 \\ 0 & 0 & \frac{\partial u_2}{\partial p} & 0 & \frac{\partial u_2}{\partial T_2} & 0 \\ 0 & 0 & \frac{\partial u_3}{\partial p} & 0 & 0 & \frac{\partial u_3}{\partial T_3} \end{vmatrix}. \tag{21}$$

4 CONCLUSIONS

The compressible density-based steam explosion simulation code ESE-2 for modelling the whole steam explosion process is being developed. It is intended to be an accurate, robust and flexible steam explosion simulation code, where different steam explosion models and steam explosion treatments will be easily incorporated. Therefore in the development of ESE-2 special attention is given to the systematic and consistent mathematical formulation, the use

of advanced accurate and time efficient numerical methods, and a clear structured coding. A quality foundation is the prerequisite for the development of a quality code with comprehensive steam explosion modelling capabilities, what is needed if we want to better understand steam explosions and simulate them more reliably.

In the paper the basic characteristics of the mathematical model and the numerical solution procedure in ESE-2 are described. The essence of the numerical treatment is that the convective terms in the multiphase flow equations are calculated with the AUSM+ scheme, which is very time efficient since no field-by-field wave decomposition is needed. The convective fluxes are calculated with second order accuracy to suppress the problematic numerical diffusion of the commonly used first order accurate discretization. Since therefore the simulation results will not be influenced so much by the extensive unphysical numerical diffusion, it will be easier to reliably estimate the appropriateness of applied steam explosion models by the comparison of simulation results to experimental measurements.

The coding of the mathematical framework and the numerical solution procedure is only the first step in the ESE-2 development. In the next step we will start gradually adding different state of the art steam explosion models in the code. After each development stage of ESE-2 we will systematically verify and validate it, starting with simple benchmark calculations and proceeding with simulations of more and more complex steam explosion experiments. Only then ESE-2 will be ready for the important and challenging task: the investigation of unresolved steam explosion issues.

ACKNOWLEDGMENTS

The author gratefully acknowledges the financial support of the Ministry of Education, Science and Sport of the Republic of Slovenia (research project number: J2-6565) and the European Commission (6.FP NoE SARNET, contract number: FI6O-CT-2004-509065).

REFERENCES

[1] G. Berthoud, “Vapor Explosions”, *Annu. Rev. Fluid Mech.,* **32**, 2000, pp. 573-611.

[2] M. Leskovar, J. Marn, B. Mavko, “The influence of the accuracy of numerical methods on steam explosion premixing phase simulation results”, *Journal of Mechanical Engineering,* **46**, 2000, pp. 607-621.

[3] M. Leskovar, B. Mavko, “An original combined multiphase model of the steam explosion premixing phase”, *Journal of Mechanical Engineering,* **48**, 2002, pp. 438-448.

[4] M. Leskovar, B. Mavko, “Simulation of the isothermal QUEOS steam explosion premixing experiment”, *Journal of Mechanical Engineering,* **48**, 2002, pp. 449-458.

[5] R. J. LeVeque, Numerical Methods for Conservation Laws, Birkhaeuser Verlag, Basel, 1992.

[6] M. S. Liou, “A Sequel to AUSM: AUSM+”, *Journal of Computational Physics,* **129**, 1996, pp. 364-382.

[7] H. Paillere, C. Corre, J. R. Garcia Cascales, “On the extension of the AUSM+ scheme to compressible two-fluid models”, *Computers & Fluids,* **32**, 2003, pp. 891-916.

[8] W. H. Press et al., Numerical Recipes in Fortran 90, Cambridge University Press, Cambridge, 1999.