9 Numerical Results and Applications

In this Chapter numerical results for various two-phase flow phenomena are presented which are governed by wave propagation phenomena. This includes the propagation of volumetric phase concentration (void waves), pressure waves, flow discontinuities and shock waves, fast depressurization processes, and related critical flow phenomena. All numerical results shown are obtained with the Advanced Two-Phase Flow Module (ATFM), as described in Chapter 8.

The examples presented fall into two different categories: (1) base-line test cases using simplified boundary conditions and constitutive modeling to provide insight into physical phenomena and to test the accuracy and robustness of the numerical method applied, and (2) engineering type applications using physically more realistic state and interfacial transport models. Where available the numerical results are compared with analytical solutions or with experimental data.

9.1 Phase separation and void waves

This is an isothermal transient test case to investigate gravity-induced phase separation and related counter-current flow conditions. It tests the ability of the methods to predict counter-current flow conditions as exist in many reactor safety-related transients. Initial conditions represent a vertical pipe of height \( h = 2.0 \) m filled with a homogeneous two-phase mixture with a void fraction of \( \alpha_g = 0.5 \). The specific challenge is the prediction of two steep void waves travelling simultaneously from the top and bottom ends into the pipe, which, when meeting at the middle section, results in the formation of a sharp interface (liquid level) after phase separation is complete. As schematically shown in Fig. 9.1, three different regions can be distinguished: single-phase gas and liquid conditions at the top and bottom part of the pipe, respectively, and a quasi-stationary two-phase flow region at the middle section.

9.1.1 Analytical model

In the undisturbed middle section of the pipe, quasi-steady-state flow conditions exist where the volumetric upward and downward fluxes of the two phases compensate each other. Neglecting the momentum flux terms and virtual mass forces, compared to the gravity and interfacial friction forces, the phasic momentum equations simplify to

\[
\alpha_g \frac{\partial p}{\partial y} = F_g^v - \alpha_g \rho_g g, \quad (9.1)
\]
With the simplified expression for the interfacial drag as specified for the ASTAR benchmark cases [2], the interfacial friction force becomes

\[ F_{v}^{g} = \frac{1}{8} C_{D} a^{\text{int}} \varrho_{m} (u_{g} - u_{l})^2, \]  

(9.3)

with the interfacial area per unit volume

\[ a^{\text{int}} = \frac{3 \alpha_{g} \alpha_{l}}{r_{p}}, \]  

(9.4)

and a unique “particle” radius \( r_{p} \). The sum and the difference of (9.1) and (9.2) result in the pressure gradient due to the buoyancy forces

\[ \frac{\partial p}{\partial y} = -\varrho_{m} g \quad \text{with} \quad \varrho_{m} = \alpha_{g} \varrho_{g} + \alpha_{l} \varrho_{l} \]  

(9.5)

and the “slip” velocity in the middle two-phase flow region as

\[ \Delta u = u_{g} - u_{l} = \sqrt{\frac{8 (\varrho_{l} - \varrho_{g}) r_{p} g}{3 C_{D} \varrho_{m}}}. \]  

(9.6)

Introducing the density values and the specified values for the “drag” coefficient \( C_{D} = 0.44 \) and particle radius \( r_{p} = 0.5 \times 10^{-3} \text{ m} \), the slip velocity becomes \( \Delta u = 0.24 \text{ m/s} \). Due to the compensating volumetric fluxes across the void wave,

\[ \bar{u} = \alpha_{g} u_{g} + \alpha_{l} u_{l} = 0 \]  

(9.7)
the propagation of the void waves can be predicted using the slip velocity as given by equation (9.6) as

\[
\begin{align*}
  u_1 &= u_g = \alpha_l \Delta u \\
  u_2 &= u_l = -\alpha_g \Delta u
\end{align*}
\]

For an initial void fraction of \( \alpha_g = 0.5 \), one obtains for the upward void front \( u_1 = 0.12 \) m/s, and for the downward void front \( u_2 = -0.12 \) m/s.

9.1.2 Numerical results

The prediction was performed for a water/air mixture in a closed pipe with the initial conditions of a constant void fraction of \( \alpha_{g0} = 0.5 \) and a pressure of \( p_0 = 1 \) bar. For the one-dimensional case a second-order Flux Vector Splitting scheme was used with 500 computational cells in the \( y \)-direction. Heat transfer between the phases as well as viscous and wall friction effects are neglected.

Calculated results for void fraction, gas and liquid velocities, and pressure distributions for various consecutive time values are shown in Fig. 9.2. As can be seen the numerical simulation largely confirms the analytical results including the positions and amplitudes of the two void waves and the (nearly) discontinuous changes of void fraction and phasic velocities across the wave fronts. The discontinuities in the pressure gradient coincides with the passage of the void waves marking the change of the gravity head between the two-phase regions and the and single-phase regions of pure liquid and pure gas. A new steady state is reached at \( t = 8.3 \) s when the two waves have merged at the middle of the pipe. The prediction does not show any anomaly or numerically induced instability during the transition from two-phase to pure single-phase gas or liquid conditions. The void wave itself is represented by two to three grid points.

During the initial phase of the transient some weak pressure wave propagation and reflection appeared in the prediction which are related to the somehow artificial (mechanical disequilibrium) initial conditions. However, these waves vanish when the nearly steady pressure gradient is reached depending on the density values in the gas, two-phase and liquid region. At the end of the transient, the pressure in the gas space has returned to the initial pressure value as expected.

The dependence of numerical results in case of a progressively increased number of grid points \( n \) is given in Fig. 9.3 for the void fraction distribution at a fixed time of \( t = 4 \) s. Figure 9.3 clearly indicates the continuous convergence toward the discontinuous analytical solution which is practically reached for \( n = 500 \). The position of the void wave remains unaffected by the change of the grid resolution.
Fig. 9.2: Phase separation in a vertical pipe due to gravity; void fraction, phasic velocities, and pressure distributions along pipe length at various time values.
This idealized test case, first proposed by Ransom and published in [1], has become a standard benchmark test case to evaluate numerical diffusion inherent in numerical solution schemes for two-phase flow. It consists in calculating a gravity driven oscillation of a water column in a U-tube manometer. The geometry of the U-tube and the initial conditions are shown in Fig. 9.4.

The initial conditions start with the maximum displacement of the water column in the left leg and with an assumed zero velocity. In the particular case that the wall friction is zero, (inviscid flow), the liquid mass oscillated indefinitely as a “rigid body” and for the whole process a simple algebraic solution exists. Any damping of the predicted oscillation can be attributed to numerical diffusion or viscosity of the finite difference or the finite volume scheme applied.
9.2.1 Analytical solution

Neglecting viscosity and wall friction effects, the oscillation frequency $\omega$ and the maximum velocity of the water column $u_{\text{max}}$ can be derived as follows:

$$\omega = \frac{1}{T} = \sqrt{\frac{g}{2\pi^2 l}}$$

and

$$u_{l_{\text{max}}} = \sqrt{\frac{2gh}{l}}.$$ (9.9)

Assuming initial conditions of zero liquid velocity everywhere and a maximum liquid level displacement $h$, the velocity at the bottom of the U-tube at time $t$ after the release is

$$u_l = u_{l_{\text{max}}} \sin \left( \frac{t}{\omega} \right).$$ (9.10)

9.2.2 Numerical results

The results shown in the following are obtained with the second-order Flux Vector Splitting technique with 200 computational cells assuming a strictly one-dimensional flow conditions.

The predicted velocity at the bottom of the U-tube (solid line) is compared with the analytical solution (dotted line) in Fig. 9.5. The practical absence of (numerical) damping indicates the low numerical viscosity of the numerical method used. The still existing small attenuation might be (at least) partially attributed to the existing differences in phasic velocities close to the moving interface and the related dissipative effects.

![Fig. 9.5: Liquid velocity at the bottom of the U-tube as a function of time; comparison of CFD calculation (solid line) with analytical solution (dotted line with circles)](image)

The predicted void fraction and pressure distribution along the U-tube for the first six oscillation cycles are given in Figs. 9.6 and 9.7. The figures show a high resolution of the moving liquid level where the discontinuities in void fraction and accompanied pressure gradient is represented by two to three grid points. The corresponding parameter profiles are maintained during various oscillation cycles, indicating a practical absence of numerical dispersion or viscosity effects. Since the liquid velocity is relatively low, the dynamic momentum contribution is negligible small and the pressure values shown in Fig. 9.7 are dominated by the gravity head determined by the actual liquid level elevation.

The successful prediction of the U-tube test case and the sedimentation case governed by counter-current two-phase flow conditions have been a milestone for the development of the hyperbolic two-fluid model as described in Chapter 5.
9.3 Pressure wave propagation phenomena

Weak pressure disturbances ($\Delta p \rightarrow 0$) in a compressible homogeneous media propagate with the speed of sound which is determined by the compressibility of the fluid and inherent inertia as given by the density. In the case of absence of viscosity and nonequilibrium effects, the sound speed is independent of the sound frequency. For the specific case of single-phase gas the sound velocity can be calculated by the isentropic relation

$$a_0 = \sqrt{\left(\frac{\partial p}{\partial \varrho}\right)_s}. \quad (9.11)$$

Assuming an ideal gas law, expression (9.11) simplifies to

$$a_0 = \sqrt{\kappa_g \varrho}, \quad \text{or equivalently} \quad a_0 = \sqrt{\kappa_g R_g T_g}, \quad (9.12)$$

with the gas constant $R_g$ and the isentropic exponent $\kappa_g$. With an increased strength of the shock wave the propagation velocity $u_{sw}$ exceeds the value of the sound velocity depending on the pressure rise $\Delta p = p_1 - p_0$

$$u_{sw} = a_1 \sqrt{1 + \frac{\kappa_g + 1}{2\kappa_g} \left(\frac{\Delta p}{p_0}\right)}, \quad (9.13)$$
For two-phase flow conditions, analytical descriptions for wave propagation phenomena with finite wave strengths do not exist, apart from the cases where extreme simplified assumptions such as homogeneous equilibrium or complete “frozen” conditions (where the algebraic mass, momentum, and energy transfer terms are set to zero) are applied.

In the following, the propagation of one-dimensional (plane) pressure waves in two-phase media are studied numerically assuming the absence of wall friction and wall heat transfer. The initial and boundary conditions are shown schematically in Fig. 9.8. At the left side of the pipe a sudden pressure increase is imposed. The calculations are terminated before the waves have reached for the far right end of the 4 m long pipe.

Before dealing with the more complex two-phase flow conditions, a few results are included here, mainly to demonstrate the capability of the Flux Vector Splitting (FVS) scheme, a numerical method that will be also used for the following two-phase cases. Predicted values for the shock wave propagation in a gas medium assuming ideal state equations are shown in Fig. 9.9 in comparison with the existing analytical solution. The calculation is performed with 1600 computational cells which corresponds to a grid spacing of \( \Delta x = 2.5 \) mm. The case selected represents a rather moderate shock strength with a shock velocity of \( u_{sw} = 473.05 \) m/s, which corresponds to a Mach number of \( M = 1.36 \) based on the sound velocity in the undisturbed region in front of the wave.

The figure indicates a high resolution of the flow discontinuities and a perfect prediction of shock velocity. Within the shown scale, there is practically no difference between the CFD calculation and the analytical solution. The calculated results are also free of any numerically induced instability and, within the predicted time frame, there is no evidence of dispersive effects. All calculated parameters across the wave including, pressure, velocity, temperature, and entropy are in good agreement with the analytical values as can be seen from Fig. 9.10. The correct prediction of temperature and entropy could be achieved only when using the full energy conservation equation.

Of particular interest with regard to the numerical feature of the FVS scheme is how the selection of the grid spacing affects the numerical results compared with the analytical solution. This is demonstrated in Fig. 9.11 showing the effect of a progressive refinement of the grid from cell sizes of 8 mm to 1 mm. The figure indicates a clear convergence of the predictions toward the discontinuous analytical solution which might be fully reached for \( \Delta x \to 0 \).
9.3 Pressure wave propagation phenomena

Fig. 9.9: Shock wave propagation in single-phase gas, second-order Flux Vector Splitting scheme with 800 cells $\Delta x = 2$ mm; comparison of CFD calculation (straight line) and analytical solution (dotted line)

9.3.2 Two-phase flow

For a two-phase test case, the pipe is assumed to be filled with a water/air mixture at equilibrium conditions with a temperature of 300 K and a void fraction of $\alpha_g = 0.05$. It is further assumed that the gas is homogeneously distributed in the form of equally sized bubbles having a bubble diameter of 4 mm. As for the previously described gas case, the shock wave is initiated by a sudden pressure rise from $p_0 = 1$ bar to $p_1 = 2$ bar. The calculations are performed with the same numerical methods as the previous case using the second-order FVS scheme. For the whole length of the pipe, 2000 computational cells are used which corresponds to a cells sizes of $\Delta x = 2$ mm. The calculated pressure wave propagation at five consecutive time values is shown in Fig. 9.12.
Fig. 9.10: Shock wave propagation in a single-phase gas, second-order FVS scheme with 800 cells ($\Delta x = 2\text{ mm}$); comparison of CFD calculation (straight line) and analytical solution (dotted line).

Fig. 9.11: Numerical simulation of a shock wave in single-phase gas media; convergence of solution in the case of grid refinement.

The figure includes the results of three calculations which differ only in the specification of the algebraic source terms describing the momentum and heat coupling between the phases:

(a) this base calculation uses a standard modeling of the momentum and energy coupling resulting in finite values for the interfacial forces and interfacial heat transfer,
9.3 Pressure wave propagation phenomena

Fig. 9.12: Shock wave propagation in two-phase media, water/air at $p_1 = 1$ bar, $T_1 = 300$ K, $\alpha_g = 0.05$; second-order FluxVector Splitting scheme with 2000 cells

(b) here partial “frozen” conditions are applied where the heat transfer between the phases is neglected, the interfacial forces are modeled as in case (a),

(c) this prediction assumes complete “frozen” conditions where both the interfacial forces and the interfacial heat transfer are set to zero. However, the nonviscous interfacial forces described by exclusively differential terms are taken into account as in the calculations (a) and (b).

Although the same sudden pressure increase is applied to initialize the shock wave, there are remarkable differences between the results with regard to the predicted wave speed and pressure profile. For fully “frozen” conditions (a) the pressure wave propagates with a constant supersonic velocity ($u_{sw} > a_0$) into the undisturbed region of the pipe, and at the same time,
the initial discontinuous pressure change is (apart from very small numerical diffusion effects) maintained.

Specifying finite values for the interfacial heat transfer and interfacial friction as in the case (a) results in a further reduction of the wave speed and, due to the inherent physical dissipation, in a transfer of the initial pressure jump into a continuous pressure profile.

A more detailed picture of the wave structure is given in Fig. 9.13 showing the governing state and flow parameters across the wave at the time $t = 30$ ms. Two different regions can be distinguished:

(1) a wave front with rather steep (but finite) parameter gradients accompanied with strong excursions for the gas velocity and temperature and resulting strong deviations from thermal and mechanical equilibrium between the phases. Within this region the effect of the algebraic source terms is practically negligible ("frozen") and the continuous change of parameters is determined by the differential coupling terms between the phasic momentum and energy equations.

(2) a relaxation zone behind the shock front with a continuous change of the flow parameters toward a new equilibrium between the phases. The width of this region is governed by the finite values for the (algebraic) terms for the interfacial friction and heat transfer and the corresponding characteristic time values. As shown in Fig. 9.13, with the present modeling assumptions the thermal equilibrium is reached considerable faster as the mechanical equilibrium between the phases.

The variation of the pressure profile relative to the shock front is presented in Fig. 9.14 for different time values after initiation of the shock wave. The figure shows that already for $t \geq 10$ ms a nearly constant wave profile is reached where dissipative effects and dynamic forces are balanced resulting in a wave structure which remains practically constant during the subsequent propagation process.

To what extent the predictions might be affected by the computational grid is illustrated in Fig. 9.15 showing the results obtained for a progressively reduced grid spacing. As indicated in Fig. 9.15, there exists a clear convergence of solution toward the continuous pressure profile which is practically reached for a grid size of $\Delta x \leq 1$ mm.

The effect of the wave strength is illustrated in Figs. 9.16 and 9.17 showing the pressure and velocity profiles at $t = 30$ ms after initiation of the shock wave. Apart from the initiating pressure $p_1$ all other initial and boundary conditions are the same as those applied before. As for single-phase gas flow, the growing shock strength results in an increase of the wave velocity accompanied with a steepening of pressure and velocity at the shock front. The figures also indicate that the homogeneous equilibrium model, indicated by the dotted line, provides a good approximation for the wave speed and the new equilibrium state downstream of the shock wave.
9.3 Pressure wave propagation phenomena

Fig. 9.13: Shock wave in two-phase media, water/air, $\alpha_g = 0.05$, parameter profiles at time $t \geq 10$ ms, second-order FVS scheme with 2000 cells, $\Delta x = 2$ mm

Fig. 9.14: Numerical simulation of a shock wave in two-phase water/air media, $\alpha_g = 0.05$, evolution of pressure profile during wave propagation, time: $0$ ms $\leq t \leq 50$ ms
Fig. 9.15: Numerical simulation of a shock wave in two-phase water/air media, $\alpha_g = 0.05$; convergence of solution in the case of grid refinement, second-order FVS scheme.

Fig. 9.16: Shock wave propagation in two-phase water/air media, $\alpha_g = 0.05$, pressure distributions at $t = 30$ ms, effect of shock strength; comparison of CFD calculation (straight line) with analytical solution for homogeneous equilibrium flow (dotted line).
9.4 Shock tube

Shock-tube devices have been extensively used to study shock wave propagation phenomena in compressible fluids like gases or gas–liquid two-phase mixtures. Usually a high (left) and a low (right) pressure region is separated by a diaphragm as schematically shown in Fig. 9.18. The transient is initiated by an instantaneous removal of the diaphragm resulting in a shock wave and rarefaction wave propagating toward the right and left ends of the pipe respectively. Assuming strictly one-dimensional flow conditions, the shock tube mathematically represents a “Riemann problem” where the initial flow velocities on both sides of the diaphragm have been set to zero.

9.4.1 Single-phase gas

For the single-phase gas case the geometry of the pipe and initial conditions are given in Fig. 9.18. For simplicity an ideal gas law is assumed with an isentropic exponent of \( \kappa = 1.4 \).

The numerical results for the shock tube problem are obtained with the ATFM code using a second-order Flux Vector Splitting scheme with 500 cells which corresponds to a grid size of 0.8 mm. Figures 9.19 and 9.20 show a comparison of the CFD results with the existing analytical solution including the pressure distribution along the pipe length at various time values (Fig. 9.19) and the parameter distribution for a fixed time of \( t = 8 \) ms (Fig. 9.20). The figures indicate a nearly perfect agreement of the CFD calculation with the analytical solution including a perfect match of the timing for wave propagation phenomena and high resolution of the shock wave and contact discontinuity.
Fig. 9.18: Shock tube problem, for single-phase gas; geometry and initial conditions

Fig. 9.19: Shock tube test problem for single-phase gas; density distribution at different time values, second-order Flux Vector Splitting scheme with 500 cells; comparison of CFD calculation (solid line) with analytical solution (dashed line)
Fig. 9.20: Shock tube test problem for single-phase gas: parameter distribution at $t = 0.8$ ms; comparison of CFD prediction (solid line) with exact solution (dashed line), dotted line: initial conditions.
9.4.2 Two-phase flow

Compared with the single-phase gas flow case, the shock tube problem becomes more complex for two-phase flow conditions. The reason for this is not only the increased number of governing flow parameters and related flow equations, but rather the presence of algebraic source terms controlling deviations between local phasic temperatures and flow velocities. As an example a two-component water/air mixture is chosen with a relatively high liquid content to exaggerate the difference to the pure gas case. Due to the large complexity, no algebraic solutions exist for the general two-phase shock tube problem. Nevertheless, for the specific condition of homogeneous equilibrium flow an iterative algebraic solution can be derived in a similar way as was described for the pure gas case in Chapter 4. The tube geometry and initial conditions as used in the predictions are given in Fig. 9.21.

![Fig. 9.21: Shock tube problem for two-phase water/air mixture; geometry and initial conditions](image)

As in the previous case, the ATFM calculations were performed with the second-order Flux Vector Splitting scheme. A relatively large number of 1000 cells was used to guarantee a converged numerical solution. The predicted pressure distributions at various time values after the rupture of the diaphragm are shown in Fig. 9.22. On first glance the results look qualitatively very similar to what was predicted for the single-phase gas, including the presence of shock and expansion waves propagating with constant velocities into the low and high pressure regions. However, as a result of the increased inertia and reduced compressibility of the two-phase mixture the wave propagation velocities are considerably lower than for the pure gas case.

More details on the wave propagation processes can be seen in Fig. 9.23 showing the distribution of governing parameters at a constant time of $t = 18$ ms. As for the pure gas case three wave propagation phenomena can be distinguished:

1. A shock wave traveling into the low pressure region which is composed of a shock front characterized by steep (but finite) gradients for all involved flow parameters followed by more of a relaxation region with moderate changes. Due to the very small time scale for crossing the shock front, all interfacial transfer processes as described by algebraic source terms are practically “frozen”, resulting in a strong deviation (overshoot) of phasic velocities and temperatures from the equilibrium conditions. The velocity of the shock front depends on the sound velocity within the undisturbed region as well as on the pressure ratio across the front which is not \textit{a priori} known. The relaxation region behind the front is governed by the interfacial heat, mass and momentum coupling driving the phase
9.4 Shock tube

Fig. 9.22: Shock tube test problem for two-phase flow of water/air mixture; pressure distribution at different time values, second-order Flux Vector Splitting scheme with 1000 cells; comparison of CFD calculation (solid line) with analytical solution for homogeneous equilibrium condition (dashed line).

parameters toward a new equilibrium state. The length of the relaxation zone depends on the intensity of the interfacial coupling terms.

2. A pressure wave followed by a “contact discontinuity” which in an ideal case marks where the two fluids were initially separated by the diaphragm. Similar to the pure gas case, the predicted pressure and mixture (to a certain extent also phasic) velocities remain equal on both sides. All the other parameters including mixture density, void fraction and phasic temperature show abrupt changes across the “contact discontinuity”. However, contrary to the gas flow case, the parameter gradients remain at finite values due to diffusion effects resulting from different local phasic velocities.
3. A smooth expansion wave traveling into the high pressure region. The front of the waves propagates with the sound velocity in the undisturbed high pressure region. The continuous dispersion of the wave is a result of the decrease of sound velocity during the expansion of the fluid.

Fig. 9.23: Shock tube test problem for two-phase water/air mixture; parameter distribution at $t = 15$ ms, comparison of CFD prediction (solid line) with algebraic solution for homogeneous equilibrium conditions (dashed line); dotted line: initial condition
In addition to the CFD prediction, Figs. 9.22 and 9.23 also include the results of an iterative analytical solution for the simplified case of homogeneous equilibrium flow. It is evident that the assumption of equal local phase velocities and temperatures suppresses all thermal and mechanical disequilibrium effects. However, there still exists a remarkable agreement with respect to pressure, mixture density, and mixture (average) velocity as well as for propagation velocities of different wave propagation processes.

9.5 Multidimensional wave propagation and explosion phenomena

The shock tube problem as described above can be extended to multidimensional “explosion” test cases, where a cylindrical or spherical high pressure core region is surrounded by a constant pressure environment as schematically indicated in Fig. 9.24. As in the shock tube problem the initial velocities in the high and low pressure regions are set to zero. As long as the fastest waves have not reached the outer walls no further specific boundary conditions are needed.

For the following numerical analysis two different computational grids will be used as shown in Fig. 9.25: (1) an equally spaced Cartesian grid (left) where, due to the expected strictly axisymmetric behavior, only one quadrant is actually used in the prediction, and (2) a quasi-one-dimensional nonuniform grid (right) which takes a full advantage of the symmetrical feature of the test case.

9.5.1 Single-phase gas flow

Before dealing with the more complicated two-phase flow conditions the numerical approach will be first tested for a pure gas case. The initial pressure and temperature values in the high pressure region are $p_1 = 5 \text{ bar}$ and $T_1 = 400 \text{ K}$, respectively. In the outer low pressure region pressure and temperature are specified as $p_0 = 1 \text{ bar}$ and $T_0 = 300 \text{ K}$. The diameter of the high pressure core is $d = 1.6 \text{ m}$.
The effect of the numerical approach on the explosion test case is shown in Figs. 9.26 and 9.27, comparing results for the pressure and density profiles obtained for different spatial resolutions. The figures include the results of three different calculations: (a) a two-dimensional calculation using a Cartesian grid of $100 \times 100 = 10000$ computational cells, (b) a quasi-one-dimensional calculation with 1000 cells (e.g., the same number of cells in the radial direction as used for the two-dimensional calculation) and (c) a quasi-one-dimensional “reference” calculation with 2000 cells. From the figures the following conclusions can be drawn:

1. in the two-dimensional calculation there is no noticeable difference whether the parameters are taken along the $x$- (or $y$-) axis or along the diagonal axis. This means that, at least for the present test case, the grid orientation effect is largely negligible,

2. the results for the two-dimensional and one-dimensional calculations are nearly identical when using the same number of cells in the radial direction,

3. the predicted wave velocities and corresponding wave locations are largely independent on the spatial resolution of the computational grid,

4. the solution with only 100 cells in radial direction did not reach spatial convergence as indicated by the poor representation of the shock wave and contact discontinuity. For the quasi-one-dimensional calculation the convergence is almost reached when 2000 cells are used in radial direction.

The figures also demonstrate a dilemma of multidimensional simulation of pressure (explosion) wave propagation problems. For a high resolution of the parameter changes in the waves, a detailed fine grid spacing would be needed only in regions of large spatial parameter variation as in the vicinity of the moving contact surface and shock wave. Using a uniform Cartesian grid as in the present case is highly inefficient and may become impractical in the case of more complex geometries.
9.5 Multidimensional wave propagation and explosion phenomena

Fig. 9.26: Explosion test case, single-phase gas flow, pressure profile in the radial direction at $t = 1.5$ ms; comparison of one- and two-dimensional calculations

Fig. 9.27: Explosion test case, single-phase gas flow, density profile in the radial direction at $t = 1.5$ ms; comparison of one- and two-dimensional calculations

Results of a “reference” calculation using a quasi-one-dimensional nonuniform grid with 2000 cells in radial direction are given in Figs. 9.28 and 9.29 showing the radial pressure and density distributions for consecutive time values during the first 2 ms of the transient. Apart from the axis symmetry the behavior is qualitatively similar to the shock tube problem including the outward propagation of a (now circular) shock wave, a circular contact discontinuity traveling with some smaller velocity in the same direction, and a circular rarefaction wave traveling toward the origin. Contrary to the strictly one-dimensional shock tube case the shock strength becomes weaker while traveling in outward direction and the velocity profile between shock wave and contact discontinuity is no longer constant.
Fig. 9.28: Cylindrical explosion test case for single-phase gas, pressure distribution at different time values, second-order Flux Vector Splitting technique with 2000 cells.
Fig. 9.29: Cylindrical explosion test case for single-phase gas, density distribution at different time values, second-order Flux Vector Splitting technique with 2000 cells
9.5.2 Two-phase flow

For the two-phase flow explosion test case a water/steam mixture is considered with the initial conditions as shown in Fig. 9.30. As in previous cases the pressure region with $p_1 = 5$ bar is surrounded by a constant ambient pressure $p_0 = 1$ bar. The gas (steam) volume fractions are $\alpha_{g,0} = 0.05$ in the high pressure region and $\alpha_{g,0} = 0.10$ on the low pressure side. In both regions thermal equilibrium is assumed with $T = T_{\text{sat}}(p)$.

How the chosen computational grid affects the calculation of the two-phase explosion test case is illustrated in Figs. 9.31 and 9.32. As for the single-phase gas case shown in Figs. 9.26 and 9.27 the results using a Cartesian grid or a quasi-one-dimensional (nonuniform) grid are nearly identical as long as the same number of grid points are used in radial directions. A converged solution is practically reached for the quasi-one-dimensional calculation for 2000 cells in radial direction which corresponds to a grid size of 1 mm.

Results for the reference calculation using a quasi-one-dimensional grid with 2000 cells are presented in Figs. 9.34 and 9.35 showing the radial profiles for pressure and void fraction.
9.5 Multidimensional wave propagation and explosion phenomena

at consecutive time values during the evolution of the transient. More detailed information on the parameter distributions at a fixed time of \( t = 40 \) ms are given in Fig. 9.33 also including phase velocities and evaporation/condensation rates. Although some common features still exist with the pure gas case as were described above, the inhomogeneity of the two-phase flow \( (u_g \neq u_l) \) and the large variation in mixture density due to the phase change processes add a considerable complexity to the wave propagation phenomena.

As in the gas case, a circular shock wave is traveling in an outward direction with a velocity of \( u_{sw} = 68.75 \) m/s which corresponds to a Mach number (based on the “frozen” sound velocity in the upstream undisturbed region) of \( M = 1.46 \). The shock wave is comprised of a leading steep wave front creating a sudden disequilibrium between the phases, and a continuous downstream relaxation region where interfacial transfer processes for mass, momentum and energy drive the flow toward a new equilibrium state. With the initial conditions chosen, the shock wave results in a complete condensation of steam which is achieved about 0.5 m downstream of the shock front.

At the same time a circular rarefaction wave is propagating into the initial high pressure core region toward the origin. The propagation velocity of this wave is largely retarded by the onset of a strong evaporation as indicated by the large increase in void fraction at the outer core region. This leads to a prolonged holdup of the pressure in the core region up to the time when most of the liquid is evaporated (not shown here).

The third wave represents a type of “contact discontinuity” showing a nearly discontinuous change in void fraction (see Fig. 9.35) from pure liquid \( (\alpha_g = 0) \) to high void fraction \( (\alpha_g > 0.8) \) two-phase conditions. The wave practically marks the boundary between the two fluids which were initially present in either the high or low pressure region. As for the gas flow the pressure remains unchanged across the contact discontinuity. The major difference to the gas case is that due to the nonhomogeneous flow conditions \( (u_g \neq u_l) \) some mixing occurs across the wave which results in penetration of vapor into the adjacent subcooled region and associated condensation (see Fig. 9.33).

The results shown here represent typical examples to demonstrate some characteristic thermal-hydraulic features of explosion phenomena in two-phase media. Nevertheless, the present modeling and numerical approach can be easily extended to other initial and boundary conditions or to diabatic flow conditions with external heat sources.
Fig. 9.33: Cylindrical explosion test case for two-phase water/steam flow, parameter distributions in radial direction at time $t = 40$ ms
9.5 Multidimensional wave propagation and explosion phenomena

Fig. 9.34: Cylindrical explosion test case for two-phase water/steam flow; pressure distribution at different time values, second-order Flux Vector Splitting technique with 2000 cells
Fig. 9.35: Cylindrical explosion test case for two-phase water/steam flow, void fraction distribution at different time values, second-order Flux Vector Splitting technique with 2000 cells.
How the multidimensional effects influence the wave propagation and attenuation is demonstrated in Figs. 9.36 and 9.37 comparing pressure and void fraction distributions at a fixed time of $t = 40 \text{ ms}$ for plane, cylindrical, and spherical configurations. The initial conditions in all the three cases are the same as used before for the cylindrical explosion cases.

**Fig. 9.36:** Explosion test case for water/steam flow; pressure profiles in the radial direction at $t = 40 \text{ ms}$ for plane, cylindrical, and spherical configuration.

**Fig. 9.37:** Explosion test case, water/steam flow; void fraction profiles in the radial direction at $t = 40 \text{ ms}$ for plane, cylindrical, and spherical conditions.

For the strictly one-dimensional conditions the “explosion case” becomes identical with the shock tube problem as was discussed in some detail in the previous section for water/air media. For the water/steam mixture, a strong shock wave is formed where in the trailing relaxation region the vapor is completely condensed. Due to the practical absence of viscosity effects (wall friction is neglected) the shock strength remains unchanged.

For the cylindrical, and even more for the spherical configuration, the continuous enlargement of the wave front while propagating in the outward direction results in a decrease of the wave intensity. On the other side, the spatial contraction to cylindrical or spherical geometries causes a faster depressurization of the core region and a more rapid evaporation as shown by the increased level of void fraction in this region.
The explosion test case as described above may also be reversed creating an implosion where an internal cylindrical or spherical core is surrounded by a high pressure region of finite thickness as schematically shown in Fig. 9.38.

Apart from the geometrical configuration, all other initial conditions for the high and low pressure regions are the same as in the previous explosion case. The quasi-one-dimensional prediction is done using the second-order Flux Vector Splitting scheme with 2000 grid points. Predicted parameter distributions for pressure and void fraction at five consecutive time values are shown in Figs. 9.39 and 9.40.

Similar to the explosion case, the onset of a strong evaporation in the initial high pressure (now outer) region creates a shock wave focusing toward the center of the sphere. The large thermal nonequilibrium in the wake of the shock leads to a complete condensation, which is practically reached within a distance of about 20 cm behind the shock front. Due to the convergence of the shock wave while propagating toward the origin the shock strength and propagation velocity continuously increase and, theoretically, an infinite pressure value would be achieved when the wave has shrunk to a single point. The prediction was terminated at \( t = 30 \) ms when the maximum pressure was \( p = 46 \) bar and the velocity of the shock wave was about \( u_{sw} = 200 \) m/s.
Fig. 9.39: Spherical implosion test case for two-phase water/steam flow, pressure distribution at different time values, second-order Flux Vector Splitting technique with 2000 cells
Fig. 9.40: Spherical implosion test case for two-phase water/steam flow, void fraction distribution at different time values, second-order Flux Vector Splitting technique with 2000 cells.
9.6 Flow through convergent–divergent nozzles

The steady state flow of compressible fluid through convergent–divergent nozzles cover various important flow phenomena like the occurrence of critical flow conditions, transition from subsonic to supersonic flow or the occurrence of flow discontinuities. For the steady state quasi-one-dimensional nozzle flow of a single-phase gas, relatively simple algebraic solutions exist as described in many textbooks of gasdynamics. For two-phase flow conditions, iterative algebraic solutions can be derived only for the rather restrictive assumption of homogeneous flow (equal local phase velocities) and thermal equilibrium between the phases as presented in Chapter 4. For the more general case of nonhomogeneous and nonequilibrium conditions, usually only numerical solutions can be obtained where the large variety of Mach number and the possibility of flow discontinuities (shock wave) represent a major challenge.

In the following various types of nozzle flows are analyzed which include different nozzle geometries, one-component (water/steam) and two-component (water/air) fluids as well as the effect of different upstream reservoir conditions and back pressure values. Where available, measured data are included for comparison. In some cases also the results from homogeneous equilibrium are included to distinguish between the effects of fluid compressibility and the contributions resulting from mechanical and thermal disequilibrium between the phases.

9.6.1 The ASTAR nozzle

Within the framework of the EU sponsored project entitled “Advanced Simulation Tool for Application to Reactor Safety” (ASTAR) (Städtke et al. [2]) various benchmark test cases have been defined to assess different approaches for the numerical simulation of two-phase flow processes. This included the stationary flow in a “smooth” convergent–divergent nozzle with the geometry shown in Fig. 9.41.

Fig. 9.41: ASTAR nozzle geometry

All calculations are related to the flow of a two-component (water/air) mixture with fixed upstream reservoir pressure and temperature values of \( p_0 = 10 \text{ bar} \) and \( T_0 = 570 \text{ K} \). The upstream gas content (gas mass fraction) has been limited to \( X_0 \geq 0.1 \), or \( \alpha_l < 0.10 \) respectively, in order to guarantee dispersed droplet flow for all the test cases. To allow a comparison with analytical solutions (e.g., for single-phase gas or liquid flows) simplified state equations are assumed such as ideal gas law and pseudo-incompressible liquid with a constant value for the sound velocity in the liquid phase. For the prediction of heat and mass transfer between
the phases the assumption of an ideal droplet flow regime is recommended based on uniform spherical droplets with a constant prescribed radius of $r_{dr} = 0.4$. The ATFM calculations shown in the following are performed using a nonuniform grid as schematically shown in Fig. 9.42.

![Fig. 9.42: ASTAR nozzle: computational grid and boundary conditions for quasi-one-dimensional flow](image)

For the prediction of the boundary conditions a one-dimensional homogeneous equilibrium flow is assumed between the reservoir and the nozzle inlet using the actual mixture velocity $u_{in}$ and mixture entropy $s_{in}$ at the first cell at the nozzle inlet

$$h_{in} = h_0 - \frac{u_{in}^2}{2} \quad (9.14)$$

$$s_{in} = s_0. \quad (9.15)$$

With the assumption of thermal equilibrium the pressure at the nozzle inlet is updated at each time step from the state equation

$$p_{in} = (h_{in}, s_{in}). \quad (9.16)$$

For the outlet boundary condition a constant ambient (exit) pressure is applied; for all other parameters the spatial gradients at the nozzle exit are assumed to be zero. The initial conditions in the nozzle are identical with the upstream reservoir conditions which implies that the transient calculation starts with a strong discontinuity at the nozzle exit. These initial boundary conditions are also applied qualitatively for the other nozzle test cases as described in this section.

**Single-phase liquid flow**

For a numerical scheme based on characteristic information, the flow of pure liquid represents a significant challenge, due to the large differences between the flow and the sound velocities. In order to test the Flux Vector Splitting technique for such conditions the flow of pure water through the ASTAR nozzle was predicted for a reservoir pressure of $p_0 = 10$ bar and an exit
pressure value of 9.99 bar $\geq p_{\text{exit}} \geq 9.80$ bar. For these conditions the maximum Mach number at the nozzle throat remains below 0.02. Predicted flow pressure values and flow velocities using 500 computational cells shown in Fig. 9.43. As indicated in the figure the CFD

![Fig. 9.43: ASTAR nozzle: stationary flow of single-phase liquid through a convergent–divergent nozzle, exit pressure: $p_{\text{exit}} = p_1$, with $p_1 = 9.99$ bar, $p_2 = 9.95$ bar, $p_3 = 9.9$ bar, $p_4 = 9.8$ bar; comparison of CFD calculation (straight line) with the results of the Bernoulli equation (triangle) calculations are in nearly perfect agreement with the analytical solution given by the Bernoulli equation. The capability to handle such low Mach number flow is a necessary prerequisite for the numerical simulation of two-phase nozzle flow with subcooled liquid conditions, as will be described later.

**Single-phase gas flow**

For the second limiting case, the flow of pure gas, the specific numerical difficulties are related to the transition through the sonic point (saddle-point singularity for $M = 1$) at the nozzle throat and the occurrence of flow discontinuities (shock waves) in the divergent part of the nozzle depending on the back pressure at the nozzle exit. The ATFM predictions are performed as for the previous liquid case with a second-order Flux Vector Splitting scheme with 500 computational cells to provide a high degree of convergence.

Figure 9.44 shows the predicted parameter distributions along the nozzle axis for various pressure values at the nozzle exit. In all the cases a nearly perfect agreement is obtained between the CFD calculation and the analytical solution, including the correct position of shock waves, and a high resolution of the corresponding flow discontinuities.
Fig. 9.44: ASTAR nozzle: flow of single-phase gas through a convergent–divergent nozzle, exit pressure $p_1 \geq p_{\text{exit}} \geq p_7$. $p_1 = 9.85$ bar, $p_7 = 0.2$ bar; comparison of results from CFD calculation (straight line) with analytical solution (dashed line).
9.6 Flow through convergent–divergent nozzles

Two-phase flow

The two-phase flow calculations are performed for two-component water/air mixtures with a gas mass fraction in the region $1.0 \geq X_0 \geq 0.10$. The predicted results for the steady state pressure and Mach number distributions for different nozzle back pressure values are shown in Fig. 9.45.

**Fig. 9.45:** ASTAR nozzle: dispersed two-phase flow of water/air mixtures through a convergent–divergent nozzle for different exit pressures $0.2 \text{ bar} \leq p_{\text{exit}} \leq 0.9 \text{ bar}$, effect of gas content $X_0$ on the location of the sonic point
As for the single-phase gas flow, the transition through the sonic point \( (M = 1) \) is characterized by a saddle-point singularity with a bifurcation of solution into a subsonic and supersonic branch separating the subsonic \( (M < 1) \) and supersonic \( (M > 1) \) regions in the divergent section, respectively. However, different to the pure gasdynamic case, the location of the singularity has moved downstream of the throat into the divergent section of the nozzle accompanied by a reduction of the critical pressure. The exact position of the sonic point depends strongly on the actual interfacial coupling between the phases as resulting from the algebraic source terms is analyzed in detail in Section 5.1.7.

![Fig. 9.46: ASTAR nozzle: dispersed two-phase of water/air, gas content \( X_0 = 0.50 \), exit pressure \( p_{\text{exit}} = 6.0 \) bar and 0.2 bar](image)

Depending on the back pressure values, shock waves occur in the supersonic region downstream of the sonic point. As already explained in Section 8.3 the shock wave structure is characterized by steep but finite parameter gradients. This “smoothing” effect results from the nonconservative terms in the phasic momentum equations which becomes more pronounced for increased liquid volume fraction. If the sonic point has moved to the nozzle exit, which in the present case is reached for \( X_0 = 0.1 \), the flow in the divergent section is free of any shock wave and the flow remains continuous up to the prescribed exit pressure.

For the pure gasdynamics case, the occurrence of critical flow conditions \( (M = 1) \) implies a maximum flow rate through the nozzle (choking condition) independent of a further reduction of the pressure at the nozzle exit. This is principally the same for two-phase nozzle
flows as shown in Fig. 9.47. For the progressive reduction of the nozzle exit pressure, two major trends are visible: (1) a continuous reduction of the exit pressure becomes necessary to achieve critical flow conditions \( M = 1 \) in the nozzle and (2) an increased retardation of the flow to asymptotically reach the maximum flow rate. This means, in particular, that a type of pre-choking might occur where the maximum flow rate is approached much earlier before the critical conditions are reached within the nozzle.

![Fig. 9.47: Flow of water/air mixtures through a convergent–divergent nozzle, mass flow rates as function of back pressure at nozzle exit, gas content \( X_0 = 0.75, 0.50, 0.25, 0.10 \)](image)

The specific peculiarities of the two-phase nozzle flow described above are largely determined by the mechanical and thermal disequilibrium as illustrated in Fig. 9.46 for a gas mass fraction of \( X_0 = 0.50 \) and exit pressure values of \( p_{\text{exit}} = 0.2 \) bar and \( 6.0 \) bar.

The strong pressure gradient and related acceleration of the flow results in an increase of the “slip velocity” which is governed by the forces acting on the dispersed droplet field. A maximum value for the velocity difference of approximately 100 m/s occurred at the middle of the divergent section. Due to a more moderate pressure decrease at the end of the nozzle, the flow shows a trend toward a mechanical equilibrium which, however, is not achieved at the nozzle exit. As a result of the intense heat transfer from the dispersed liquid to the gas phase, the thermal disequilibrium is less pronounced and toward the nozzle exit a new thermal equilibrium is practically achieved.

For an exit pressure of \( p_{\text{exit}} = 6 \) bar, a moderate shock wave is formed in the divergent section of the nozzle with an abrupt decrease of gas velocity and increase of gas temperature. Resulting from the continuous heat transfer to the gas phase, the gas temperature at the shock wave is much higher than the value predicted by an isentropic gas flow, and therefore, it is not surprising that the shock wave exhibits a peak gas temperature above the temperature at the reservoir. Due to the thermal and mechanical inertia, the liquid velocity and liquid temperature are practically “frozen” across the shock wave which leads to a reverse of thermal and mechanical disequilibrium immediately downstream of the shock. The region behind the shock is characterized by a relaxation region superimposed with the effect resulting from the change of the nozzle cross section in the flow direction. Within the relaxation zone, the flow is approaching a new thermal and mechanical equilibrium which is achieved at the nozzle exit.
As already mentioned the deviations from thermal and mechanical equilibrium between the phases are largely determined by the modeling details for the algebraic source terms describing interfacial transfer processes for momentum and energy. The validity of the coupling terms will be indirectly tested for the following nozzle test case by comparing with experimental data.

Two-dimensional nozzle flow

For the relatively large L/D ratio of the ASTAR nozzle geometry essentially one-dimensional flow conditions are expected for the single-phase flow of gases. However, this may no longer be the case for dispersed droplet flows due to the large density ratio between the liquid and gas phases as will be shown in the following. In order to investigate multidimensional effects, two-dimensional calculations have been performed for a planar nozzle with a body-fitted computational grid as schematically shown in Fig. 9.48.

![Fig. 9.48: ASTAR nozzle: computational grid for two-dimensional calculations (schematically)](image)

Actually a computational grid of $20 \times 200 = 4000$ cells are used for the second-order Flux vector Splitting scheme. At the nozzle inlet a gas content of $X_0 = 0.5$ is assumed which corresponds with a void fraction of $\alpha_{g,0} = 0.98$. The calculations were performed for two different exit pressure values of $p_{exit} = 1.0$ bar and $p_{exit} = 6$ bar.

Calculated values for the liquid volume fraction $\alpha_l$ and corresponding vector fields of liquid mass flow densities $\alpha_l\nu_l$ are shown in Fig. 9.49. The figure indicates a large enrichment of liquid near the wall region in the convergent section of the nozzle which, due to the large curvature near the nozzle throat, detaches from the wall and penetrates toward the nozzle axis. This creates a layer structure for the liquid fraction in the divergent section which remains evident up to the nozzle exit as indicated in Figs. 9.50 and 9.51.

Figure 9.50 provides spectral plots for the pressure distributions as were obtained for two different pressure values at the nozzle exit of $p_{exit} = 0.2$ bar and $p_{exit} = 6$ bar resulting either in a continuous depressurization to the ambient pressure ($p_{exit} = 1$ bar) or in the formation of a shock wave in the divergent section followed by a continuous pressure increase up to the exit pressure value of $p_{exit} = 6$ bar. The cross-sectional distributions of liquid volume fraction $\alpha_l$ as shown in the lower part of Fig. 9.50 clearly reflect the redistribution of liquid concentration
from a liquid enriched wall region in the convergent part to a gas enriched wall region in the divergent section of the nozzle.

The nonhomogeneous phase distribution over the nozzle cross-sectional area also affects the Mach number distribution as indicated in Fig. 9.51. This results from the large sensitivity of the sound velocity with regard to changes in the volume concentration for high void fraction (as in the present case) or low void fraction.
Fig. 9.50: ASTAR nozzle: results of two-dimensional calculation for $p_0 = 10$ bar and $X_0 = 0.5$; pressure distribution (top) and liquid volume fraction profiles at the convergent section, nozzle throat, and divergent section (bottom); second-order FVS scheme with $20 \times 200 = 4000$ cells
Fig. 9.51: ASTAR nozzle: results of two-dimensional calculation for $p_0 = 10$ bar and $X_0 = 0.5$; Mach number distribution (top) and Mach number profiles at the convergent section, nozzle throat, and divergent section (bottom); second-order FVS scheme with $20 \times 200 = 4000$ cells
9.6.2 Deich nozzle tests

The experimental program for the investigation of single component water/steam mixtures through a convergent–divergent (naval) nozzle as reported by Deich et al. [3] covers a wide spectrum of gas contents and exit pressure values. The experiments were performed with wet steam for a region of liquid contents \( Y_0 \) (wetness) ranging from \( Y_0 = 0 \) (slightly superheated vapor) up to a maximum liquid content of \( Y_0 = 0.83 \). The geometry of the nozzle as shown in Fig. 9.52 consists of a circular inlet section with a radius of 28 mm, followed by a cone with a constant angle of aperture \( \Phi_i = 3.3^\circ \) and a length of 122 mm. The nozzle inlet pressure was fixed at 1.2 bar, the outlet pressure was progressively reduced down to 0.05 bar. The measured data including static pressure values along the nozzle axis and mass flow rates of liquid water and vapor should be preferably considered as a qualitative measure for the flow behavior.

As an example a comparison of measured and predicted pressure values along the nozzle and corresponding Mach numbers are shown in Fig. 9.53 for an inlet liquid content (wetness) of \( Y_0 = 0.83 \) and progressively reduced pressure values at the nozzle exit.

Fig. 9.52: Deich nozzle geometry

Fig. 9.53: Deich nozzle; parameter distribution along the nozzle axis for different exit pressure values \( 0.1 \text{ bar} \leq p_{\text{exit}} \leq 0.95 \text{ bar} \); liquid mass fraction (wetness) at the reservoir \( Y_0 = 0.83 \)
For all exit pressure values the pressure and the Mach number distributions change continuously and are free of any discontinuity. The steep pressure and Mach number gradient at the nozzle exit for $p_{\text{exit}} = 0.1$ bar as shown by the predictions and the measured pressure values suggest that critical conditions have been reached for an exit pressure of $p_{\text{exit}} = 0.1$ bar. Nevertheless, as also shown in Fig. 9.53, the conditions at the nozzle throat no longer change for $p_{\text{exit}} < 6.0$ bar, which indicates that a constant (maximum) flow rate through the nozzle already occurred before critical conditions were achieved in the nozzle exit area. This is confirmed by Fig. 9.54, where the calculated mass flow rate is given as a function of the exit pressure.

![Fig. 9.54: Deich nozzle: comparison of measured and predicted mass flow rates as a function of the back pressure at the nozzle exit](image)

In order to investigate the sensitivity of the nozzle flow with respect to the nozzle geometry various calculations have been performed for a wetness of $Y_0 = 0.43$ where the angle of aperture for the divergent section is varied in the region of $0^\circ \leq \Phi_i \leq 6^\circ$. The exit pressure for all calculations was $p_{\text{exit}} = 0.1$ bar to guarantee that critical conditions are achieved in all cases.

The predicted pressure and Mach numbers as shown in Fig. 9.55 indicate that for all cases a critical state has been achieved in the divergent section of the nozzle. Any reduction of the angle $\Phi_i$ results in downstream movement of the critical cross-section from a position close to the throat for $\Phi_i = 6^\circ$ toward the nozzle exit which is reached for values $\Phi_i \leq 1^\circ$. For the experimental nozzle configuration of $\Phi_i = 3.3^\circ$ the predicted pressure distribution is in good agreement with the corresponding measured data which is also the case for the critical mass flow as given in Fig. 9.56.
Fig. 9.55: Deich nozzle: critical flow of water/steam mixture; liquid mass fraction at the reservoir \( Y_0 = 0.57 \), effect of angle of aperture in divergent section, triangles represent measured data for \( \Phi_i = 3.3^\circ \).

Fig. 9.56: Deich nozzle: mass flow rate as a function of the angle of aperture \( \Phi_i \) in the divergent section, liquid mass fraction at reservoir \( Y_0 = 0.83 \).
9.6 Flow through convergent–divergent nozzles

9.6.3 Moby–Dick nozzle tests

The Moby–Dick nozzle test program [4] was performed at the Centre d’Etude Nucleaire (CEA) de Grenoble as part of the qualification of the French Nuclear Thermal Hydraulic code CATHARE [5]. The tests were designed to study two-phase critical flow conditions which are of particular importance for the analysis of hypothetical Loss of Coolant Accidents (LOCA) in Pressurized Light Water reactors. Such accidents might be initiated by a structural failure of the high pressure primary system of a PWR resulting in a fast depressurization of the coolant system and in a degradation of the heat removal from the reactor core.

![Moby–Dick nozzle geometry, all dimensions in mm](image)

The Moby–Dick nozzle as shown in Fig. 9.57 has a total length of about 1 m and consists of a smooth convergent section, a relatively long cylindrical throat and a conical divergent section with an angle of aperture of $7^\circ$. The nozzle inlet conditions range from subcooled liquid with different degrees of subcooling to saturated conditions with different vapor mass fractions. From the large experimental program, two tests are selected with subcooled conditions at the nozzle entrance. The upstream reservoir pressure is in both cases $p_0 = 20$ bar with a degree of subcooling of $\Delta T_{\text{sub}} = 2$ K and 25 K, respectively. In the experiments the pressure downstream of the nozzle was continuously reduced up to a point (or even below) where a maximum flow rate was obtained through the nozzle. In the ATFM calculation the measured pressure at the nozzle exit is used as a boundary condition. Predicted parameter distributions for steady state conditions are given in Figs. 9.58 and 9.59 including experimental data for pressure and void fraction (not for all tests available) as well as analytical results based on the homogeneous equilibrium assumptions.

For the low degree of subcooling (Fig. 9.58) the flow in the convergent section remains pure liquid. The evaporation starts immediately at the entrance to the cylindrical throat section followed by a moderate acceleration of the fluid and a related drop of pressure. At the inlet to the divergent section the further expansion of the fluid becomes more pronounced leading to an increased acceleration of the fluid with maximum flow velocities for gas and water of $u_g = 240$ m/s and $u_l = 150$ m/s. The flow remains always subsonic and, therefore, is free of any discontinuous (or near discontinuous) parameter change. The good agreement with measured pressure and void fraction data suggests that the prediction gives a fair picture of the flow behavior. The analytical solution assuming homogeneous equilibrium flow largely differs from the experimental data and shows the presence of an unrealistic shock wave in the divergent section of the nozzle.

For the high degree of subcooling (Fig. 9.59) the behavior of the nozzle flow becomes slightly different. The flow remains pure liquid up to the near end of the cylindrical section where a strong evaporation (flashing) starts, possibly triggered by the frictional pressure drop.
Nevertheless, the void fraction is somewhat lower as for the previous case with near saturated inlet conditions and consequently the flow shows a more moderate acceleration with the maximum phase velocities $u_g = 90$ m/s and $u_l = 70$ m/s. Also in this case the flow in nozzle remains subsonic and, therefore, is free of shock waves.

The fact that in both of the Moby–Dick test cases shown above the flow remained everywhere subsonic and therefore, the question arises whether the condition for “choking” has been obtained where the flow through the nozzle becomes independent of the exit pressure. This is demonstrated in Fig. 9.60 for the high degree of subcooling ($\Delta T = 25$ K) showing the distributions of governing flow parameters for progressively reduced pressures at the nozzle exit $p_{\text{exit}}$. The figure indicates that for $p_{\text{exit}} = 16$ bar any further reduction has no effect on the flow parameter in the convergent part and in cylindrical throat section of the nozzle, indicating that the mass flow through the nozzle has practically reached a maximum value. Any further reduction of back pressure pushed the region of influence toward the nozzle exit and at $p_{\text{exit}} = 1$ bar, the flow in the whole nozzle is unaffected by any further change of the back pressure.
The effect of “pre-choking” is also seen on the total mass flow rate through the nozzle as a function of the exit pressure as shown in Fig. 9.61. Already at a rather moderate pressure reduction at the nozzle exit a practically constant mass flow is achieved for values much higher than those used in the experiment. The figure also indicates the correct prediction of the measured mass flow for both cases of subcooling at the nozzle entrance.
Fig. 9.60: Moby–Dick nozzle: $p_0 = 20$ bar, $T_0 = 461$ K, effect of back pressure on the nozzle flow, $19 \text{ bar} \geq p_{\text{exit}} \geq 0.2 \text{ bar}$

Fig. 9.61: Moby–Dick nozzle: $p_0 = 20$ bar; effect of back pressure on mass flow rate; comparison of prediction (straight line) with measured data (triangles)
9.7 Blowdown phenomena

The fast depressurization of pressure vessels or piping systems containing subcooled or saturated liquids is of large interest for the safety analysis of industrial installations. Such “blowdown” processes might originate by a structural failure or by an operational opening of safety valves to prevent damage to the plant. In particular for the safety analysis of Light Water Reactor (LWR) safety analysis, blowdown phenomena have been extensively studied. This included the event of the rupture of a main coolant pipe in the primary system of a pressurized LWR often postulated as a most severe credible accident for the design of emergency cooling systems and accident management procedures. Since for obvious reasons, full scale experiments are not feasible, complex thermal-hydraulic computer codes have been developed to describe such phenomena and their consequences for a safe shutdown of the plant. In order to assess these codes a number of standard test cases were defined by the Committee for the Safety of Nuclear Installation (CSNI) [6] which cover a wide spectrum of physical phenomena involved at different geometrical scales.

9.7.1 Edwards’ pipe blowdown

A standard test case for thermal-hydraulic codes has been the blowdown of an initially hot pressurized liquid from a pipe of approximately 4 m length, known as the CSNI standard problem No. 1, also known as Edwards’ pipe blowdown [7] (Fig. 9.62). The water in the pipe has an initial pressure of 7.0 MPa and a temperature of 502 K which corresponds to an initial subcooling of 56.8 K. The geometrical configuration is given in Fig. 9.63. The transient is initiated by the rupture of a bursting disk allowing the rapid discharge to the environment at atmospheric pressure.

Most of existing calculations for this test use a constant (atmospheric) pressure as a boundary condition immediately downstream of the pipe. This seems to be doubtful, especially in the cases where the flow in the pipe remains subsonic and the high pressure difference between the pipe exit area results in continuation of the evaporation process downstream of the exit. In the calculation presented here, the specification of boundary conditions at the very sensitive area at the pipe exit is avoided by enlargement of the numerical simulation to include the expansion of the two-phase mixture and jet formation downstream of the pipe. This is done by the modeling as an axisymmetric, quasi-two-dimensional flow process near the pipe exit with a constant (atmospheric) far-field pressure boundary. The computational scheme used in the following calculations is shown in Fig. 9.63.
With regard to the governing phenomena of the blowdown process two different time periods can be distinguished:

(1) A short time period mainly characterized by wave propagation and reflection phenomena shown in Fig. 9.64. Immediately after the removal of the rupture disk, a sudden pressure drop occurs at the pipe exit resulting in the onset of a violent evaporation of liquid which limits the pressure decrease to a value slightly below the saturation pressure according to the initial liquid temperature. This pressure value is nearly maintained during the first 10 ms period of the transient characterized by the propagation of a rarefaction wave propagating with the speed of sound of the liquid phase into the pipe. The reflection of this wave at the left closed end of the pipe at about 3 ms results in pressure undershoot limited by the accompanied evaporation process. This forms a moderate pressure wave which travels back toward the pipe exit which is reached by about 6 ms. After the pressure wave has returned to the exit, the transient continues with the bulk evaporation over the full pipe length leading to a more moderate depressurization.

(2) A long time period showing a more steady transient governed by a continuous bulk evaporation as shown in Fig. 9.65. As shown in Figs. 9.64 and 9.65, the flow in the pipe remains subsonic over the whole transient, however, supersonic ($M > 1$) conditions occur temporarily in a region slightly downstream of the pipe. The governing process controlling the discharge from the pipe is the short region with extremely large evaporation rates close to the exit as created by the steep pressure gradient in this region.
9.7 Blowdown phenomena

The long time blowdown behavior is governed by the discharge from the pipe, the continuous evaporation of liquid and to a lesser extent by the frictional forces at the pipe walls. With a further decline in pressure the flow velocities start to decrease up to the end of the blowdown at $t = 0.5\text{ s}$ when atmospheric pressure is reached in the pipe.

A comparison of the calculated values for the pressure at the pipe head and for the void fraction at the pipe middle section is given in Fig. 9.66. The rather good agreement with the corresponding measured data suggests that the governing phenomena are correctly described.
Fig. 9.65: Edwards' pipe blowdown: parameter distributions during the long time period at time values $0.01 \, \text{s} \leq t \leq 0.5 \, \text{s}$

Fig. 9.66: Edwards' pipe blowdown: comparison of predicted and measured values; pressure at pipe head (left) and void fraction at pipe middle section (right)
9.7.2 Canon experiment

The Super-Canon test program was performed at the Centre d’Etude Nucleaire (CEA) de Grenoble with the aim to enlarge the experimental database for the assessment of thermal-hydraulic computer codes developed for the safety analysis of Light Water Reactors. The experiments were performed in a similar way as already described for Edwards’ pipe, using the horizontal pipe of 4.39 m length and an internal diameter of 0.1 m. Compared with Edwards’ pipe a more detailed instrumentation was used providing information on pressure and temperatures at different positions of the pipe and to a lesser extent on the void fraction. The geometry of the pipe and the measurement positions are given in Fig. 9.67.

From the Super-Canon test program [8], an experiment has been selected with an initial pressure of $p_0 = 150 \text{ bar}$ and a temperature of $T_0 = 507 \text{ K}$ (equivalent to a subcooling of 42 K). Due to the extremely high initial pressure, critical flow conditions are expected to exist at the pipe exit during most of the blowdown period. Therefore, it seems to be justified to assume atmospheric pressure at the exit of the pipe. The computational grid and initial conditions as used in the calculations are schematically shown in Fig. 9.68.

The predicted behavior during the blowdown as shown in Figs. 9.69 and 9.70 is qualitatively very similar to that obtained for Edwards’ pipe. This includes the wave propagation and reflection phenomena during the first 10 ms of the transient when the strong evaporation (flashing) upstream of the pipe exit prevents the pressure from dropping below the saturation
Different to Edwards’ pipe, critical flow conditions \((M = 1)\) occurred immediately after the removal of the rupture disk and were also maintained as long as the pressure in the pipe considerably exceeded the atmospheric pressure.

Fig. 9.69: Canon blowdown test case; parameter distribution for the short term period, time values; \(0.1 \text{ ms} \leq t \leq 7 \text{ ms}\)

A comparison with the measured data for pressure and void fraction is given in Fig. 9.71. Although the figure indicates that the general trends of the experiment are reasonable well predicted, a more qualitative evaluation is only partially possible due to the large scatter in the measured data (in particular for the void fraction).
9.7 Blowdown phenomena

Fig. 9.70: Canon blowdown test; parameter distribution for the long term period, time values: $0.01 \, \text{s} \leq t \leq 0.375 \, \text{s}$

Fig. 9.71: Canon blowdown test: comparison of prediction with measured data; left: pressure at the pipe head (1), pipe middle section (4), and near pipe exit (6), right: corresponding void fraction values
9.7.3 Two-vessel test case

This purely hypothetical test case is included to demonstrate the capabilities of the presented modeling and numerical strategies for the numerical simulation of more complex multidimensional two-phase processes as are also of interest for many industrial applications. The assumed facility consists of two cylindrical vessels connected by a horizontal stand pipe schematically shown in Fig. 9.72. The high pressure container on the left side is partially filled with saturated liquid with a pressure of 10 bar whereas the right vessel contains pure vapor at atmospheric pressure. Both vessels are separated by a diaphragm at the exit of the connecting pipe which is assumed to be removed instantaneously at time zero.

Since the major parameter changes are expected in the \(x-y\) plane, the problem is treated as a pseudo two-dimensional case where some three-dimensional effects are taken into account by a variable “depth” in the \(z\)-direction. The corresponding computational grid as used in the calculation is shown schematically in Fig. 9.73.

![Fig. 9.72: Two-vessel test case: geometrical configuration and initial conditions, dimensions: \(H = 1.8\) m, \(D = 0.6\) mm, \(L = 1.0\) m, \(d = 0.01\) m](image1)

![Fig. 9.73: Two-vessel test case: computational grid for a quasi-two-dimensional calculation (schematically)](image2)
In the actual calculations a hexagonal grid is used within the $x$-$y$ plane as indicated in Fig. 9.74. This has the advantage that every cell has common interfaces with all neighboring cells, which provides a reduction of the grid dependence of solution compared with a Cartesian grid.

![Diagram of two-vessel test case: hexagonal grid at symmetry plane and reference data positions](image)

In the following the results of two calculations are presented including a completely closed system where the valve on top of the right (low pressure) vessels remains closed during the whole transient and (b) and a vented system, where the valve is opened simultaneously with the removal of the diaphragm in the connecting pipe at time zero.

**Closed system**

A qualitative picture of the transient might be obtained from Figs. 9.79 and 9.80 showing the void fraction distribution and the vector field for the gas mass flow at various consecutive time values. A more detailed information is presented in Figs. 9.75 and 9.76 for the pressure values and Mach numbers in the vessels and in the pipe during the short time ($0.0 \text{ s} \leq t \leq 0.1 \text{ s}$) and long time ($0.1 \text{ s} \leq t \leq 10 \text{ s}$) periods:

(a) a rapid boil-off and swelling of the water pool in the left vessel due to fast evaporation,

(b) transition from single-phase vapor to two-phase flow and choking in the interconnecting pipe,

(c) jet formation in the right (low pressure) vessel, jet impingement at the vessel wall and a strong re-circulating flow pattern,

(d) gravity-induced phase separation,

(e) liquid collapse and a formation of residual liquid pools in the two vessels.
The transient is terminated at about 12 s when a new equilibrium state is reached in the whole system and the vapor and liquid phases in both vessels are completely separated. As can be seen from Fig. 9.76 a large amount of liquid is finely transported into the right vessel.

**Open system**

As long as there exists critical flow conditions in the connecting pipe during the short time period, the behavior of the vented system is nearly identical with those predicted for the closed system and, therefore, is not explicitly shown here. Shortly after the flow in the connecting pipe turns to subsonic condition the pressure in the right vessel reached a maximum value of about $p_4 = 3$ bar when the volumetric flow in the connecting pipe and the discharge through the valve are at the same order of magnitude (see Fig. 9.77). This pressure then remains nearly constant for a certain period of time before, due to the dominating effect of discharge to the
atmosphere, a continuous depressurization of both vessels occurs up to the time when the atmospheric pressure is reached at about \( t = 12 \) s.

![Graph showing pressure and Mach number during blowdown phenomena.](image)

**Fig. 9.77:** Two-vessel test problem, open conditions: pressure and Mach number during the long time period at the top of the left vessel (1), inlet (2) and outlet (3) of the connecting pipe, and at the top of the right vessel (4)

Predicted values for pressure and mass inventories in both pressure vessels are compared in Fig. 9.78 for closed and open conditions. The figure indicates that in the case of closed conditions, the transient results mainly in a redistribution of the mass inventory and the final equilibrium pressure appears only slightly below the initial pressure of the left vessel. For the open conditions, a large amount of water is finally ejected from the system and only small liquid pools remained in both vessels at the end of the transient.

![Graph comparing pressure and mass inventory for closed and open conditions.](image)

**Fig. 9.78:** Two-vessel test problem, comparison of results for closed and open conditions: pressure and mass inventory for the left (solid line) and right (dashed line) vessel as a function of time
Fig. 9.79: Two-vessel test problem: void fraction distribution and vector field for gas velocity for short time period
Fig. 9.80: Two-vessel test problem: void fraction distribution and vector field for gas velocity during long time period
References


