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MODELLING OF ORIFICE FLOW IN COMPLEX THERMODYNAMIC CYCLE SIMULATIONS

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Summary: *The present paper is aimed at the modelling of compressible gases in axi-symmetric pipes exhibiting sudden changes (discontinuities) of diameter. These parts of pipes are called orifices. The modelling of orifice flow is problematic due to its complicated and genuinely spatial character. Moreover, due to the fact that the presented flow problem builds only a small part of a complex thermodynamic cycle simulation, we are requested to get satisfactory results using only as few degrees of freedom as possible. We develop several simplified models of the orifice flow and test their quality numerically. Results of numerical experiments are presented and discussed.*

Key words: *Orifice, pipe, flow, quasi one-dimensional, finite volume method, compressible Euler equations.*

1 Introduction and the aim of the study

There are many scientific papers where the precise resolution of the flow is of paramount (and often the only) interest. Usually, one uses fine grids, higher-order finite volume or finite element schemes, and possibly error indicators and adaptivity in space and sometimes also in time. In addition, one uses high-level computers, usually workstations and sometimes also parallel supercomputers with hundreds of megabytes or maybe giga- or terabytes of memory. Computing times often do not play a crucial role.

The situation dramatically changes when the scientific methods should be transmitted into engineering practise. Suddenly, one has limited resources both in time and in money. Often, the only possibility to sell a numerical software to the customers is to design it for a PC with a very limited memory and speed. Moreover, in many engineering applications the computational fluid dynamics is only a part of a more complex simulation.

This paper is devoted to the modelling and numerical simulation of inviscid compressible gas flow in pipes which exhibit sudden changes (discontinuities) of diameter. Sudden changes of pipe diameter are called *orifices* in our contribution. We model the flow using the compressible Euler equations for a perfect gas. As our method will be used in the framework of complex thermodynamic cycle simulation, where a lot of unknowns are occupied by the thermodynamics, we can dispose only with an extremely low number of degrees of freedom. Standard quasi-1D finite volume method (see e.g. [2], [4]) can be applied to pipe sections where no discontinuity of diameter occurs. The quasi-1D finite volume method requires only three degrees of freedom (fluid density, velocity and pressure) in each element, and this is the minimum we can achieve. Unfortunately, the quasi-1D finite volume method behaves very poorly at orifices.

Therefore, our task is to model the flow in the neighbourhood of an orifice as precisely and using as few degrees of freedom as possible. The situation is depicted in the following Figure 1.

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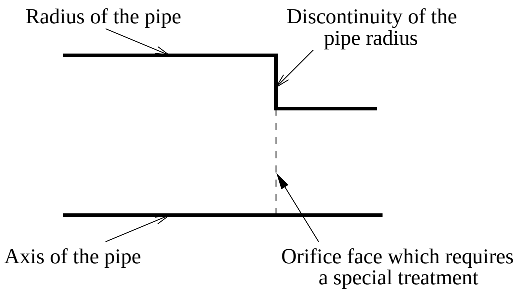

Figure 1: Discontinuity of the pipe radius and the orifice face.

It is our aim to develop a coupled finite volume scheme which is quasi one-dimensional within flat pipe sections (i.e. within pipe sections where the diameter of the pipe is continuous), and which is sufficiently precise in the close neighbourhood of the orifices.

2 Model problem - a Laval nozzle

We are going to propose, test and discuss several models of the orifice flow in the following sections. For the purpose of comparison, it is suitable to choose a model problem, the precise results of which can be measured or computed. According to engineering practice, the value of stationary mass flux resulting from a prescribed pressure drop between the ends of the pipe, and an inlet temperature, is of key importance for the judgment of quality of orifice flow models.

We choose a Laval nozzle shown in Figure 2, which is described by a poly-line given by the points $[-0.08, 0.025]$, $[0.0, 0.025]$, $[0.0, 0.005]$, $[0.02, 0.005]$, $[0.2, 0.015]$. Boundary conditions are chosen as follows: inlet pressure 50000 Pa, inlet temperature 358.16 K and the outlet pressure 15000 Pa. The perfect gas is characterized by the constants $\kappa = 1.39970094478$ and $R = 287.09$.

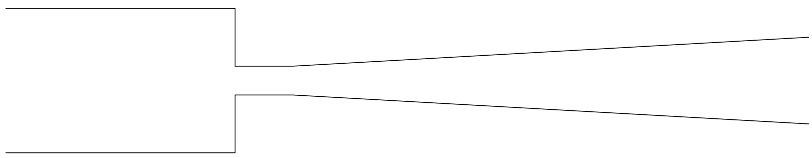

Figure 2: Geometry of the benchmark Laval nozzle.

We have solved this example using the three-dimensional compressible Euler equations, discretized by the 3D axi-symmetric finite volume method. The resulting stationary pressure distribution is shown in the following Figure 3.

We used a sequence of several unstructured triangular meshes (the three finest ones contained 9140, 36560 and 146240 triangles) to quarantee the convergence of the method. We can state that on the finest mesh, the 3D axi-symmetric compressible Euler equations are resolved precisely. The difference between the values of the stationary mass flux computed on the two finest meshes is less than 10^{-3} kg/hour.

The most precise value of the stationary mass flux is 24.5137 kg/hour. Measurements confirmed that for the above boundary data, the presented value of the stationary mass flux is very close to the reality.

3 Why quasi-1D modelling is not sufficient

In this section we present our experience with the quasi-1D modelling of the flow in the orifice region. With respect to the standard quasi-1D finite volume method, there will be only a difference in the quasi-1D element (let us call it *left-hand-side (LHS) orifice element*), which

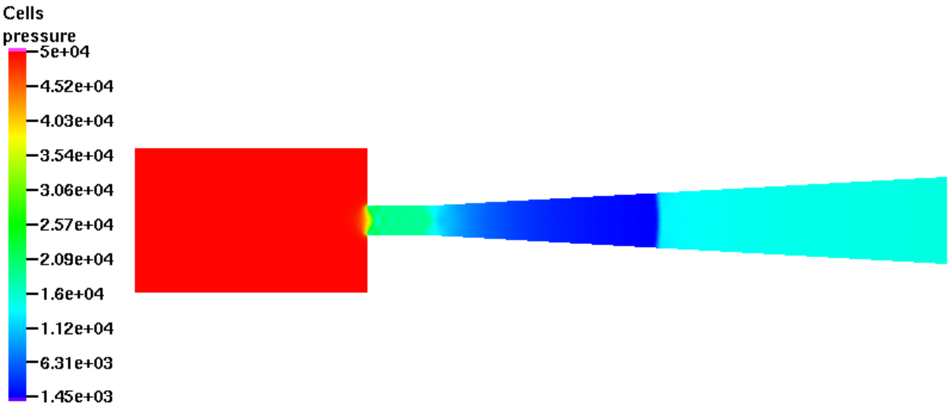

Figure 3: Precise 3D axi-symmetric stationary solution (pressure).

contains the part of the impermeable wall that is perpendicular to the x-axis. In the following Figure 4, the LHS orifice element is shown.

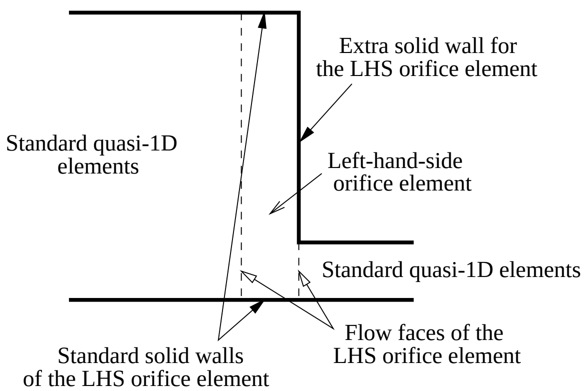

Figure 4: Special treatment of the LHS orifice element.

One face of the LHS orifice element is built partially by an impermeable wall and partially by a flow face shared with its adjacent element (on its right-hand-side in the Figure 4). We solve the Riemann problem only on the flow part of the combined face, meanwhile standard solid-wall numerical flux is used for its impermeable part. We show results of several computations in the following Table 1.

Division (elements)	Mass flux (kg/hour)
13	16.6772
130	16.6119
260	16.6110
520	16.6105

Table 1: Stationary mass flux for the quasi-1D orifice flow model.

The reader can see that the mass flux is more than 32% underestimated with respect to the precise axi-symmetric 3D computation.

The reason for these large errors is the complexity of the flow in the orifice region covered with the LHS orifice element. In the upper part of the element, the flow moves with a small velocity, meanwhile in the orifice region the velocity of the flow becomes sonic. As the approximate quasi-1D solution in the radial direction is constant, it offers only a mean value, which is far from both extrems. Moreover, we should not forget that in this case the flow velocity is considered one-dimensional. Therefore, for our purposes it is not suitable to model orifices by means of quasi-1D finite volume schemes.

4 3D axi-symmetric modelling

In this section, we will model the orifice region by means of a 3D axi-symmetric finite volume scheme. According to what we said above, our aim is to couple the axi-symmetric model of the orifice region with the standard quasi-1D finite volume scheme in the rest of the pipe. Resolution of the flow around the radius jump has a crucial influence on the value of the mass flux.

To demonstrate the behaviour of the proposed coupled technique, we use several mixed quasi-1D/axi-symmetric grids, In the following five figures, each rectangle represents four first-order quasi-1D elements meanwhile triangles represent first-order axi-symmetric rings.

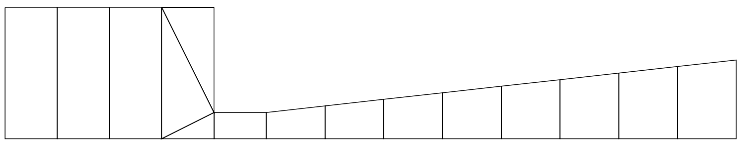

Figure 5: Mesh 1 with 3 axi-symmetric and 48 quasi-1D elements.

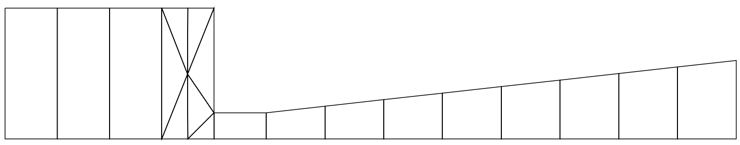

Figure 6: Mesh 2 with 7 axi-symmetric and 48 quasi-1D elements.

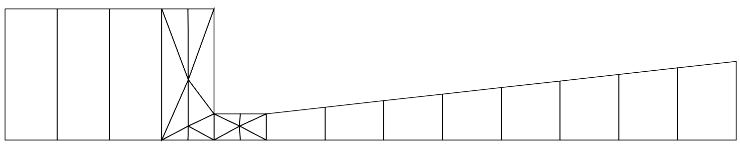

Figure 7: Mesh 3 with 14 axi-symmetric and 44 quasi-1D elements.

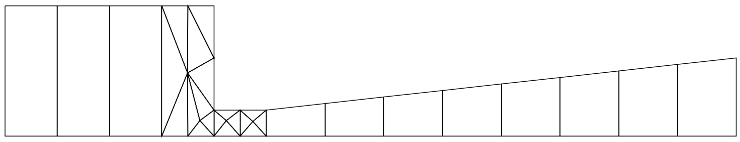

Figure 8: Mesh 4 with 18 axi-symmetric and 44 quasi-1D elements.

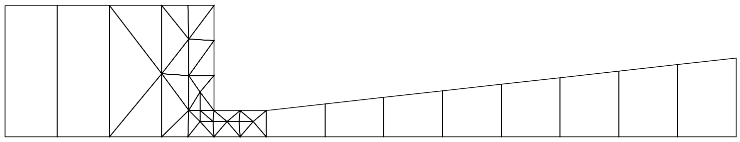

Figure 9: Mesh 5 with 25 axi-symmetric and 44 quasi-1D elements.

In the following Table 2 we present the stationary inlet and outlet mass fluxes corresponding to the above meshes. The axi-symmetric version of the FVM is non-conservative. This effect disappears on fine meshes as the numerical error of the integration of involved source terms vanishes. Nevertheless, our meshes are very coarse and therefore the values of inlet and outlet mass fluxes are not identical. In Table 2, the reader can see that the rate of non-conservativity doesn't vanish even if the resolution near the corner is improved. The reason is that the rate of non-conservativity depends on the coarsest axi-symmetric elements in the grid.

Mesh	Rings	Inlet mass flux (kg/hour)	Outlet mass flux (kg/hour)
1	3	22.64	23.345
2	7	22.88	23.60
3	14	23.67	24.42
4	18	23.84	24.62
5	25	24.08	24.86

Table 2: Stationary mass flux for the above five coupled quasi-1D/axi-symmetric models.

The reader can see that the difference between the inlet and outlet mass fluxes does not exceed 5 %. In comparison with the precise value of the stationary mass flux (24.5137 kg/hour), our worst results (Mesh 1) differ no more than 8 %. Another way leading to an improvement of conservativity of this coupled technique would be to avoid large axi-symmetric elements. It is not necessary that the interface between the quasi-1D and axi-symmetric 3D parts of the mesh is built with exactly one axi-symmetric ring.

Nevertheless, from the point of view of computational efficiency for desired applications, it is not possible to use grids which are so fine that the effect of non-conservativity vanishes. We shall turn our attention to conservative schemes.

5 Topologically simplified 3D modelling

In the computational fluid dynamics, difficult problems sometimes can be approximated on simplified topologies. By *simplified topology* we mean another shape of the computational domain, which leads to an easier application of the numerical method. In our compressible inviscid case, the topologically changed domain must be related to the original one in such a way, that the machinery of characteristics and other non-trivial flow phenomena stay unchanged, or nearly unchanged.

Simplifying the topology of the problem, one must be careful to conserve all important flow phenomena. Sometimes, it can be difficult to decide, which flow phenomena are important. The goal is to find such geometrical properties of the problem that make the solution difficult and that, on the other hand, have no crucial influence on the observed properties of the solution.

In our case, the most important phenomenon characterizing the flow restriction is the impermeable solid wall which is perpendicular to the x-axis and which is acting as an obstacle to the flow. The fact that the real geometry of the channel is axi-symmetric, is not so important for our purposes.

In our case, a suitable topological simplification of the axi-symmetric flow restriction is shown in the following Figure 10. It conserves the volume of the original flow restriction, the sizes and normal angles of the inlet and outlet faces and of the impermeable solid walls. The distance between the inlet and the orifice is also conserved.

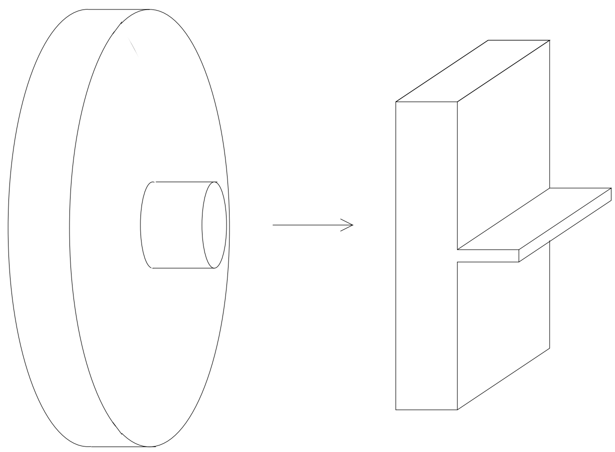

Figure 10: Topological simplification of the problem.

The reader can see the greatest advantage immediately: the flow within the changed topology is obviously three-dimensional, but as it does not depend on the third direction, two-dimensional finite volume method can be used for its solution. Moreover, the simplified model is plane-symmetric, which reduces the computational costs once more, by a factor of two.

For readers who are not familiar with this technique we remark, that in the framework of the quasi-1D finite volume method, both the original axi-symmetric geometry and the topologically simplified one are exactly equivalent. In addition to this fact, involving three-dimensional effects, the new model will be definitely closer to the reality than the quasi-1D simulation.

We shall present a numerical example documenting how the model treats the most important of the observed quantities - the stationary mass flux.

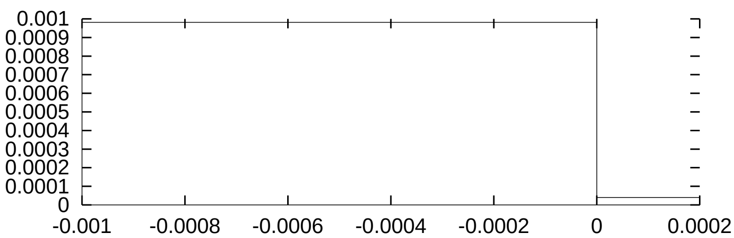

Figure 11: 2D geometry used for the precise computation of the stationary mass flux in the orifice region corresponding to the simplified topology.

As the outlet in this case is sonic, we only need to prescribe the boundary conditions along the inlet (left) part of the domain boundary.

The 2D domain shown in the Figure 11 is covered with a sequence of unstructured triangular grids which are strongly refined in the orifice region. These computations lead us to the precise value of the mass flux, which is 25.1168 kg/hour. Thus, by changing the topology of the problem, we overestimate less than 2.4603 % in this case.

Additional important questions are: Would coarse meshes on the 2D segment still give a reasonable value of the stationary mass flux? Does the length of the 2D segment influence the approximate stationary mass flux? What about the representation of other flow quantities in the domain?

Analogously as in the previous sections, two-dimensional finite volumes discretizing the region in front of the orifice are coupled with quasi-1D finite volumes covering the rest of the geometry. The 2D segment of the used mixed mesh is shown in the following Figure 12.

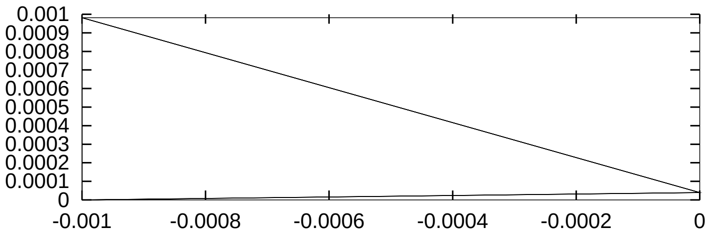

Figure 12: 2D mesh covering one symmetric half of the xy-cut through the orifice region corresponding to the topologically changed 3D geometry.

As computed in Section 2, the precise value of the stationary mass flux is 24.5137 kg/hour. The stationary mass flux obtained on a mixed quasi-1D/2D mesh containing the above 2D segment is 24.0806 kg/hour, which means that our new model lies within a tolerance of 1.77 % with respect to the precise result of the 3D axi-symmetric computation. Moreover, the dependence of this value on the length of the topologically simplified segment of the geometry turned out to be very small.

6 Coarse 3D modelling

In this section, we mention our experience with the finite volume approximation of the orifice flow by coarse 3D meshes. It is sufficient to cut off a part of the axi-symmetric 3D geometry corresponding to a reasonably small angle ϕ, as indicated in the following Figure 13. Obviously, to extend the computed value of the mass flux to the correct one, we have to multiply by the fraction of the original cross-section and the current one. Our mesh consists of 15 tetrahedra, thus we use 75 degrees of freedom. The fraction of the original circular cross-section and the computational one is 36.183459. The resulting stationary mass flux in this case is 0.6765 kg/hour, which means 24.514293 kg/hour after the extension to the original geometry. This value of the stationary mass flux lies only 0.00611 % from the value 24.5157 kg/hour obtained by our most precise computations on very fine axi-symmetric meshes in Section 2.

The coarse 3D approximation of the flow restriction gives very good results, at least concerning the mass flux, but on the other hand we need much more degrees of freedom with respect to the topologically simplified geometry (where 12 DOF's have been enough).

We can conclude that the technique based on topological simplification of the problem, which was introduced in Section 5, turns out to be the most promising one among all models discussed in this paper.

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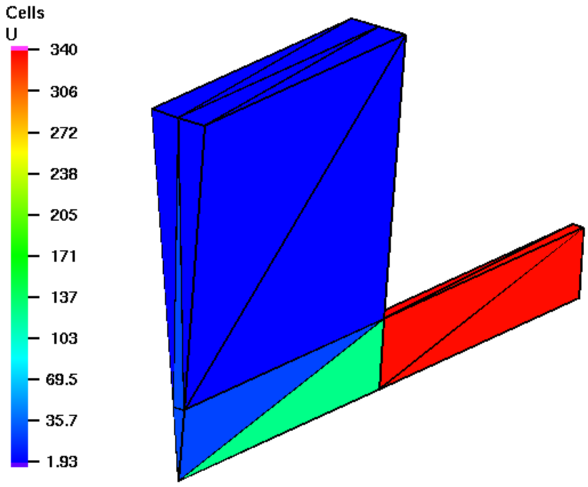

Figure 13: Coarse 3D approximation of the orifice region - stationary pressure distribution in the 3D part of the quasi-1D/3D mixed mesh.

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