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A non-linear quasi-3D model with Flux-Corrected-Transport for engine gas-exchange modelling

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Abstract

Modelling has proven to be an important tool in the design of manifolds and silencers for internal combustion engines. Although simple 1D models are generally sufficiently precise in the case of manifold models, they would usually fail to predict the high frequency behaviour of modern compact manifold designs and, of course, of a complex-shaped silencing system. Complete 3D models are able to account for transversal modes and other non-1D phenomena, but at a high computational cost. A suitable alternative is provided by time-domain non-linear quasi-3D models, whose computational cost is relatively low but still providing an accurate description of the high frequency behaviour of certain elements. In this paper, a quasi-3D model which makes use of a non-linear second order time and space discretization based on finite volumes is presented. As an alternative for avoiding overshoots at discontinuities, a Flux-Corrected Transport technique has been adapted to the quasi-3D method in order to achieve convergence and avoid numerical dispersion. It is shown that the combination of dissipation via damping together with the phoenical form of the anti-diffusion term provides satisfactory results.

Keywords: Gas exchange, Quasi-3D model, Flux-Corrected-Transport

1. Introduction

Engine modelling has become in recent years an essential tool in the design of reciprocating internal combustion engines, as it allows reducing considerably the development time and costs. Classical design methodologies are based on prototype manufacturing and trial-and-error tests. Currently, most of those tests have been replaced by numerical computations, so that only the most promising design options are actually tested on engine bench.

For years, 1D gas dynamics codes in the time domain [1] have offered sufficiently good solutions for modelling both engine performance and intake and exhaust noise. The choice of 1D models is justified because in most ducts present in engine intake and exhaust systems it can be assumed that there is only one flow direction. However, for a more demanding level of design, a 1D representation may not be sufficient to describe accurately the flow in certain elements. This is especially important in the case of silencers, where the 1D assumption can only be applied to simple geometries [2] and, even in that case, suitable results can only be obtained for frequencies below the cut-off frequency of higher order modes [3], but also in the case of duct junctions, where the existence of complex 3D flow structures sets the applicability limit for a simple zero-

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dimensional description [4]. In view of these limitations, the first option would typically be the use of a computational fluid dynamics (CFD) model; however, the application of such a model to a complete intake or exhaust system entails an excessive computational time.

A possible solution comes from the use of a 3D model only locally at those parts in which 3D effects are relevant, through the coupling between 1D and 3D models. Such coupling can be done directly in the time domain [5] or by means of time-frequency hybrid schemes [6] in which the element information is obtained from 3D or quasi-3D linear models [7], although the use of hybrid schemes is hampered by their very slow convergence.

An alternative compromise solution is given by quasi-3D models, in which the momentum equation is solved in a simplified way on a staggered mesh [8]. A good quasi-3D model should be able to offer almost as good results as a CFD tool, at least for the particular problem for which it was designed, while reducing greatly the computation time. Such solutions have become standard in commercial codes, and have been successfully applied to silencers with perforated tubes and/or absorbing material, both in the acoustic regime [9] and in real engine conditions [10]. It is well known, however, that such methods do not satisfy the stability requirement, especially in cases where pressure gradients are significant, unless some additional term is included in the momentum equation, be it either an equivalent friction force [8] or a momentum diffusion term [11].

The main objective of this paper is to evaluate the possibility of avoiding such additional terms by means of the use of a Flux Corrected Transport (FCT) methodology [12], which has proven to be a suitable solution to avoid overshoots at discontinuities when the flow equations are solved with finite differences schemes, even in ducts with non-uniform cross-section [13].

The paper is organized as follows: First, in section 2 the method is described, including the discretization of the equations and the formulation of the FCT method. Then, in section 3 the stability and convergence of the method are tested on the shock-tube problem. Finally, in section 4 the conclusion of the work are summarized.

2. Description of the method

When trying to determine the reasons why 3D methods need high computational resources and, if possible, to reduce those needs, it is readily concluded that the main problem lies in the momentum equation. Even neglecting any viscosity terms, it is a vector equation and thus a system of three equations has to be solved, in addition to the mass and energy equations, in each cell for each time step. Therefore, this is the aspect addressed when considering a quasi-3D approach, as described in the following.

2.1 Mesh elements

Two types of basic elements are considered that henceforth will be referred to as volumes and connectors. Volumes contain information about scalar magnitudes such as pressure, density or temperature, and of course of the cell volume itself, whereas connectors contain information on vector quantities (flow velocity or momentum), on their own orientation in space also some scale information (the connector area). A connector always connects two volumes, whereas a volume may be attached to as many connectors as required by the problem.

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In Figure 1, two volumes connected by a connector are shown. The volumes are represented by cubes, although they do not actually have any defined shape, in the same way as the connector is simply an area across which the flow passes between the two volumes.

2.2 Discretization of the basic equations

The starting point of the method are the usual Euler equations for the 3D case. However, in the context of the quasi-3D method the key issue is where and how those equations are solved. Initially, from the initial conditions defined, the mass equation:

$$\partial\rho/\partial t + \nabla\cdot(\rho\vec{u}) = 0 \tag{1}$$

where ρ is the density and $\vec{u}$ is the flow velocity, is solved in the volumes, so that after discretization one gets

$$\rho^{n+1} = \rho^{n} + \frac{\Delta t}{V}\sum_{c=1}^{N_c}\rho_c^n u_c^n A_c \tag{2}$$

where the superscript n indicates the time step, Δt represents the time interval, V the volume of the cell, N_c the number of connectors and subscript c indicates that the variable is taken at the connectors. Variables without that subscript refer to the volumes.

After solving this equation, the equation of energy is considered:

$$\partial(\rho e_0)/\partial t + \nabla\cdot[(\rho e_0 + p)\vec{u}] = 0 \tag{3}$$

where p is the pressure and e_0 is the specific internal energy, defined as:

$$e_0 = c_v T + u^2/2 \tag{4}$$

Equation (3) is also solved in the volumes, and now discretization gives:

$$(\rho e_0)^{n+1} = (\rho e_0)^{n} + \frac{\Delta t}{V}\sum_{c=1}^{N_c}\rho_c^n e_0^n u_c^n A_c + \frac{\Delta t}{V}\sum_{c=1}^{N_c}p_c^n u_c^n A_c \tag{5}$$

Notice that in the energy equation no source terms, such as heat transfer, have been initially considered, and thus only adiabatic cases will be addressed in the rest of the paper.

Regarding the momentum equation:

$$\partial(\rho\vec{u})/\partial t + \nabla(p + \rho\vec{u}\vec{u}) = 0 \tag{6}$$

it is simplified as follows: Momentum is calculated at the connectors, rather than at the volumes, only in the direction orthogonal to the connector surface by projecting the flow velocity in the connected volumes onto that direction, as depicted in Figure 1, where the velocity u_c in the connector, and the projections of the volume flow velocity, u_{Ln} and u_{Rn}, are shown. Based on this assumption, it follows that one can calculate the momentum in the connector from a one-dimensional momentum equation as:

$$\partial(\rho u)/\partial t + \partial(\rho u^2 + p)/\partial x = 0 \tag{7}$$

A discretization similar to that used in the previous equations gives:

$$(\rho_c u_c A_c)^{n+1} = (\rho_c u_c A_c)^{n} + (\Delta t/\Delta L)[(\rho u_n^2 + p)_L + (\rho u_n^2 + p)_R]A_c \tag{8}$$

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Here, u_n is the velocity projection onto the direction orthogonal to the connector surface and subscripts R and L make reference to the volumes at the right and left of the connector, respectively.

It is important to notice that, with this simplification, only an equation for each connector must be solved, instead of three equations for each volume, which significantly reduces the computation time.

Finally, the momentum associated with the volumes is calculated by distributing the connector momentum between the two adjacent volumes. If the mesh is uniform, each volume will be assigned half the momentum of the connector. Knowing also the orientation of the connectors, a vector sum can be performed to obtain the momentum vector of each volume, as:

$$(\rho_c \vec{u} V)_v^{n+1} = \frac{1}{2}\sum_{c=1}^{N_c} (\rho \vec{u}_c A_c \Delta L)_c^{n+1} \tag{9}$$

Summarizing, the method is a second order method based on an explicit scheme with a staggered grid.

2.3 Flux-Corrected-Transport formulation

Here, first the formulation of the method for finite differences schemes will be outlined, and then its adaptation to the quasi-3D method described in section 2.2 will be described.

FCT consists of three stages [12]: The first stage is a transport stage based on the second order scheme considered. Next, a diffusion stage is performed which aims at reducing the numerical dispersivity introduced in the transport stage. With this purpose, a linear operator is defined that is introduced in the scheme in conservative form and allows to reduce or eliminate any unphysical numerical oscillations produced in the transport stage, thus reducing the accuracy to first order. The diffusive operator is defined as:

$$D_j(W) = \theta\left(W_{j+1/2}\right) - \theta\left(W_{j-1/2}\right) \tag{10}$$

where

$$\theta\left(W_{j+1/2}\right) = \left(W_{j+1} - W_j\right)\vartheta/4, \;\; \vartheta \in \mathbb{R}^+ \tag{11}$$

Here, W_j represents the conservative variable calculated in the transport stage at cell j, subscripts $j \pm 1/2$ denote the value of the variable corresponding to the midpoint between cells j and $j \pm 1$. The factor ϑ is taken to be $\vartheta \geq 1/2$ to avoid introducing any instability. This intermediate step is similar to the calculation of the connectors in the quasi-3D method. The guessed value $\bar{W}_j$ of the variable W_j may be computed in two ways: applying diffusion via smoothing, so that:

$$\bar{W}_j^{n+1} = W_j^{n+1} + D_j(W^{n+1}) \tag{12}$$

or applying diffusion via damping, in which case one has:

$$\bar{W}_j^{n+1} = W_j^{n+1} + D_j(W^{n}) \tag{13}$$

Finally, an anti-diffusion stage is applied, where the accuracy of the scheme used in the transport stage in those cells where the solution is smooth is restored, but preserving the

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accuracy of the diffusion operator in the neighbourhood of discontinuities occur. With this purpose, a non-linear operator A_j is defined as:

$$A_j(W) = \Psi(W_{j-1/2}) - \Psi(W_{j+1/2}) \tag{14}$$

Using the anti-diffusive limited flow defined in [14] one has:

$$\Psi(W_{j-1/2}) = s\max\left[0, \min\left((5/8)s\,\Delta W_{j-1/2}, (1/8)\left|\Delta W_{j+1/2}\right|, (5/8)s\,\Delta W_{j+3/2}\right)\right] \tag{15}$$

Here, s=sign$(\Delta W_{j-1/2})$, $\Delta W_{j-1/2} = W_j - W_{j-1}$, $\Delta W_{j+1/2} = W_{j+1} - W_j$ and $\Delta W_{j+3/2} = W_{j+2} - W_{j+1}$. Then, depending on the information used, one can devise different forms for this step, from which the two following ones will be used here: the Naive form:

$$\bar{\bar{W}}_j^{n+1} = \bar{W}_j^{n+1} + A_j(W^n) \tag{16}$$

and the Phoenical form:

$$\bar{\bar{W}}_j^{n+1} = \bar{W}_j^{n+1} + A_j(W^{n+1}) \tag{17}$$

As defined, flux correction techniques are conservative at the interior mesh points, since all the corrections are cancelled out along the duct except at the ends, where the anti-diffusion operator can be defined by evaluating the differences present in each case, i.e.:

$$\Psi(W_{j+1/2}) = s\max\left[0, \min\left((5/8)s\,\Delta W_{j-1/2}, (1/8)\left|\Delta W_{j+1/2}\right|,\right)\right] \tag{18}$$

for the right end, and

$$\Psi(W_{j-1/2}) = s\max\left[0, \min\left((1/8)\left|\Delta W_{j-1/2}\right|, (5/8)s\Delta W_{j+1/2},\right)\right] \tag{19}$$

for the left end.

The application of the FCT technique to a quasi-3D method poses some problems in the case of the mass and energy equations, as they both are calculated in the volumes, and it is not evident from which of the possible six connectors should the required data be taken. However, it is known that overshooting problems are related only with the momentum equation, which is computed at the connectors; since a connector always connects two volumes, the method can be adapted so that the FCT cells correspond to the connectors, and for the intermediate steps $j \pm 1/2$ the projection of the variables corresponding to the volumes connected by connector j are used. For instance, the equation for conservation of momentum with diffusion via damping would be as follows:

$$(\overline{\rho u_c A_c})_j^{n+1} = (\rho u_c A_c)_j^{n+1} + D_j(\rho u_c A_c)_j^n \tag{20}$$

and thus the diffusive term becomes:

$$D_j(\rho u_c A_c)_j^n = \theta(\rho u_n A_c)_{j+1/2}^n - \theta(\rho u_n A_c)_{j-1/2}^n \tag{21}$$

where

$$\theta(\rho u_c A_c)_{j+1/2}^n = \left[(\rho u_n A_c)_{j+1}^n - (\rho u_n A_c)_j^n\right]\vartheta/4 \tag{22}$$

For the anti-diffusion stage, equations (14) to (19) can be adapted in a similar way, so that the FCT technique can be readily adapted to a quasi-3D model.

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3. Stability and convergence analysis

In order to establish the stability and convergence of the method, the first step is to ensure that the CFL condition is satisfied. This condition, obtained by Courant, Friedrichs and Lewy [15] in the context of the demonstration of the existence of a solution to certain partial differential equations (PDE), establishes that, for any numerical method, the domain of dependence of the method should include the domain of dependence of the PDE, at least in the limit when the mesh size Δx and the time step Δt tend to 0. This condition is usually expressed in term of the Courant number C as:

$$C = \lambda \Delta t / \Delta x < 1 \tag{10}$$

where λ is the propagation speed of the signal, which typically corresponds to the addition of the speed of sound and the flow velocity. In the case of the quasi-3D model presented, the CFL condition is slightly modified as:

$$C = \lambda \Delta t A_c / V < 1 \tag{11}$$

After securing the CFL condition, the method described is applied to the simple case of the shock-tube problem [16], often used as to validate computational methods and to demonstrate their predictive capabilities under singularities associated with the different types of waves that may appear in an unsteady problem.

In this problem, two gases with different thermo- and fluid-dynamic states are put into contact. To some extent, when unsteady flow is solved with the type of methods discussed in this paper, such a problem is solved in each cell. In Figure 2(a) an outline of the initial state of the problem is shown. After a certain time, the contact discontinuity has travelled with the flow velocity, whereas a shock wave has travelled in the same direction with the speed of sound plus the flow velocity, and a rarefaction wave has travelled in the opposite direction at the speed of sound minus the flow velocity. These perturbations divide the duct into four zones with different thermo- and fluid-dynamic fluid states, as shown in Figure 2(b).

The initial conditions in the present case were: $p_1 = 5$ bar, $p_4 = 1$ bar, $T_1 = 1200$ K, $T_4 = 300$ K, and $u_1 = u_4 = 0$ ms^{-1}. A 1D mesh was used, with 100 volumes 1 cm long. The results obtained with the raw method (without FCT) are shown in Figure 3, together with the theoretical solution available in the literature [16]. Two main differences can be observed: on one hand, the expected overshooting associated with the propagation of the shock wave can be clearly seen; on the other hand, it appears that the method introduces some diffusion in the contact discontinuity, which spreads in space. This is obviously related with the solution procedure used for the mass and energy equations, and need not be a serious shortcoming of the method, as sharp discontinuities as those seen in the theoretical solution do not exist in real flow situations.

Once the main features of the solution provided by the method were identified, different formulations of the FCT method were tested, considering the possible combinations of the different versions of the diffusion stage (damping or smoothing) and of the anti-diffusion stage (naive or phoenical). In all the cases, the minimum possible value of $\vartheta = 1/2$ was used, in order to avoid excessive dissipation.

First, in Figures 4 and 5 results of introducing the diffusion via smoothing are shown; for brevity, only results for pressure and velocity, i.e. those variables directly affected by the

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momentum equation on which the FCT has been applied, are plotted. Both the results of considering only the diffusion stage and of considering also the anti-diffusion stage are shown. It can be seen that, even if the phoenical form (Figure 5) is rather more efficient than the naive form (Figure 4) in removing the overshoots at the shock wave, the remaining instabilities are excessive, thus indicating that diffusion via smoothing is not well adapted to the basic computational method. In fact, the application of the anti-diffusion stage does not introduce any improvement on the shock wave description, as this is better when only the diffusion stage is considered. However, it is precisely the anti-diffusion step who provides a suitable description of the rarefaction wave.

If the diffusion is introduced via damping, the results are in general much better. Using the naive form in the anti-diffusion stage, the results shown in Figure 6 are obtained. It can be observed that just a small and local overshoot remains, but this overshoot virtually disappears when the phoenical form is used in the anti-diffusion stage, as shown in Figure 7, where the four relevant magnitudes are shown as in Figure 3. It can be seen that, for the four variables, the shock wave is correctly described, and only some very small perturbations can be observed in the tail of the rarefaction wave. Therefore, one may conclude that the application of the FCT method to the momentum equation, given that diffusion is incorporated via damping, and the phoenical form of the anti-diffusion stage is used, provides a suitable alternative to the introduction of an artificial momentum diffusion term or an equivalent dissipative force into the momentum equation.

Summary and conclusions

A quasi-3D model which makes use of a non-linear second order time and space discretization based on finite volumes has been developed. Such methods are affected by the occurrence of overshoots in the vicinity of discontinuities in the flow variables and do not satisfy the stability requirement, even if the CFL criterion is accomplished. It has therefore been mandatory that some additional term, such as an equivalent friction force or a momentum diffusion term, is included in the momentum equation.

Seeking for an alternative allowing avoidance of overshoots at discontinuities, a Flow Corrected Transport technique has been adapted to the quasi-3D method presented. Thanks to the staggered mesh which the method is based on, it has only been necessary to apply the FCT technique to the momentum equation, so that the resulting method can be directly apply to three-dimensional cases without further developments.

However, in order to highlight the relevant aspects of the method, it was validated in the one-dimensional case of the well-know shock-tube problem. The four possible combinations of diffusion stage (smoothing and damping) and anti-diffusion stage (naive and phoenical) were checked, with the results that the combination of dissipation via damping together with the phoenical form of the anti-diffusion term provides satisfactory results. Therefore, such a method represents a suitable alternative for the computation of gas flows in intake and exhaust systems of internal combustion engines.

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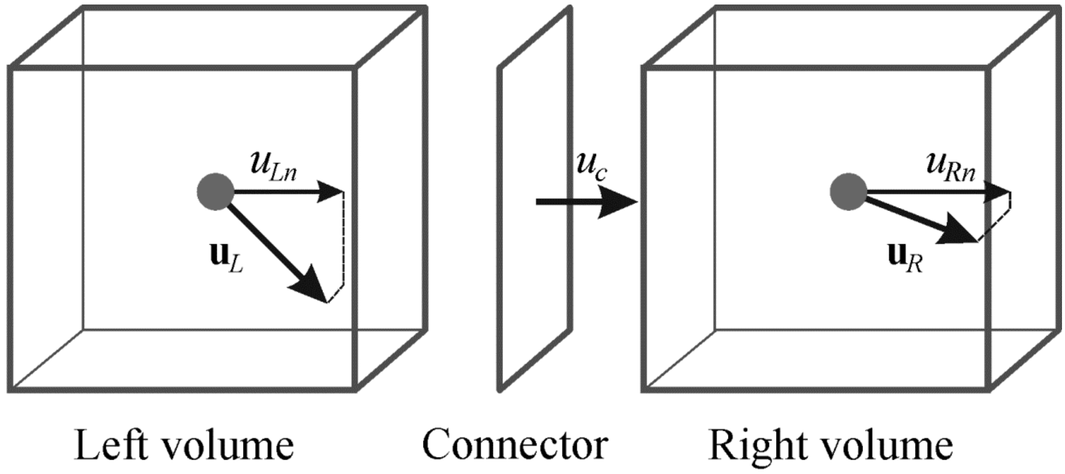

Figure 1: Basic mesh elements and definition of velocity projections.

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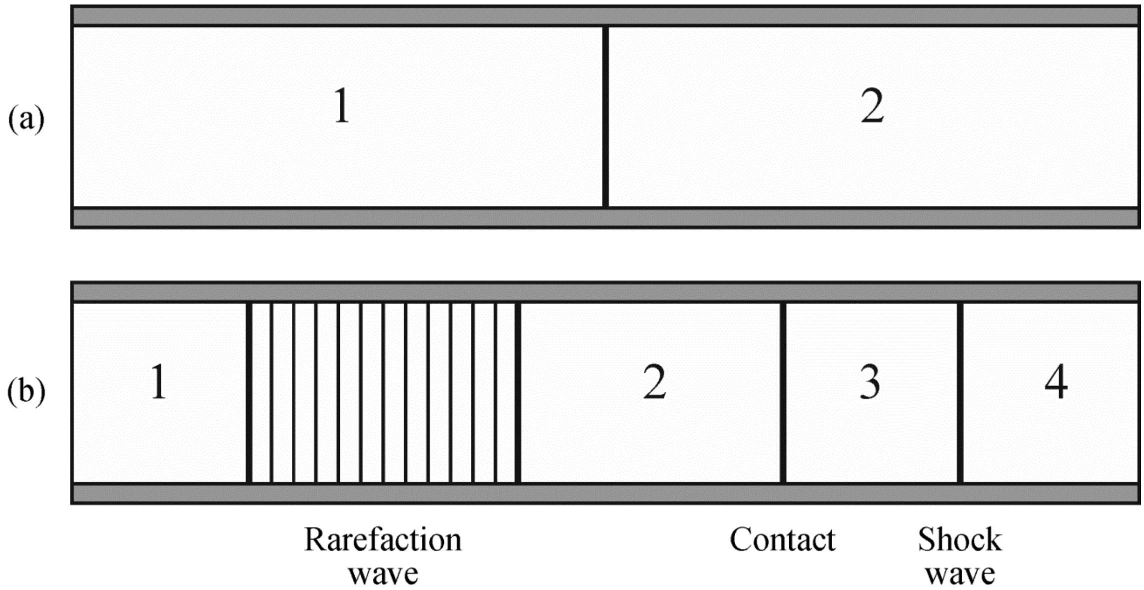

Figure 2: Initial state of the shock-tube problem (a) and scheme of the solution structure after a certain time (b).

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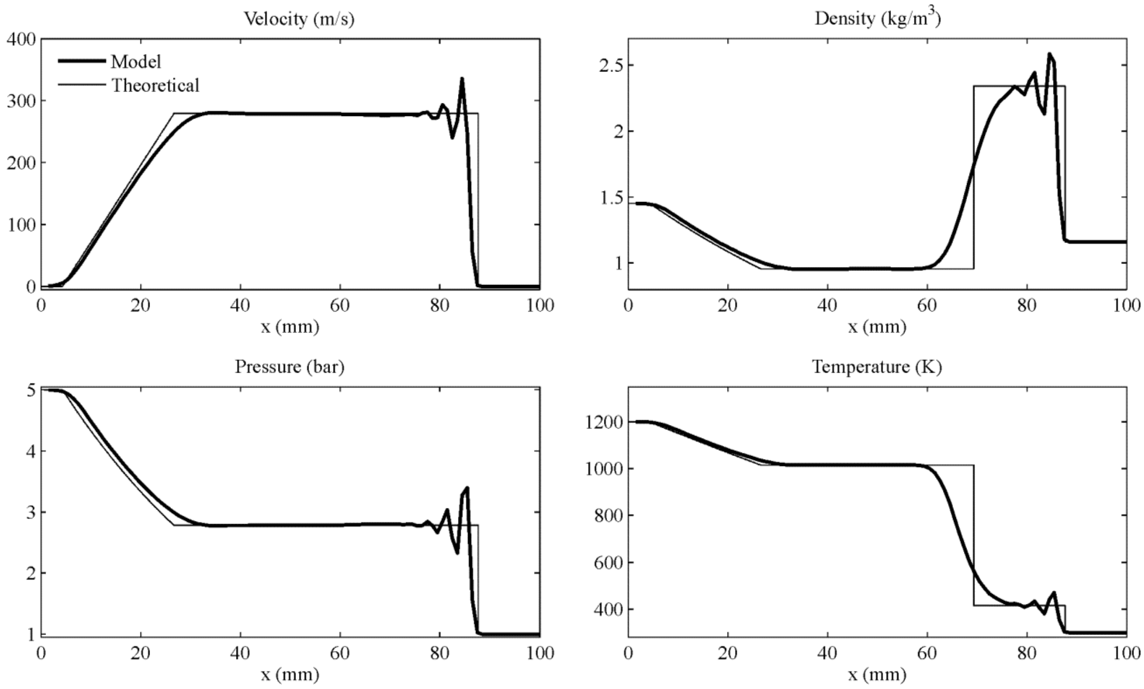

Figure 3: Comparison of the solution obtained without FCT and the theoretical solution of the shock-tube problem.

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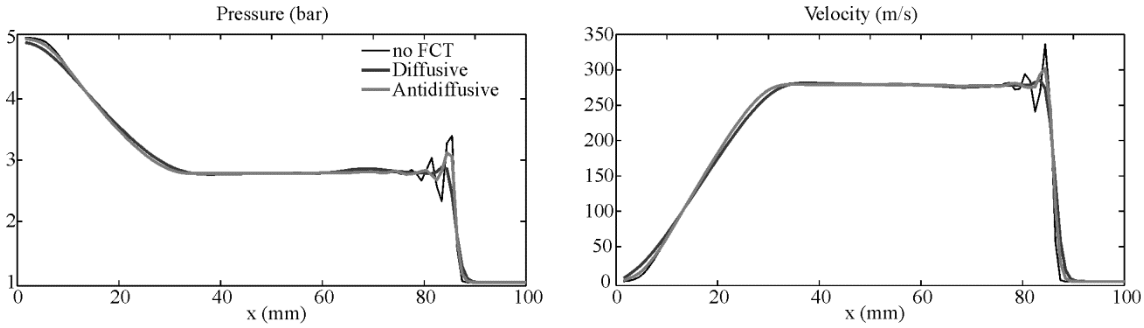

Figure 4: Comparison of the solution obtained for the shock-tube problem without FCT and with FCT with smoothing diffusion and naive anti-diffusion.

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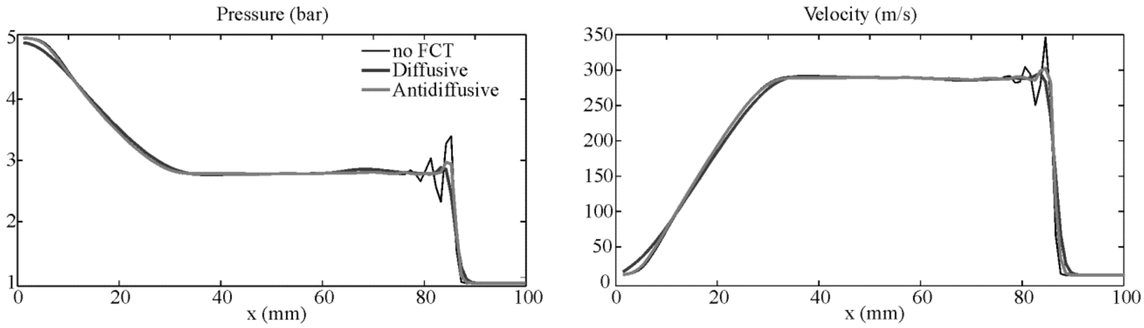

Figure 5: Comparison of the solution obtained for the shock-tube problem without FCT and with FCT with smoothing diffusion and phoenical anti-diffusion.

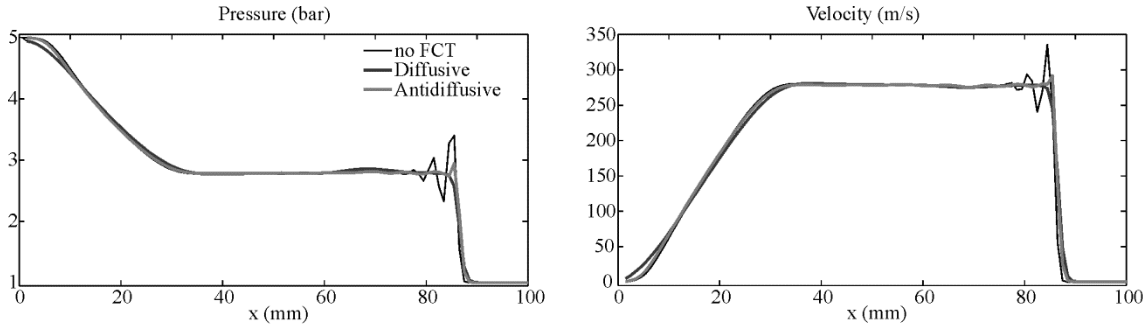

Figure 6: Comparison of the solution obtained for the shock-tube problem without FCT and with FCT with damping diffusion and naive anti-diffusion.

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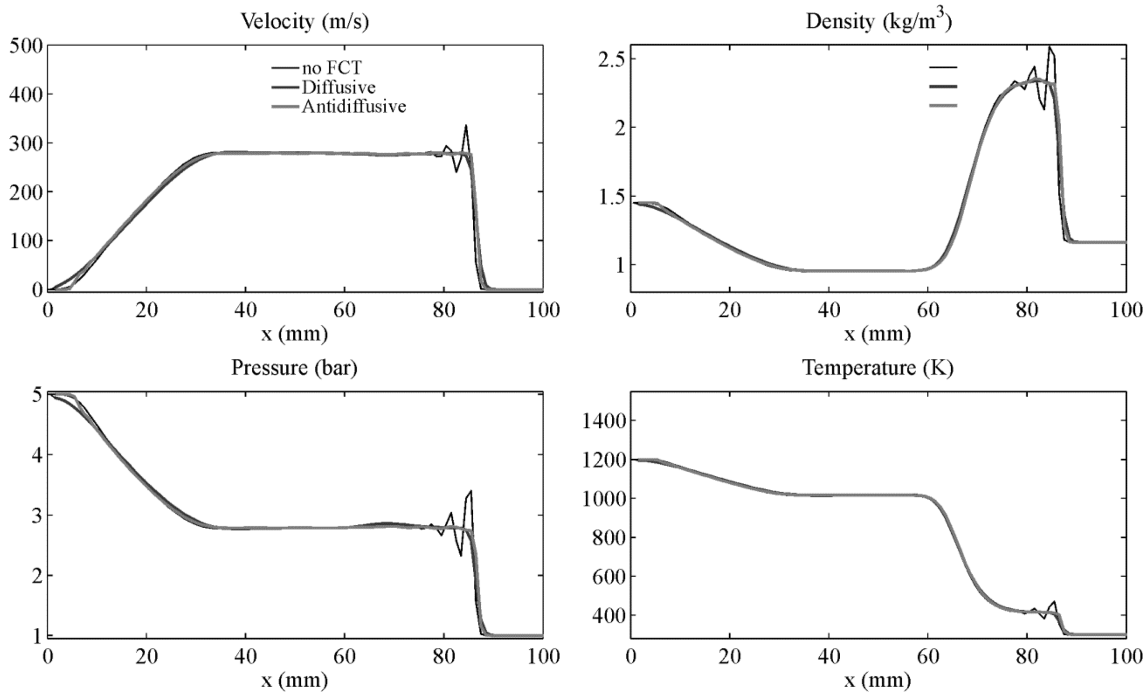

Figure 7: Comparison of the solution obtained for the shock-tube problem without FCT and with FCT with damping diffusion and phoenical anti-diffusion.

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