

Document downloaded from:

<http://hdl.handle.net/10251/60419>

This paper must be cited as:

Serrano Cruz, JR.; Climent, H.; Piqueras, P.; Garcia Afonso, O. (2013). Analysis of shock capturing methods for chemical species transport in unsteady compressible flow. *Mathematical and Computer Modelling*. 57(7-8):1751-1759. doi:10.1016/j.mcm.2011.11.026.



The final publication is available at

<http://dx.doi.org/10.1016/j.mcm.2011.11.026>

Copyright Elsevier

Additional Information

Analysis of shock capturing methods for chemical species transport in unsteady compressible flow

J. R. Serrano, H. Climent, P. Piqueras*, O. García-Afonso

Universitat Politècnica de València, CMT-Motores Térmicos, Camino de Vera s/n, 46022 Valencia, Spain.

Abstract

This paper presents a chemical species transport model to account for variable composition and gas properties along the flow path in internal combustion engines. It is described the numerical solution to adapt the gas dynamic model to chemical species transport in boundary conditions by means of the Method of Characteristics and in volumes by means of a filling and emptying model. The performance for chemical species transport in 1D elements of shock-capturing methods, such as the two-step Lax&Wendroff method and the Sweby's TVD scheme considering several flux limiter definitions, is carried out by means of shock-tube tests. The influence of the fluid modelling as perfect or non-perfect gas on the numerical methods features and the flow characteristics on shock-tube results is analysed.

Keywords: gas dynamics, chemical species, finite difference, thermal properties, internal combustion engines

1. Introduction

During the last years, the aftertreatment systems have become a new standard element of internal combustion engines. For the case of diesel engines, the current and future emission regulations have led manufacturers and researchers to the use of diesel oxidation catalysts, diesel particulate filters and selective catalyst reduction systems. The influence of all these elements in the gas flow path, whose analysis is essential for the optimization of the engine performance [1], justifies their integration into gas dynamic codes. Additionally, the inclusion of specific models for every of these elements involves the modeling of the chemical species transport. It is needed for the subsequent calculation of the chemical kinetics in the aftertreatment systems to evaluate the heat released across these systems and to predict the engine emissions.

The solution of the conservation equations system in gas dynamic codes with transport of chemical species has been approached by several authors. Winterbone and Pearson [2] applied flux-corrected transport (FCT), the Davis's TVD algorithm and artificial compression terms to try to mitigate spurious oscillations produced at discontinuities by second order symmetric finite difference numerical methods. Later, Onorati *et al.* applied the chemical species transport to ignition combustion engines [3]. In these works, several numerical methods are applied: the

*P. Piqueras. CMT-Motores Térmicos, Universitat Politècnica de València.
Camino de Vera s/n, 46022 Valencia, Spain. Phone: +34 963877650 Fax: +34 963877659 e-mail: pedpicab@mot.upv.es
Preprint submitted to Mathematical and Computer Modelling *November 11, 2011*

CE-SE method, the MacCormack predictor-corrector method with the addition of flux-limiting techniques and the Galerkin finite element method. Yuhua and Reitz [4] proposed a 1D model for EGR level prediction applying the Method of Characteristics. Finally, Arnau *et. al* [5] applied a semi-implicit CE-SE method to chemical species transport in tapered ducts of ICE.

In this work, a chemical species transport model is proposed to be integrated in an open source gas dynamic model so-called OpenWAMTM [6, 7]. The chemical species are tracked across any element of the engine. These elements are represented by 1D elements, 0D elements, boundary conditions or a combination of them. The conservation equations are solved in every of these elements with specific methods which need to be adapted to chemical species transport: shock-capturing methods in 1D elements, such as the two-step Lax&Wendroff method [8] and the Sweby's TVD scheme [9], a filling and emptying model in 0D elements [7] and the Method of Characteristics in boundary conditions [10]. The influence of the shock-capturing method in the solution of chemical species transport is analysed by means of representative shock-tube test in ICE. In the case of the Sweby's TVD scheme, the effect of several flux limiters is also evaluated. Furthermore, the transport of chemical reactions allow to model the fluid as a perfect or non-perfect gas, so that the influence of variable gas composition and temperature on numerical solution and flow characteristics along ICE can be assessed.

2. Chemical species transport model

Wave actions models consider the flow to be essentially one-dimensional in nature. This statement is right when the length-to-diameter is high enough and the turbulent flow is totally developed. The governing equations for one-dimensional unsteady compressible non-homentropic flow, i.e. the mass, momentum and energy conservation equations, form a hyperbolic system of partial differential equations in the vector form of equation (1). The vectors are represented in strong conservative form in equation (2):

$$\frac{\partial \mathbf{W}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \mathbf{C}_1 + \mathbf{C}_2 = 0, \quad (1)$$

$$\begin{aligned} \mathbf{W}(x, t) &= \begin{bmatrix} \rho F \\ \rho u F \\ F \left(\rho \frac{u^2}{2} + \frac{p}{\gamma-1} \right) \end{bmatrix} & \mathbf{F}(\mathbf{W}) &= \begin{bmatrix} \rho u F \\ (\rho u^2 + p) F \\ u F \left(\rho \frac{u^2}{2} + \frac{\gamma p}{\gamma-1} \right) \end{bmatrix} \\ \mathbf{C}_1(x, \mathbf{W}) &= \begin{bmatrix} 0 \\ -p \frac{dF}{dx} \\ 0 \end{bmatrix} & \mathbf{C}_2(\mathbf{W}) &= \begin{bmatrix} 0 \\ g \rho F \\ -q \rho F \end{bmatrix}. \end{aligned} \quad (2)$$

In equations (1) and (2), \mathbf{W} represents the solution vector; \mathbf{F} is the flux vector (mass, momentum and energy); \mathbf{C}_1 and \mathbf{C}_2 include the source terms that take into account the effects of area changes, friction and heat transfer.

The combined solution of equation (1) and the state equation of the ideal gases allows obtaining the flow properties at every node of the duct and time instant considering different numerical methods, time marching and spatial discretization techniques in the solution [11, 12, 13, 14]. Additionally, it is possible to consider the inclusion of the chemical species transport equation to the governing equations system without any change in the solution procedure and the order of accuracy of the applied numerical methods.

The solution of the chemical species transport along the 1D elements requires the addition of $n - 1$ equations of chemical species conservation in the governing equations system, where n is the number of chemical species to be transported. The chemical species conservation equation in vector form is

$$\frac{\partial(\rho\mathbf{Y}F)}{\partial t} + \frac{\partial(\rho u\mathbf{Y}F)}{\partial x} = \rho F \dot{\mathbf{Y}}, \quad (3)$$

where \mathbf{Y} is a vector including the mass fraction of $n - 1$ different chemical species. The mass fraction of the chemical species n is given by the compatibility equation

$$Y_n = 1 - \sum_{j=1}^{n-1} Y_j. \quad (4)$$

Equation (3) considers the convective transport and the effect of conversion rate because of chemical reactions. The term due to diffusion between chemical species is not considered because its influence is negligible in comparison with the velocity transport in ducts of internal combustion engines.

Taking into account the transport of chemical species transport in 1D elements, the governing equations system in vector and strong conservative form is formulated as

$$\begin{aligned} \mathbf{W}(x, t) &= \begin{bmatrix} \rho F \\ \rho u F \\ F \left(\rho \frac{u^2}{2} + \frac{p}{\gamma-1} \right) \\ \rho F \mathbf{Y} \end{bmatrix} & \mathbf{F}(\mathbf{W}) &= \begin{bmatrix} \rho u F \\ (\rho u^2 + p) F \\ u F \left(\rho \frac{u^2}{2} + \frac{\gamma p}{\gamma-1} \right) \\ \rho u F \mathbf{Y} \end{bmatrix} \\ \mathbf{C}_1(x, \mathbf{W}) &= \begin{bmatrix} 0 \\ -\rho \frac{dF}{dx} \\ 0 \\ 0 \end{bmatrix} & \mathbf{C}_2(\mathbf{W}) &= \begin{bmatrix} 0 \\ g \rho F \\ -q \rho F \\ \rho F \dot{\mathbf{Y}} \end{bmatrix}. \end{aligned} \quad (5)$$

2.1. Adaptation of numerical methods for chemical species transport

The solution of the governing equations system with chemical species transport needs the adaptation of the numerical methods. In the case of the finite difference numerical methods applied in this work, the following considerations have to be taken into account:

- In the case of the two-steps Lax&Wendroff method [8], the $n - 1$ equations of chemical species transport are discretized in the same way than the mass conservation equation. The only difference is that both the solution and the flux terms have to be multiplied by the mass fraction of the chemical species i , Y_i .
- In the case of the Sweby's TVD scheme [9] the transport of chemical species requires to consider that the vector formulation of the method evaluates the Jacobian matrix of the governing equations system. The introduction of the chemical species conservation equations does not introduce new eigenvalues to the equations system. Therefore, the vector formulation of the Sweby's TVD scheme is applied to the solution of the mass, momentum and energy conservation equations, whereas every chemical species conservation equation is solved applying the scalar formulation.

2.2. Chemical species transport in boundary conditions and 0D elements

The transport of chemical species in 1D elements can be performed solving the governing equations system by means of finite difference numerical methods. However, wave action models consider other types of elements that can be found in internal combustion engine: cylinders, turbine, compressor, diesel particulate filters, intercoolers, volumes, etc. All this kind of systems are modelled as boundary conditions, 0D elements or a combination of these with 1D elements.

Boundary conditions

The numerical methods applied to know the fluid conditions in 1D elements allow obtaining them only in the internal nodes. The solution of the end nodes of 1D elements requires to consider the boundary conditions, which are solved applying the Method of Characteristics (MOC) [10, 15]. The inclusion of the chemical species transport does not affect the solution procedure of the MOC but can modify the value of the Riemann variables and the entropy level. Therefore, next aspects have to be considered:

- The chemical species are tracked from the point (y, t) to the end of the duct across the path-lines.
- As solution in this work the MOC formulation for perfect gas is applied but the gas properties are calculated as function of composition and temperature at time t both in point (y, t) , from which the characteristic lines or the path-line leaves, and at the end node to obtain the flow conditions in time $t + \Delta t$. In this way it is obtained an improvement in the evaluation of the friction and heat transfer influence along the characteristic lines or the path-line without a substantial increase of complexity and computation effort because of the non-perfect formulation of the MOC.

0D elements

The 0D elements are those which are able to accumulate flow being the flow conditions constant in all its volume at each calculation instant. This is the case of the cylinders, turbine or other volumes in intercoolers, aftertreatment devices, etc. This kind of elements are solved by means of a filling and emptying model [7] that includes the mass and energy conservation equations for open systems combined with the ideal gas state equation.

The chemical species transport across 0D elements involves the addition of $n - 1$ mass conservation equations to calculate the mass fraction of $n - 1$ chemical species,

$$\Delta m_{iny_j} = \sum_i \dot{m}_i Y_{jcc_i} \Delta t, \quad (6)$$

where m_{iny_j} is the mass of the chemical species j inside the 0D element and Y_{jcc_i} is the mass fraction of the chemical species j entering to or exiting from the 0D element through the boundary condition i . Finally, the mass fraction of the chemical species j at time instant will be

$$Y_j = \frac{m_{iny_j} + \Delta m_{iny_j}}{m_{in} + \Delta m_{in}}. \quad (7)$$

As in the case of the 1D elements, the mass fraction of the chemical species n is given by the compatibility equation (4).

3. Results and discussion

This section is focused on the evaluation of the two-step Lax&Wendroff method and the Sweby's TVD scheme to solve the governing equations with chemical species transport. These methods are applied to shock-tube tests derived from the Riemann problem. The simulations are performed assuming homentropic flow (no friction, no heat transfer and no area changes) because with this assumption the Riemann problem has exact solution, which can be obtained solving the Rankine-Hugoniot equations iteratively.

Case I: Thermal and composition contact discontinuity

Case I is a shock-tube test which consists of a duct with a diaphragm separating two regions where the flow has different conditions in pressure, temperature and composition. When the diaphragm is removed, the initial conditions generate a shock wave and a strong thermal and composition contact discontinuity.

The separation between both flow regions is imposed in the centre of the domain defined as $D = \{x : x \in [-1, 1]\}$, which is expressed in meters. The diaphragm is removed at instant $t = 0$ s. The spatial mesh size is 20 mm. The initial conditions in every region have been taken from the works of Winterbone y Pearson in [2] and are detailed in Table 1. These conditions are not representative of flow in internal combustion engine. However, they are very useful to assess numerical methods and the influence of the gas properties on the mass, momentum and energy transport.

The exact solution of the problem, which is represented in Figures 1 and 2 by the solid line, has been obtained considering the fluid to be a perfect gas with a molar composition $X_{N_2} = 0.7$ and $X_{CO_2} = 0.3$ and at 300 K. At these conditions, it is given that $\gamma = 1.36$, $R = 253.41$ J/kgK and $c_p = 959.5$ J/kgK. These properties have been applied to obtain the numerical solution with the assumption of perfect gas for the case of the two-step Lax&Wendroff method and the Sweby's TVD scheme, which are represented in Figure 1 and Figure 2 respectively.

Figure 1 shows the results corresponding to the two-step Lax&Wendroff method. As common in symmetric shock-capturing methods of second or higher order, the solution is dispersive and spurious around the discontinuities. This behavior also appears in the transport of chemical species. Furthermore, it is proved that the mass fraction of any chemical species can be lower than 0.

Regarding the numerical solution considering variable gas properties depending on the gas temperature and composition, it is worth to note that the main differences with respect to the exact solution appear in the left side. It is because of the fact that the exact solution has been obtained with the fluid properties of the right side. The flow which is being transported is such in the left side. Its composition and temperature impose $\gamma = 1.21$ and lead to sound differences.

The differences affect mainly the propagation velocity of the rarefaction wave, since it is the discontinuity more exposed to fluid properties with respect to the exact solution. A slight influence appears also in the region between the contact discontinuity and the shock wave because of the temperature effect.

The same simulations have been performed with the Sweby's TVD scheme applying the Van Leer flux limiter, as discussed in section 3.1. As shown in Figure 2, the use of this method allow removing the spurious oscillations around the discontinuities, independently of the perfect or non-perfect gas assumption. The reason is the reduction of the method accuracy to first order in the region of the discontinuity by means of the flux limiter application. However, this approach involves numerical diffusion around the discontinuity, which is typical from first order methods.

With respect to the transport of chemical species, the numerical diffusion affects the mass fraction solution mainly in the region of the contact discontinuity but influences also in the proximity of the shock wave and the end of the rarefaction wave. As Winterbone and Pearson suggest in [2], these features of high-resolution schemes can be related with its development to have specific characteristics in the solution of scalar conservation laws. Its application to the solution of the governing equations with the use of the scalar formulation for chemical species equation can prompt that this kind of schemes be not able to provide results in agreement with the TVD condition under some flow conditions.

Case II: Contact discontinuity in ICE

This case is devoted to evaluate the order of magnitude of the influence of the non-perfect gas assumption in the solution of the governing equations under representative flow conditions in internal combustion engines.

A shock-tube test is approached to analyse the transport of a contact discontinuity between a wave of exhaust gas and fresh air (intake flow). The test consists again of a duct with a diaphragm separating two regions where the flow has different conditions in pressure, temperature and composition, which are described in Table 2. The problem is simplified to steady flow in order to isolate the propagation of the contact discontinuity from pulsating phenomena. It makes possible to study the effect of the flow properties modeling on the propagation of the shock and rarefaction waves.

The fluid at the left of the diaphragm is composed of burned gases at 773 K in temperature. When the diaphragm is removed, the fluid moves towards the right, moving the air on this side of the diaphragm, which is at 333 K, due to the pressure gradient. It has been set to 0.45 bar in order to represent a gradient between the peak pressure of a exhaust pressure pulse and the intake pressure.

The exact solution for this test has been obtained considering that the fluid is a perfect gas whose properties are $\gamma = 1.4$, $R = 287 \text{ J/kgK}$ and $c_p = 1004.5 \text{ J/kgK}$. The numerical solution has been calculated with the two-step Lax&Wendroff method and the Sweby's TVD scheme with a spatial mesh size of 20 mm. In the case of the numerical solution, the properties of the gas has been considered to be variable with temperature and composition.

The results are shown in Figure 3 and evidences that the variable gas properties calculation brings noticeable differences in the prediction of temperature, pressure and velocity around thermal and composition contact discontinuities typical from ICE. At the same time, these variations affects the propagation velocity of shock and rarefaction waves and the position of the contact discontinuity.

These effects are disguised in the case of the Sweby's TVD scheme because of the non-physical diffusion. Nevertheless, although the two-step Lax&Wendroff method produces spurious oscillations, the lack of non-physical diffusion in this method allow to state that the propagation velocity of the rarefaction and shock waves is lower when variable gas properties are considered.

3.1. Effect of flux limiter of Sweby's TVD method on chemical species transport

The results of the Sweby's TVD scheme shown in Case I and Case II have been obtained adopting the flux limiter proposed by Van Leer [16]. There are available other flux limiters, but usually without important effects on the solution.

This general conclusion is extended in this work to the specific problem of chemical species transport in non-perfect ideal gases. Figure 4 represents the results regarding pressure, temperature and velocity for Case I that are obtained by the Sweby's TVD method with every second order flux limiter defined in Table 3.

The flux limiter definition does not equally influence all the physical magnitudes and waves. In the case of the pressure, there is not any effect on the solution. However, the temperature solution is sensitive to the flux limiter definition around the contact discontinuity. As pointed out in Figure 4, the region affected for the numerical diffusion can reach a length greater than 50 mm before and after the discontinuity depending on the flux limiter. This region would be larger if the spatial mesh size were increased. Finally, the velocity profile is only slightly affected around the rarefaction wave.

The effect of every flux limiter on the transport of chemical species is analysed in Figure 5. It is only represented the transport of N_2 , whereas the CO_2 is the complementary according to equation (7). The numerical diffusion affects around the contact discontinuity in a similar way than in the case of the temperature. It is observed that those flux limiters causing less numerical diffusion generate a slight spurious oscillation in the proximity of the discontinuity. On the other hand, the most diffusive flux limiters (Roe's *minmod* on the left and Van Albada's flux limiter on the right) do not show any oscillation and its solution achieve a better performance of the TVD condition.

According to these results, the use of the flux limiter with the optimum balance between numerical diffusion and spurious oscillation around discontinuities is advisable. The Van Leer's flux limiter has shown the best compromise between these characteristics when assuming variable gas properties and composition.

4. Summary and conclusions

The paper presents a chemical species transport model for gas dynamic calculation. The model has been integrated into OpenWAM and adapted to the solution of the governing equations system in 1D elements, which are solved applying shock-capturing methods, 0D elements and boundary conditions, which have required the adaptation of a filling and emptying model and the Method of Characteristics respectively.

The two-step Lax&Wendroff method and the Sweby's TVD scheme considering several flux limiters have been adapted to the transport of chemical species. The two-step Lax&Wendroff method has shown typical spurious oscillations of second order symmetric schemes. On the other hand, the Sweby's TVD scheme mitigates this effect but introduces numerical diffusion around the discontinuities with dependency on the flux limiter definition. Influence of the rarefaction and shock waves has been also identified on the chemical species transport.

The transport of the chemical species has additionally allowed the solution of the governing equations considering non-perfect ideal gas. The shock-tube tests results have shown that variable gas properties as function of temperature and composition affect the values of gas conditions and wave propagation velocity at typical ICE operating conditions with respect to the perfect gas assumption.

Acknowledgements

This work has been partially supported by the spanish Ministerio de Ciencia e Innovación through grant number DPI2010-20891-C02-02.

- [1] V. Bermúdez, J. R. Serrano, P. Piqueras, O. García-Afonso, Assessment by means of gas dynamic modelling of a pre-turbo diesel particulate filter configuration in a turbocharged HSDI diesel engine under full-load transient operation, *Proceedings of the Institution of Mechanical Engineers, Part D: Journal of Automobile Engineering* 225 (9) (2011) 1134–1155.
- [2] D. E. Winterbone, R. J. Pearson, Calculating the effects of variations in composition on wave propagation in gases, *International Journal of Mechanical Science* 35 (6) (1993) 517–37.
- [3] A. Onorati, G. Ferrari, Modeling of 1-D unsteady flows in I.C. engine pipe systems: numerical methods and transport of chemical species, in: *SAE Technical Paper 980782*, 1998.
- [4] Z. Yuhua, R. Reitz, A 1-D gas dynamics code for subsonic and supersonic flows applied to predict egr levels in a heavy-duty diesel engine, *International Journal of Vehicle Design* 22 (1999) 227–252.
- [5] J. M. Arnau, S. Jerez, L. Jódar, J. V. Romero, A semi-implicit Conservation Element-Solution Element method for chemical species transport simulation to tapered ducts of internal combustion engine, *Mathematics and Computers in Simulation* 73 (2006) 28–37.
- [6] Openwam website, CMT-Motores Térmicos (Universitat Politècnica de València). www.openwam.org (2011).
- [7] J. Galindo, J. R. Serrano, F. J. Arnau, P. Piqueras, Description and analysis of a one-dimensional gas-dynamic model with Independent Time Discretization, in: *Proceedings of the Spring Technical Conference of the ASME Internal Combustion Engine Division*, 2008, pages 187-197.
- [8] P. D. Lax, B. Wendroff, Systems of conservation laws, *Communications on Pure and Applied Mathematics* 17 (1964) 381–398.
- [9] P. K. Sweby, High resolution schemes using flux limiters for hyperbolic conservation laws, *SIAM Journal of Numerical Analysis* 21 (5) (1984) 995–1011.
- [10] R. S. Benson, *The thermodynamics and gas dynamics of internal-combustion engines*, Vol. 1, Clarendon Press, New York, 1982.
- [11] J. R. Serrano, F. J. Arnau, P. Piqueras, A. Onorati, G. Montenegro, 1D gas dynamic modelling of mass conservation in engine duct systems with thermal contact discontinuities, *Mathematical and Computer Modelling* 49 (5-6) (2009) 1078–1088.
- [12] J. Galindo, J. R. Serrano, F. J. Arnau, P. Piqueras, High-frequency response of a calculation methodology for gas dynamics based on Independent Time Discretisation, *Mathematical and Computer Modelling* 50 (5-6) (2009) 812–822.
- [13] J. Galindo, J. R. Serrano, F. J. Arnau, P. Piqueras, Description of a Semi-Independent Time Discretization methodology for a one-dimensional gas dynamics model, *Journal of Engineering for Gas Turbines and Power* 131 (2009) 034504.
- [14] A. J. Torregrosa, J. R. Serrano, F. J. Arnau, P. Piqueras, A fluid dynamic model for unsteady compressible flow in wall-flow diesel particulate filters, *Energy* 36 (2011) 671–684.
- [15] J. M. Desantes, J. R. Serrano, F. J. Arnau, P. Piqueras, Derivation of the method of characteristics for the fluid dynamic solution of flow advection along porous wall channels, *Applied Mathematical Modelling*, (2011), doi:10.1016/j.apm.2011.09.090.
- [16] B. Van Leer, Towards the ultimate conservative difference scheme. ii. Monotonicity and conservation combined in a second order scheme, *Journal of Computational Physics* 14 (1974) 361–370.
- [17] B. Van Leer, Towards the ultimate conservative difference scheme. iii. Upstream-centered finite-difference schemes for ideal compressible flow, *Journal of Computational Physics* 23 (1977) 263–275.
- [18] P. L. Roe, Characteristic-based scheme for the Euler equations, *Annual Review of Fluid Mechanics* 18 (1986) 337–365.
- [19] S. R. Chakravarthy, S. Osher, High resolution applications of the osher upwind scheme for the euler equations, in: *Proc. AIAA 6th Computational Fluid Dynamics Conference*, pp. 363-373, 1983.
- [20] N. P. Waterson, H. Deconinck, A unified approach to the design and application of bounded higher-order convection schemes, in: *Proceedings of the Ninth International Conference on Numerical Methods in Laminar and Turbulent Flow*, Atlante, Pineridge Press, 1995.
- [21] G. D. Van Albada, B. Van Leer, W. W. Roberts, A comparative study of computational methods in cosmic gas dynamics, *Astronomy and Astrophysics* 108 (1) (1982) 76–84.

NOTATION

0D	zero-dimensional
1D	one-dimensional
c_p	specific heat at constant pressure
\mathbf{C}	source term vector
CE-SE	Conservation-Element Solution-Element
EGR	exhaust gas recirculation
F	cross-section area
FCT	Flux-Corrected Transport
\mathbf{F}	flow term vector
g	friction term
ICE	internal combustion engine
\dot{m}	mass flow
MOC	Method of Characteristics
n	number of chemical species
p	gas pressure
q	heat per unit of time and area
R	specific gas constant
t	time dimension
TVD	Total Variation Diminishing
u	gas velocity
\mathbf{W}	field variable vector
OpenWAM	Open source code Wave Action Model
x	axial dimension
X	molar fraction
Y	mass fraction
\mathbf{Y}	mass fraction vector
$\dot{\mathbf{Y}}$	vector of rate of mass fraction variation

Greek letters

γ	specific heat ratio
ψ	flux limiter
ρ	gas density

Table 1: Case I: Initial conditions.

Property	Left	Right
p [bar]	5	1
T [K]	1000	300
u [m/s]	0	0
X_{N_2} [-]	0.3	0.7
X_{CO_2} [-]	0.7	0.3

Property	Left	Right
p [bar]	1.45	1
T [K]	773	333
u [m/s]	0	0
Y_{N_2} [-]	0.733	0.7686
Y_{O_2} [-]	0.0663	0.2314
Y_{H_2O} [-]	0.0525	0
Y_{CO_2} [-]	0.1482	0

Table 3: Flux limiters applied to the Sweby's TVD scheme.

Flux limiter	$\psi(r)$
MC [17]	$\max[0, \min(2r, 0.5(1+r), 2)]$
Minmod [18]	$\max[0, \min(r, 1)]$
Osher [19]	$\max[0, \min(r, \beta_{lf})]$ $1 \leq \beta_{lf} \leq 2$
Ospre [20]	$\frac{1.5(r^2+r)}{r^2+r+1}$
Superbee [18]	$\max[0, \min(2r, 1), \min(r, 2)]$
Sweby [9]	$\max[0, \min(\beta_{lf}r, 1), \min(r, \beta_{lf})]$ $1 \leq \beta_{lf} \leq 2$
Van Leer [16]	$\frac{r+ r }{1+r}$
Van Albada [21]	$\frac{r^2+r}{r^2+1}$

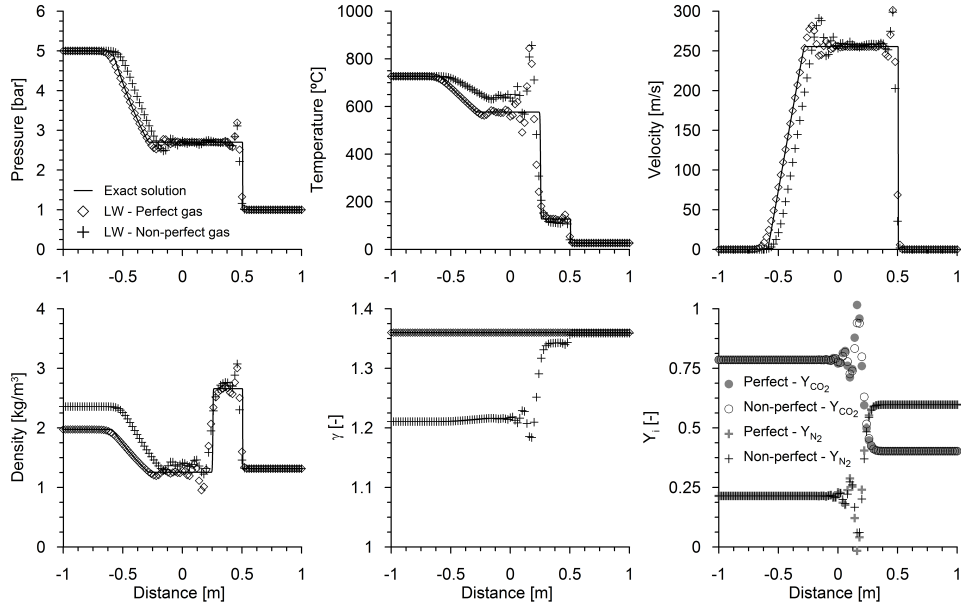


Figure 1: Case I. Results of the two-step Lax&Wendroff method with chemical species transport. Time $t = 0.001s$.

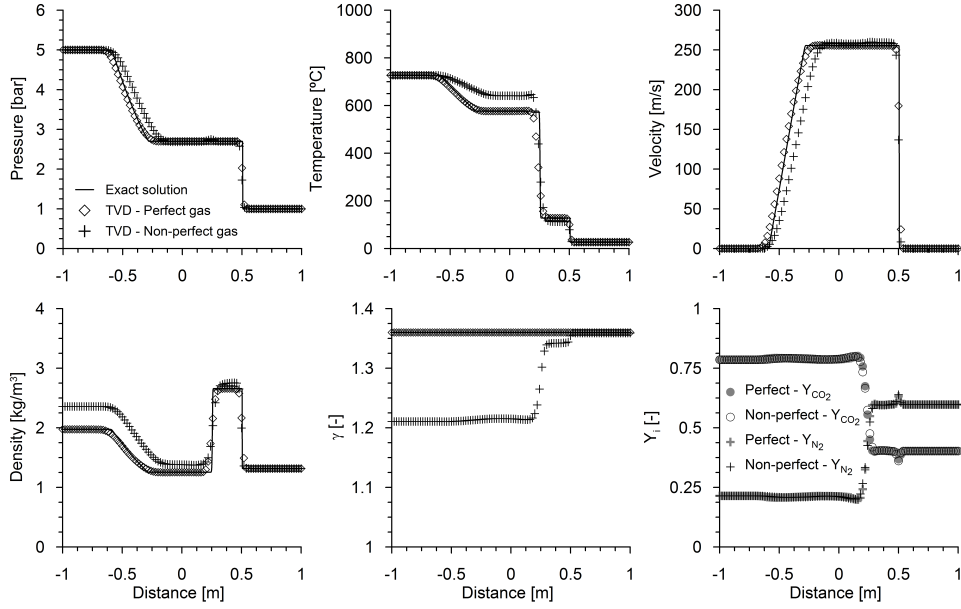


Figure 2: Case I. Results of the Sweby's TVD scheme with chemical species transport. Time $t = 0.001$ s.

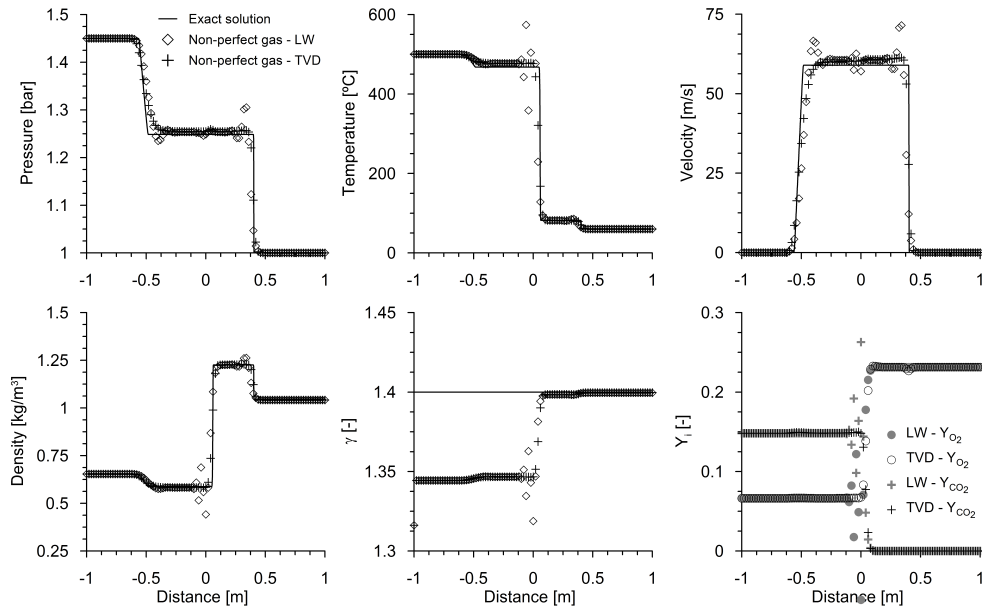


Figure 3: Case II. Results of the two-step Lax&Wendroff method and the Sweby's TVD scheme with chemical species transport considering variable gas properties (non-perfect gas). Time $t = 0.001$ s.

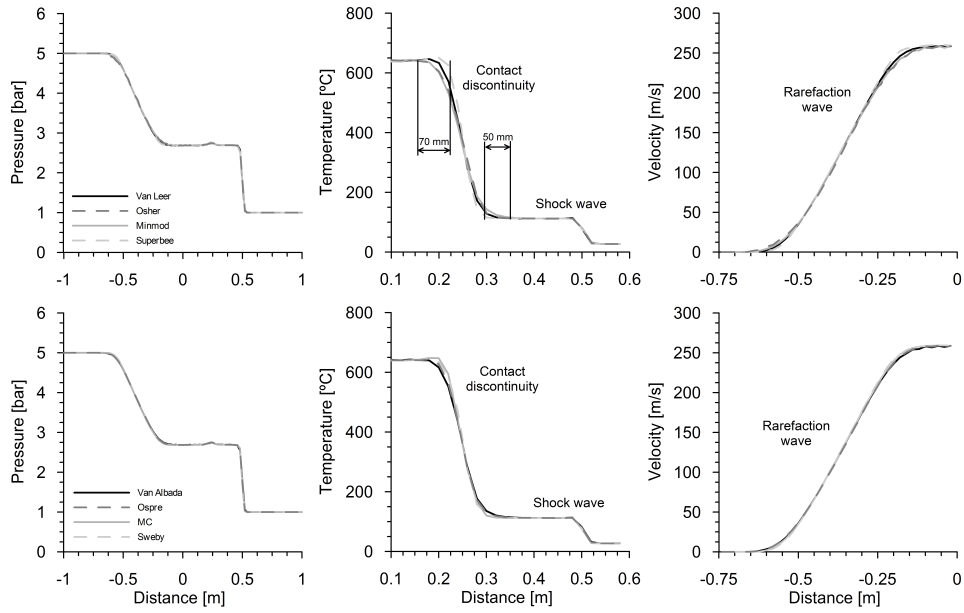


Figure 4: Effect of the flux limiter on pressure, temperature and velocity with the Sweby's TVD scheme and variable gas properties. Instant $t = 0.001$ s.

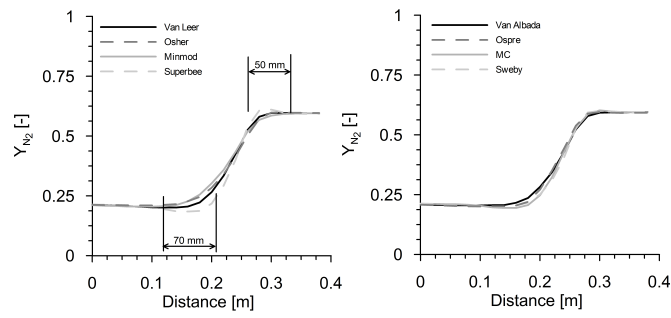


Figure 5: Effect of the flux limiter on chemical species transport with the Sweby's TVD scheme and variable gas properties. Instant $t = 0.001$ s.