A Parametric Study of Shock Wave Simulations with Help of COMSOL Multiphysics®

Fabio Ferrero*, Ronald Meyer, Martin Kluge, Volkmar Schröder
BAM Federal Institute for Materials Research and Testing
*Corresponding author contacts: Fabio Ferrero, Unter den Eichen 87, 12205 Berlin, fabio.ferrero@bam.de

Abstract: Shock wave simulations have been carried out with COMSOL Multiphysics® v4.2 with the "High Mach Flow Module", in order to better appreciate experimental results from adiabatic compression tests with tetrafluoroethylene. The shock wave generation and propagation has been properly computed and it was possible to perform a parametric study to analyze the effect of the pipe diameter and length on the shock wave evolution. The simulations were useful for the definition of a further test series yet to be performed, with the aim of achieving reproducible ignitions of tetrafluoroethylene induced by adiabatic compression.

Keywords: adiabatic compression, shock wave, High Mach Module, pipes.

1. Introduction

Adiabatic compression of gases can work as an ignition source and is still one of the main causes of accidents in chemical plants processing tetrafluoroethylene (Reza and Christiansen, 2007). The ignition of tetrafluoroethylene induced by adiabatic compression has been studied experimentally with a setup which allowed for the rapid opening of a high speed valve connecting two portions of a pipeline at different initial pressures (Meyer, 2009). Due to the fast opening time and to the high pressure difference, a shock wave in the pipeline was generated. The propagation of the shock wave and its reflection at the end of the pipeline caused pressure and temperature increase. This led to some ignitions in the experiments performed. Nonetheless, in some tests an ignition was not achieved, even if this was expected according to the theoretical temperatures predicted by the Rankine-Hugoniot equations (see Lamnaouer, 2004 or McMillan, 2004 for the shock tube theory).

In order to understand the discrepancy between the experimental results and the theoretical predictions, shock wave simulations have been carried out with COMSOL Multiphysics® v4.2. The current paper describes the results achieved in the simulations.

2. Model definition

2.1 Geometry and mesh

The geometry and mesh used for the first case simulated (0.2-m-pipe with 20 mm diameter) are shown in Figure 1 In order to reduce computing times 2D axial symmetric geometries were considered. Triangular elements were chosen and the default option physics-controlled mesh with finer elements was employed. Reflecting the experimental conditions from Meyer (2009), the following domains were computed:

- a zone with gas at high pressure;
- a zone with gas at low pressure;
- the pipe walls (material: steel);
- a nylon end plate.

In the simulations the pipe diameter and the pipe length were varied in order to perform a parametric study. The mesh properties for the different geometries analyzed are presented in Table 1.

2.2 General assumptions and equations

The *High Mach Flow Module* was used, since it solves the coupled heat and impulse equations for fast flows. The governing equations of the model are shown in Table 2, while the boundary settings selected are summarized in Table 3.

The following settings were considered in the simulations:

- high pressure section: nitrogen initially at 20 bara;
- low pressure section: nitrogen initially at 1 bara;
- initial temperature of the system: 23.5 °C;
- adiabatic walls to the outside;
- flow slip condition at the inner walls;
- laminar flow.

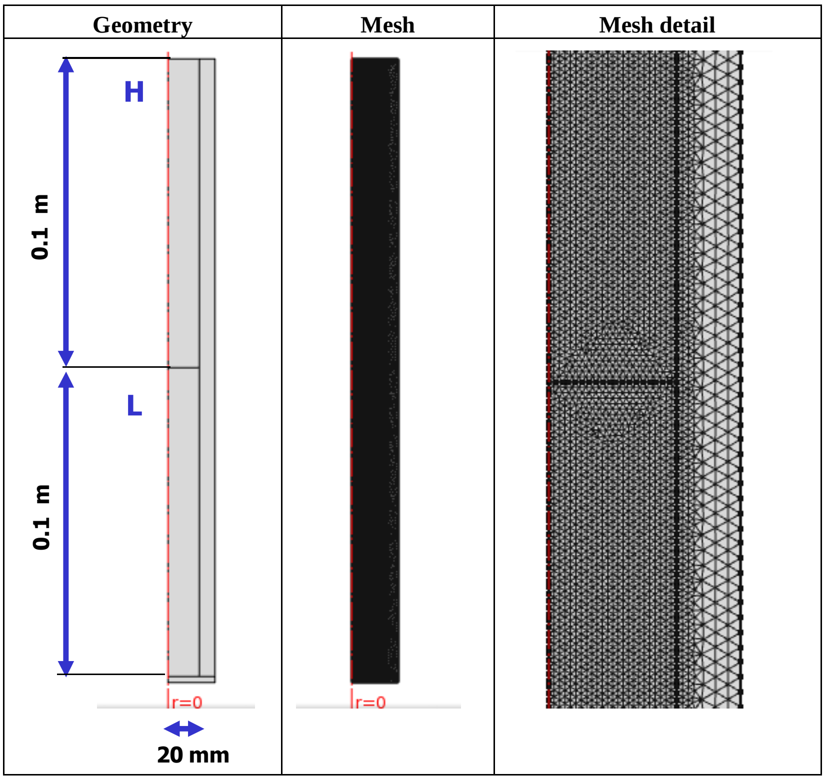


Figure 1. Geometry and mesh used in the simulations of a 0.2-m-pipe with a diameter of 20 mm (H = high pressure zone, L = low pressure zone).

Table 1. Mesh properties.

Pipe length	**Pipe diameter**	**Minimum element quality**	**Number of elements**
[m]	[m]	[-]	[-]
0.2	20	0.8096	22534
0.2	40	0.8470	15378
2	20	0.8777	79088

Table 2. Governing equations.

	Gas domain (nitrogen)	**Solid domains (walls and end plate)**
Momentum equation	$\rho_{N_2} \frac{\partial \vec{u}}{\partial t} + \rho_{N_2} (\vec{u} \cdot \nabla)\vec{u} = -\nabla p + \eta_{N_2} \nabla^2 \vec{u}$	not applicable
Continuity equation	$\frac{\partial \rho_{N_2}}{\partial t} + \nabla \cdot \left(\rho_{N_2} \vec{u}\right) = 0$	not applicable
Heat transfer equation	$\rho_{N_2} c_{P,N_2} \frac{\partial T}{\partial t} = \mathrm{div}\left(\lambda_{N_2}\ \mathrm{grad}\, T\right) - \rho_{N_2} c_{P,N_2}\ \vec{u} \cdot \mathrm{grad}\, T$	$\rho_{solid}\, c_{P,solid} \frac{\partial T}{\partial t} = \mathrm{div}\left(\lambda_{solid}\ \mathrm{grad}\, T\right)$
Ideal gas law	$\rho_{N_2} = p / \left(\mathrm{R}_s T\right)$	not applicable

Table 3. Boundary settings in the performed simulations.

	Momentum Equation	**Heat Transfer Equation**
High to low pressure zone interface	continuity	continuity
Pipe/end plate inner walls	slip	continuity
Pipe/end plate outer walls	not applicable	thermal insulation / constant temperature
Symmetry axis	axial symmetry	axial symmetry
Upper boundary	slip / inlet	thermal insulation / constant temperature

Divergence problems occurred when trying to add turbulence to the system and strange temperature and profiles after the shock wave reflection were achieved if the no slip condition at the walls was chosen. Therefore a laminar flow with slip at the wall was selected for preliminary computations.

The material properties of nitrogen, steel and nylon have been taken from the internal COMSOL Multiphysics® library.

3. Discussion

As at start of the simulation (representing the moment where the high speed valve in the experiments is opened), the pressure discontinuity will generate a shock wave which pressure and temperature increase of the gas initially at low pressures. The Rankine-Hugoniot equations can be used to predict the highest temperature near the compression pipe end, which is achieved for a short time after the shock wave is reflected at the pipe end (Lamnaouer, 2004; McMillan, 2004). The Rankine-Hugoniot equations are expressed in Table 4, where the standard symbologies are used.

Table 4. Rankine-Hugoniot equations

Calculation of the shock wave Mach number from the initial pressure ratio
$\frac{p_4}{p_1}=\frac{2\gamma_1 M_s^2-(\gamma_1-1)}{\gamma_1+1}\left[1-\frac{\gamma_4-1}{\gamma_1+1}\frac{a_1}{a_4}\left(M_s-\frac{1}{M_s}\right)\right]^{\frac{-2\gamma_4}{\gamma_4-1}}$
Calculation of the reflected temperature from the shock wave Mach number
$\frac{T_5}{T_1}=\frac{\left[2(\gamma_1-1)M_s^2+(3-\gamma_1)\right]\left[(3\gamma_1-1)M_s^2-2(\gamma_1-1)\right]}{(\gamma_1+1)^2 M_s^2}$

In Table 4 for the sake of conciseness only the equation for the calculation of the reflected temperature is presented. Equations for the calculation of the other shock wave physical properties are to be found in the mentioned literature.

Figure 2 and Figure 3 show, respectively, the velocity and temperature distribution over time for a simulation in a 0.2-m-pipeline of 20 mm in diameter for the shock analyzed. The shock wave generation and propagation has been properly computed and the physical properties of the shock wave reflected the prediction of the Rankine-Hugoniot equation presented in Table 5.

Table 5. physical properties predicted by the Rankine-Hugoniot equations for the analyzed shock (initial conditions: nitrogen at 23.5 °C, pressure ratio of 20).

Zone	**T [°C]**	**p [bar(a)]**	**v [m/s]**
1: undisturbed gas at low pressure	23.5	1	0
2: gas being travelled by the shock wave	186	3.6	365
3: gas after the shock wave	-89	3.6	365
4: undisturbed gas at high pressure	23.5	20	0
5: reflection zone	373	10.8	0

Therefore the model was considered to be validated and it was possible to perform a parametric study in order to analyze the effect of the pipe diameter and length on the shock wave evolution.

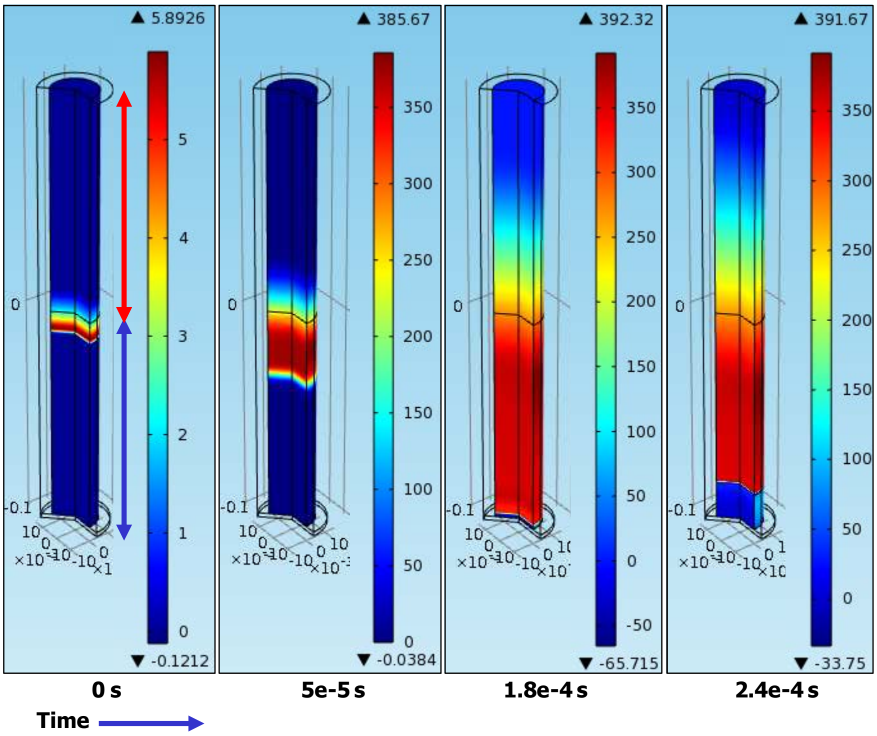


Figure 2. Simulated velocity (m/s) distribution in the pipeline over time.

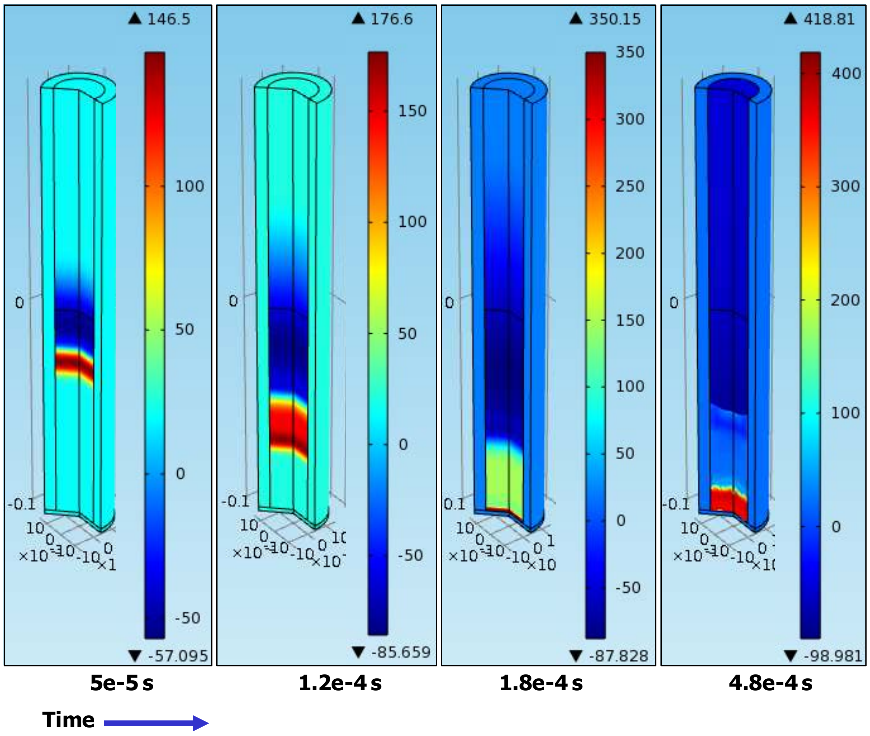
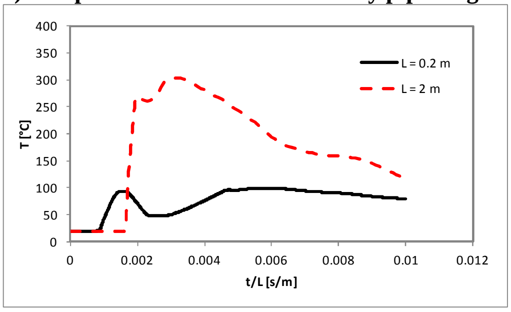


Figure 3. Simulated temperature (°C) distribution in the pipeline over time.

Details on the parametric study are presented in the following paragraphs:

1. analysis of the pipe length effect: simulations in the original pipe were compared with computations in a longer pipe (total length: 2 m; high pressure zone length: 1 m; low pressure zone length: 1 m), considering adiabatic walls. Figure 4 shows a comparison of the temperature averaged in the volume corresponding to the last 50 mm from the pipe end for both cases. For simplicity in Figure 4a) the average temperature is plotted against the time divided by length of the low pressure zone pipe, so that the peaks due to compression approximately start at the same moment for both computations. It is shown that the average temperature in the longer pipe is higher, meaning a high temperature is achieved in a larger portion of the pipe. Figure 4b) presents the average temperature evolution over time, where it can be seen that in the larger pipe the high temperature is also kept over a larger time. It is therefore proven that in a longer pipe, higher tendency to ignition can be given, since higher temperature are maintained over a longer time, provided the process is so fast that the heat losses are negligible;

a) Temperature over time divided by pipe length



b) Temperature evolution over time

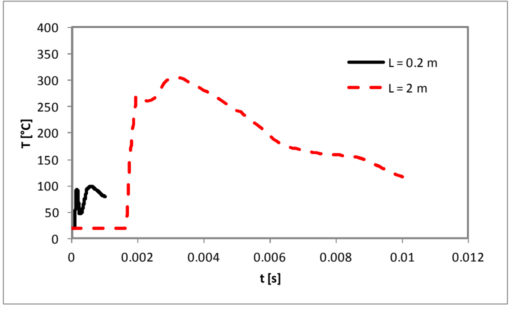


Figure 4. Average temperature in the 50 mm zone above the end plate for simulations of pipelines with two different lengths.

2. analysis of the pipe diameter effect: simulations with constant wall temperatures of 20 °C for pipes with L = 0.2 m and diameters of 20 and 40 mm were performed. Figure 5 presents the temperatures on the pipe axis at 5 mm from the pipe end for both cases considered. It is shown that in the pipe with smaller diameter the temperature is dissipated faster than in the pipe with larger diameter. This means, even is the shock wave process is very fast, if the diameter is too small heat losses to the surroundings might not be negligible.

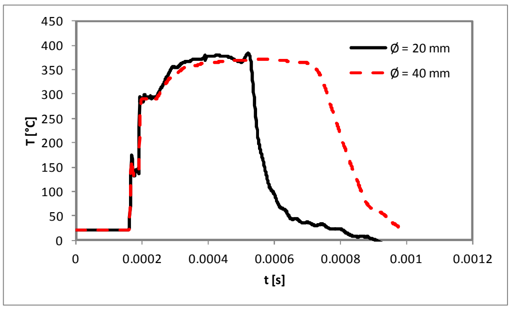


Figure 5. Temperature over time on the pipeline axis at 5 mm from the end plate for simulations with two different diameters. The plateaus in the curves indicate the predicted temperatures of the reflected wave.

Considering that in the experiments performed by Meyer (2009) pipe diameters up to 20 mm were employed, the simulations suggest that the pipe geometry was probably not optimal for the achievement/conservation of high temperatures and might explain the difficulty in inducing ignitions of tetrafluoroethylene by adiabatic compression. According to the results of the current work, a further series of tests with larger pipe diameters and lengths has been planned.

4. Conclusions

Shock wave simulations have been performed with COMSOL Multiphysics® v4.2. Various geometries were considered, in order to analyze the effects of the pipe diameter and length on the shock wave generation and propagation. The computations realized show that pipes of larger diameter and/or length could be keener to achieve and maintain higher temperatures over a larger portion of the pipe. This is of extreme relevance when dealing with gases like tetrafluoroethylene, which could experience an explosive decomposition induced by the temperature/pressure increase caused by the shock wave. In particular, the simulations might explain why in adiabatic compression tests with tetrafluoroethylene with pipes with diameters up to 20 mm (Meyer, 2009) it was difficult to achieve reproducible decompositions. A series of experiments to be performed in the near future with enhanced geometries is tended to confirm the finding of the computations.

5. References

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6. Acknowledgements

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7. Nomenclature

Symbols

Symbol	Description	Unit
a	Sonic speed	m/s
c_{P,N_2}	Specific heat of nitrogen	J/(kg·K)
$c_{P,solid}$	Specific heat of solid	J/(kg·K)
L	Pipe length	m
$\mathrm{M_s}$	Mach number of the shock wave, -	-
p, p	Pressure	Pa, bar(a)
R_s	Specific gas constant of nitrogen	J/(kg·K)
T, T	Temperature	K, °C
t, t	Time	s
$\vec{u}$	Velocity field vector	m/s
λ_{N_2}	Heat conduction coefficient of nitrogen	W/(m·K)
λ_{solid}	Heat conduction coefficient of solid	W/(m·K)
η_{N_2}	Dynamic viscosity of nitrogen	Pa·s
ρ_{N_2}	Density of nitrogen	kg/m^3
ρ_{solid}	Density of steel	kg/m^3
Ø	Diameter	mm
γ	Isentropic coefficient	-

Subscripts

Subscript	Description
1	Properties in the low pressure zone
4	Properties in the high pressure zone
5	Properties in the reflection zone