COMSOL Multiphysics as a Tool to Increase Safety in the Handling of Acetylene Cylinders Involved in Fires

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Abstract: In this paper a mathematical model for predicting the heating-up of an acetylene cylinder involved in a fire is presented. In the simulations polynomial functions were used to describe the temperature dependency of the thermal properties of the cylinder interior, which is a complex system composed by a solid porous material, a solvent (typically acetone) and acetylene dissolved in it. Model equations covered heat conduction in the cylinder interior and at its walls, while the fire surrounding the cylinder was simulated by solving the coupled heat transfer (convection and conduction) and the momentum equation (Navier-Stokes). Results of the calculations and the effects of some model parameters are discussed. Furthermore, the model is used to determine how long a cooling with water has to be applied, so that the system is brought again under a non critical temperature.

Keywords: acetylene, safety, heat transfer, momentum transfer

1. Introduction

Acetylene (chemical formula C_2H_2) is an unstable gas, which is commonly used for cutting and welding purposes, since its combustion releases a large amount of heat (1.300 kJ/mol). The instability of acetylene lays in its capability of decomposing explosively into carbon and hydrogen, reaction which is initiated at sufficiently high temperature and pressure. For this reason the storage of acetylene in gas cylinders occurs normally at relatively low pressures. As to increase the storage capacity acetylene is dissolved in a solvent (typically acetone, chemical formula C_3H_6O). The amount of solvent cannot exceed defined values, as to prevent the hydraulic rupture of the cylinder due to contained heating (for example during the filling of acetylene) and this limits the maximum pressure in the gas phase to 25 bara. As a further safety measure, the interior of such cylinders is filled with a porous material, which can prevent the appearance of convective currents and stop the propagation of the decomposition reaction. Furthermore, due to the presence of the porous material, the solvent/acetylene solution is homogenously distributed and the appearance of local hot spots is reduced. Anyway, if a cylinder comes in contact with a strong heat source, for example a fire, decomposition of acetylene can still happen and propagate, causing pressure increase and eventually leading to the break-up of the vessel, often with generation of a fireball. Consequences of this kind of explosions can be serious damages to buildings and injuries to people (Schutterwald, 1994 and Brisbane, 1999). Therefore, it is important to predict the heating-up of an acetylene cylinder involved in a fire, in order to know if the critical temperature for the explosive decomposition, which is also pressure dependent, is reached. Since the decomposition, once initiated, could continue even if the fire already extinguished, it is important to determine how long firemen have to apply a cooling with water, so that the system is brought again to non critical conditions.

COMSOL Multiphysics was used to solve a mathematical model to predict the heating-up of an acetylene cylinder involved in a fire and the successive cooling process.

The paper describes the main equations of the developed model and discusses the results of the calculations performed.

2. Numerical Model

2.1 Equations

The mathematical model made the following assumptions:

- in the cylinder interior and at its walls only heat conduction was considered. The assumption for the interior is justified by the presence of the porous material, which prevents convection. Also in the cavity with free acetylene on the cylinder shoulder no convection was taken into account, due to the small disposable space;
- in the fluid surrounding the cylinder the coupled heat transfer (convection and conduction) and momentum equation (Navier-Stokes) were solved;
- for the calculations of the heating-up, the fire was simulated with an air flow with a maximum temperature of 1000 °C. The flow development was generated by the concomitance of the upward gas velocity and of the side wind speed. In this phase, the compressible Navier-Stokes equations were solved;
- when simulating the cooling of the acetylene cylinder, a downward water flow at the cooling temperature was considered. In this phase, the incompressible Navier-Stokes equations were solved;
- the dilatational viscosity in the momentum equation was neglected;
- the density driven volume forces were neglected, since they were supposed to be smaller than the ones generated by the assumed air flow;
- material properties in the cylinder interior were considered temperature dependent and were described by polynomial functions either taken from Yaws (2003) or determined experimentally. As solvent, acetone was considered;
- wall material properties have been taken from the internal COMSOL library (Steel AISI 4340);
- air properties were considered to be temperature dependent for the heat transfer equation, but not for the momentum equation;
- water properties were considered to be temperature dependent for the heat transfer equation and the momentum equation.

Thus, the model equations are written. Equation (1) describes the heat transfer by conduction, valid for the cylinder interior (free cavity and system composed of porous material, acetone and dissolved acetylene) and at the cylinder walls:

$$\rho_i c_{p,i} \frac{\partial T}{\partial t} = \lambda_i \,\mathrm{div}\,\mathrm{grad}\, T \qquad (1)$$

where the subscript i represents the substance/material for which the equation is written.

The heat transfer by conduction and convection in the surroundings of the acetylene cylinder (air simulating a fire during the heating-up or water during the cooling) is expressed by equation (2), where the subscript j represents air or water.

$$\rho_j c_{P,j} \frac{\partial T}{\partial t} = \lambda_j \,\mathrm{div}\,\mathrm{grad}\, T - \rho_j c_{P,j}\, \vec{u} \cdot \mathrm{grad}\, T \qquad (2)$$

The momentum equations for air and water are written in the following form:

$$\rho_j \frac{\partial \vec{u}}{\partial t} + \rho_j\, \vec{u} \cdot \nabla \vec{u} = -\nabla p + \eta_j \nabla^2 \vec{u} \qquad (3)$$

and are completed by the corresponding continuity equations:

$$\frac{\partial \rho_j}{\partial t} + \nabla \cdot \left(\rho_j\, \vec{u}\right) = 0 \qquad (4)$$

The boundary conditions selected for the calculations during the heating and cooling are summarized in **Table 1**. It can be seen that the velocity profiles at the boundary have been described by functions of the r and z direction respectively. The optimal function for the application is still under investigation. In the calculations performed in this paper, a parabolic profile was used, as expressed in equations (5) and (6) for the side wind speed and the upward gas velocity, respectively.

$$u = u(z) = -4u_{\max} z(1-z) \qquad (5)$$

$$v = v(r) = 4v_{\max} r(1-r) \qquad (6)$$

Furthermore, in order to avoid steep temperature gradients, in the simulations of the cylinder heating it was considered that the fire reached its maximum temperature not instantaneously but in a short fixed time, in which the temperature rose from the initial temperature of the acetylene cylinder to the maximum value. Similarly, in the cooling calculations water temperature was supposed to decrease from the initial temperature of the acetylene cylinder to the cooling temperature in a short interval. This arrangement helped in preventing divergence problems and did not show relevant effects on the model outputs.

2.2 Geometry

Figure 1 shows the geometry used during the calculations, where the acetylene cylinder is represented by the colored area. In the simulations, due to axial symmetry only the half of the 2D section along the r-z plane could be considered, as to reduce computing times. The white zone surrounding the cylinder defines the domain with air (heating-up) or water (cooling).

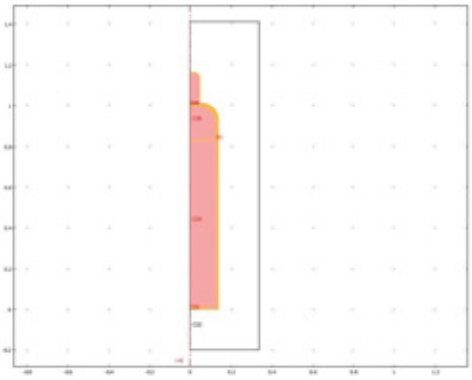

Figure 1. Geometry used in the calculations.

In the model geometry it was also considered that, due to the construction procedure, a small cavity without porous material is formed on the cylinder shoulder: this free space is critical, since acetylene could gather in it, increasing the risk of explosion. In **Figure 2** the cavity containing free acetylene is highlighted. In our simulations a 4 mm wide cavity was considered.

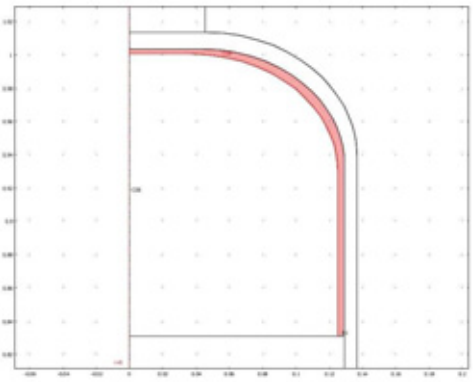

Figure 2. Detail of the geometry used in the calculations (gas cavity in color).

Figure 3 shows the mesh normally used in the calculations, which consisted of 10740 triangular elements, corresponding to 6045 nodes. By further reduction of the mesh elements dimension, no changes in the output results were stated, which means that the mesh was adequate for the calculations. In the results presented in the paper a 50L cylinder was considered, but the model can be also applied to other volumes.

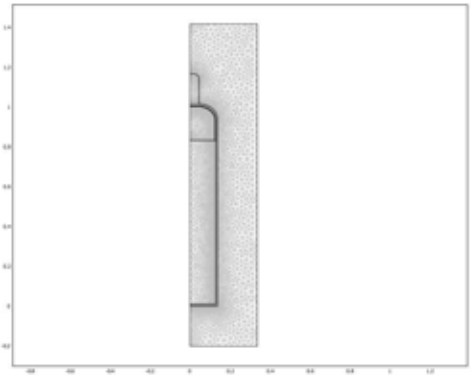

Figure 3. Mesh used in the calculations.

3. Results and Discussion

3.1 Heating-up

Figure 4 and **Figure 5** show the temperature in the middle of the cavity with free acetylene for a time corresponding to 640s and 1800s from the start of the fire, for a simulation of a 50L acetylene cylinder with a start temperature of 15°C. Temperature data are presented as a function of the maximum wind speed and of the maximum upward velocity. For the current analysis maximum wind speed was chosen in the range 0-2 m/s (typical values). The maximum upward velocity was estimated between 0 and 5 m/s, according to the results of the works of Thomas (1963), McCaffrey (1995), Ferrero (2007).

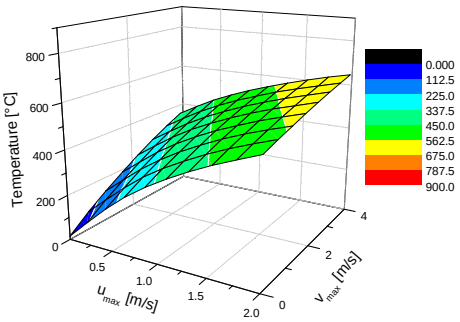

Figure 4. Temperature in the gas cavity after 640 s as a function of the upward gas velocity and of the side wind speed [initial temperature 15°C].

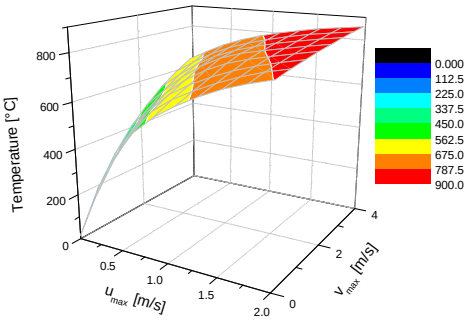

Figure 5. Temperature in the gas cavity after 1800 s as a function of the upward gas velocity and of the side wind speed [initial temperature 15°C].

From both graphs it can be seen that the computed temperatures in the gas cavity increase if the upward velocity and/or the wind speed are increased. The maximum temperatures which can be potentially achieved are much higher than the acetylene decomposition temperature (about 370°C at 10 bara, BAM, 2008), which can lead to the break up of the cylinder. The calculation could therefore be used to predict if (and when) an explosion can occur by analyzing if (and when) the critical temperature is reached.

3.2 Cooling down

In the calculations of the cooling, it was considered that the acetylene cylinder has an initial temperature of 400°C. This is a conservative assumption, since at this temperature the cylinder would have exploded, due to the pressure increase. Anyway, for preliminary calculations the assumption is satisfactory. Table 2 shows the times required to cool the whole acetylene cylinder down to 350 and 300°C for different cooling water temperatures, which ranged between 20 and 80°C, under consideration that water in the extinguishment system can have come in contact with heat sources. Also, simulations with different values of the initial time by which water effectively reaches the cooling temperature (see 2.1) were performed and showed no big effect on the calculated times, justifying the assumption. The determined times range between 10 and 16 hours, in dependence with the final temperature of the acetylene cylinder and of the water temperature.

4. Conclusions

A mathematical model to predict the heating-up of an acetylene cylinder involved in a fire and its afterward cooling by means of water was developed. The system of equations was solved with help of COMSOL Multiphysics. The model could help in predicting if an acetylene cylinder exposed to fire can explode, due to the achievement of a critical temperature, by which acetylene decomposition starts.

Furthermore, the model could help in predicting how long a heated cylinder must be cooled, as to bring it again under a non critical temperature, by which an initiated decomposition would be quenched.

The possibility of simulation of the pressure in the cylinder inside and the inclusion of the acetylene decomposition reaction in the model are currently under study, since this would provide further information about the burst processes.

5. References

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Appendix

Table 1: Boundary settings.

	Heat Transfer	
	Heating	*Cooling*
Cylinder wall	$T^+ = T^-$	$T^+ = T^-$
Boundary H1	$T = T_{hot}$	Convective Flux
Boundary H2	Convective Flux	$T = T_w$
Boundary V1	$T = T_{hot}$	Convective Flux
Boundary V2	Convective Flux	Convective Flux
	Momentum Equation	
	Heating	*Cooling*
Cylinder wall	not active	not active
Boundary H1	$v = v(r)$	$p = p_0$
Boundary H2	$p = p_0$	$v = v(r)$
Boundary V1	$u = u(z)$	Slip/Simmetry
Boundary V2	Slip/Simmetry	Slip/Simmetry
	Legend	
Boundary H1	Lower horizontal boundary of the cylinder surroundings	
Boundary H2	Upper horizontal boundary of the cylinder surroundings	
Boundary V1	Lower vertical boundary of the cylinder surroundings	
Boundary V2	Upper vertical boundary of the cylinder surroundings	

Table 2: Calculated cooling times for a 50L acetylene cylinder.

	T_0	T_w	t_w	$t_{cool,1}$	$t_{cool,2}$
	[°C]	[°C]	[s]	[h]	[h]
Initial Case	400	20	120	10.1	13.8
Case 1	400	20	60	10.1	13.8
Case 2	400	20	30	10.1	13.8
Case 3	400	30	120	10.3	14.1
Case 4	400	80	120	10.5	15.5

Table 3: Nomenclature.

Symbol	Description	Unit
c_p	Specific heat	J/(kg·K)
p	Pressure	Pa
p_0	Start pressure	Pa
T	Temperature	K
T_0	Start temperature	°C
T_{hot}	Flame temperature	°C
T_w	Cooling water temperature	°C
T^+, T^-	Temperature at the two sides of a boundary (for definition of continuity)	°C
t	Time	s
t_w	Time by which water reaches the cooling temperature	s
$t_{cool,1}$	Time by which no spot in the cylinder exceeds 350 °C	h
$t_{cool,2}$	Time by which no spot in the cylinder exceeds 300 °C	h
$\vec{u}$	Velocity field vector	m/s
u	Wind speed	m/s
$u_{\max}$	Maximum wind speed	m/s
v	Upward gas velocity	m/s
$v_{\max}$	Maximum upward gas velocity	m/s
λ	Heat conduction coefficient	W/(m·K)
η	Dynamic viscosity	Pa·s
ρ	Density	kg/m^3