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

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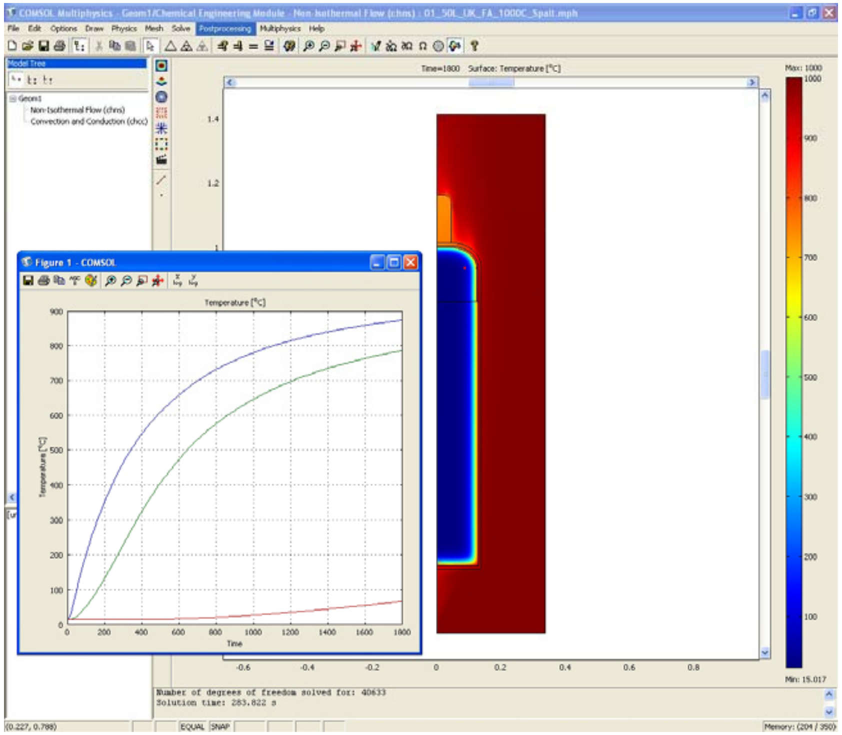

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COMSOL MULTIPHYSICS

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Background

- Acetylene (C_2H_2) is commonly used for cutting and welding purposes
- Normally stored in compressed gas cylinders
- Acetylene cylinders involved in fire can burst

Explosion of a fully charged 40 dm^3 acetylene cylinder (bonfire test)

- Previous accidents:
  - Schutterwald, Germany, accident in a private workshop (1994)
  - Brisbane, Australia, accident in an acetylene factory (1999)
  - Dallas, USA, accident in a gas factory (2007)

Consequences → Economical and human losses (fireball, ejection of fragments)

Objectives

Important to know:

- *heating up process*
  - time to explosion

- *critical temperature / pressure in the cylinder*
  - acetylene can decompose with high heat release (226 kJ/mol)

- *cooling with water*
  - the cylinder can be safely handled after the fire

→ experiments and/or <u>simulations</u>

A mathematical model to predict the heat transfer in the acetylene cylinder has been developed and solved in COMSOL Multyphysics

Acetylene Cylinder

Acetylene cylinder:

- steel wall

- the inside is not a free space, but a complex system

Acetylene Cylinder

Composition cylinder inside:

- porous material
- acetone (liquid/vapour)
- acetylene (free/dissolved)

Acetylene Cylinder

Composition cylinder inside:

- porous material
- acetone (liquid/vapour)
- acetylene (free/dissolved)

Free space

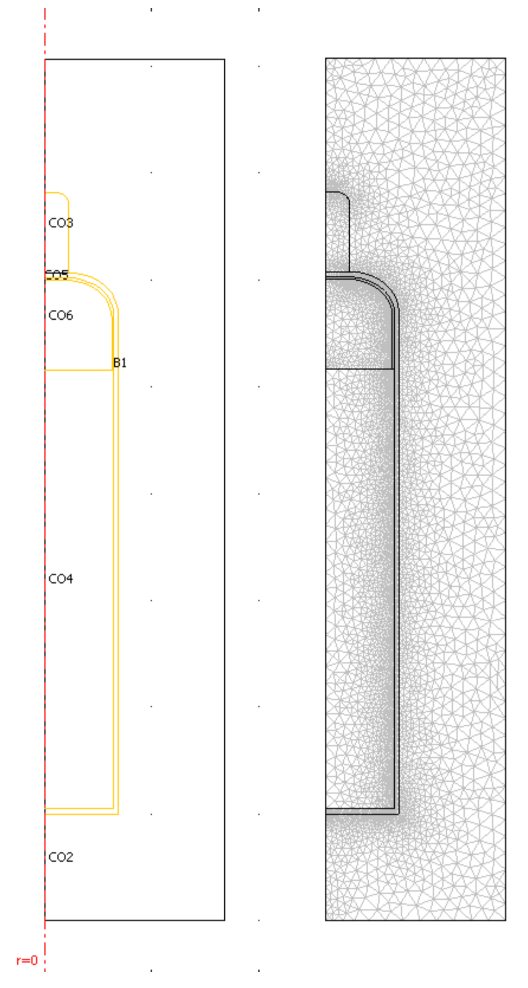
- free acetylene
- acetone vapour

Simulation: geometry & mesh

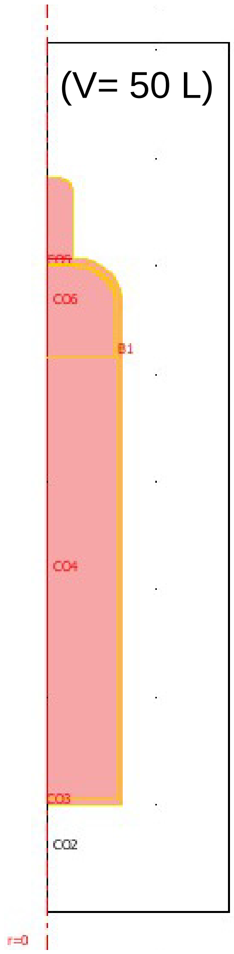
Implementation in COMSOL

Geometry (50 dm^3):
2D Axial symmetric (computing time reduction)

Mesh
- elements: 10740
- nodes: 6045
- degrees of freedom: 40633



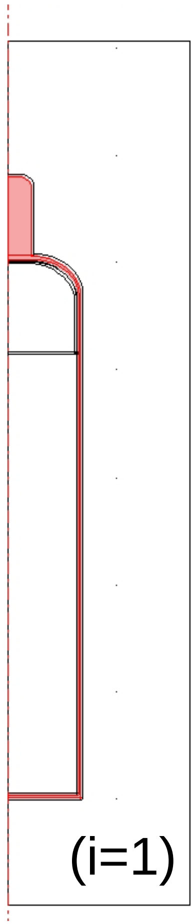
Simulation: domains and equations



Heat transfer through conduction

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

Simulation: domains and equations

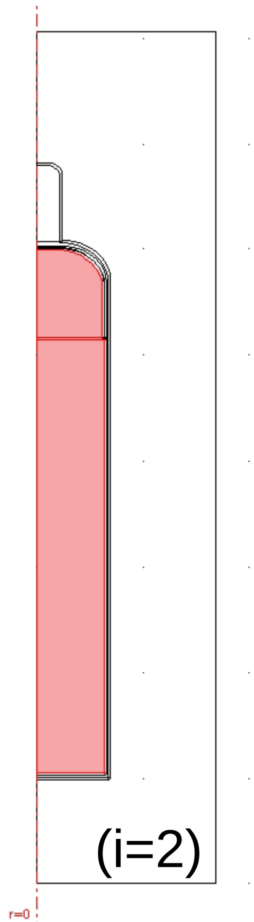


Heat transfer through conduction

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

i=1 steel wall (COMSOL library)

Simulation: domains and equations



Heat transfer through conduction

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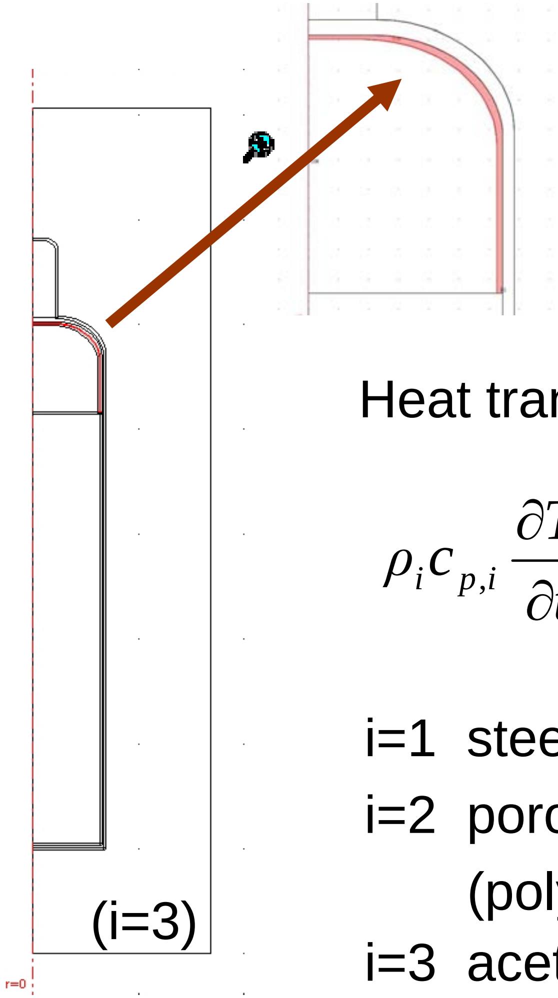
i=1 steel wall (COMSOL library)

i=2 porous material / acetone (g,l) / acetylene (d,f) (polynomial functions)

Simulation: domains and equations



Heat transfer through conduction

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i=1 steel wall (COMSOL library)

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i=3 acetylene (g) (polynomial functions)

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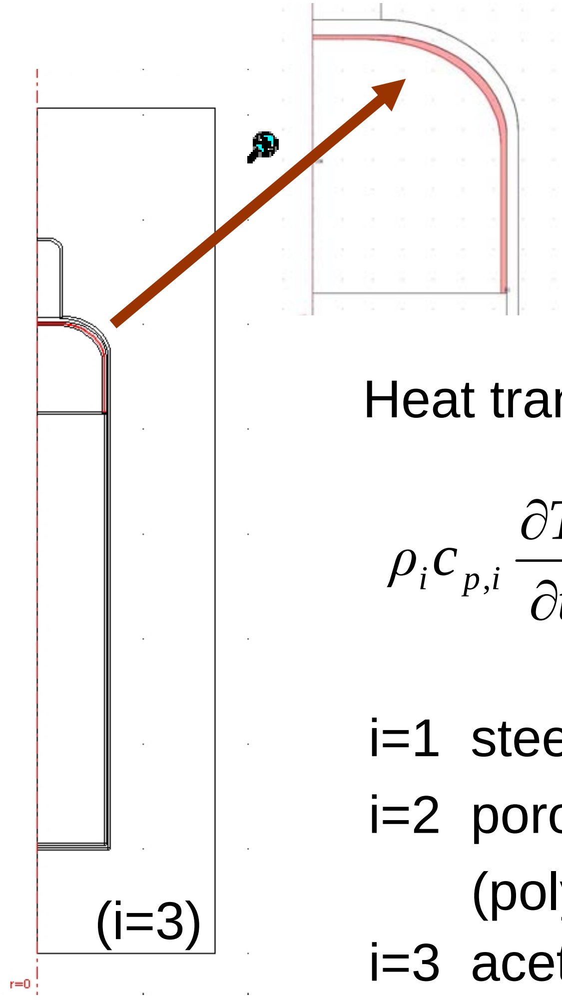
Simulation: domains and equations



No decomposition / No pressure

Heat transfer through conduction

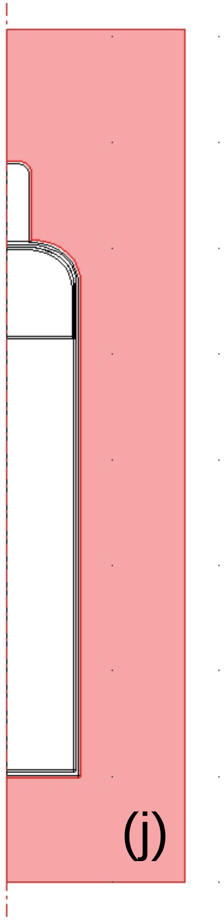
$$\rho_i c_{p,i} \frac{\partial T}{\partial t} = \lambda_i \operatorname{div} \operatorname{grad} T \qquad (1)$$

i=1 steel wall (COMSOL library)

i=2 porous material / acetone (g,l) / acetylene (d,f) (polynomial functions)

i=3 acetylene (g) (polynomial functions)

Simulation: domains and equations



Heat transfer through conduction/convection

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

Momentum equation (Navier Stokes)

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

Continuity equation

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

j=1 air (heating up)

j=2 water (cooling)

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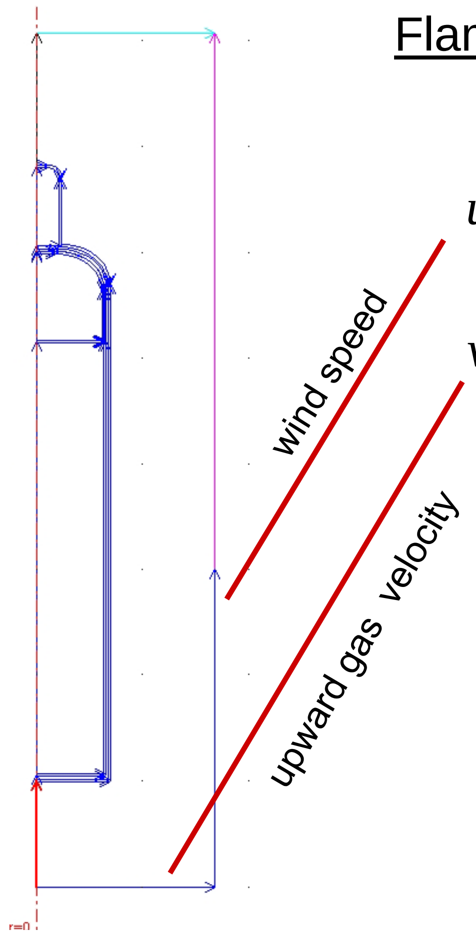
Simulation: boundary settings (heating)



Flame velocity field

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

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

Both currents are at T_{flame} = 1000°C

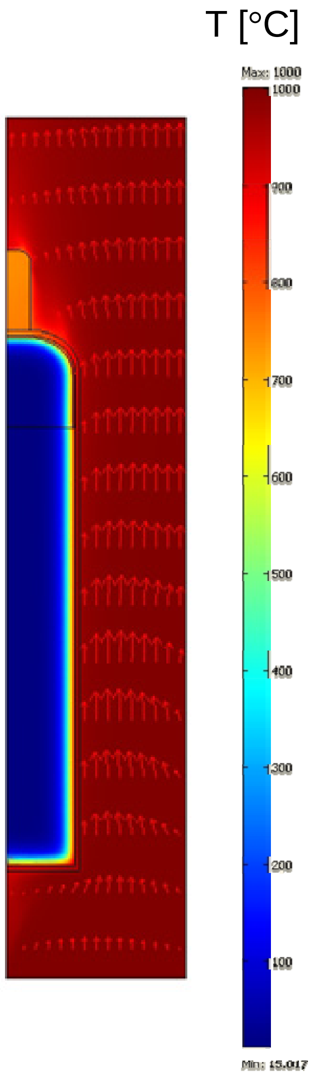
Simulation: results (heating)

Initial temperature: 15°C

u_{max} = 2 m/s

v_{max} = 5 m/s

t = 1800 s



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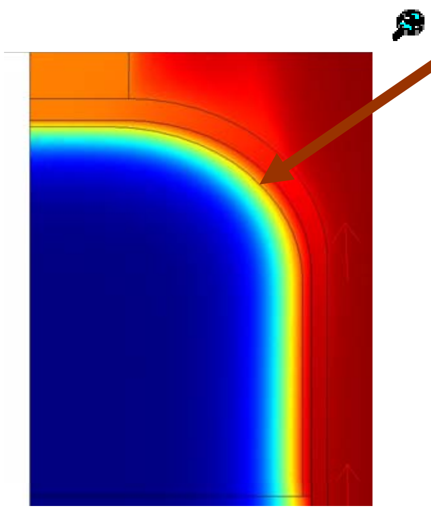

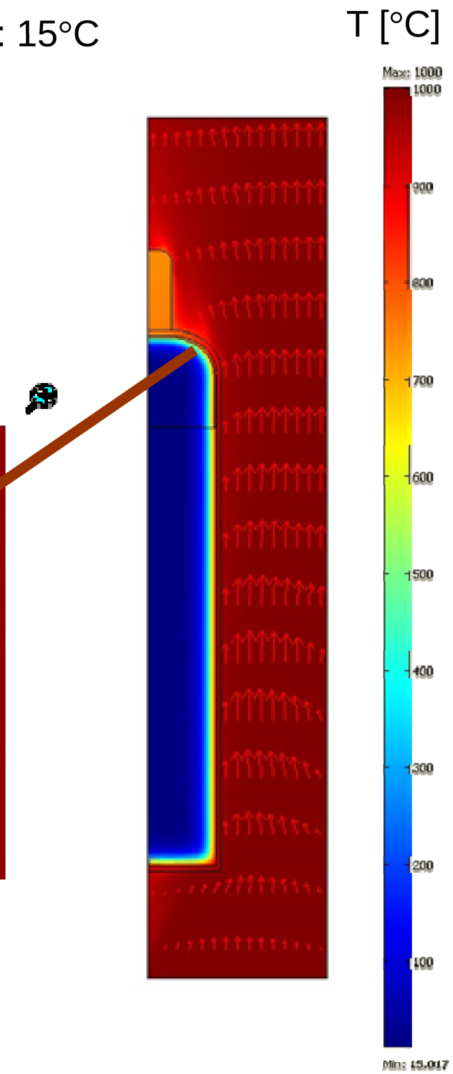

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Simulation: results (heating)

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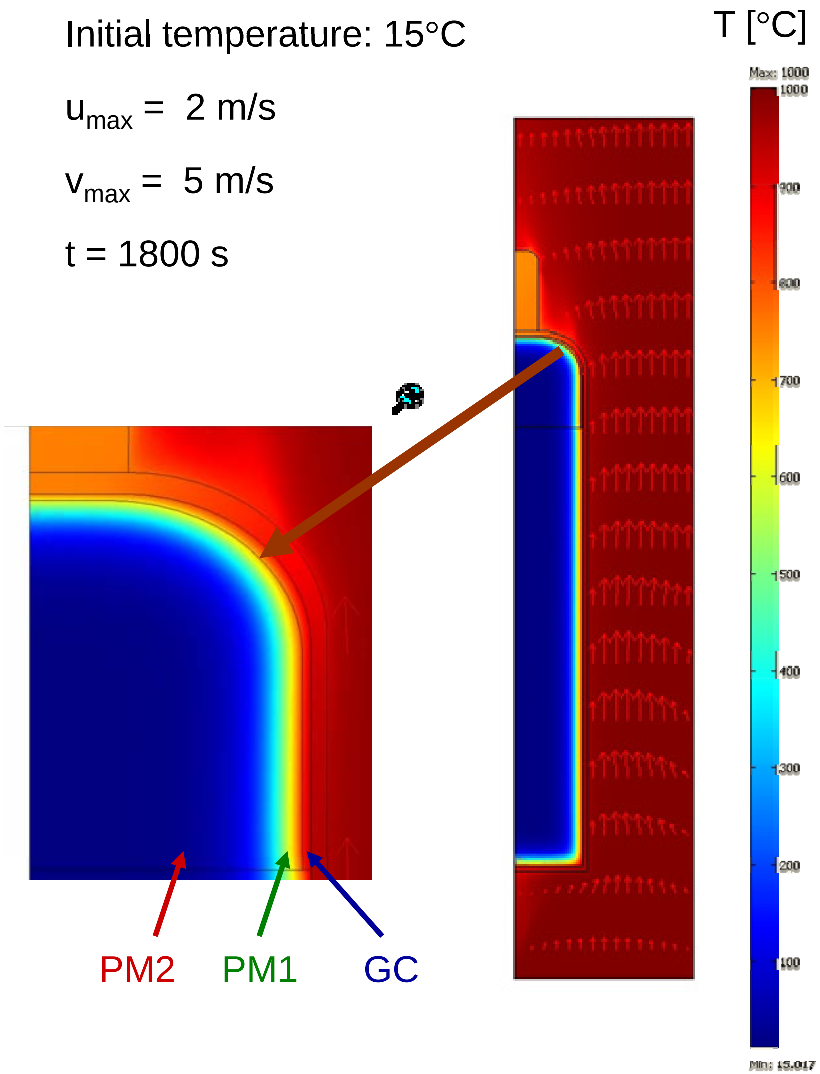

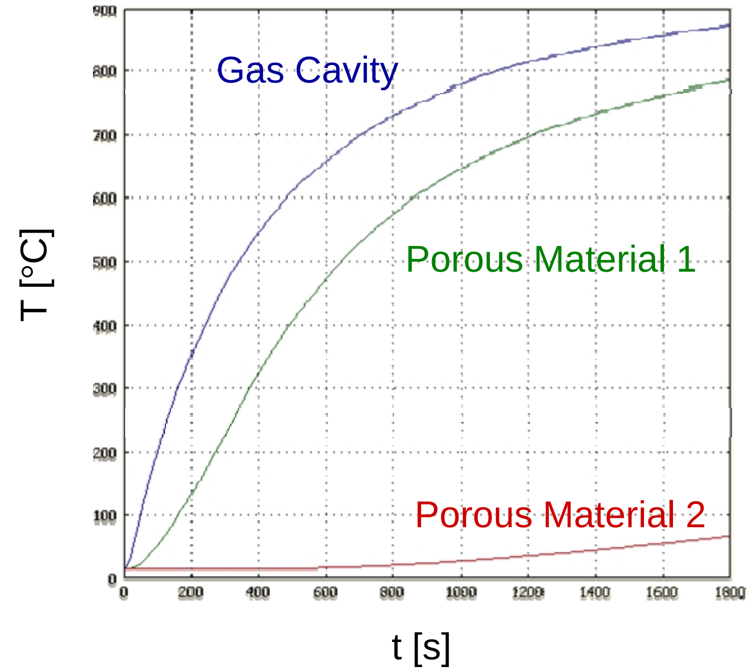

Critical temperatures can be achieved

p_0 = 10 bara, T=370°C ($V= 3\ dm^3$)

Simulation: results (heating)

Initial temperature: 15°C

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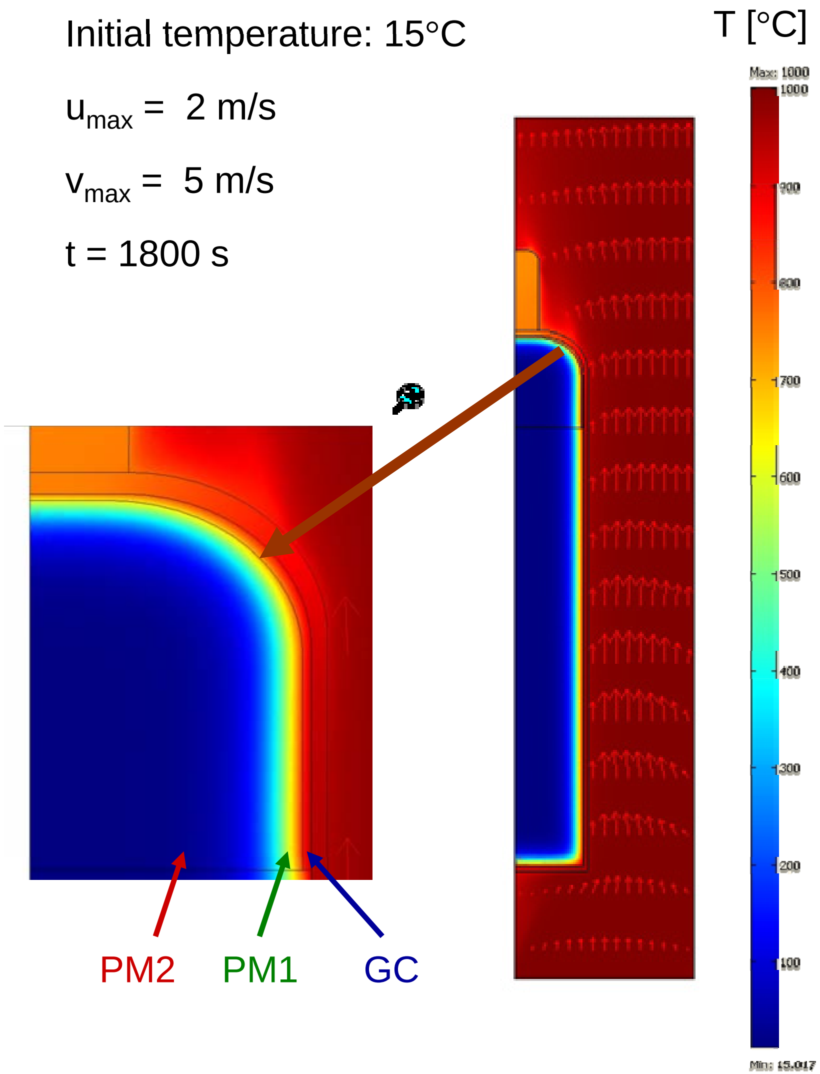
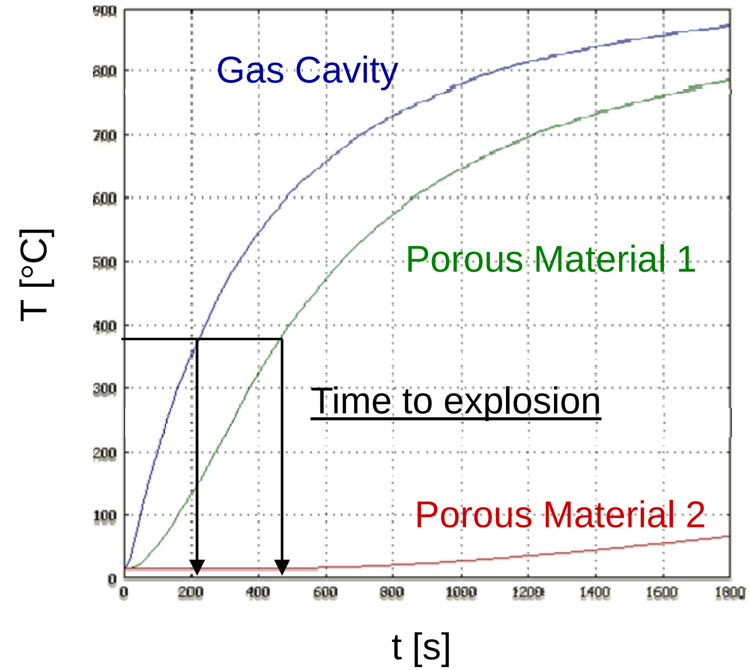
v_{max} = 5 m/s

t = 1800 s





Critical temperatures can be achieved

p_0 = 10 bara, T=370°C

(V= 3 dm^3)

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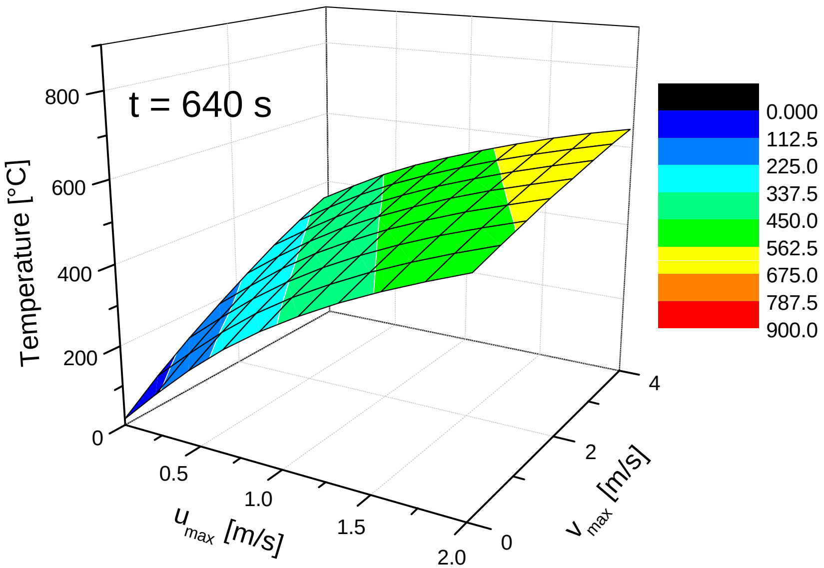
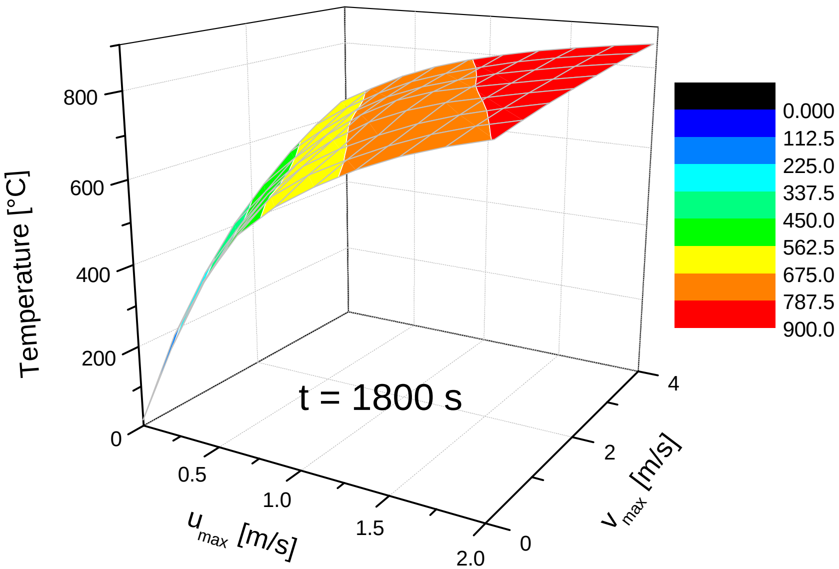
Simulation: results (heating)

Temperature in the gas cavity as a function of: - upward gas velocity (range 0-4 m/s)
- side wind speed (range 0-2 m/s)



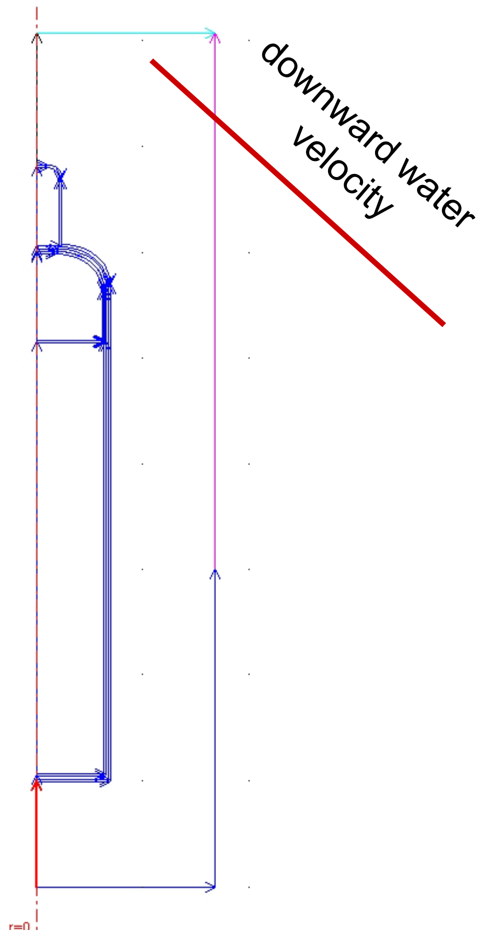


[initial temperature: 15°C]

Strong effects on the simulations

→ find optimum values

Simulation: boundary settings (cooling)

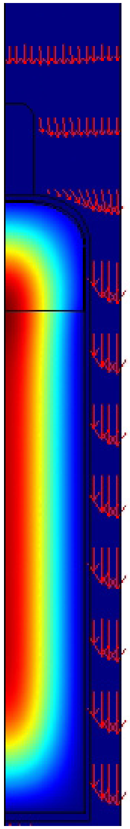


Water velocity field

$$v = v(r) = -4v_{max} r(1-r) \quad \text{or } v_{max} \tag{7}$$

The current is at T_{water} = 20-80°C

Simulation: results (cooling)



v_{max} = 1 m/s

Initial temperature	Water temperature	Time to 350°C	Time to 300°C
[°C]	[°C]	[h]	[h]
400	20	10.1	13.8
400	30	10.3	14.1
400	80	10.5	15.5

Take with caution:

- 400°C may be too conservative
- include acetylene reaction (decomposition)

Conclusions / Future Work

Conclusions

COMSOL Multiphysics can help in increase the safe handling of acetylene cylinders involved in fire by predicting the:

- time to explosion due to fire exposure
- duration of the cooling with water after the fire

Future work

- comparison with experiments (some have been already performed)
- determination of critical temperatures/pressures for the decomposition
- inclusion of the pressure in the model
- inclusion of the decomposition reaction

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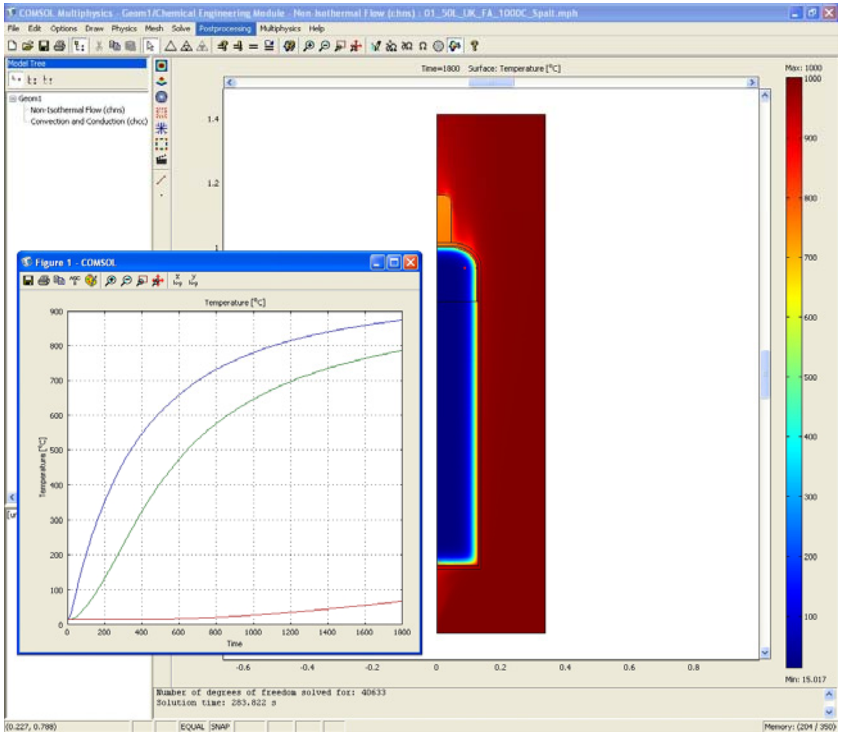

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