Numerical Study of the Self-ignition of Tetrafluoroethylene in a 100-dm^3-reactor

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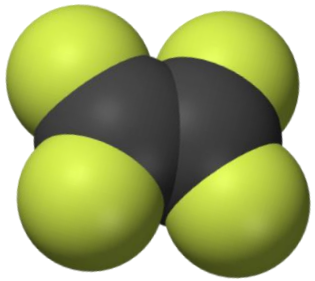
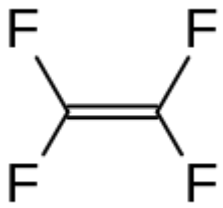
COMSOL CONFERENCE ROTTERDAM2013

What is tetrafluoroethylene (TFE)?





- Tetrafluoroethylene (C_2F_4) is a colorless gas
- TFE has a wide commercial relevance
  - PTFE (Teflon®)
  - PTFE Co-polymers
- TFE is a chemically unstable gas → explosive decomposition without oxidant (accidents in chemical plants*)
- Focus: ignition of TFE caused by contact on hot surfaces (self-ignition)

* Reza, A., Christiansen, E., A Case Study of a TFE Explosion in a PTFE Manufacturing Facility, *Process Safety Progress*, 26(1), 77-82 (2007)

Main reactions

TFE at high pressure comes in contact with hot surfaces

DIMERIZATION

$$C_2F_4 \Leftrightarrow 0.5\ c-C_4F_8$$

$$\Delta H_R = -103\left(kJ/mol_{TFE}\right)$$

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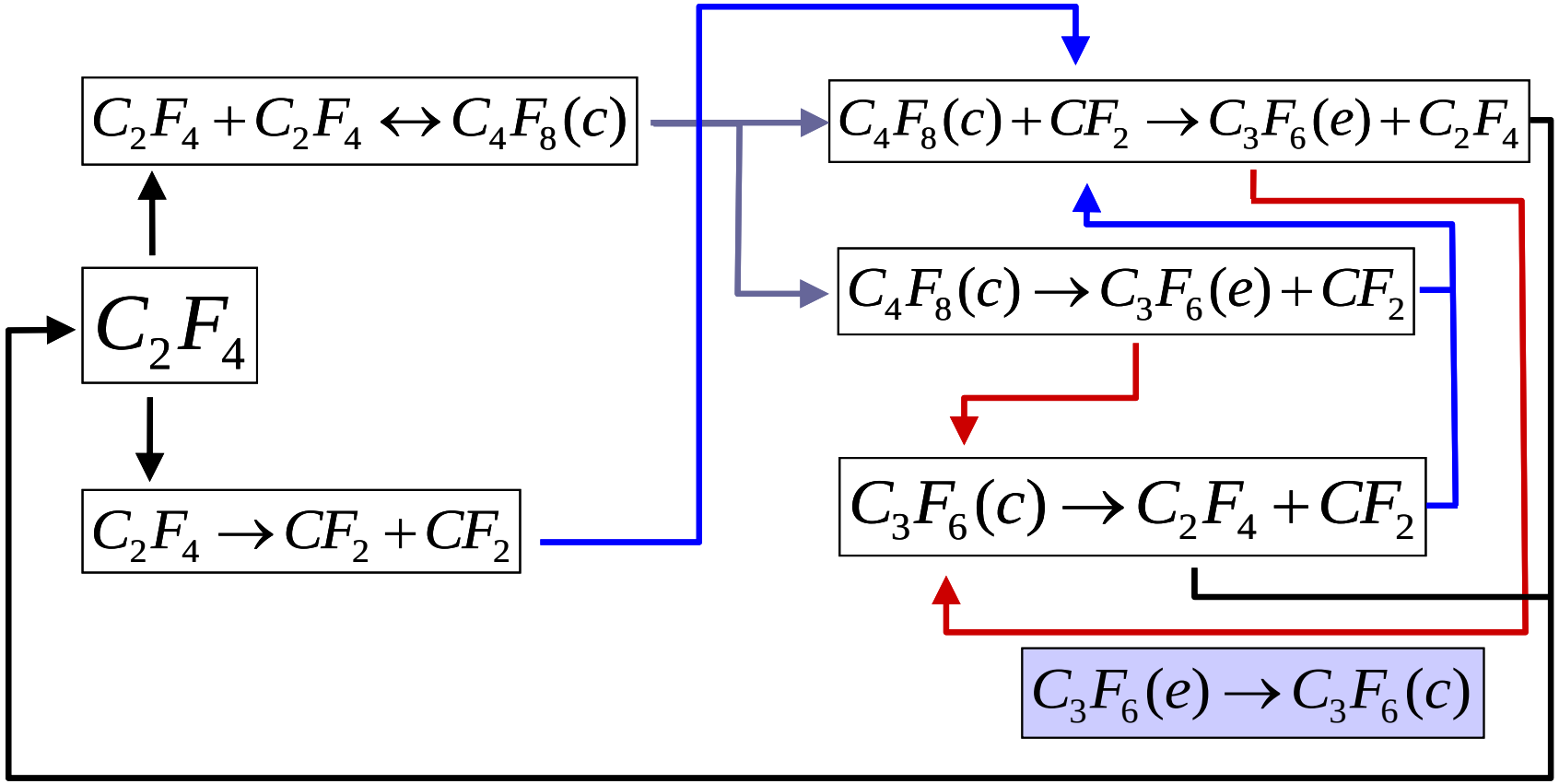
DECOMPOSITION

$$C_2F_4 \Rightarrow CF_4 + C(s)$$

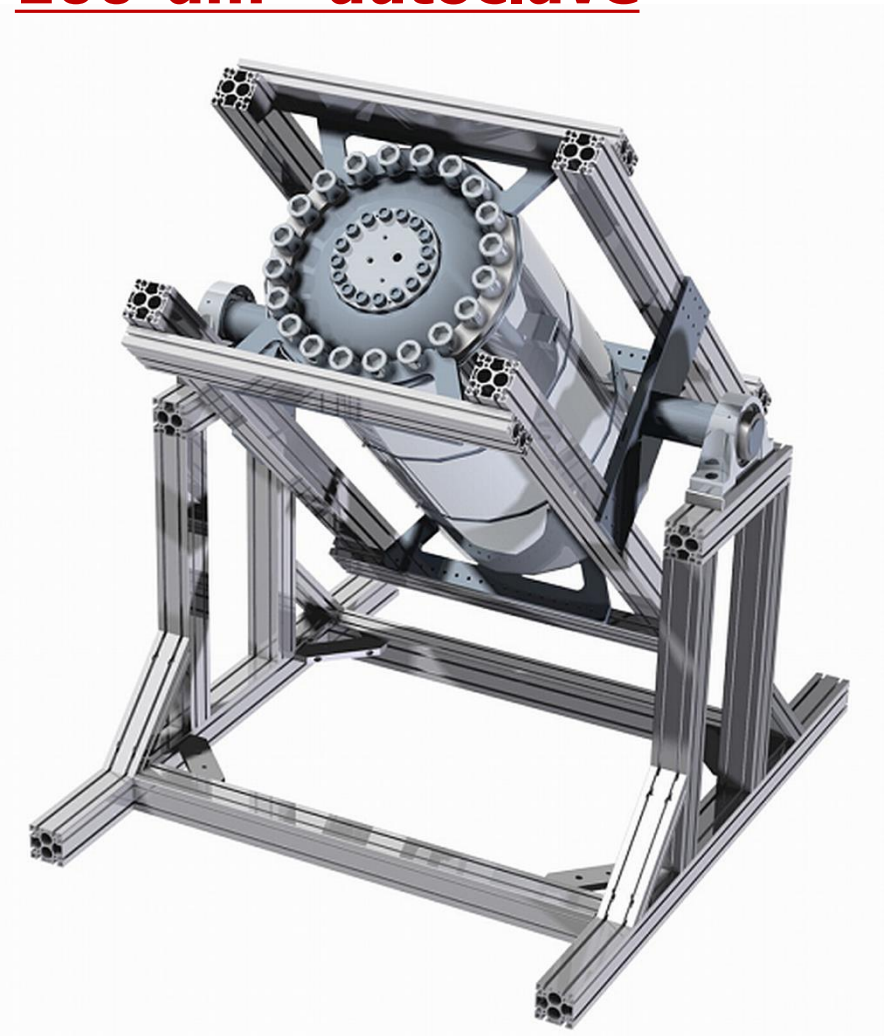
$$\Delta H_R = -257\left(kJ/mol_{TFE}\right)$$

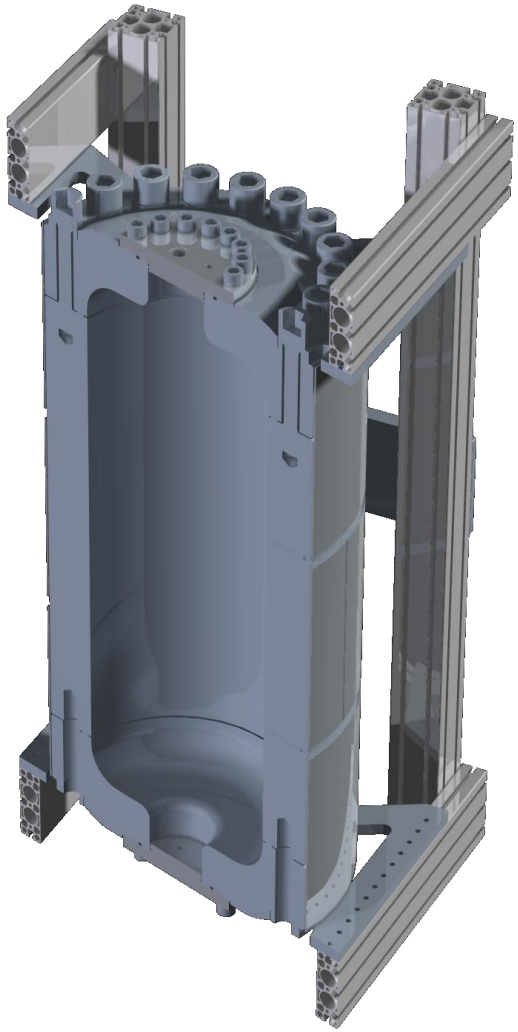
Extended reaction net*



*Bauer, S.H., Javanovic, S., The Pyrolysis of Octafluorocyclobutane - Revisited, *International Journal of Chemical Kinetics*, 30, 171-177 (1998)

100-dm³-autoclave

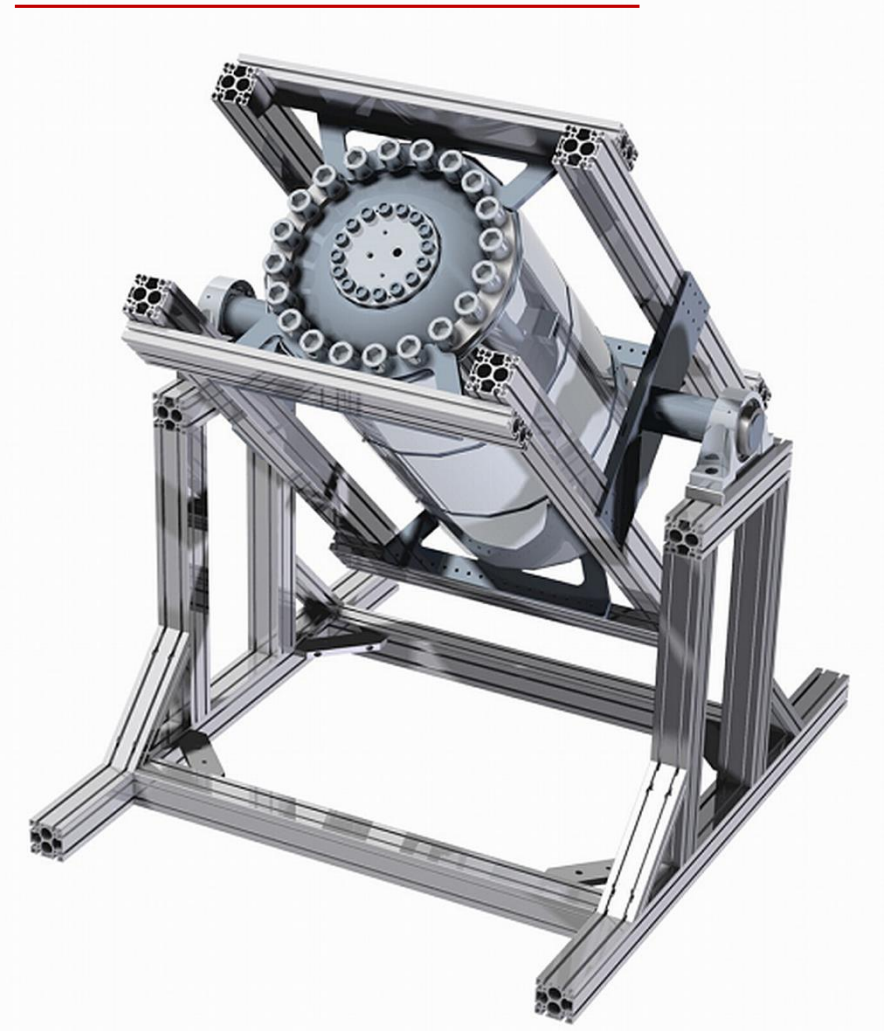




Properties: • stainless steel • 1200 kg • 360° rotation • 345 bar(a) at 20 °C

Measurements: • temperature (up to 3 TC) • pressure

100-dm³-autoclave



Tests:

- p_0 = 5, 10 and 20 bar(a)
- $T_{wall,0}$ is varied

=> lowest $T_{wall,0}$ with an ignition

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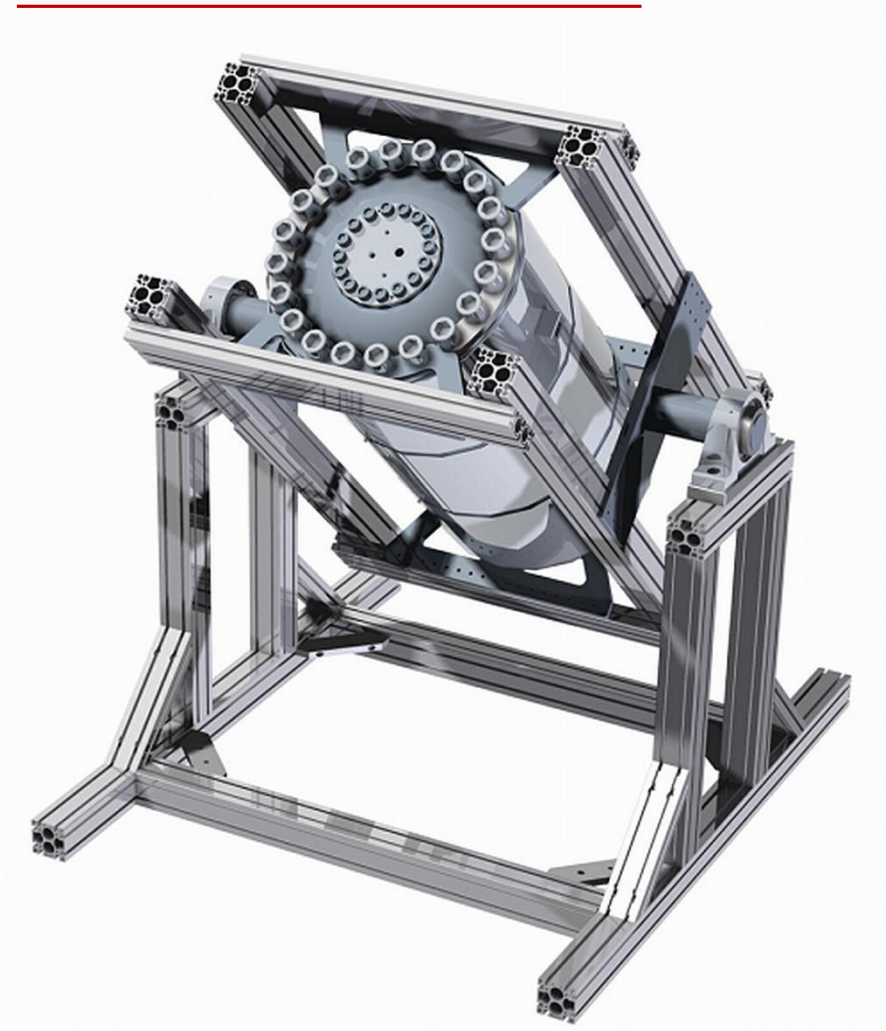

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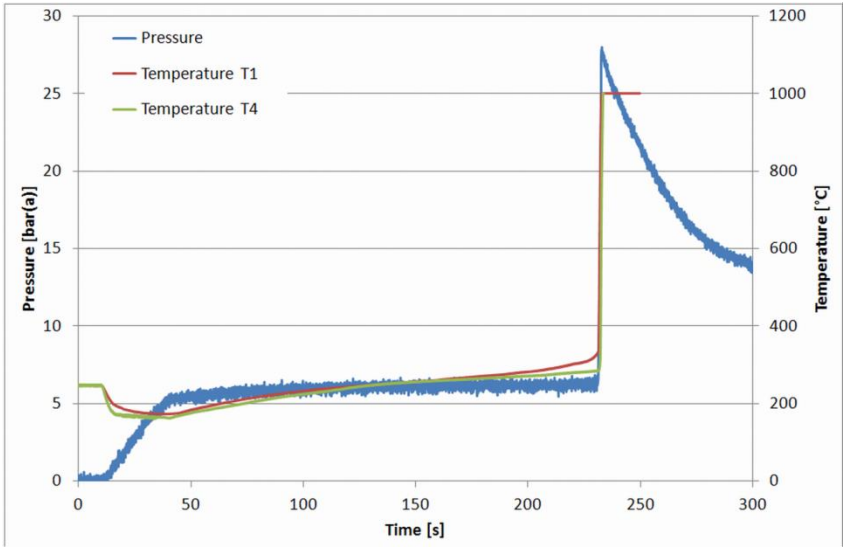

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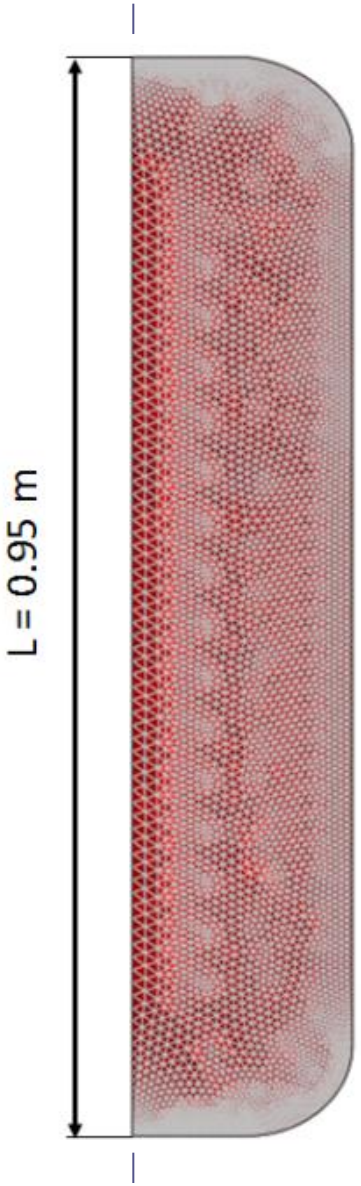
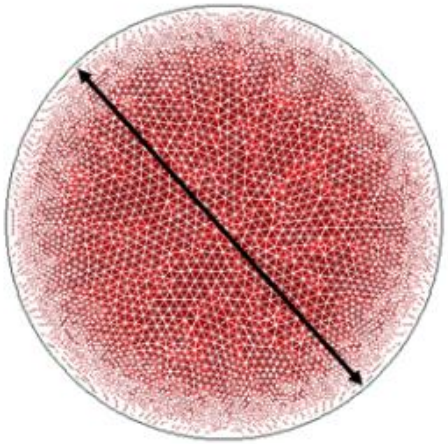
Meshes (2D): only the TFE domain is computed



▼ horizontal vessel (xy)



Ø = 0.385 m

◀ vertical vessel (rz)

Quality > 0.85

Equations

$$\rho\frac{\partial\vec{u}}{\partial t}+\rho(\vec{u}\cdot\nabla)\vec{u}=-\nabla p+\eta\nabla^2\vec{u}+\vec{F}$$ **Momentum**

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\vec{u})=0$$ **Continuity**

$$\rho c_P\frac{\partial T}{\partial t}=\nabla\cdot(\lambda\nabla T)-\rho c_P\vec{u}\cdot\nabla T+S_T$$ **Heat transfer**

$$\frac{\partial C_k}{\partial t}=\nabla\cdot(\mathrm{D}_k\nabla C_k)-\vec{u}\cdot\nabla C_k+S_{C_k}$$ **Mass transfer**

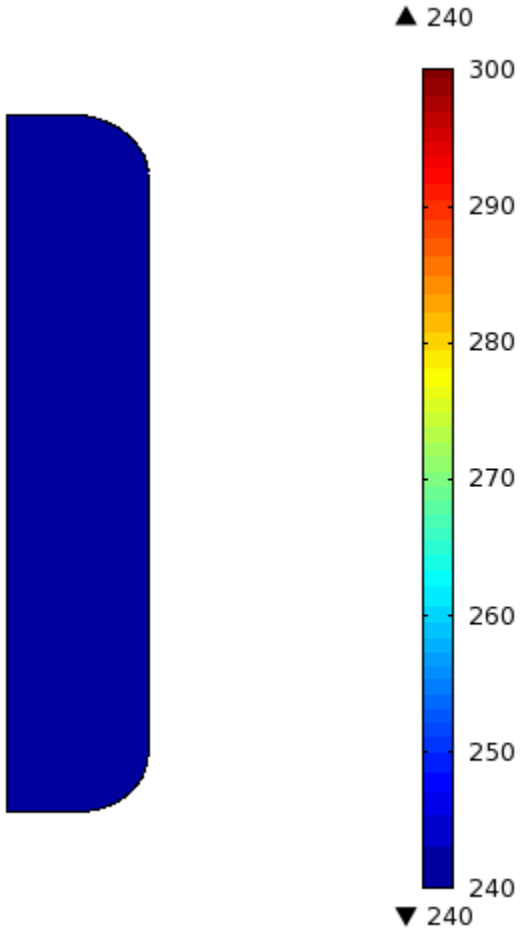
$$\rho=p/(\mathrm{R}_s T)$$ **Ideal gas law**

Chemical Engineering Module:

- *non-isothermal flow mode (chns)*
- *convection and conduction mode (chcc)*
- *convection and diffusion mode (chcd)*

Vertical Reactor

p_0 = 11 bar(a)
T_0 = 240 °C



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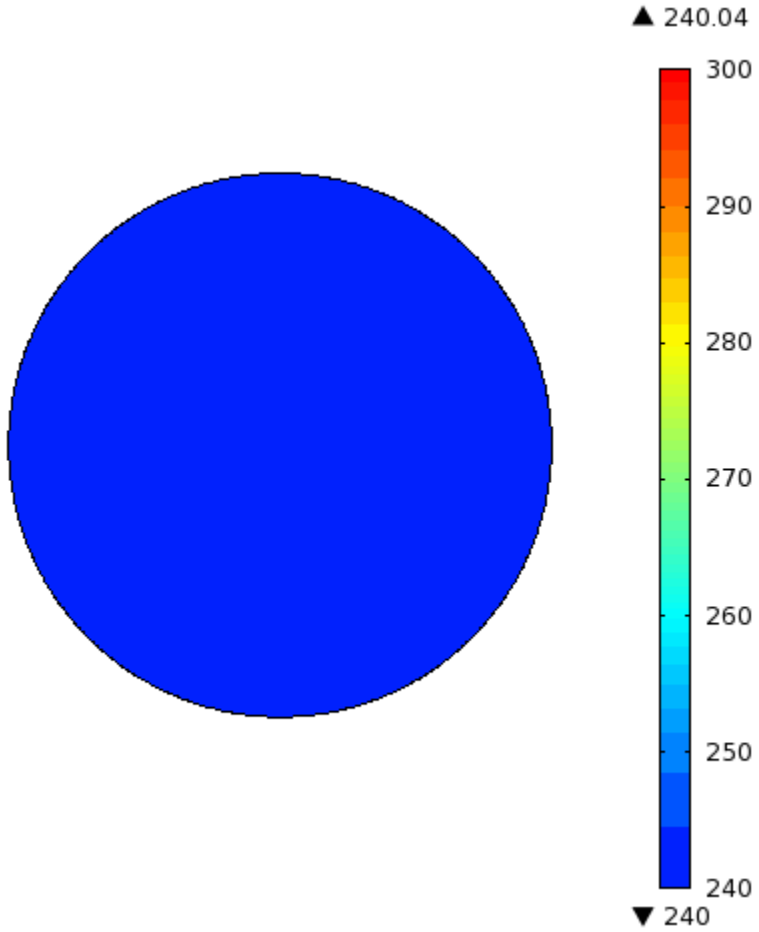
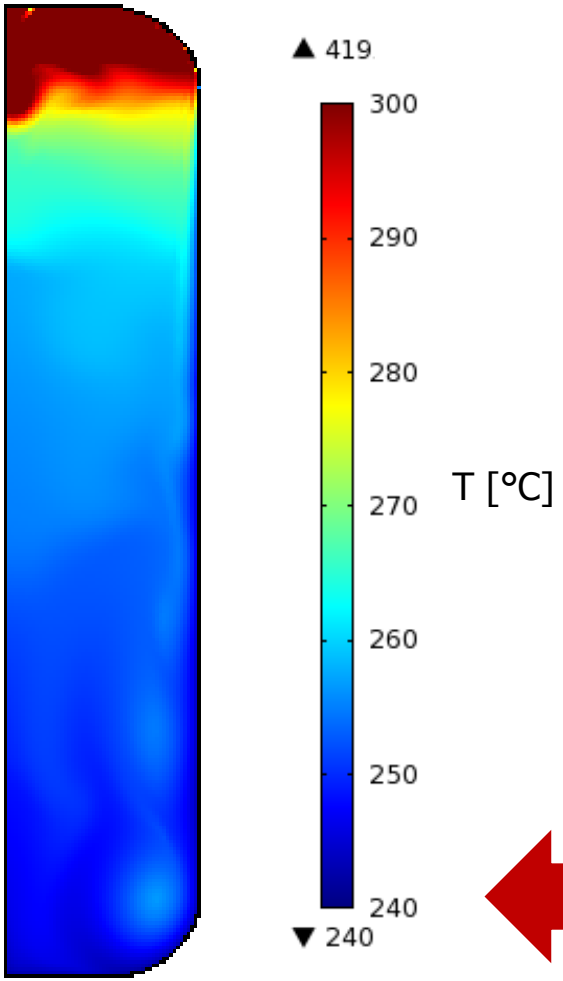


Time=0 Surface: Temperature (degC)

Vertical Reactor

p_0 = 11 bar(a)
T_0 = 240 °C
t = 54 s



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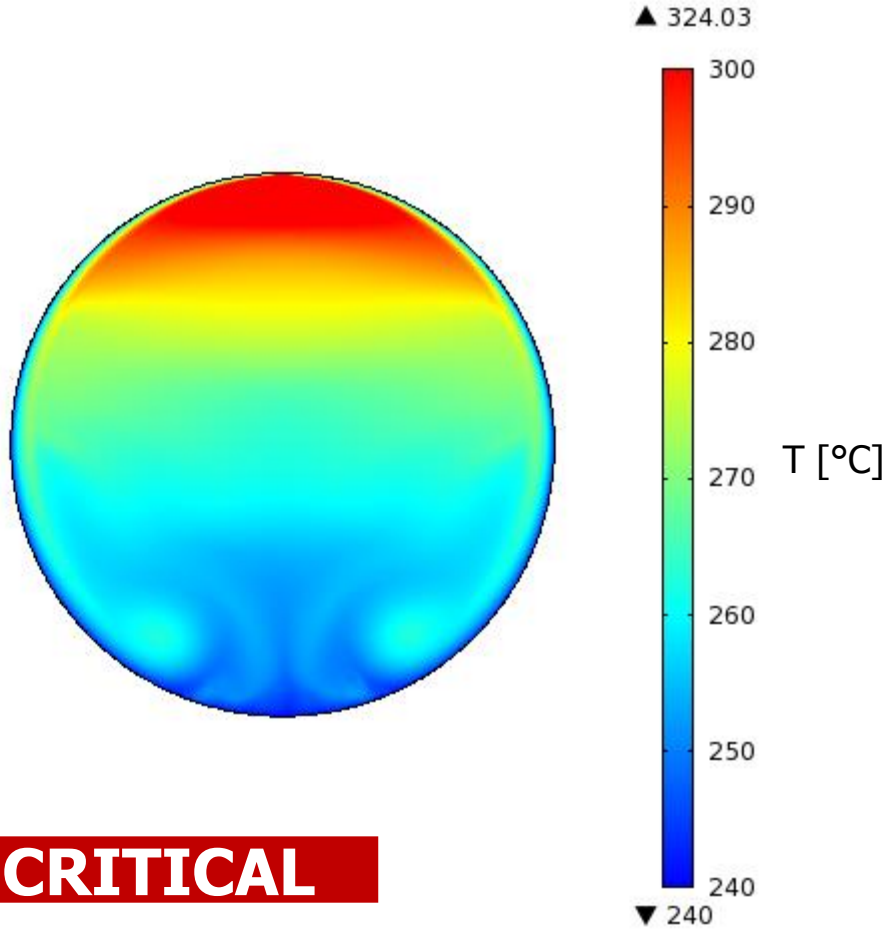
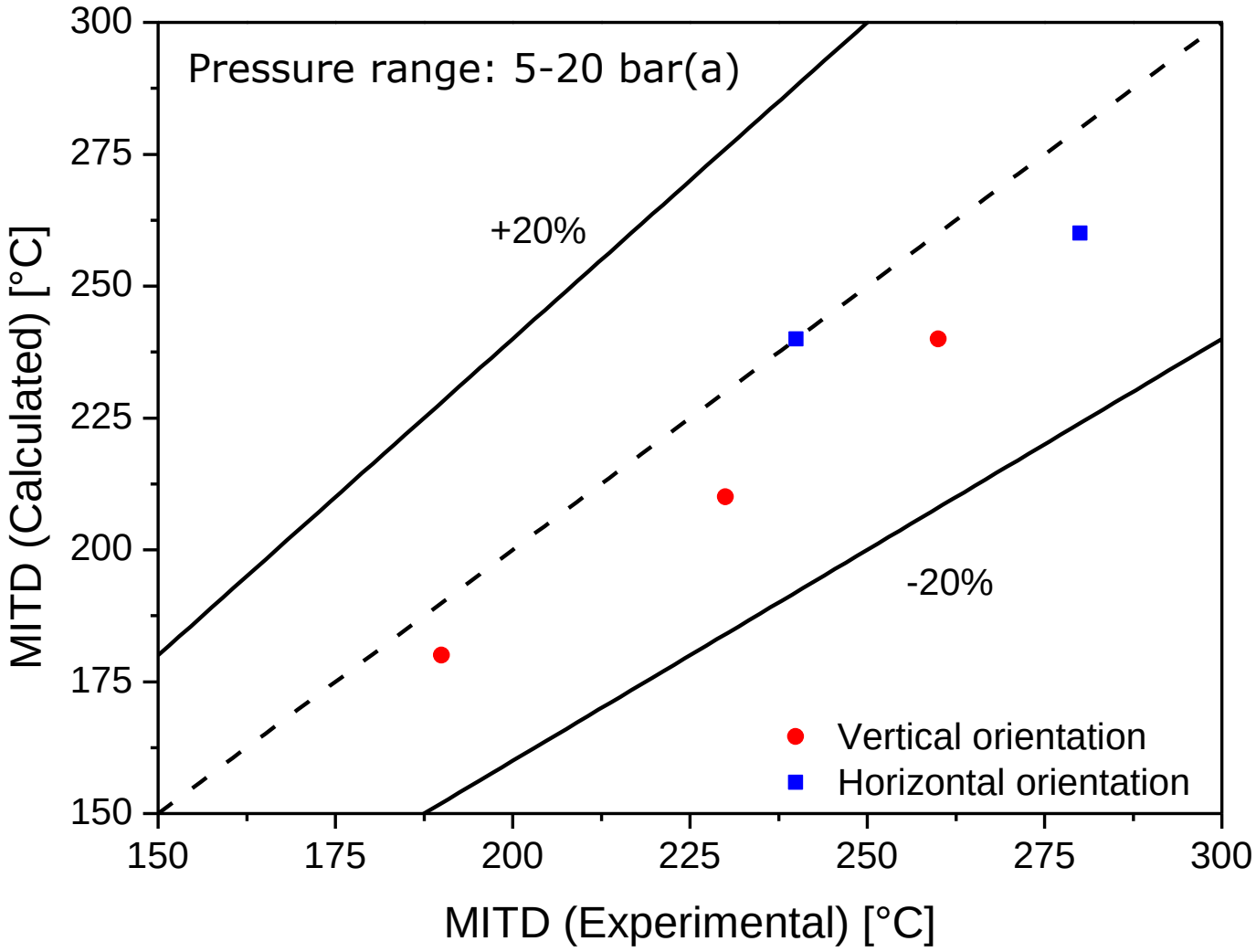


MORE CRITICAL

Prediction accuracy of TFE ignition temperatures (MITD)



- simulations of the self-ignition of TFE in a large scale vessel (100 dm³) were performed
- a good agreement with experimental data was observed
- in particular ignition temperatures of TFE were well predicted
- the model is considered validated for large geometries

QUESTIONS

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