CENTER FOR SUSTAINABLE FUTURE TECHNOLOGIES

CFD Modeling Of A Laboratory-scale Setup for Thermochemical Materials Performance Analysis

S. Salviati[1], N. Vasile[1], F. Carosio[2], G. Saracco[2], A. Fina[2]

[1] *Center for Sustainable Future Technologies, Istituto Italiano di Tecnologia, 10144, Torino, Italy*

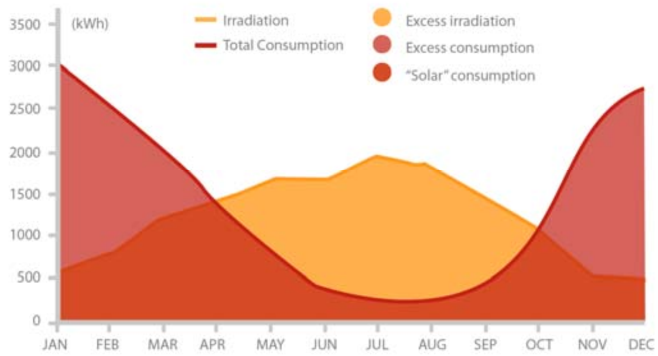
[2] *Dipartimento di Scienza Applicata e Tecnologia, Politecnico di Torino, 15121, Alessandria, Italy*

COMSOL CONFERENCE
2018 LAUSANNE

ISTITUTO ITALIANO DI TECNOLOGIA

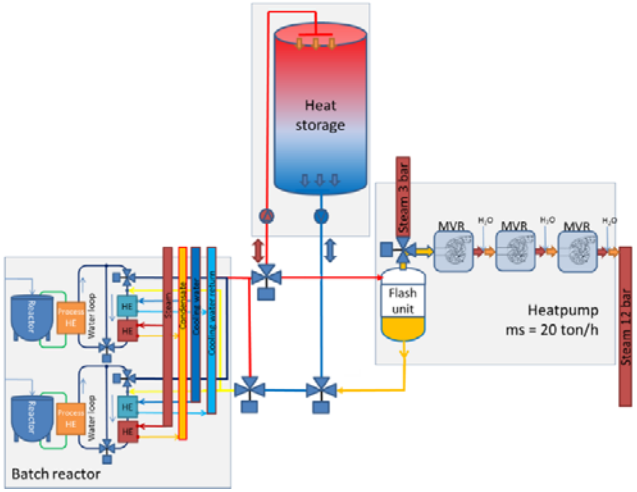
Open issues in Thermal Energy Storage

Seasonal storage in buildings



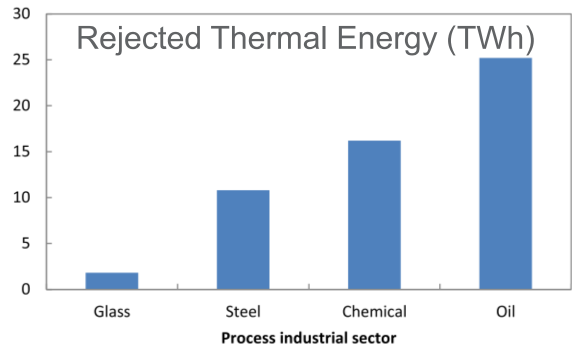
COMTES project
http://comtes-storage.eu/

Heat management in batch processes



Robert de Boer / 12th IEA Heat Pump Conference (2017)

Low grade waste heat reuse

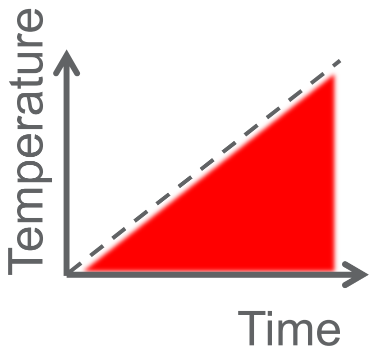


D.M. van de Bor et al. / Energy (2015)

Thermal Storage Technologies

Sensible heat

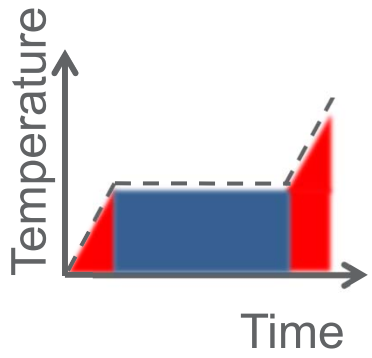
$$Q = mC_p\Delta T$$



Latent heat

$$Q = mC_p\Delta T + mL$$

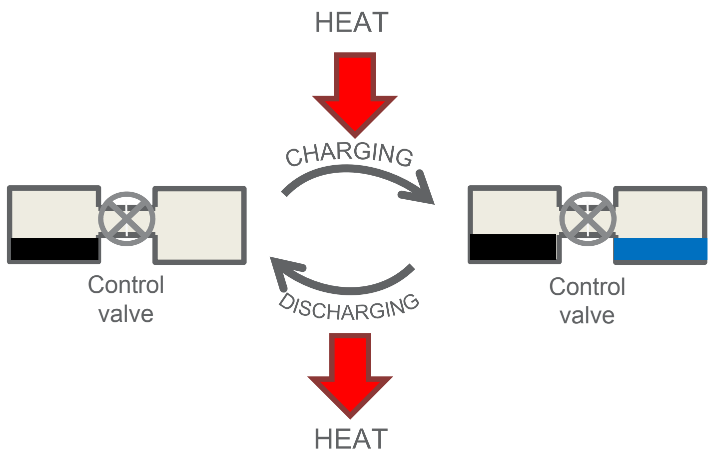
Phase Change Materials (PCMs)



$$L = \Delta H_{phase\ change}$$

Thermochemical materials (TCMs)

$M_nA_m \cdot XH_2O + Q \rightleftharpoons M_nA_m \cdot (X\text{-}Y)H_2O + YH_2O$



$$L = \Delta H_{reaction}$$

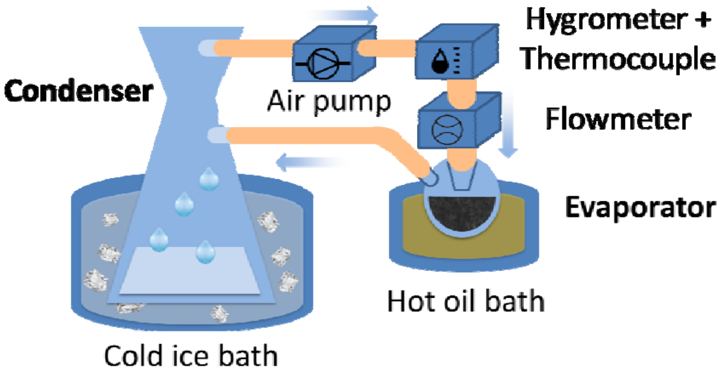
Termochemical storage

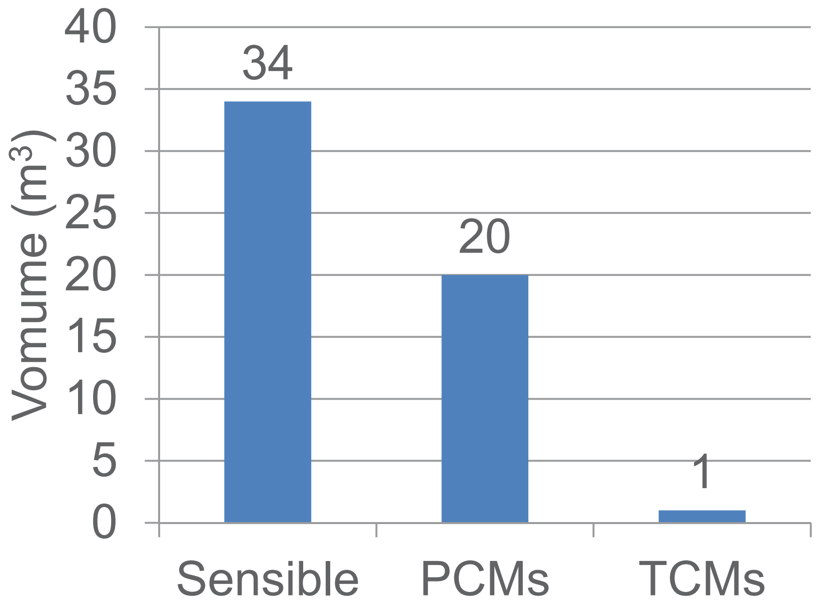
Advantages

- High heat storage density
- Controllable charge/discharge cycles

Disadvantages

- Materials issues: corrosion, low cyclability, difficulty to characterize materials properties
- Device issues: need to identify the best design to maximize heat and mass exchange





Active material volume required to store 1850 kWh (1 year household supply)

N. Yu et al. / Progress in Energy and Combustion Science (2013)

Experimental data fitting

0D component used to calculate reactions constant values
to be used in 3D model using Levenberg-Marquardt method.

Evaporator reaction

$H_2O_{cry} \rightarrow H_2O_{vap}$

$r = k_1 [H_2O_{vap}]$

Condenser reaction

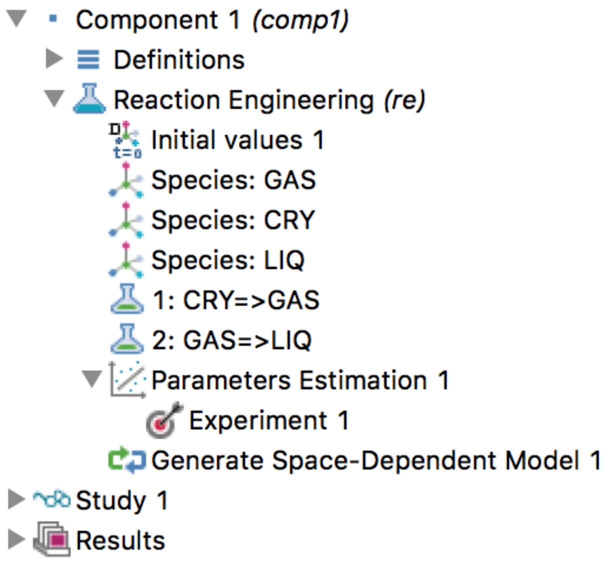
$H_2O_{vap} \rightarrow H_2O_{liq}$

$r = k_2 (1/[H_2O_{vap}])$

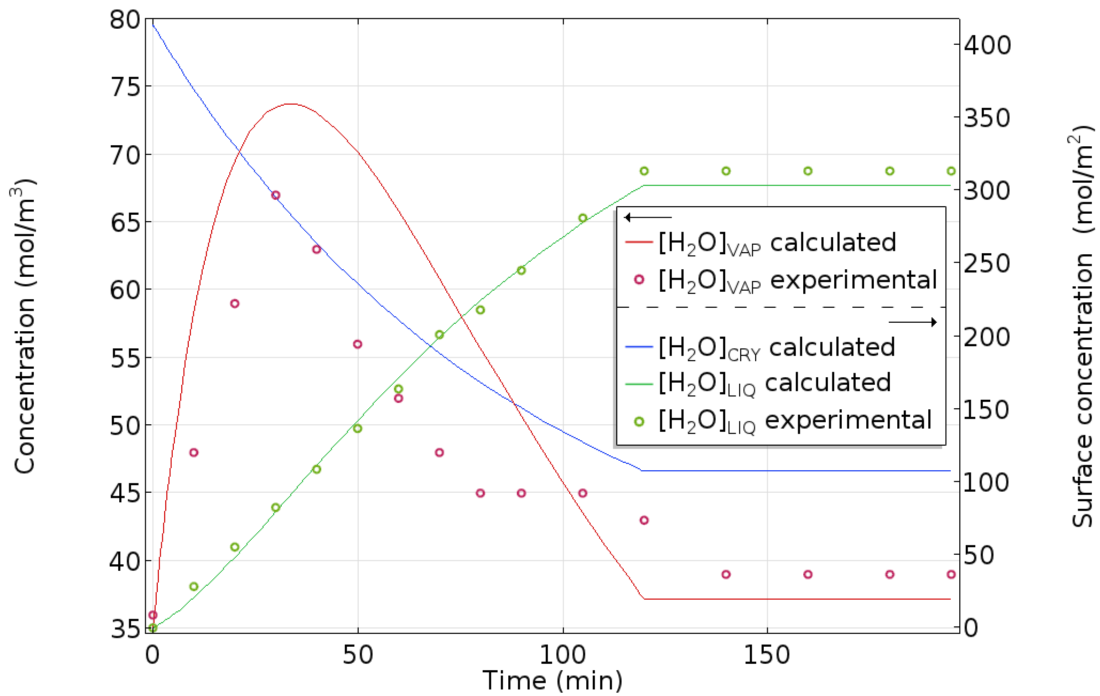
Calculated reaction constants

k_1=0.043 1/s

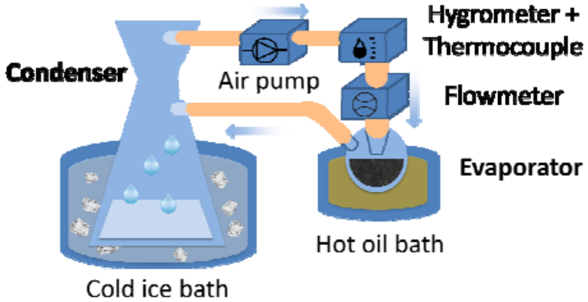
k_2=0.0112 1/s

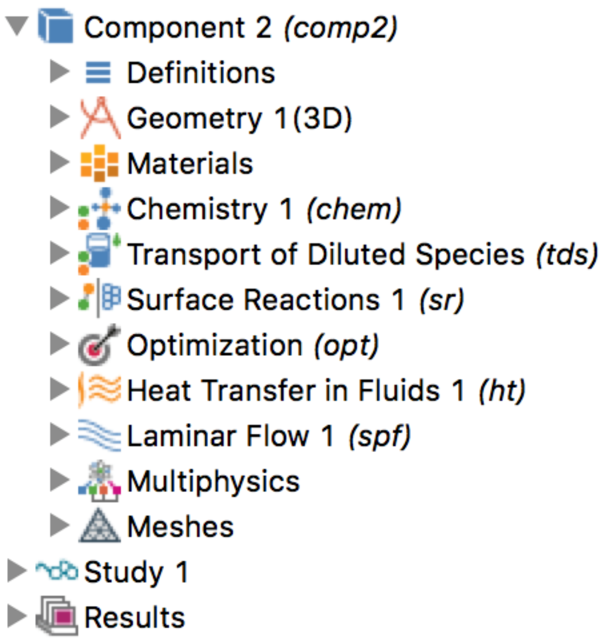


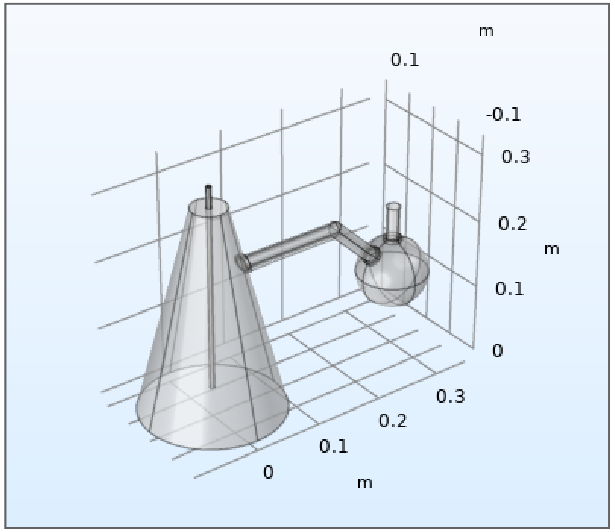
Thermochemical material:
$SrBr_2 \cdot 6H_2O$/graphite
composite

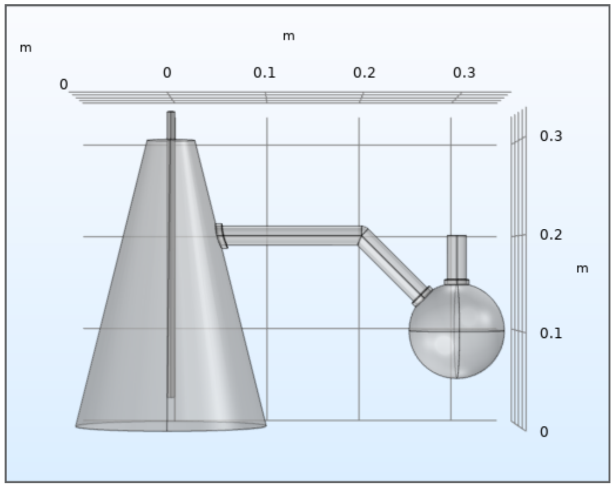


Thermochemical reactor design





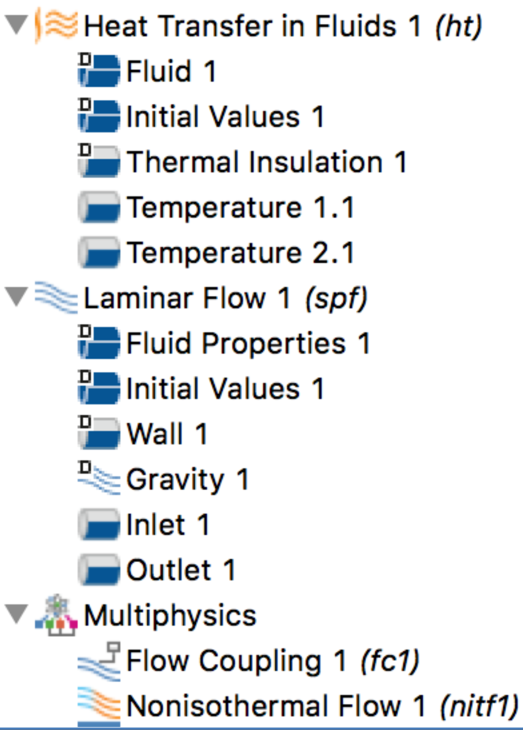


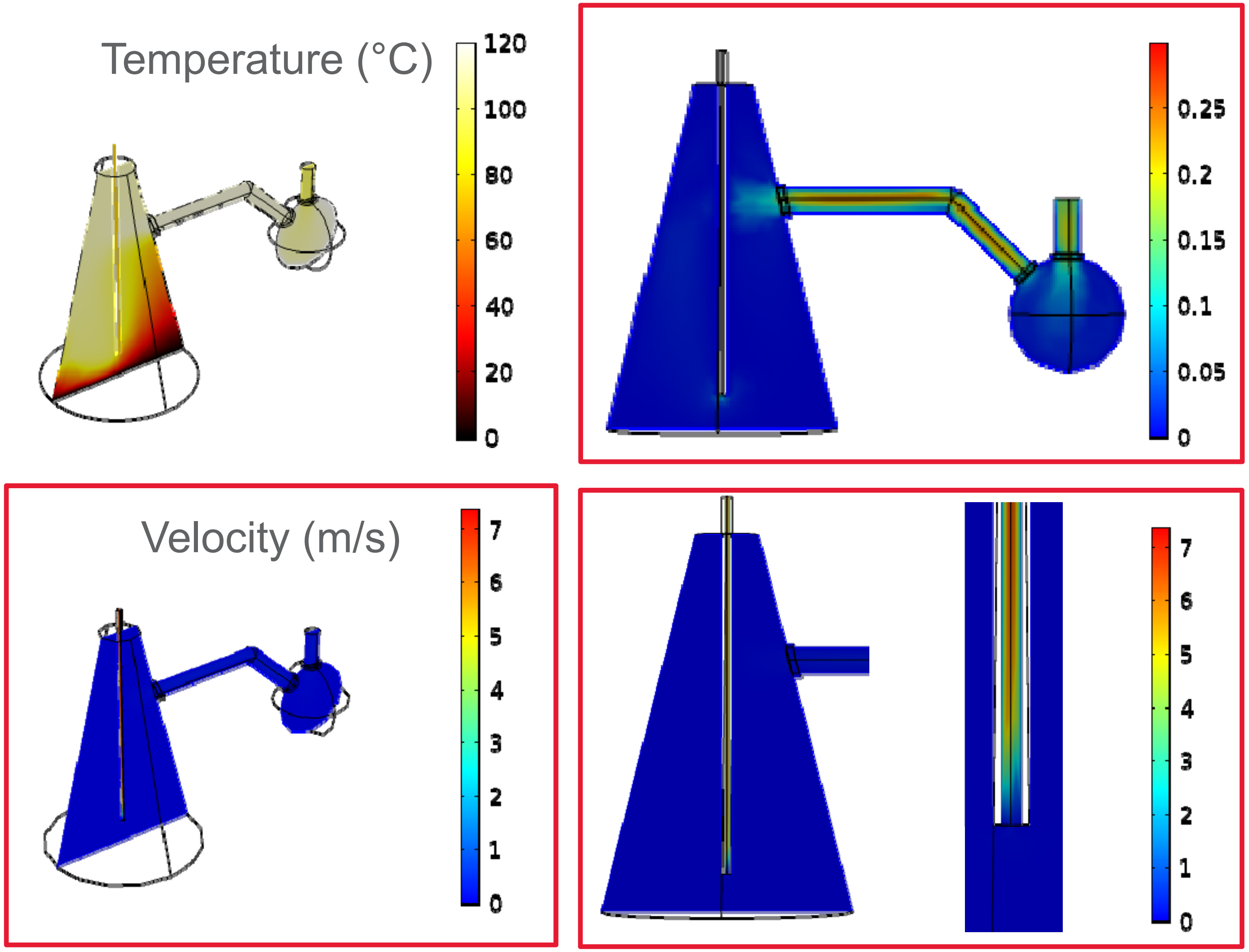


COMSOL® applications «Degradation of DNA in Plasma» and «Protein Adsorption» were used as examples

Thermo-fluid dynamics

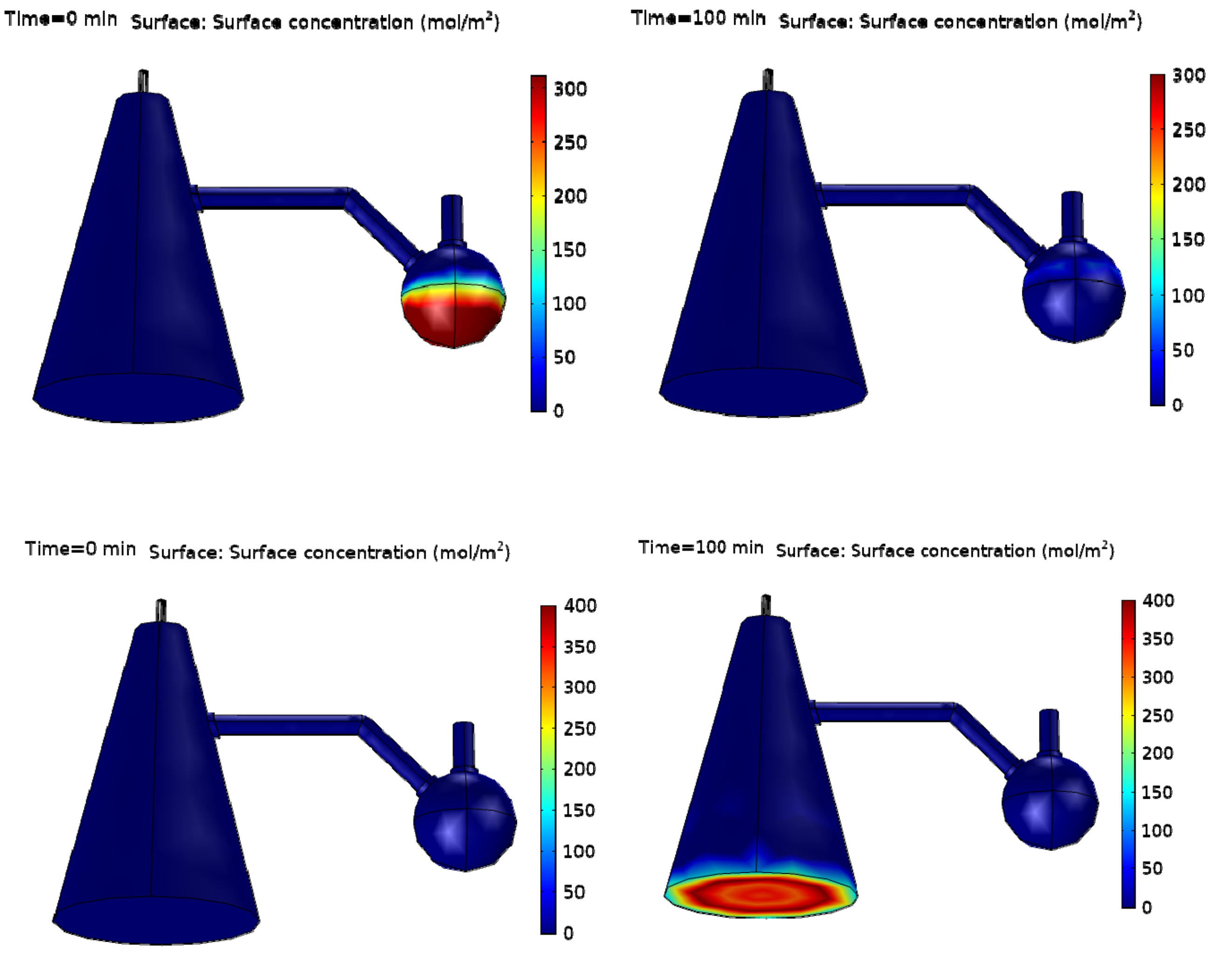
Parameter	Value
Inflow velocity	1.5 m/s
Evaporator temperature	120 °C
Condensator temperature	0 °C





Surface reactions

- Chemistry 1 *(chem)*
  - 1: Surface: CRY(ads)=>GAS
  - Surface species: CRY(ads)
  - Species: GAS
  - 2: Surface: GAS=>LIQ(ads)
  - Surface species: LIQ(ads)
- Transport of Diluted Species *(tds)*
  - Transport Properties 1
  - No Flux 1
  - Initial Values 1
  - Reactions 1_CRY
  - Inflow 1
  - Outflow 1
  - Reactions 2_LIQ
- Surface Reactions 1 *(sr)*
  - Surface Properties 1
  - No Flux 1
  - Initial Values 1
  - Reactions 1
  - Reactions 2
  - Initial Values 2_CRY
  - Initial Values 3_LIQ



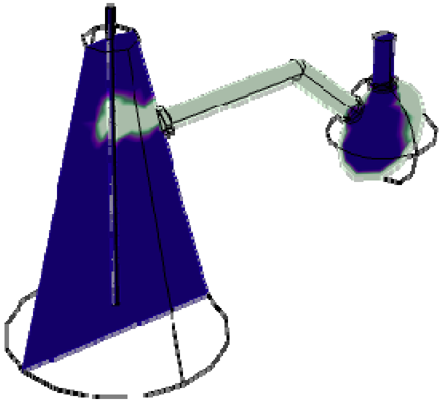
Condensation area

$$RH = \frac{p(T)}{p_{sat}(T)} = \frac{cRT}{20.386 - (\frac{5132}{T})}$$

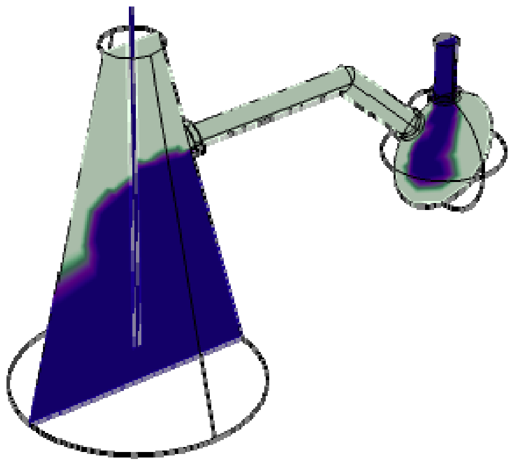
RH>100%

RH<100%

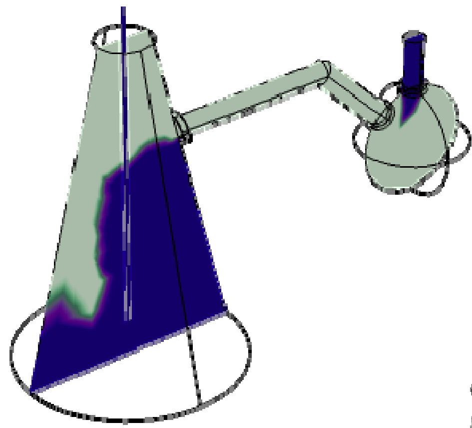
Time=10 min



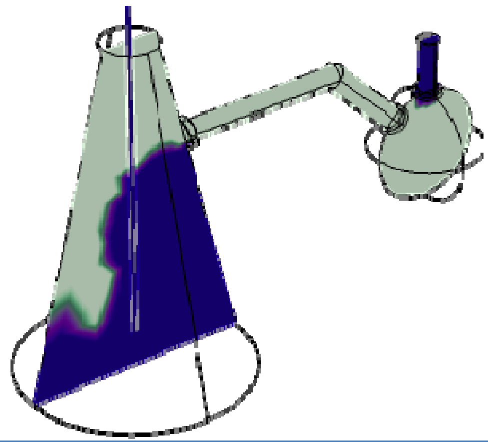
Time=30 min



Time=70 min



Time=100 min



Conclusions and outlook

- Assembly and testing of a lab scale thermochemical reactor
  in the charging step
- Realization of a working 3D model using COMSOL® evaluating thermo-fluid dynamics, reactions evolution and water vapor transport
- Study of RH surface to guide geometry improvement

- Design improvement towards an application-ready geometry
- Implementation of condensation on reactor surfaces
- Normalization of reaction constants *k* over geometry to compare different materials performance

Thanks for your kind attention

Any questions?