COMSOL
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Thermal Modeling of Chlorination Reactor

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OVERVIEW

- Introduction
- Numerical model
  - Main features of the model
  - Geometry & Meshing
  - Governing equations
  - Boundary Conditions
- Numerical results
- Conclusions

Chlorination Reactor

❑ **Salt handling and purification system**

❑ **Electrorefiner**

N_2 atm glove box

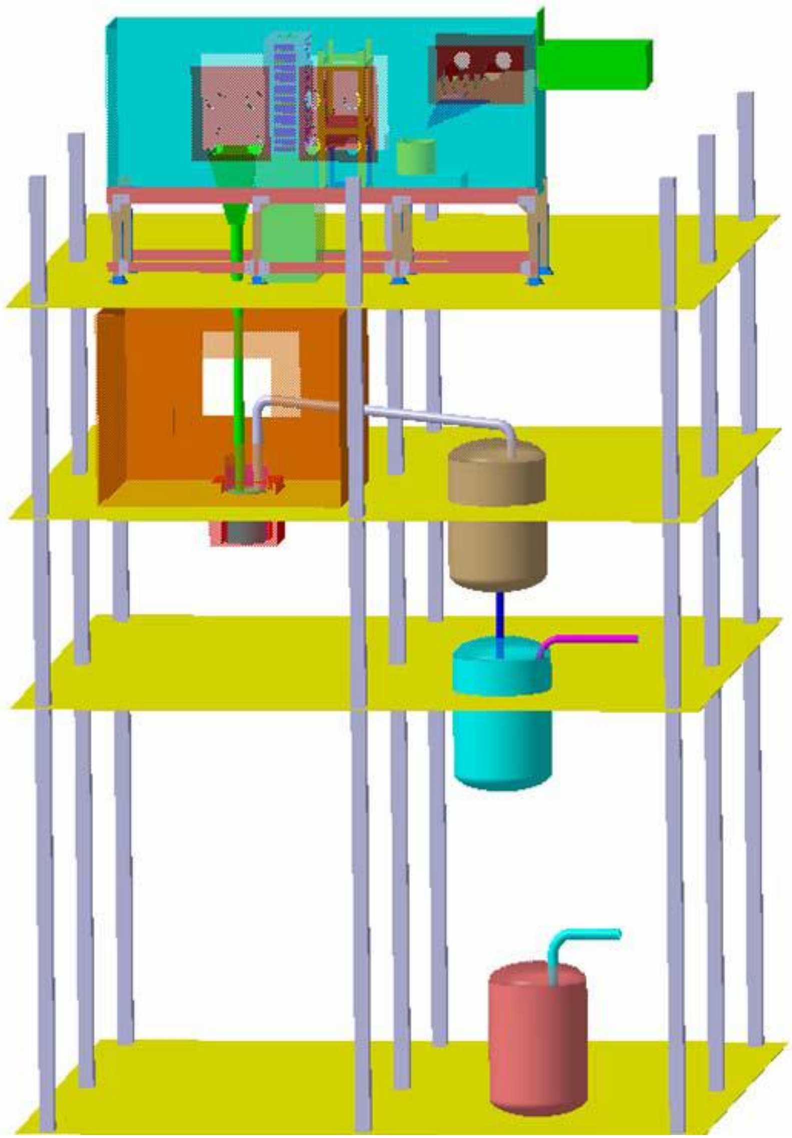
vacuum oven

Chlorination Reactor

Intermediate Vessel

Transfer Vessel

Spent salt vessel



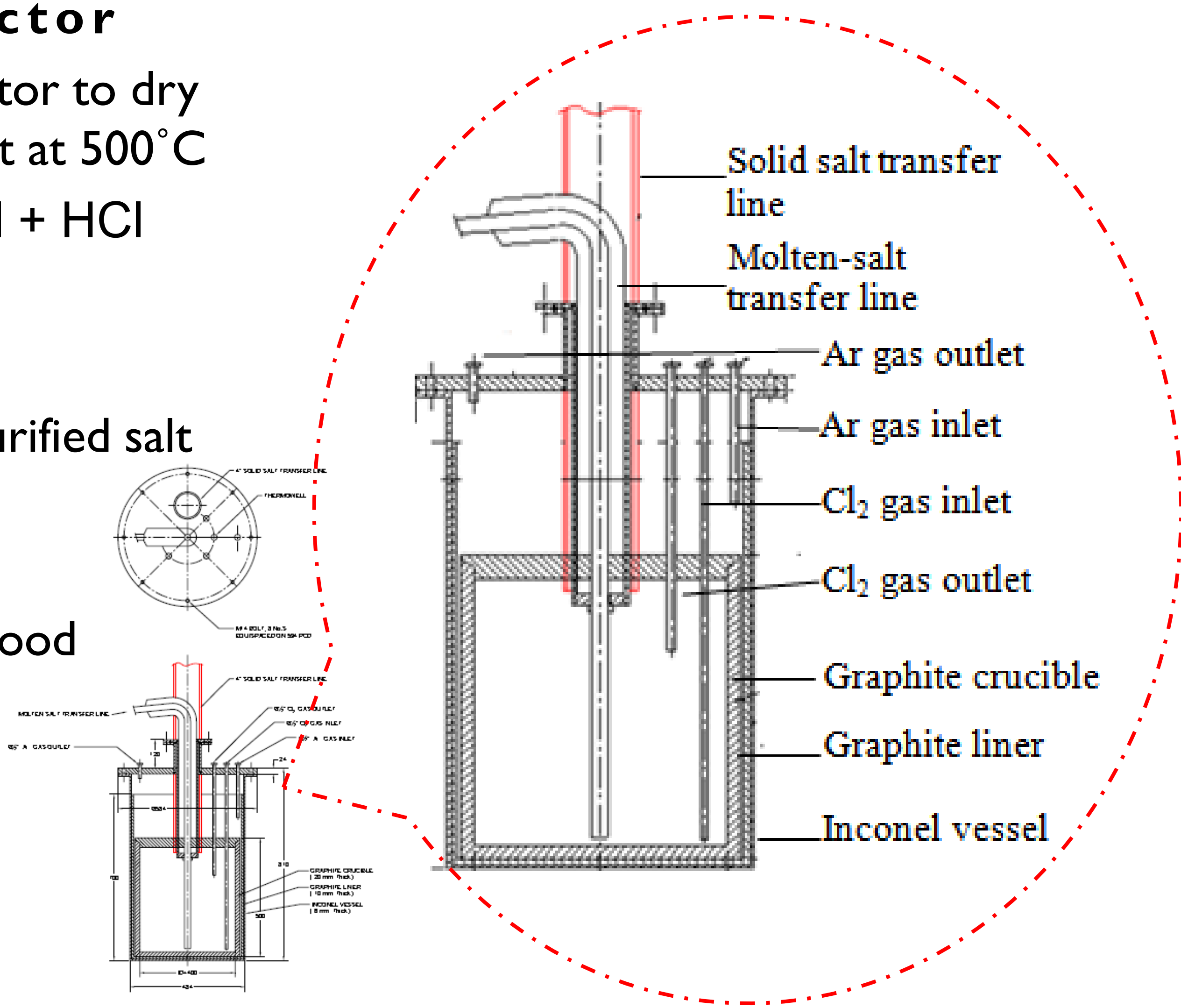
❑ Chlorination Reactor

It is a high temperature reactor to dry molten LiCl-KCl eutectic salt at 500˚C

$Cl_2 + LiOH \rightarrow LiCl + HOCl + HCl$

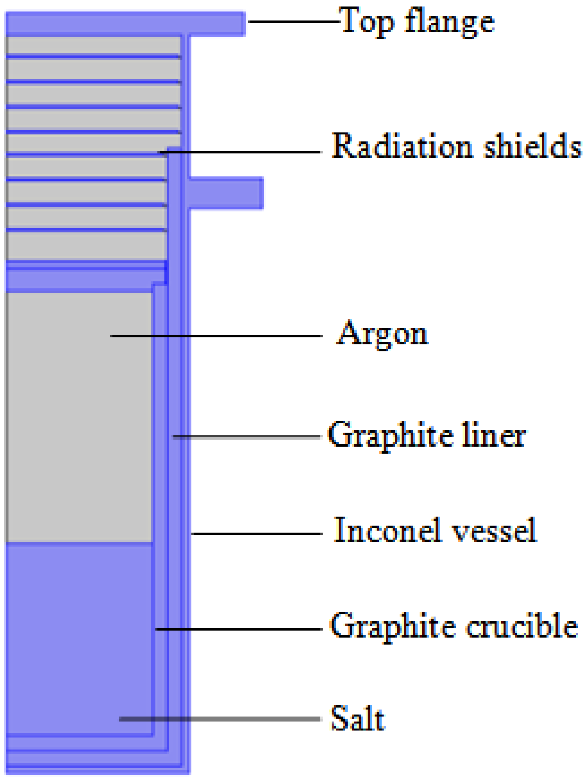
Functions :

- Melts the solid salt and purified salt transfer
- Chlorination Reaction
- Operates in inert fume hood
- Resistance heating



- ✓ Multiphysics problem-
- ✓Non linear properties
- ✓1:1 scale model
- ✓Axi-symmetric model
- ✓Steady state
- ✓Conjugate heat transfer
- ✓buoyancy driven flow using volumetric force term
- ✓Effective thermal conductivity model

- Physics –controlled fine triangular mesh



2D-axisymmetric COMSOL model of chlorination reactor

❑ GOVERNING EQUATIONS AND BOUNDARY CONDITIONS

Fluid Flow- Continuity and Momentum equations

$$\frac{1}{r}\frac{\partial}{\partial r}(ru) + \frac{\partial}{\partial z}(v) = 0$$

$$\rho u \frac{\partial u}{\partial r} + \rho v \frac{\partial u}{\partial z} = -k\frac{\partial p}{\partial r} + \mu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}(ru)\right) + \frac{\partial^2 u}{\partial z^2}\right]$$

$$\rho u \frac{\partial v}{\partial r} + \rho v \frac{\partial v}{\partial z} = -k\frac{\partial p}{\partial z} + \mu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}(rv)\right) + \frac{\partial^2 v}{\partial z^2}\right] + \rho(T)g_z$$

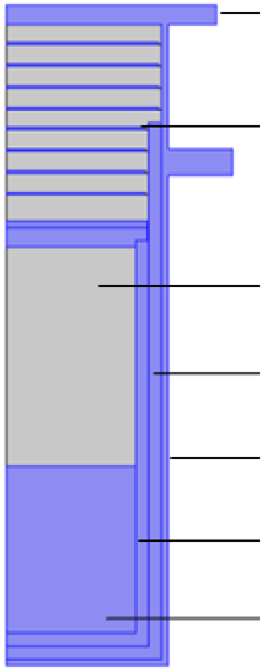
- **These equations are solved in fluid computational domains of model.**
- **The boundary conditions imposed for fluid flow are no slip and pressure point constraint.**

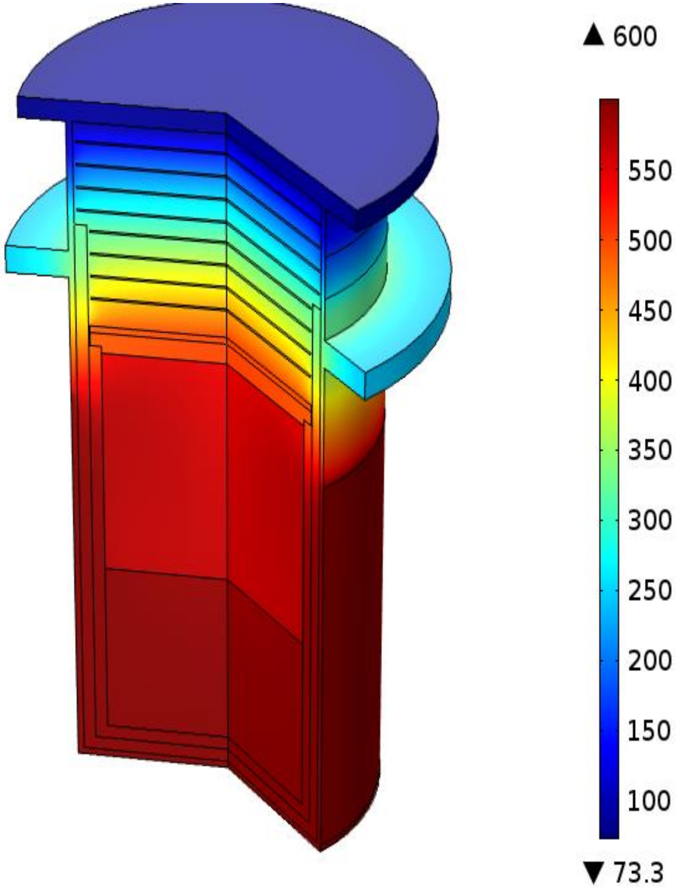
❑ GOVERNING EQUATIONS AND BOUNDARY CONDITIONS

Thermal field – Energy equation

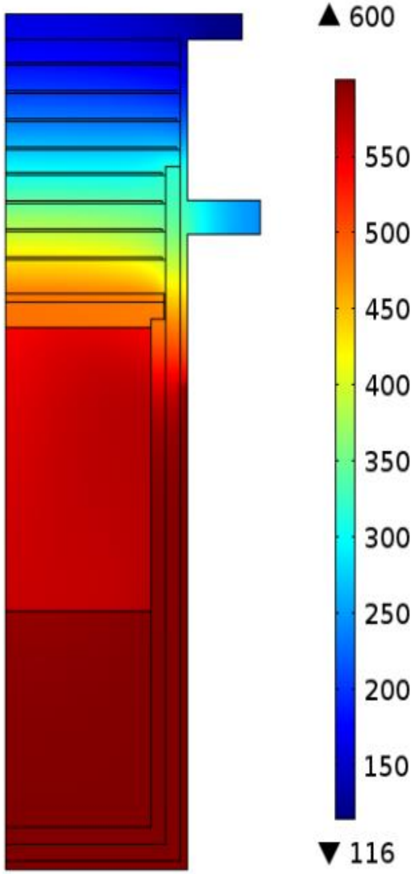
$$\rho c_p u \frac{\partial T}{\partial r} + \rho c_p v \frac{\partial T}{\partial z} = k\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial z^2}\right]$$

- All domains computational domains of the model,
- All the initial temperatures are set to 30°C
- All the inside free surfaces in the model are allowed to participate in surface to surface radiation.
- The outer vessel wall surfaces are allowed to participate in surface to ambient radiation and convective cooling using suitable values of *h*.
- *Dirichlet b.c. for vessel wall*
- Water cooling on the vessel wall near the top flange is given as convective cooling boundary condition.

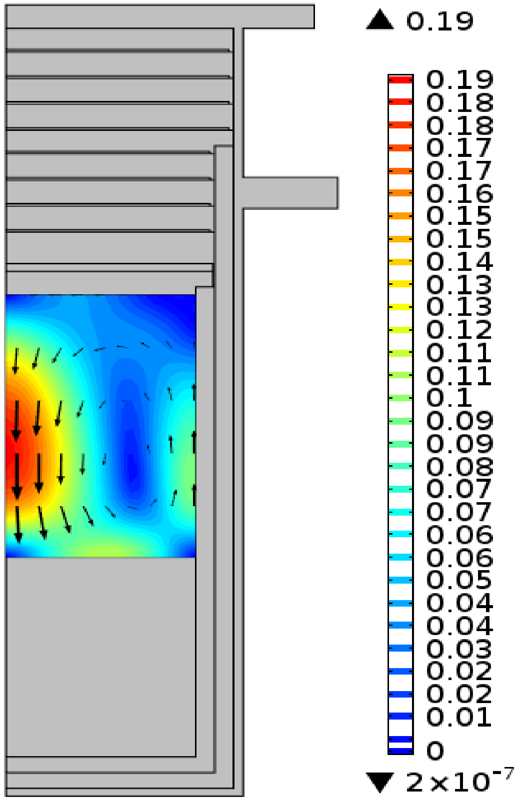




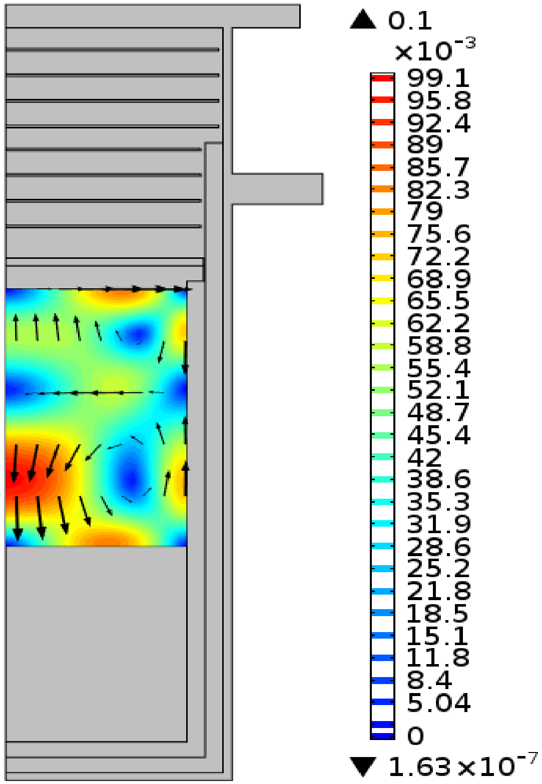
3D Temperature distribution in the chlorination reactor



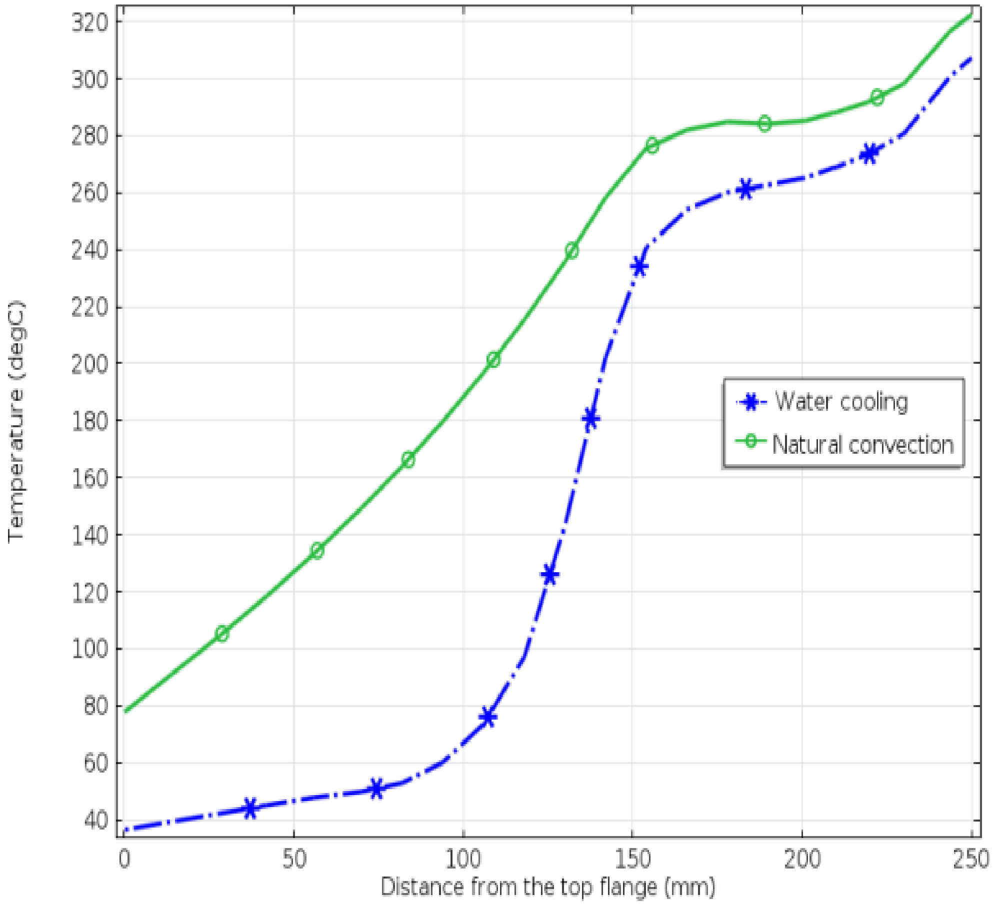
2D Temperature distribution in the chlorination reactor

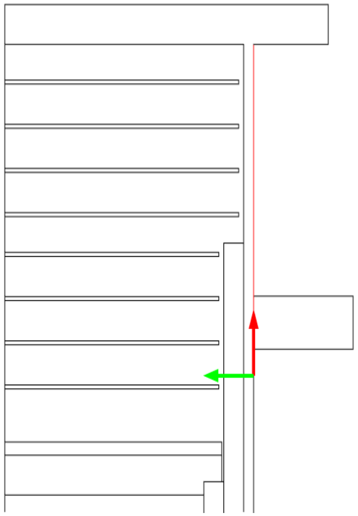


Velocity distribution in the cover gas
(Natural convection case)



Velocity distribution in the cover gas
(Forced convection case)

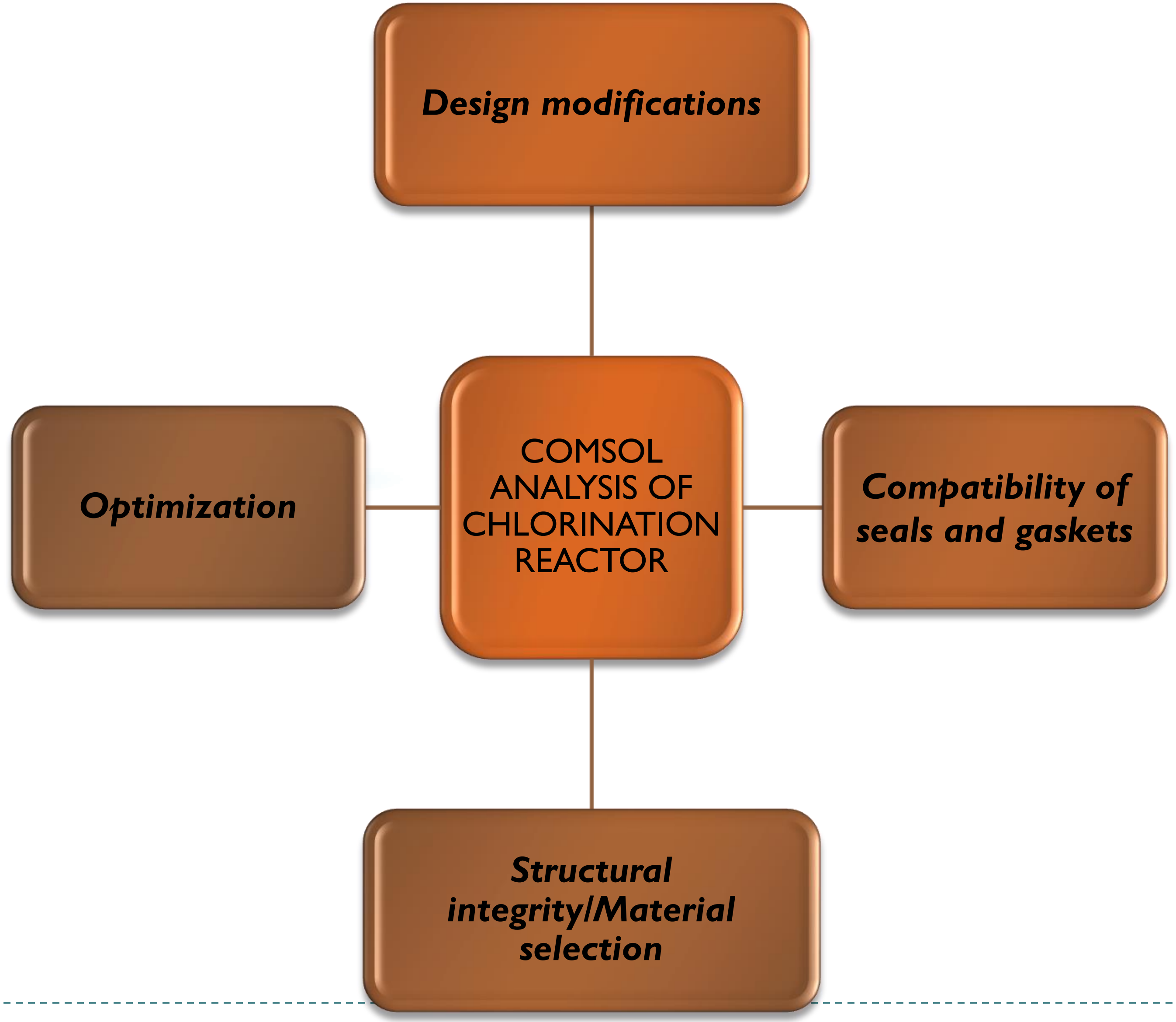




Temperature profile in top portion of outer vessel.

- ✓ 2D axisymmetric model of Chlorination Reactor.
- ✓ Solution of heating problem in the Chlorination Reactor.
- ✓ Evaluation of Temperature and Velocity field.
- ✓ The results of this study have shown that furnace temperature of 600 °C is sufficient to maintain the salt phase at temperature of about 500 °C.
- ✓ The water cooling, if attempted for the vessel, will change temperature distribution in the reactor and result in steep thermal gradients in the vessel wall hence calling for thermal stress analysis of the components.
- ✓ The radiation shields provided and with natural convection cooling of the vessel wall, the top flange temperature is reasonable to allow smooth operation of the reactor.

Importance



COMSOL ANALYSIS OF CHLORINATION REACTOR

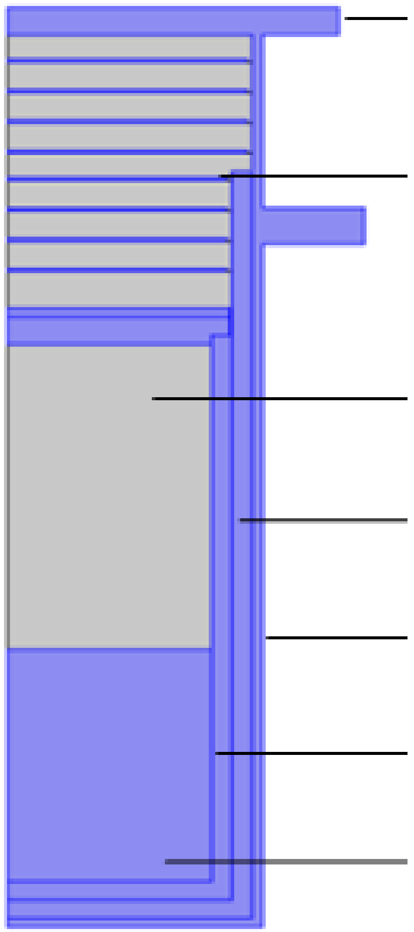
Design modifications

Optimization

Compatibility of seals and gaskets

Structural integrity/Material selection

Future Work



Parametric Studies for number of baffles

Chlorine Transport and Chemical Reaction

Melting and solidification

References

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5. COMSOL Multiphysics, User Manual, Modules and Model Library, Comsol 4.4a

Thanks for your attention............