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Evaporation of Liquid Chlorides in Closed Tanks using the PHOENICS Code

Presentation of a Rigid Interface Model (RIModel)

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SUMMARY

1 - INTRODUCTION

2 - EVAPORATION OF LIQUIDS - *Theorical Background*

3 - RIModel (Rigid Interface Model)

- *Governing Equations and Characteristics*
- *Application with the PHOENICS Code*
- *Boundaries Conditions for Parametric Study*
- *Simulated Cases*
- *Exemple of Results*

4 - RIModel VALIDITY LIMIT - *Subcooled Pool Boiling Situation*

5 - CONCLUSION

INTRODUCTION

1 - Optical Fiber Industry

- Liquid ($SiCl_4$, $GeCl_4$, ...) changed into Vapor and Oxydized (SiO_2, GeO_2, ...)
- Mainly used Current Technique : Bubbling $\Rightarrow$ Carrier Gas send into Liquid
- Intended Technique : Direct Liquid Evaporation for Higher Vapor Flow expected

2 - Prediction of Evaporation Phenomenon means turn to Numerical Simulation

- Hydrodynamic and Thermal Phenomena Simulation inside Closed Tanks
- Start from Equilibrium Situation and Simulation of Flow Requirements for Optical Fiber Production

INTRODUCTION

3 - Specific Model for prediction of Evaporation Process in closed Tanks

- Multi-Domain Method

⇒ Resolution of each Phase separately

⇒ *Two Phases linked by Boundaries Conditions at the Interface*

- Use CHAM's CFD PHOENICS

⇒ Computation of a Specific Model for Evaporation in Closed Tanks

⇒ Interface taken as a Rigid Plate with a Moving Speed

⇒ *RIModel (acronym of Rigid Interface Model)*

EVAPORATION OF LIQUIDS - *Theorical Background*

1 - Two kinds of Evaporation Processes for Liquids

- Vapor directly produced at Liquid / Vapor Interface *(Radiative Heating for instance)*
- Vapor produced by Bubbles starting at Immersed Solid Heated Surface *(Pool Boiling)*

2 - Pool Boiling $\Rightarrow$ *4 Boiling Mechanisms*

- Subcooled Boiling $\Rightarrow$ *No bubbles (or Recondense near Heated Surface)*
- Boiling with Net Evaporation $\Rightarrow$ *Nucleate Boiling Region*

  $\Rightarrow$ *Partial Film Boiling Region (or Transition)*

  $\Rightarrow$ *Film Boiling Region*

EVAPORATION OF LIQUIDS - *Theorical Background*

3 - How to predict Evaporation Phenomenon in Closed Tanks ?

⇒ ASSUMPTION :

Pool Subcooled Boiling ⇒ *Pressure Stability, Avoiding Decay of Liquid Precursors*

⇒ CONSEQUENCE :

Two Phases Liquid and Vapor strictly separated : Analogy with Melting Process

⇒ Two Regions with Different Thermodynamic Properties separated by a Moving Interface

⇒ Heat Exchange at the Interface according Heat Conduction with Release *(Solidification or Condensation Process)* or Absorption of Heat *(Melting or Evaporation Process)*

RIModel - *Governing Equations and Characteristics*

4 - Implement Features with PHOENICS ⇒ *Rigid Interface Model (RIModel)*

- *Vapor Quantity Calculation by a Mass Balance and the Perfect Gas Law :* **Mvap (t)**

  Mvap (t) = Mvap(t = 0) – Mcoll (t) + Mint (t) ⇒ **Pvap**

- *Liquid Interface Temperature Calculation with Antoine's Equation (SiCl4) :* **Ts**

  Pvap = 10^[4.09777 – 1200 / (Ts – 37)] ⇒ **Ts**

- *Mass Exchange Calculation at the Interface :* **qint (t)**

  qint (t) . ΔHvap = [λvap . (∂T/∂z) – λliq . (∂T/∂z)] ⇒ **qint (t)**

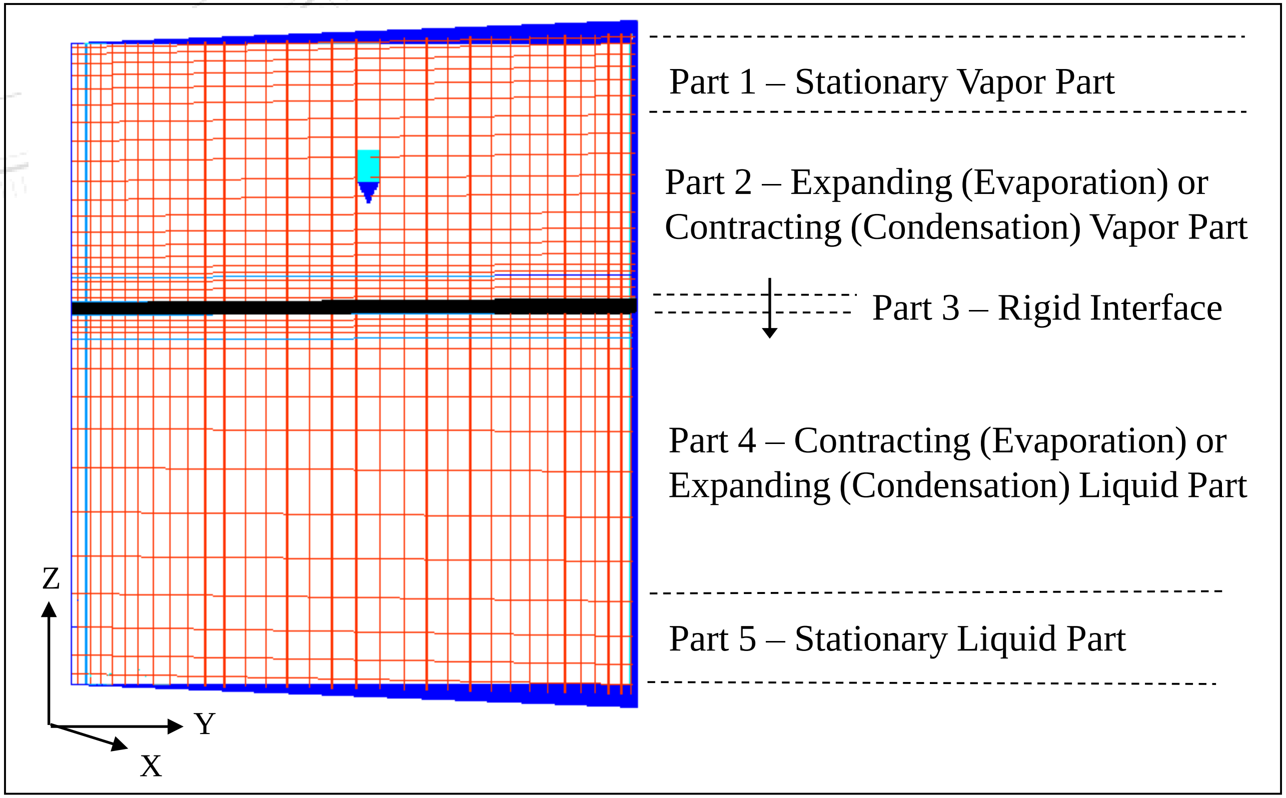
- *Interface taken as Rigid Plate with Moving Speed equal to Evaporation Speed*

- *Friction at the Vapor Side of the Plate and Slip without Friction at the Liquid Side of the Plate*

RIModel - *Application with the PHOENICS Code*

1 - Moving Grid Option ⇒ *ZMOVE function of PHOENICS*

2 - Tank Internal Domain splitted in 5 Zones



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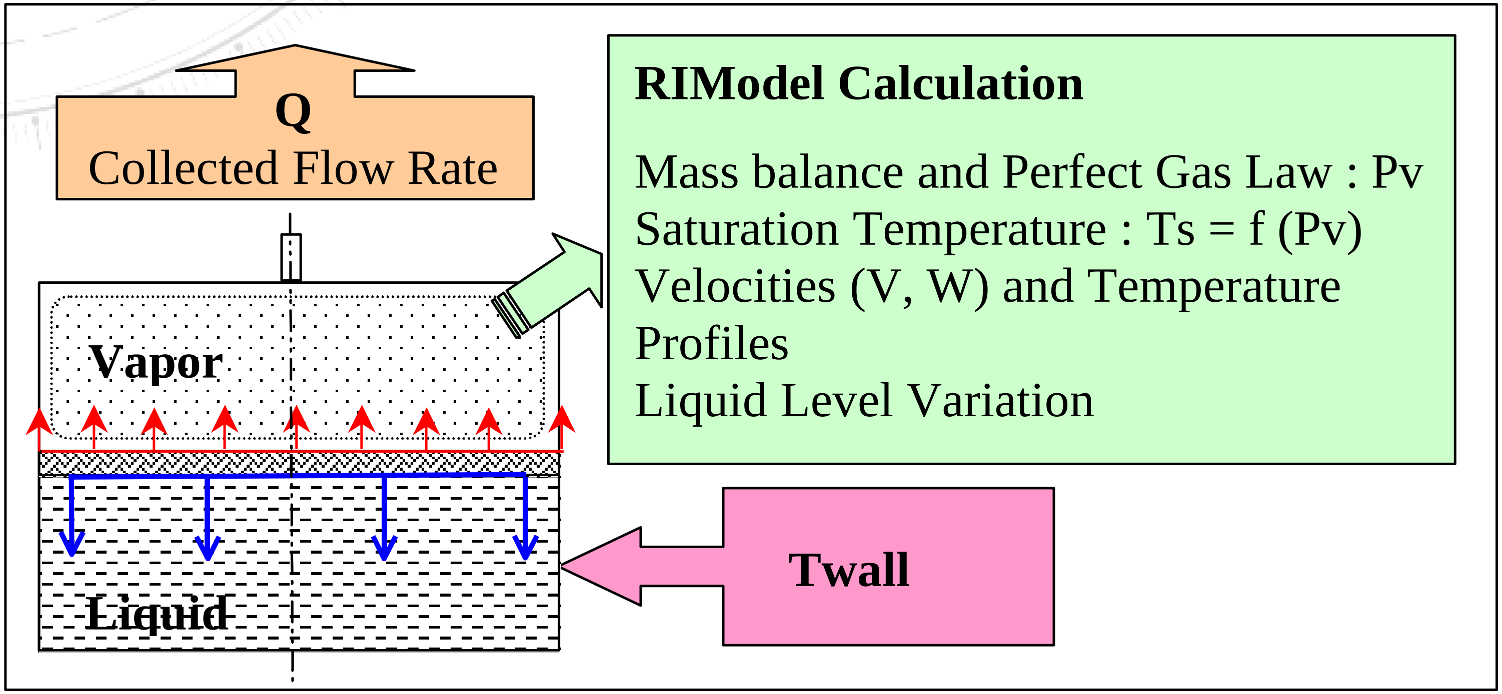
RIModel - *Boundaries Conditions for Parametric Study*

3 PARAMETERS FOR PARAMETRIC STUDY

⇒ Q *(Collected Vapor Flow)*

⇒ S *(Size of Evaporation Surface)*

⇒ Twall *(Fixed Wall Temperature)*



RIModel - *Simulated Cases*

		S1	S2 = 2 x S1	S3 = 5 x S1
		Geometry n°1 (S1 = 5.6 dm^2)	Geometry n°2 (S2 = 11.2 dm^2)	Geometry n°3 (S3 = 28 dm^2)
Q1	Vapour Flow n°1 (Q1 = 6.5 gr/min)	Case n°1	Case n°4	Case n°7
Q2 = 2 x Q1	Vapour Flow n°2 (Q2 = 13 gr/min)	Case n°2	Case n°5	Case n°8
Q3 ≈ 5 x Q1	Vapour Flow n°3 (Q3 = 30 gr/min)	Case n°3	Case n°6	Case n°9

And for Every Case :

⇒ Same Tank Internal Volume (29 Liters) and Liquid Quantity (20 Liters)

⇒ Fixed Wall Temperature (Twall) fixed by “Empiric” Determination

RIModel - *Exemple of Results for Case n°5*

1 - Boundary Conditions

⇒ *Collected Vapor Flow : Q2*

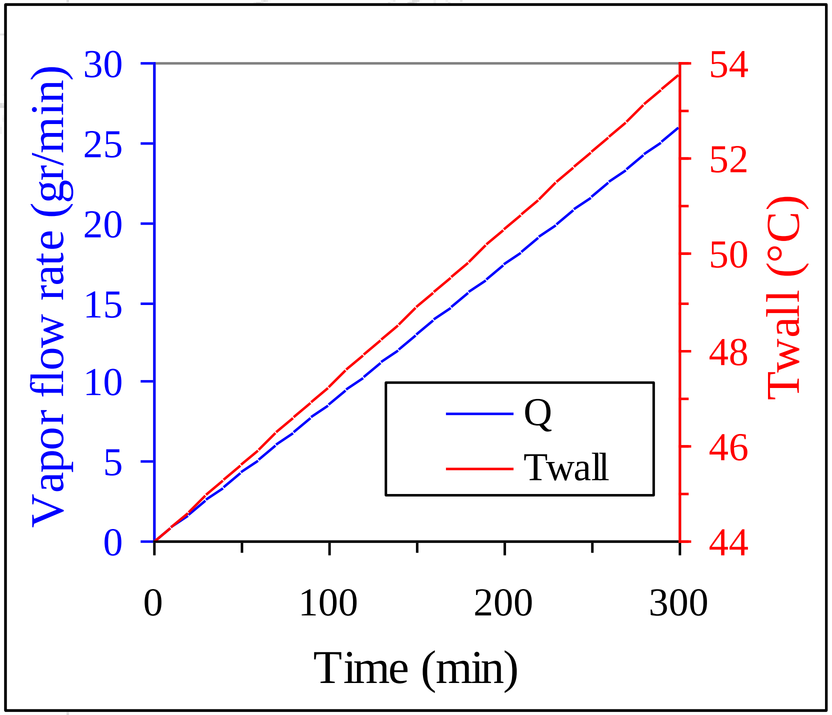
⇒ *Evaporation Surface : S2 = 11.2 dm²*

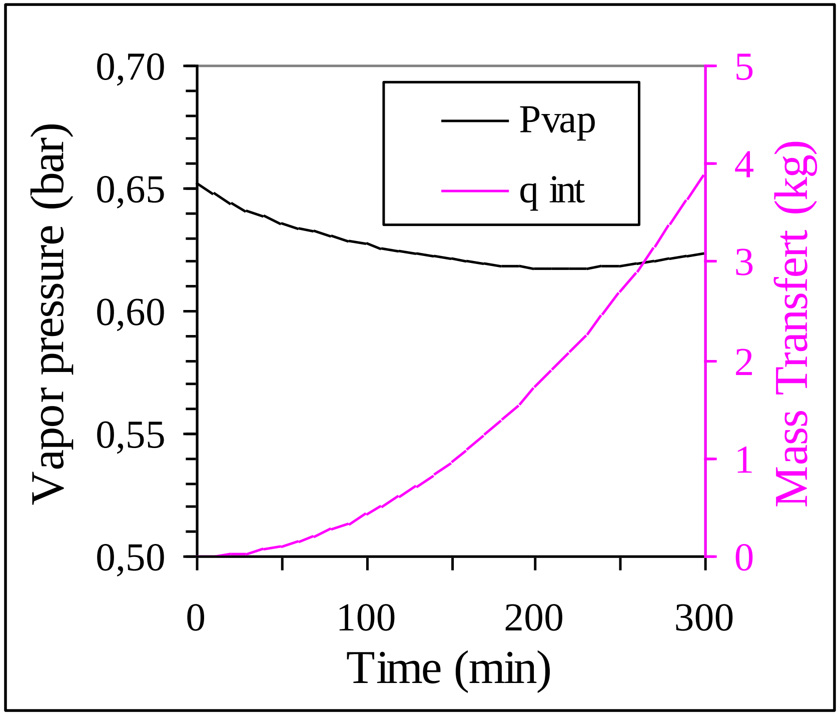
⇒ *Fixed Wall Temperature : Twall*

2 - Simulation Results *(start from 44°C)*

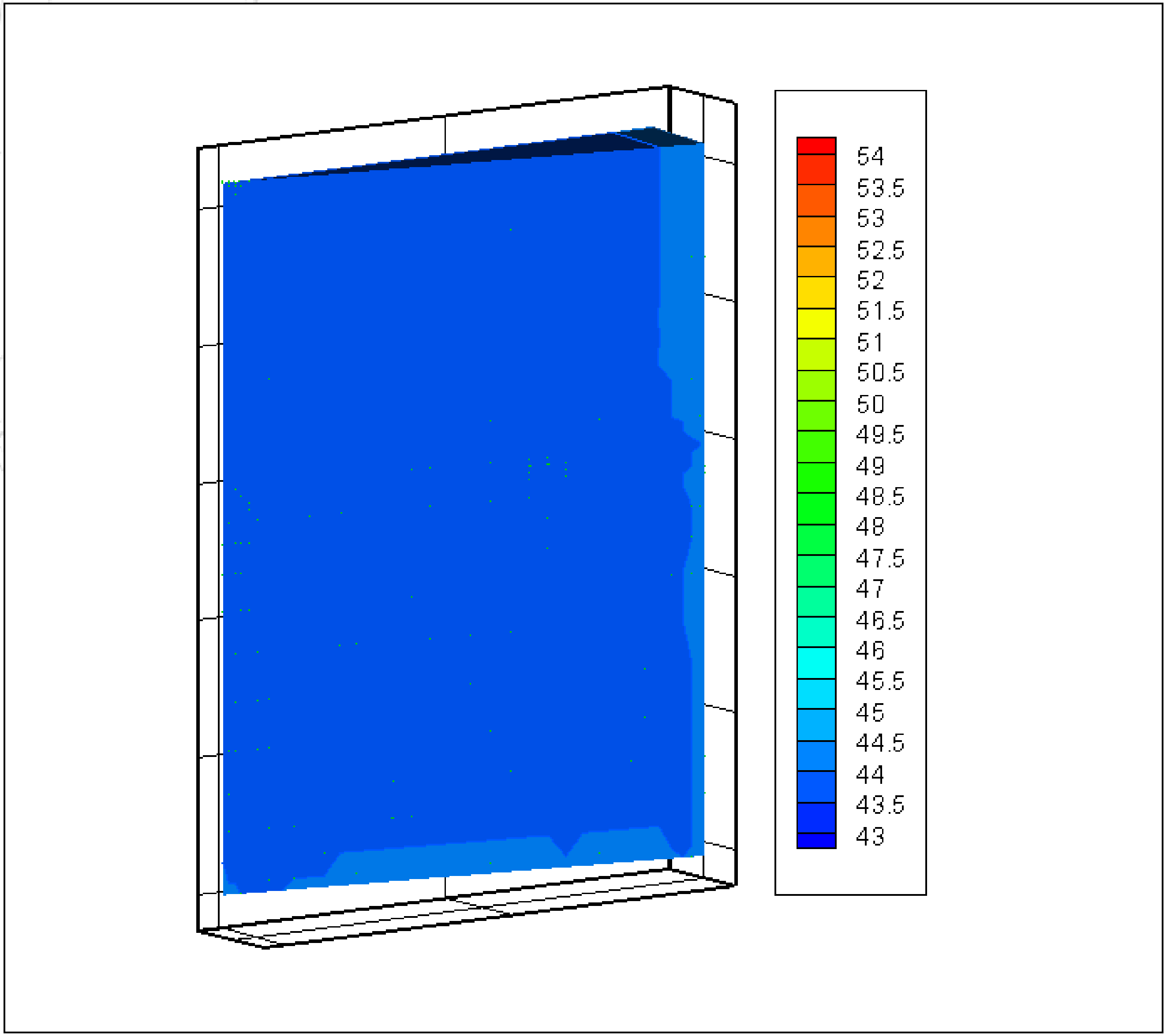
⇒ *Vapor Pressure : Pvap*

⇒ *Interfacial Mass Transfert : q int*





Temperature



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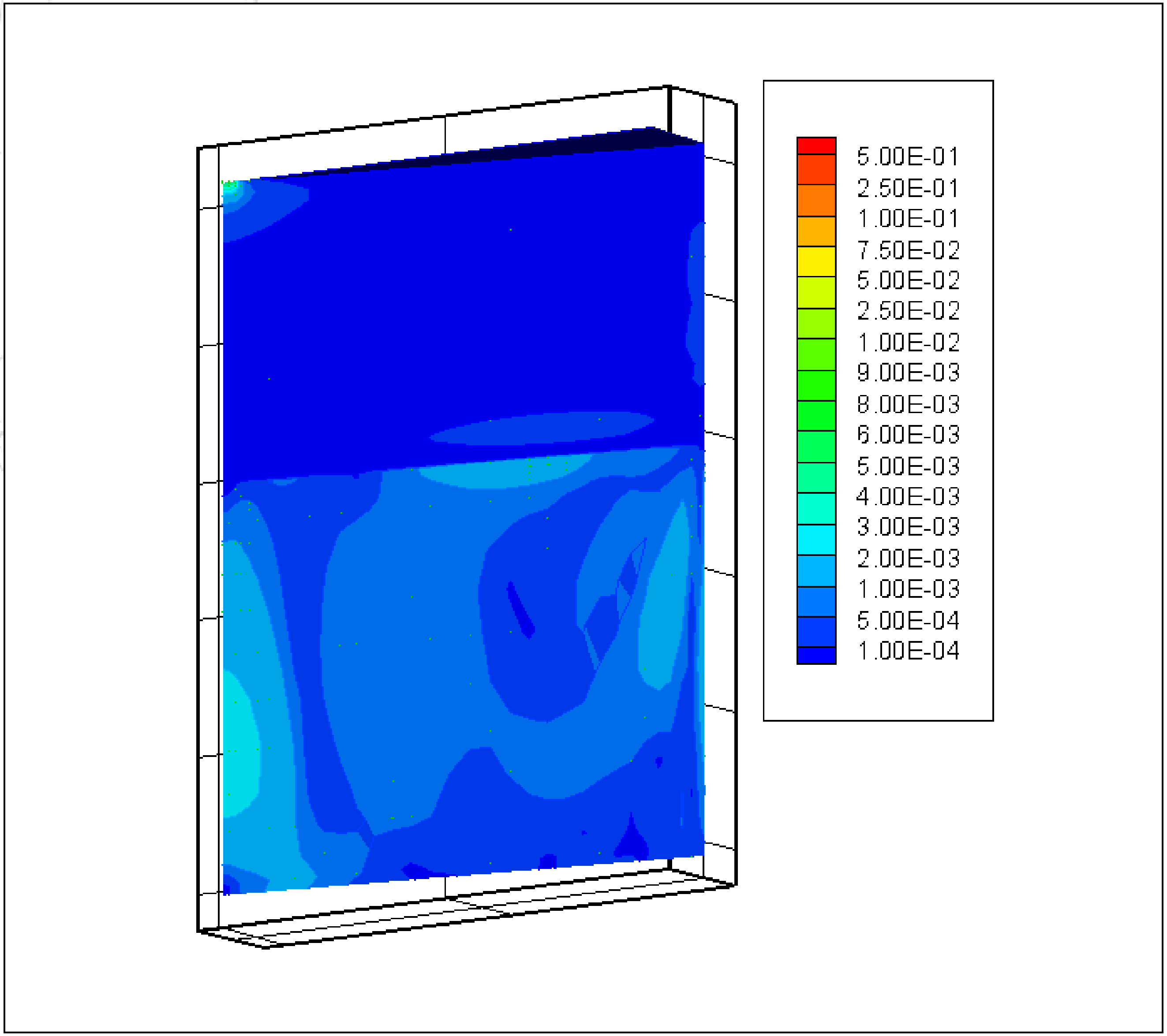
Velocity



RIModel VALIDITY LIMIT - *Subcooled Pool Boiling*

1 - The RIModel $\Rightarrow$ *Assumes Pool Subcooled Boiling Situation*

2 - The Transition Pool Subcooled Boiling to Nucleate Boiling

$\Rightarrow$ *Depend on Gap between Wall and Saturation Temperatures*

$$\Delta T = Twall - Tsat = [\ 2\ .\ \sigma\ .\ Tsat\ ]\ /\ [\ \rho vap\ .\ \Delta Hvap\ .\ R\ ]$$

$\Rightarrow$ *Depend on Nucleation Cavity Radius*

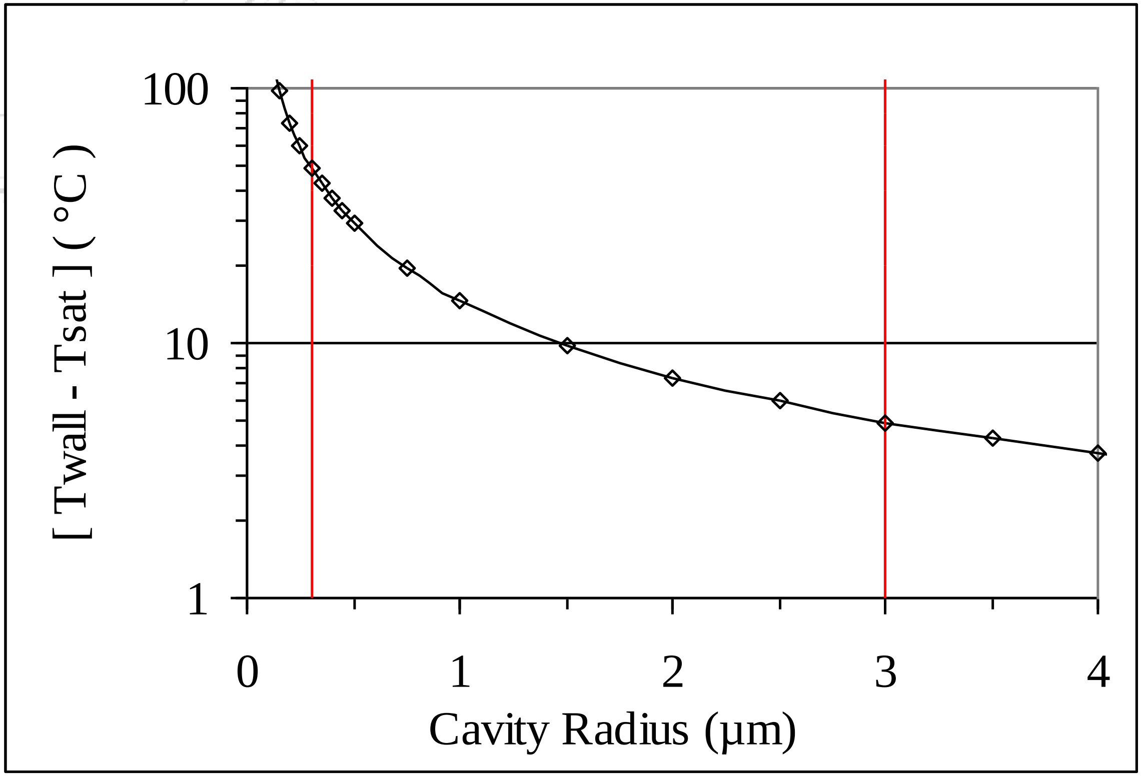
3 - Typical Cavity Radius in the µm Range

$\Rightarrow$ *0.3 µm < Cavity Radius : R < 3 µm* $\Rightarrow$ *50 °C >* ΔT *> 5 °C*

$\Rightarrow$ *CONSEQUENCE : RIModel valid for Temperature Gap of about 20°C (and even more : no major disturbance induced by Beginning of Nucleate Boiling)*

RIModel VALIDITY LIMIT - *Subcooled Pool Boiling*

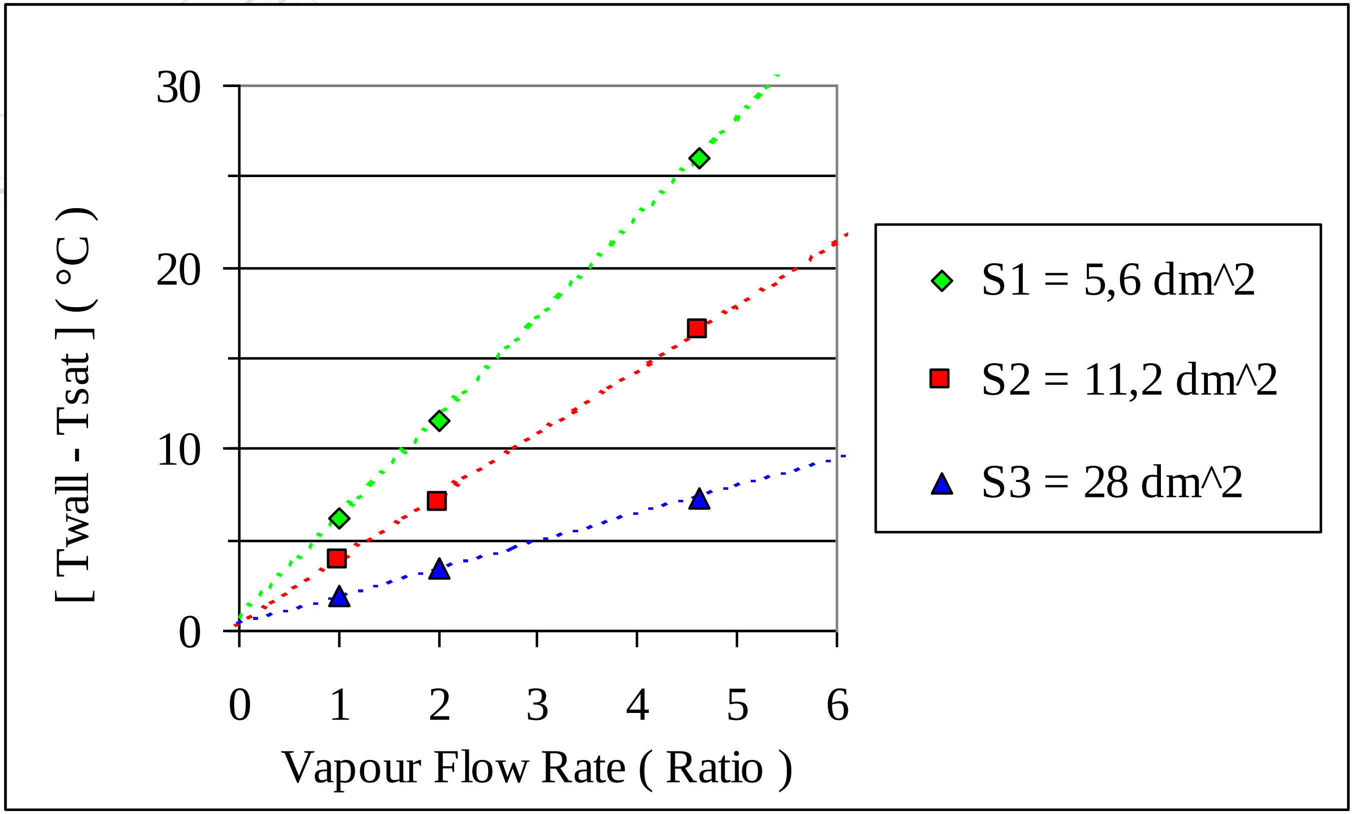
⇒ *Onset of Heterogeneous Nucleation ⇒ Δ T = f (Cavity Radius)*



RIModel - *Parametric Study Results - Temperature Gap*

⇒ *Temperature Gap Dependence with Vapor Flow Rate (Q)*

and Evaporation Surface Size (S)



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CONCLUSION

1 - The RIModel for Evaporation of Liquids in Closed Tanks is :

⇒ Based upon Heat Conductivity at Liquid / Vapor Interface by analogy with Melting or Solidification Process

⇒ Assuming Pool Subcooled Boiling Situation

⇒ Assuming to preserve Plane Interface during Evaporation

2 - The Parametric Study ⇒ *Quantify influence of Boundary conditions (Q, S, Twall)*

⇒ For same couple (Q, Twall) ⇒ The larger (S) ⇒ The bigger (Pvap)

⇒ For same couple (Q, Pvap) ⇒ The larger (S) ⇒ The smaller (Twall)

3 - Critical discussion of Numerical Results

⇒ With features of Boiling Process and Mechanism of Bubbles Generation

⇒ *RIModel Limit of Validity*