Two-Phase Evaporation/Boiling/Condensation Mechanism in Phoenics

This report details the development and implementation of a two-phase evaporation, boiling, and condensation mechanism within Phoenics. While this implementation is focused on two phases, adjustments will be required for a three-phase model, which is outside the current scope.

1. Overview of Cases

The developed model is applied to two scenarios:

- **Film Boiling**
- **Bulk Boiling / Condensation**

These cases differ in their respective evaporation rate formulations.

2. Methodology

The implementation leverages the existing Volume of Fluid (VOF) method within Phoenics, assuming incompressible fluids. Below are the general governing equations, followed by specific adjustments for each problem.

3. General Equations

The governing equations for the model include:

- **Momentum Equation:**

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla.(\rho \boldsymbol{u}\boldsymbol{u}) = [-\nabla p + \nabla.\mu(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)] + \rho \vec{g} + (\sigma \kappa \boldsymbol{n} - \nabla_s T)\delta$$

- **Continuity Equation:**

$$\nabla.\boldsymbol{u} = S_m\left(\frac{1}{\rho_L} - \frac{1}{\rho_v}\right)$$

This source term accounts for the evaporation rate, and is introduced in **GXEVAP** (Group 8, Section 7). The GXEVAP subroutine is invoked in GREX3 when EVAP is true.

- **VOF (Volume of Fluid) Equation:**
  Conservative form:

$$\frac{\partial \alpha}{\partial t} + \nabla.(\alpha \boldsymbol{u}) = \frac{S_m}{\rho_L}$$

Non-conservative form:

$$\frac{\partial \alpha}{\partial t} + \boldsymbol{u}\nabla \alpha = \frac{S_m}{\rho_L} - \alpha \nabla.\boldsymbol{u} = \frac{S_m}{\rho_L \rho_v}\rho$$

The non-conservative form is preferred for phase change problems, set by enabling NONCON=T in the **Q1** file.

The source term is introduced in GXEVAP group 13. Depending on the value of NONCON one of or the other source is introduced.

- **Energy Equation:**

$$\frac{\partial \rho C_p T}{\partial t} + \nabla.\left(\rho C_p T \boldsymbol{u}\right) = \nabla.(k\nabla \mathrm{T}) + Sh$$

After transformation (valid for two and three phases).

$$\frac{\partial(\rho Cp_G T)}{\partial t} + \nabla\cdot(\rho Cp_G VT) = \nabla.(\lambda\nabla T) - \frac{\partial(\rho_L(Cp_L - Cp_G)*\Phi T)}{\partial t} - \nabla\cdot(\rho_L(Cp_L - Cp_G)*\Phi VT) + Sh =$$
$$\nabla.(\lambda\nabla T) - \rho_L(Cp_L - Cp_G)*\Phi*\left(\boldsymbol{\frac{\partial T}{\partial t}} + \boldsymbol{V\nabla T}\right) + Sh - \rho_L(Cp_L - Cp_G)*T*\frac{S_m}{\rho_L}$$

where S_h accounts for latent heat as an energy source. If Cp_L=Cp_G, extra terms vanish, and if no evaporation occurs, S_m=0.

The source term Sh and the source term $-\rho_L(Cp_L - Cp_G)*T*\frac{S_m}{\rho_L}$ are introduced in GXEVAP group 13.

4. Volumetric interface mass transfer:

The volumetric interface mass transfer, S_m, is modeled using either the Lee model or a modified version, as described below.

- **Phase change model:**

The mass source term S_m simulates phase change according to the following conditions:

4.1 For film boiling/Condensation:

$$T_{cell}\ temperature\ inside\ the\ control\ volume$$

When $T_{cell} < T_{sat}\ and\ 0 \leq \alpha < 1$ then

$$\boldsymbol{S_m = \rho Cp * \frac{T_{sat} - T_{cell}}{\Delta t L}}$$ **source term corresponding to condensation**

Δt time step, L latent heat

When $T_{cell} > T_{sat}\ and\ 0 < \alpha \leq 1$ then

$$\boldsymbol{S_m = \rho Cp * \frac{T_{sat} - T_{cell}}{\Delta t L}}$$ **source term corresponding to evaporation**

Otherwise**, S_m=0; S_h=S_m*L**

4.2 For bulk boiling/Condensation (Fahdl model):

Working with α color function to be liquid.

When $T_{cell} < T_{sat}$ then

$$\boldsymbol{S_m = -\beta\rho_V(1-\alpha) * \frac{T_{sat} - T_{cell}}{T_{sat}}}$$ **source term corresponding to condensation**

When $T_{cell} > T_{sat}$ then

$$\boldsymbol{S_m = -\beta\rho_L\alpha * \frac{T_{sat}-T_{cell}}{T_{sat}}}$$ **source term corresponding to evaporation**

Otherwise S_m=0

S_h=S_m*L

$$\beta = Evapco = 0.1\ (in\ the\ Fadhl\ case) not\ used\ in\ film\ boiling$$

$$\boldsymbol{\rho Cp = \rho_L Cp_L\alpha + \rho_V Cp_V(1-\alpha)}$$ **(L for Liquid, v for vapor)**

The evaporation rate is computed in GXEVAP group 19.

In order to have a smoother convergence, the evaporation rate is smoothed in group 19 of GXEVAP.

5. Implementation in Phoenics of sources

GXSURF.FOR has been modified to account correctly for the non-conservative approach. The temperature equation inside gxsurf.for has also been modified to account for the new formulation of the energy equation.

To implement the mass source term related to the continuity equation:

$$\nabla.\boldsymbol{u} = S_m(\frac{1}{\rho_L} - \frac{1}{\rho_v})$$

We use the following in GXEVAP.FOR group 8, section 7

```
C   * ------------------- SECTION 7 ---- Volumetric source for gala
          IMEVA=LBNAME('MEVA')       !represent the Sm term
          RHOL=F(INDPRTB(IPRPSA,0)+1)
          RHOV=F(INDPRTB(IPRPSB,0)+1)
          ACOEF=(1.0/RHOL-1.0/RHOV)
          CALL FN53(LSU,IMEVA,VOL,acoef) ! VAL=val + ACOEF*IMEVA*VOL
      RETURN
   88 CONTINUE
```

For the problem of film boiling, the properties have been set in Q1.

For the problem of bulk boiling the properties are set in the PROPS file.

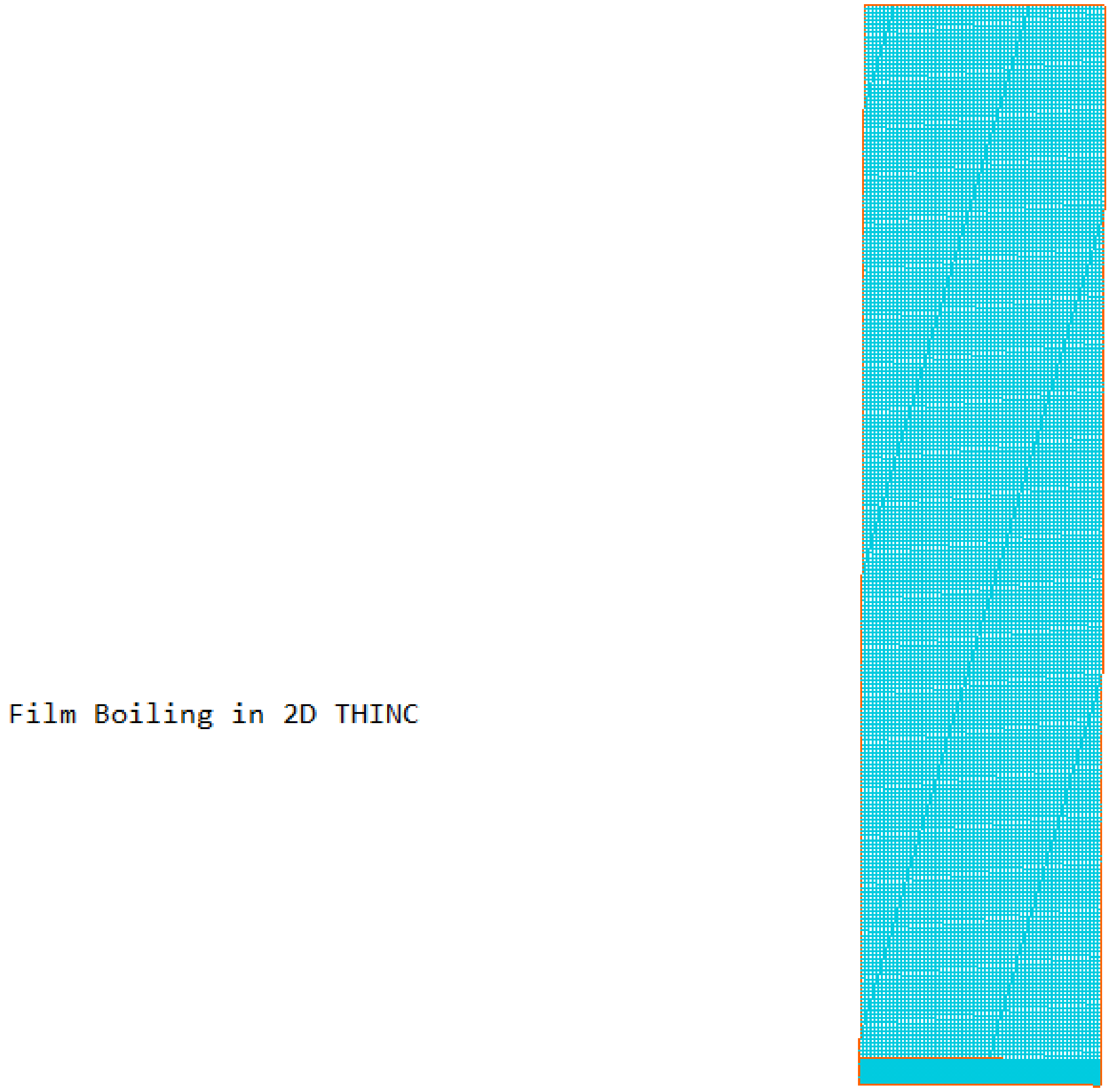
6. Film boiling in Phoenics

In this study, we replicate the example case from Hajime Onishi et al. (International Journal of Heat and Mass Transfer, Volume 186, 1 May 2022, 122429).

The surface tension for this case is a constant equal to 0.1. The properties are introduced through Q1. The case has been solved using the VOF THINC model.

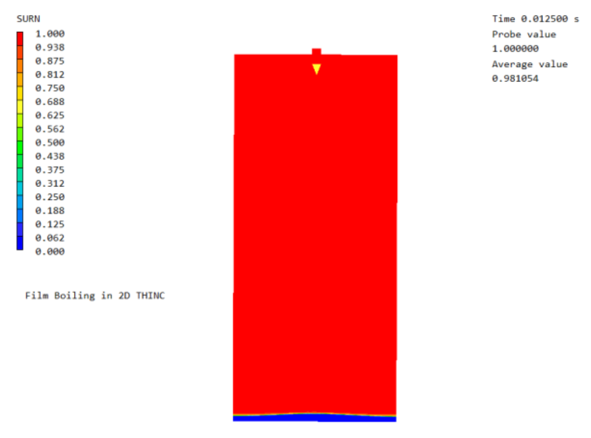
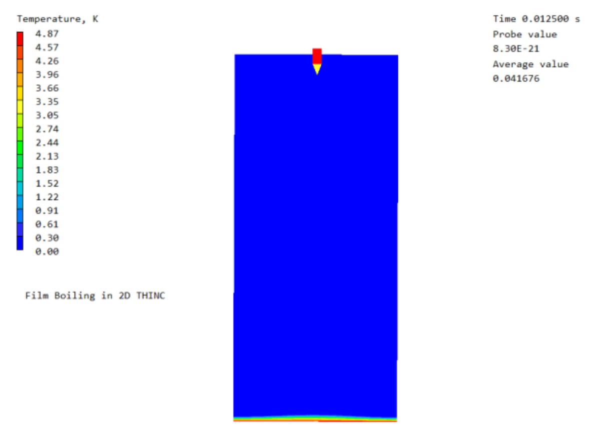
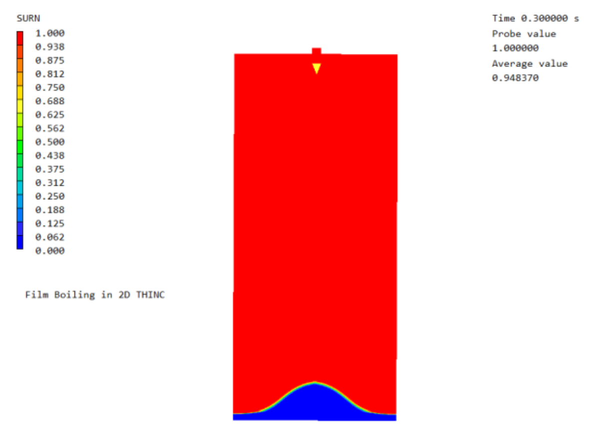
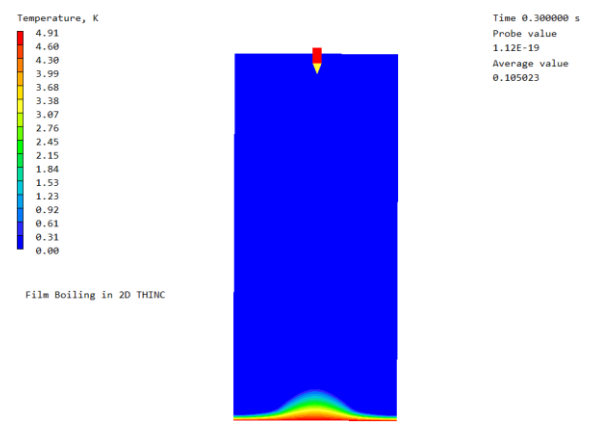
```
  Group 9. Properties
*  List of user-defined materials to be read by EARTH
    MATFLG=T;IMAT=2
```

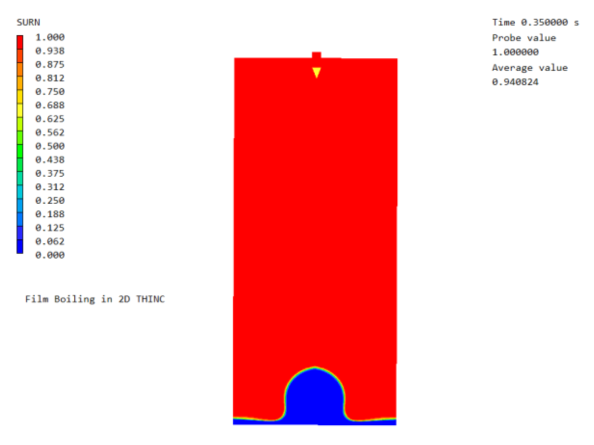
```
   *  Name
   *Ind. Dens.  Viscos.  Spec.heat  Conduct.  Expans.  Compr.
   *  <VAPOR>
    34 5.0 1.0E-3 200.0 1.0 3.33E-3
   *  <LIQUID>
    78 200.0 5.0E-4 400.0 40.0 1.18E-4
 ************************************************************
  Group 19. EARTH Calls To GROUND Station
IEVAP=2          !if >0 then true then evaporation - else false no
evaporation
LATH=1.0E+04     !latent heat
TSAT=0.0         !Tsat
NONCON=T         ! Non-conservative formulation
EVAPCO=0.1       ! Lee coefficient
```

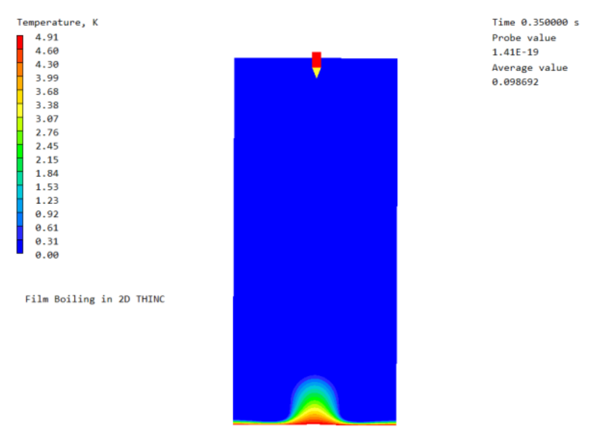


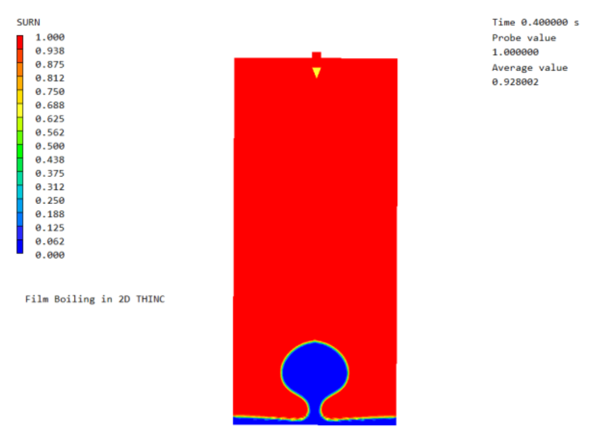
The grid is finer in a lower region where the interface between the liquid and the vapor lies. This is in order to have a better profile of the initial curvature. The domain size is 0.039342 m x 0.177039 in X & Y. The meshes in X & Y are 64 x 289. The refined region in Y is of size 0.004317 m and has 24 cells.

Here is a series of snapshot of the color function and of the temperature:

Color function	Temperature
	
	


SURN
1.000
0.938
0.875
0.812
0.750
0.688
0.625
0.562
0.500
0.438
0.375
0.312
0.250
0.188
0.125
0.062
0.000
Film Boiling in 2D THINC
Time 0.350000 s
Probe value
1.000000
Average value
0.940824


Temperature, K
4.91
4.60
4.30
3.99
3.68
3.38
3.07
2.76
2.45
2.15
1.84
1.53
1.23
0.92
0.61
0.31
0.00
Film Boiling in 2D THINC
Time 0.350000 s
Probe value
1.41E-19
Average value
0.098692


SURN
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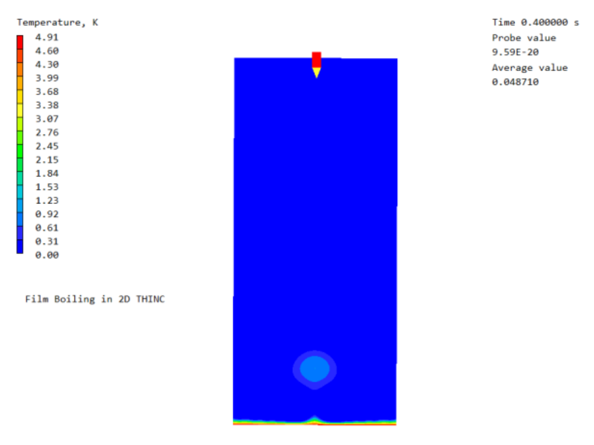
0.938
0.875
0.812
0.750
0.688
0.625
0.562
0.500
0.438
0.375
0.312
0.250
0.188
0.125
0.062
0.000
Film Boiling in 2D THINC
Time 0.400000 s
Probe value
1.000000
Average value
0.928002


Temperature, K
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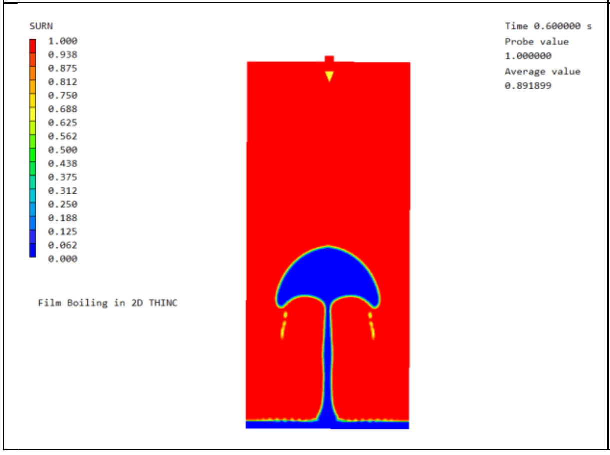
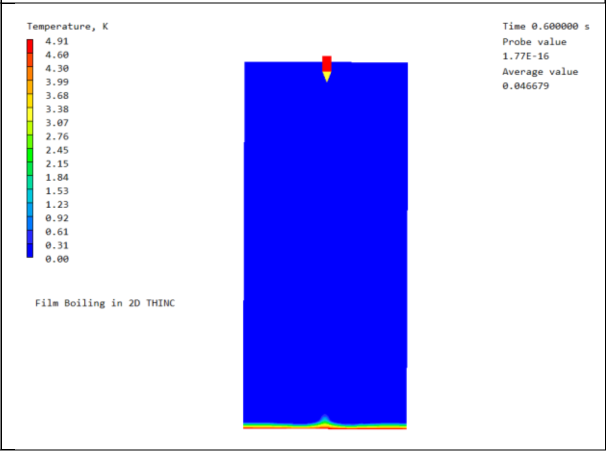
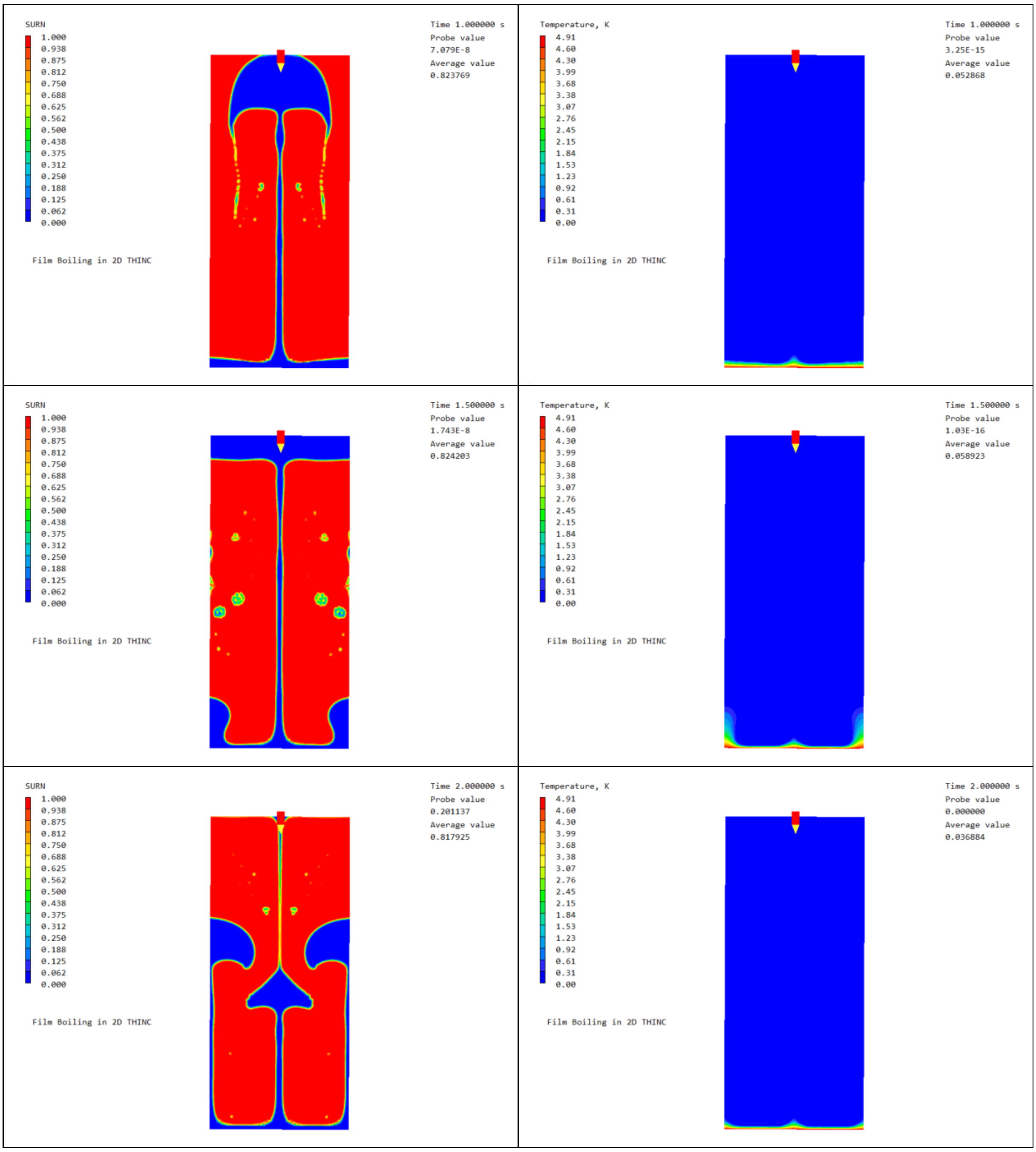
4.60
4.30
3.99
3.68
3.38
3.07
2.76
2.45
2.15
1.84
1.53
1.23
0.92
0.61
0.31
0.00
Film Boiling in 2D THINC
Time 0.400000 s
Probe value
9.59E-20
Average value
0.048710


SURN
1.000
0.938
0.875
0.812
0.750
0.688
0.625
0.562
0.500
0.438
0.375
0.312
0.250
0.188
0.125
0.062
0.000
Film Boiling in 2D THINC
Time 0.600000 s
Probe value
1.000000
Average value
0.891899


Temperature, K
4.91
4.60
4.30
3.99
3.68
3.38
3.07
2.76
2.45
2.15
1.84
1.53
1.23
0.92
0.61
0.31
0.00
Film Boiling in 2D THINC
Time 0.600000 s
Probe value
1.77E-16
Average value
0.046679



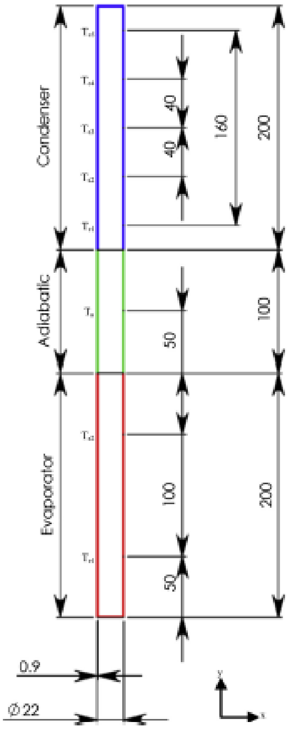
This case is included in the Option – Advanced multi-phase - VOF library as case P140. An animation of the evolution of color function can be found here cham.co.uk/phoenics/d_polis/d_applic/d_vof/film-surn.gif.

7. Bulk Boiling/condensation

In the following, we tackle the model developed in Fluent and used by Fadhl & al (PHYSICS OF FLUIDS **26**, 024114 (2014)).

7.1 Description of the model

The geometry consists of a 2D rectangular domain in the X and Y directions, following the setup in Fadhl et al. The figure below illustrates the various sections of the domain. A 36x900 mesh is used, with 36 cells along the X-axis and 900 along the Y-axis. In the X direction, boundary layers are applied at both the West and East boundaries, each with a thickness of 7.7 x 10^{-4} m, divided into 5 cells within each boundary layer region.



The primary difference from the approach used by Fadhl et al. is that here, we consider fully incompressible fluids, allowing us to apply the traditional Volume of Fluid (VOF) method. In contrast, Fadhl et al. employ a weakly compressible VOF approach that incorporates the full continuity equation and a color function specifically for the vapor phase.

In the approach by Fadhl et al., the liquid density is modeled as a second-order polynomial function of temperature. This allows for a more precise representation of density variations with temperature changes in the liquid phase, accounting for thermal effects in a dilatable context.

The surface tension is expressed here as: $\sigma = \sigma_0 - \gamma(T - T_r) + \gamma_2(T - T_r)^2$; This has been coded in gxsurfts.for to add the $\gamma_2(T - T_r)^2$ term.

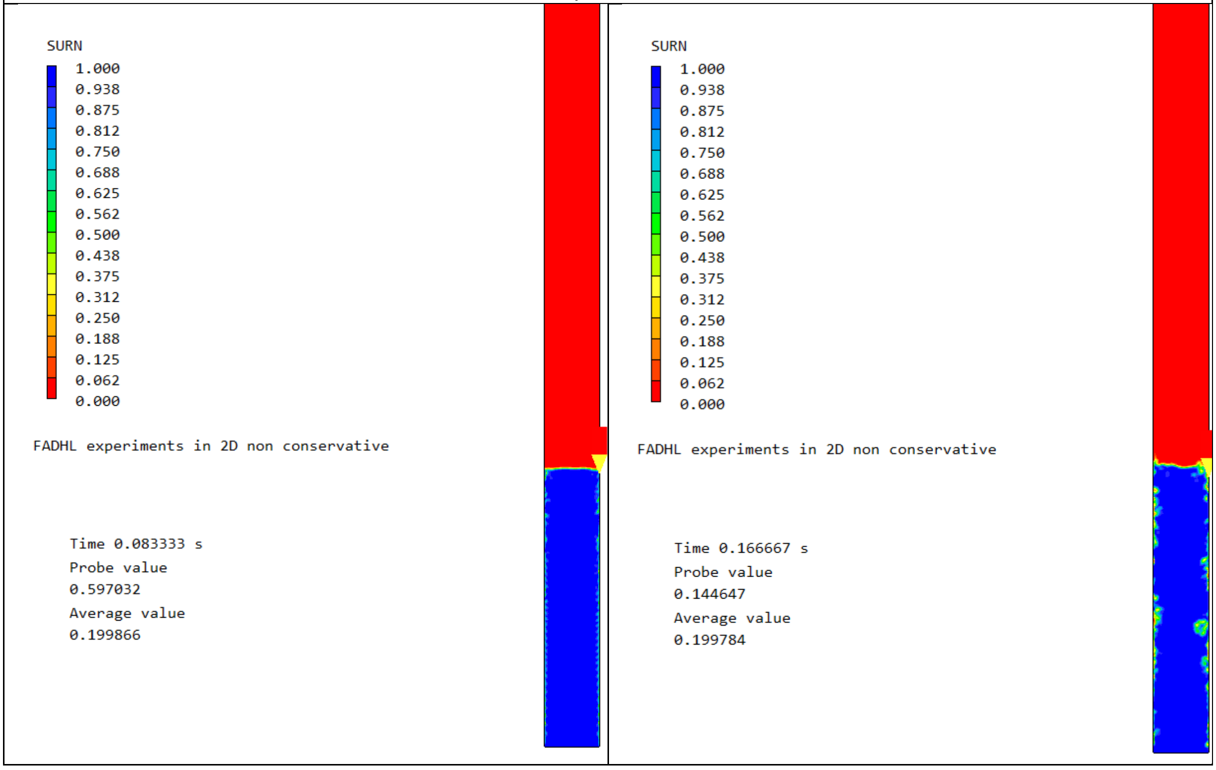
with indices r, l, v, are for a reference temperature of 99.85°C, liquid, and v vapor, respectively.

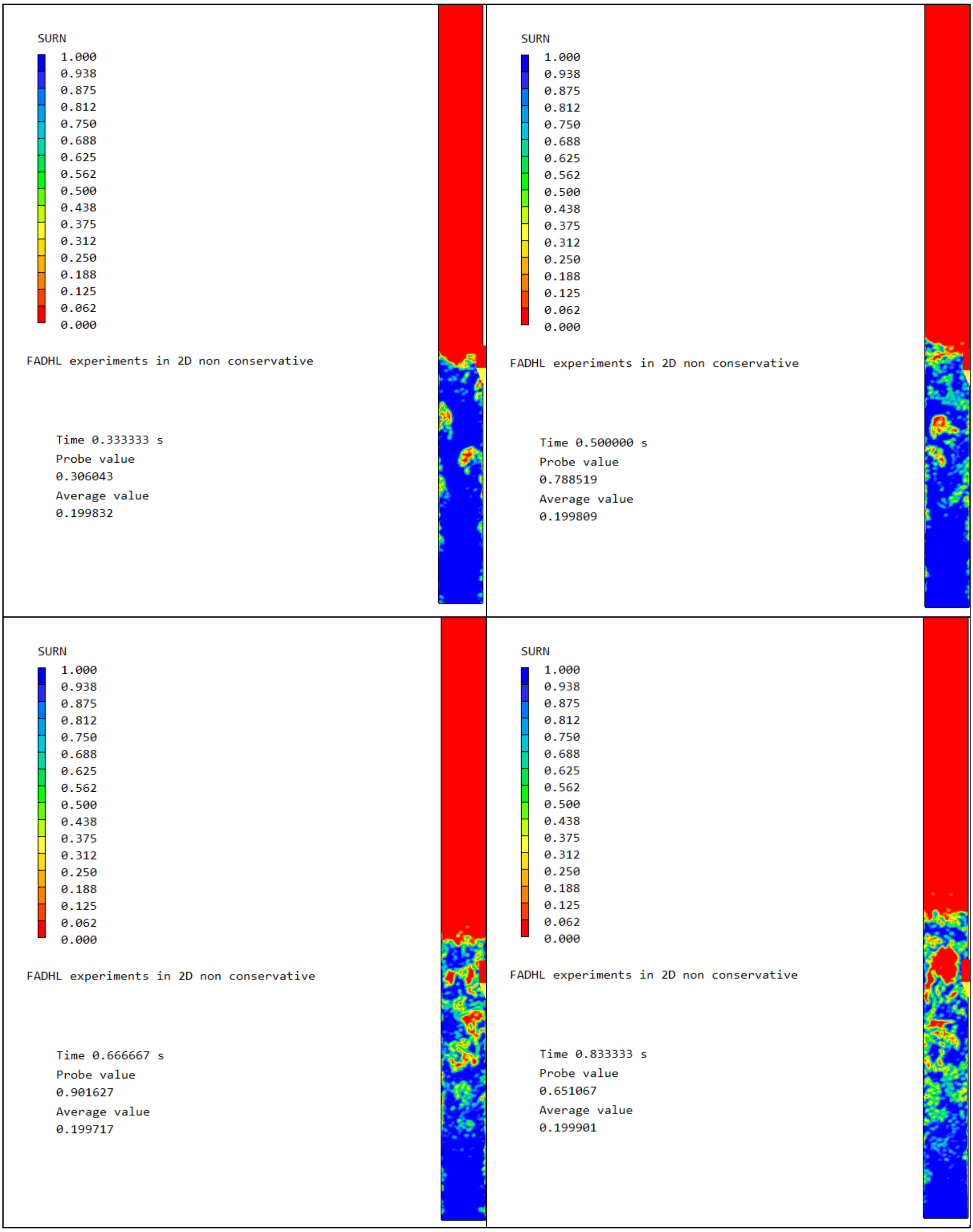
7.2 Physical properties in terms of mass fraction for the liquid (water) and vapor (Steam) :

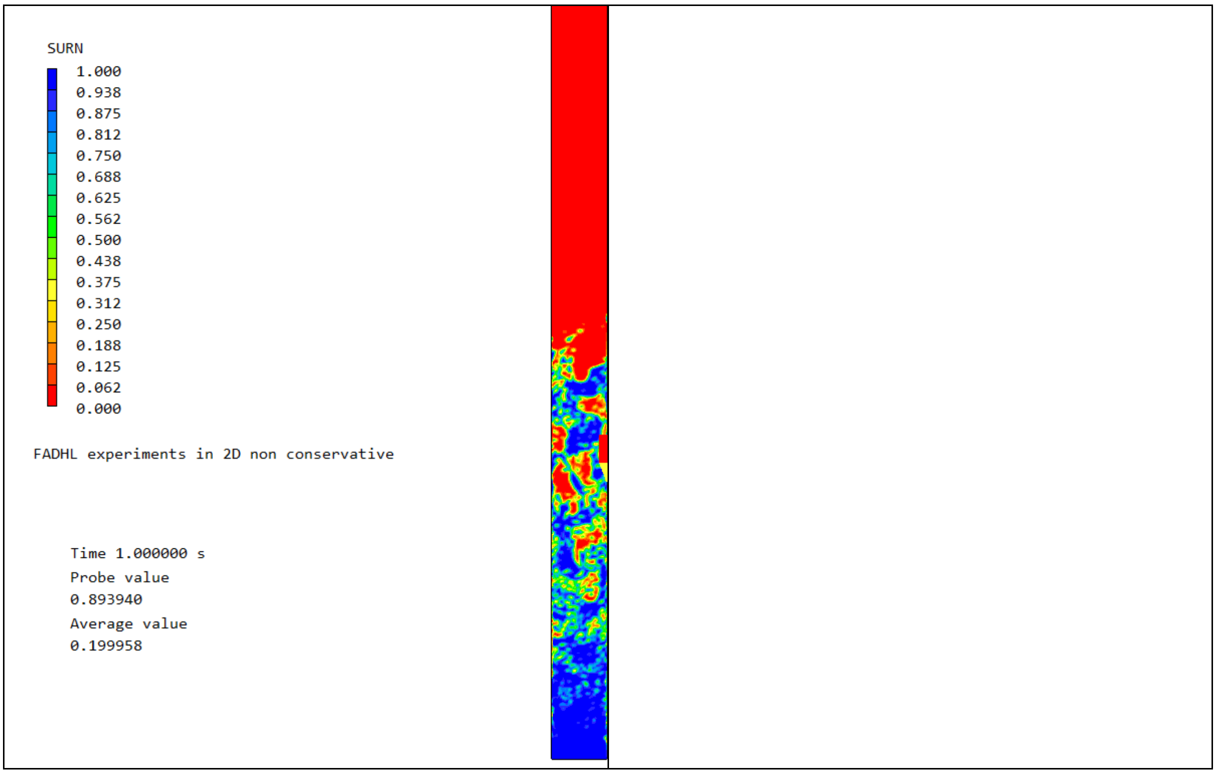
In the following table the values and names of physical properties at 1 atm.

		Liquid	Vapor
Density	$\rho\ (kg\ m^{-3})$	998.23	0.5863
Kinematic Viscosity	$\nu\ (m^2\ s^{-1})$	$1.006\ 10^{-6}$	$2.168\ 10^{-5}$
Thermal conductivity	$k\ (W\ m^{-1}\ K^{-1})$	0.597	0.0246
Specific Heat	$Cp\ (J\ kg^{-1}\ K^{-1})$	4181.8	2060.0
Thermal Expansion	$\beta\ (K^{-1})$	$1.18\ 10^{-4}$	$2.68\ 10^{-3}$
Surface Tension	$\sigma\ (N\ m^{-1})$	0.098058	
Surface Tension coefficient	$\gamma\ (N\ m^{-1}\ K^{-1})$	$-1.845\ 10^{-5}$	
Surface Tension coefficient 2	$\gamma_2\ (N\ m^{-1}\ K^{-1})$	$-2.3\ 10^{-7}$	
Latent Heat	$\Delta h_v\ (J\ kg^{-1})$	$2.455\ 10^{6}$	

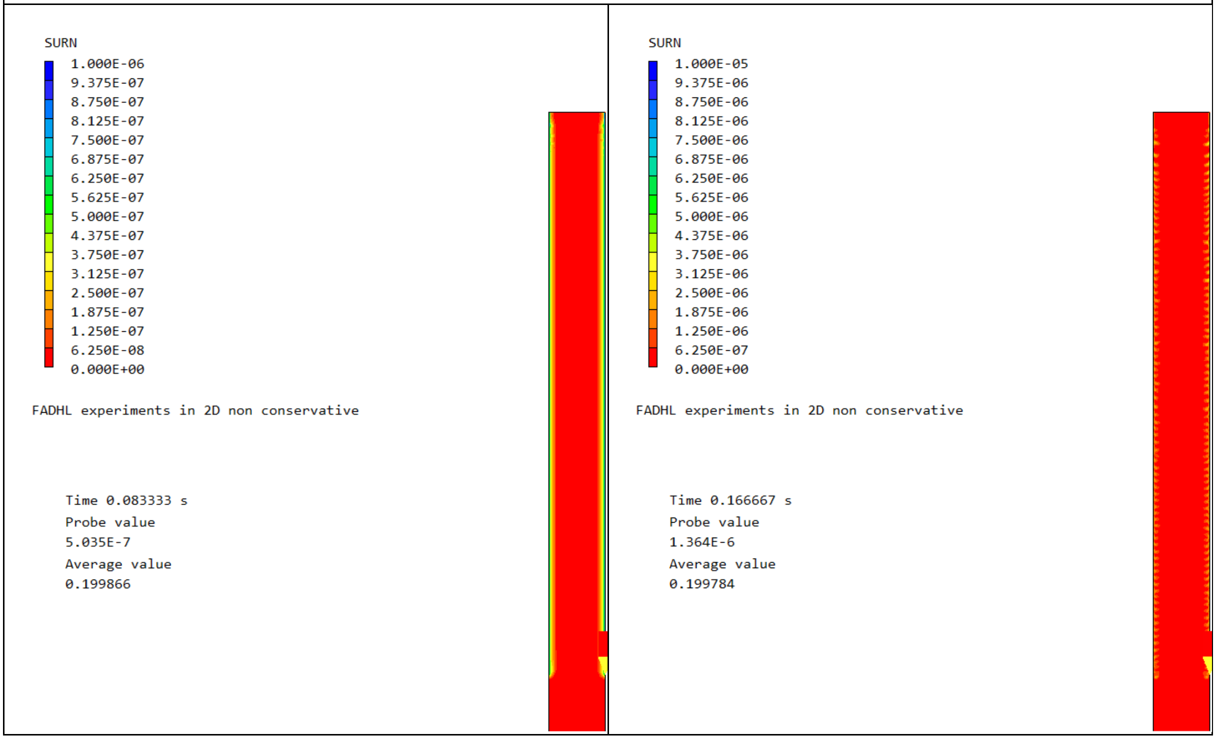
Color function at different timesteps in the Evaporator domain

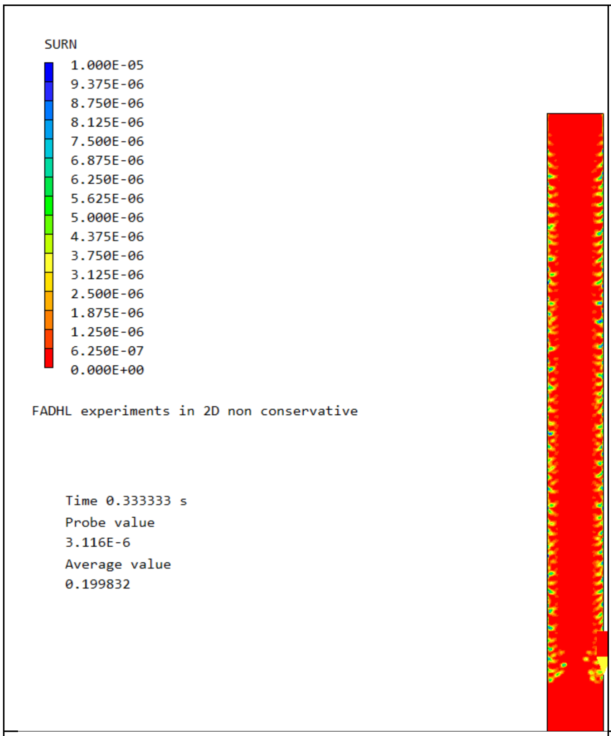



SURN
1.000
0.938
0.875
0.812
0.750
0.688
0.625
0.562
0.500
0.438
0.375
0.312
0.250
0.188
0.125
0.062
0.000
FADHL experiments in 2D non conservative
Time 0.333333 s
Probe value
0.306043
Average value
0.199832
SURN
1.000
0.938
0.875
0.812
0.750
0.688
0.625
0.562
0.500
0.438
0.375
0.312
0.250
0.188
0.125
0.062
0.000
FADHL experiments in 2D non conservative
Time 0.500000 s
Probe value
0.788519
Average value
0.199809
SURN
1.000
0.938
0.875
0.812
0.750
0.688
0.625
0.562
0.500
0.438
0.375
0.312
0.250
0.188
0.125
0.062
0.000
FADHL experiments in 2D non conservative
Time 0.666667 s
Probe value
0.901627
Average value
0.199717
SURN
1.000
0.938
0.875
0.812
0.750
0.688
0.625
0.562
0.500
0.438
0.375
0.312
0.250
0.188
0.125
0.062
0.000
FADHL experiments in 2D non conservative
Time 0.833333 s
Probe value
0.651067
Average value
0.199901



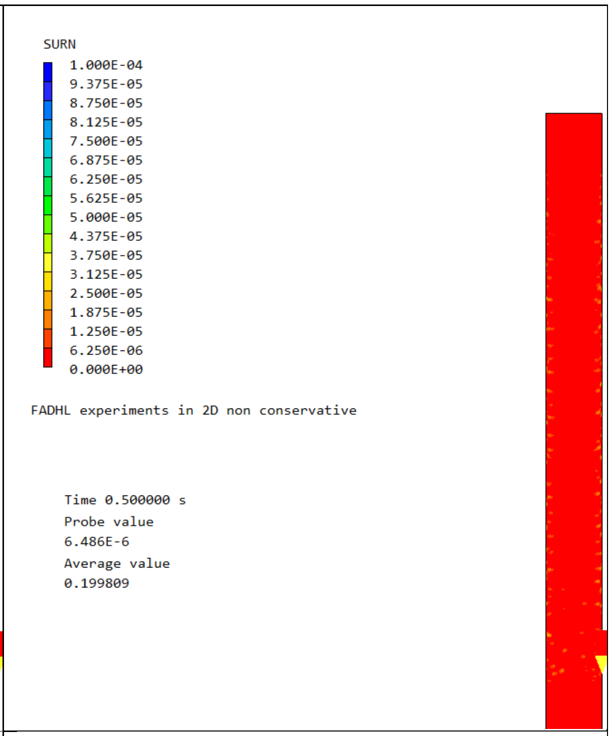
Color function at different timesteps
in the Condensation domain





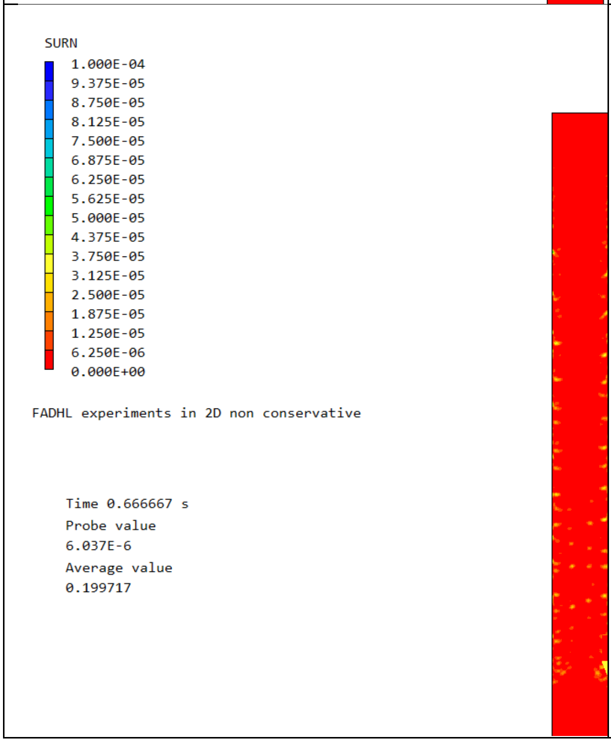
```
FADHL experiments in 2D non conservative

Time 0.333333 s
Probe value
3.116E-6
Average value
0.199832
```



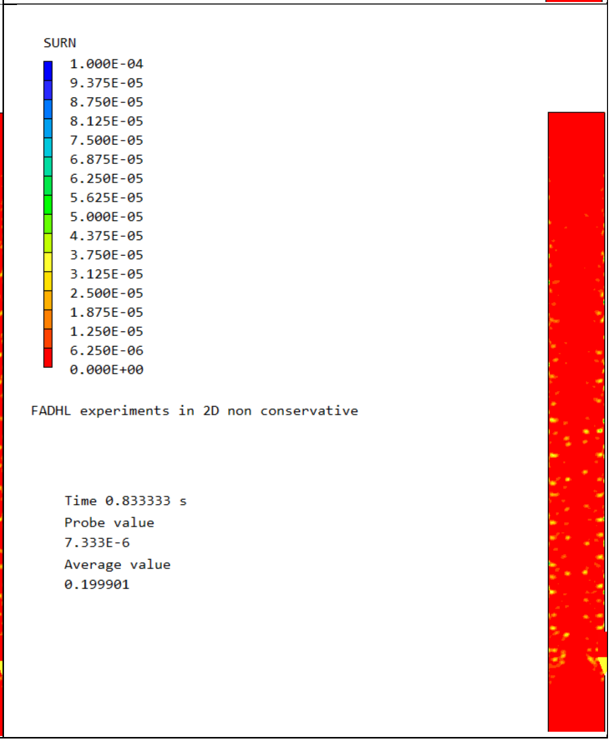
```
FADHL experiments in 2D non conservative

Time 0.500000 s
Probe value
6.486E-6
Average value
0.199809
```



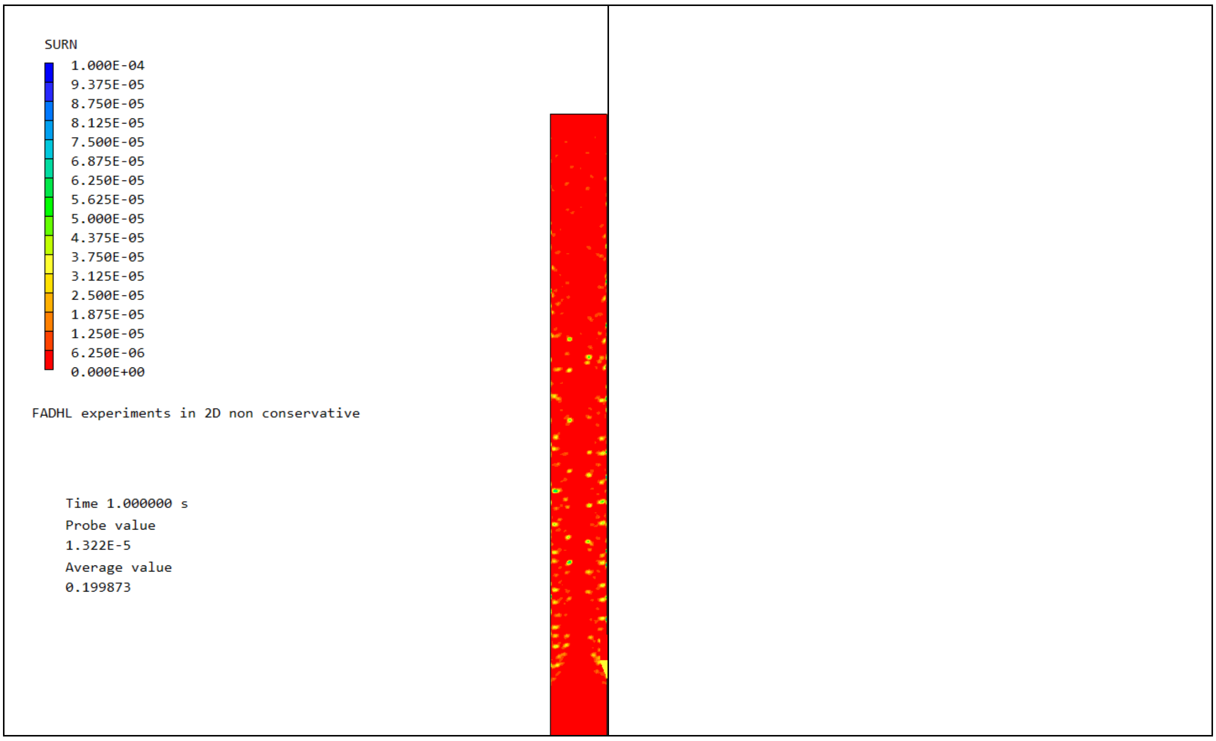
```
FADHL experiments in 2D non conservative

Time 0.666667 s
Probe value
6.037E-6
Average value
0.199717
```



```
FADHL experiments in 2D non conservative

Time 0.833333 s
Probe value
7.333E-6
Average value
0.199901
```



In the tables above, the colors have been reversed for easier comparison with the data from Fadhl et al. Additionally, in the condensation regions, the figures have been rescaled to highlight the subtle variations occurring in the early stages of the process.

This case is included in the Option – Advanced multi-phase - VOF library as case P139.

An animation of the evolution of color function in the evaporation section can be found here cham.co.uk/phoenics/d_polis/d_applic/d_vof/fadhl-evap.gif,

and in the condensation section here cham.co.uk/phoenics/d_polis/d_applic/d_vof/fadhl-condens.gif

For this case, are attached the gxsurf.for, gxsurfts.for, gxevap.for, grex3.for files, the properties file EPRP and the Q1 file. An animation of color function in the evaporator.

8. Conclusion

The development of the evaporation and condensation models in the existing VOF framework of Phoenics has been challenging due to the ambiguity in the methodology used by Fadhl et al. and the incomplete implementation of the continuity equation. With these improvements, the current model is now operational and offers a foundation for further enhancements. Future developments could include the integration of a Fickian diffusion model for evaporation and condensation, which would be particularly beneficial for processes at temperatures well below the boiling point. Such extensions could expand the model's applicability to various experiments involving droplet and film evaporation.