Complete Transient Droplet Evaporation Modelling: Deviation from the d^2 Law under Cryogenic Conditions

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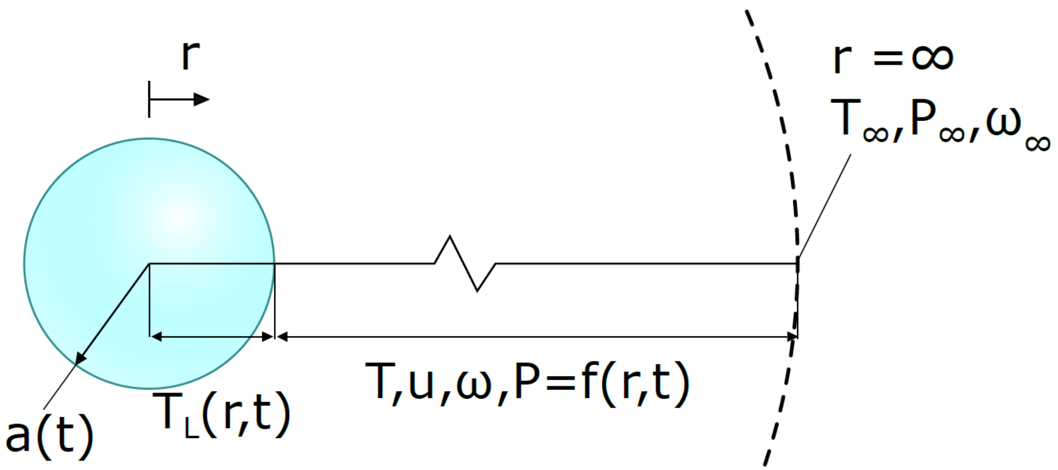
1. Problem Definition

Single liquid droplet in quiescent, infinite gaseous medium



Assumptions:

1. Spherical droplet
2. Microgravity → symmetric
3. Local phase equilibrium at droplet surface
4. Thin phase transition zone
5. Soret/ Dufour effect neglected
6. Radiative heat transfer neglected
7. Incompressible liquid
8. Ideal gas mixture
9. Pure conduction within liquid (no convection)

Not a limitation of the presented model

10. Constant specific heats
11. Constant transport properties
12. Incompressible gas phase
13. Negligible viscous/ pressure work

~~14. Quasi-steady gas phase~~
~~15. Quasi-steady liquid phase~~

2. Governing Equations

Dimensionless variables

Mass

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

$$\frac{\partial\tilde{\rho}}{\partial\tilde{t}} + \tilde{\boldsymbol{\nabla}}\cdot(\tilde{\rho}\tilde{\boldsymbol{u}}) = 0$$

Species

$$\rho\frac{D\omega}{Dt} = \boldsymbol{\nabla}\cdot(\Gamma\boldsymbol{\nabla}\omega)$$

$$\tilde{\rho}\frac{D\tilde{\varphi}}{D\tilde{t}} = \tilde{\boldsymbol{\nabla}}\cdot\left(\tilde{\Gamma}\,\tilde{\boldsymbol{\nabla}}\tilde{\varphi}\right)$$

Microgravity $\boldsymbol{Fr} = \frac{\rho_\infty^2 a_i^3 g}{\Gamma_\infty^2} \ll \mathbf{1}$

Momentum

$$\rho\frac{D\boldsymbol{u}}{Dt} = -\boldsymbol{\nabla}P + \boldsymbol{\nabla}\cdot\boldsymbol{\tau} + \rho\boldsymbol{g}$$

$$\tilde{\rho}\frac{D\tilde{\boldsymbol{u}}}{D\tilde{t}} = -\tilde{\boldsymbol{\nabla}}\tilde{P} + Sc\,\tilde{\boldsymbol{\nabla}}\cdot\tilde{\boldsymbol{\tau}} + \cancel{Fr}\,\tilde{\rho}\tilde{\boldsymbol{g}}$$

Negligible work terms $\boldsymbol{Ec} = \frac{\left(\frac{\Gamma_\infty}{\rho_\infty a_i}\right)^2}{c_{p\infty}(T_\infty - T_{QS})} \ll \mathbf{1}$

Energy

$$\rho c_p\frac{DT}{Dt} - \frac{DP}{Dt} = \boldsymbol{\nabla}\cdot(\lambda\boldsymbol{\nabla}\mathrm{T}) + \Delta c_p\Gamma\boldsymbol{\nabla}\omega\cdot\boldsymbol{\nabla}T + \boldsymbol{\tau}:\boldsymbol{\nabla}\boldsymbol{u}$$

$$(1+\chi\tilde{\varphi})\tilde{\rho}\frac{D\tilde{\theta}}{D\tilde{t}} - \cancel{Ec}\,\frac{D\tilde{P}}{D\tilde{t}} = Le\,\tilde{\boldsymbol{\nabla}}\cdot\left(\tilde{\lambda}\tilde{\boldsymbol{\nabla}}\tilde{\theta}\right) + \chi\tilde{\Gamma}\tilde{\boldsymbol{\nabla}}\tilde{\varphi}\cdot\tilde{\boldsymbol{\nabla}}\tilde{\theta} + Sc.\cancel{Ec}\,\tilde{\boldsymbol{\tau}}:\tilde{\boldsymbol{\nabla}}\tilde{\boldsymbol{u}}$$

State (ideal gas)

$$P = \rho RT$$

$$1 + \cancel{Ma}^2\tilde{P} = \tilde{\rho}(1 + C_\varphi\tilde{\varphi})(1 + C_\theta\tilde{\theta})$$

Incompressible Ma $= \frac{\Gamma_\infty}{\rho_\infty a_i}\sqrt{\frac{\rho_\infty}{P_\infty}} \ll \mathbf{1}$

Energy (liquid)

$$\rho_l c_l\frac{\partial T}{\partial t} = \boldsymbol{\nabla}\cdot(\lambda_l\boldsymbol{\nabla}\mathrm{T})$$

$$\frac{\partial\tilde{\theta}}{\partial\tilde{t}} = \frac{Le}{\alpha_r}\tilde{\nabla}^2\tilde{\theta}$$

Dimensionless variables:

$$\tilde{\theta} = \frac{T - T_\infty}{T_\infty - T_{QS}}$$

$$\tilde{\varphi} = \frac{\omega - \omega_\infty}{\omega_{QS} - \omega_\infty}$$

$$\tilde{P} = \frac{P - P_\infty}{P_o - P_\infty}$$

$$\tilde{r} = r/a_i$$

$$\tilde{a} = a/a_i$$

$$\tilde{u} = u\rho_\infty a_i/\Gamma_\infty$$

$$\tilde{t} = \frac{t\Gamma_\infty}{\rho_\infty a_i^2}$$

$$\tilde{\rho} = \rho/\rho_\infty$$

3. Modelling Procedure

Inputs

Dimensionless Fluid Properties:

$\cancel{Ma, Ec, Fr,}$ $Sc = \mu_\infty / \Gamma_\infty$

$Le = \dfrac{\lambda_\infty}{c_{p\infty}\Gamma_\infty}$, $Ja = \dfrac{c_{pA}T_{BP}}{L}$

$\gamma_A = c_{pA}/c_{vA}$, $\varepsilon = M_A/M_B$

$c_{pr} = c_{pA}/c_{p\infty}$,

$\rho_r = \rho_\infty/\rho_l$, $c_r = c_{pA}/c_l$

$\lambda_r = \lambda_\infty/\lambda_l$

Dimensionless Boundary Conditions

$\tilde{T}_{ex} = T_\infty/T_{BP}$, $\delta = 1 - \omega_\infty$

Initial Fields

$\tilde{\theta}, \tilde{\varphi}, \cancel{\tilde{P}, \tilde{u}}$ for $\tilde{r} > 1$

$\tilde{\theta}$ for $\tilde{r} \leq 1$

Derived Constants

Spalding numbers

$$B_M = \frac{\omega_{QS} - \omega_\infty}{1 - \omega_{QS}}$$

$$B_T = \frac{c_{pA}}{L}\left(T_\infty - T_{QS}\right)$$

Function

- Numerical model
- Finite element method
- Spatial and temporal discretisation
- Moving mesh to accommodate droplet shrinkage

Outputs

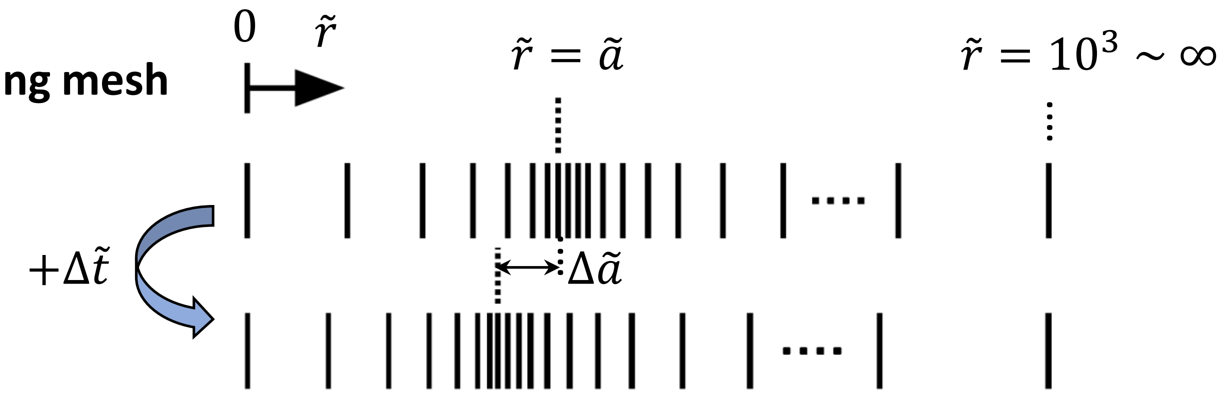
Field variables as function of space $\tilde{r}$ and time $\tilde{t}$

$\tilde{\theta}, \tilde{\varphi}, \tilde{\rho}, \tilde{u}, \tilde{P}$ for $\tilde{r} > \tilde{a}$

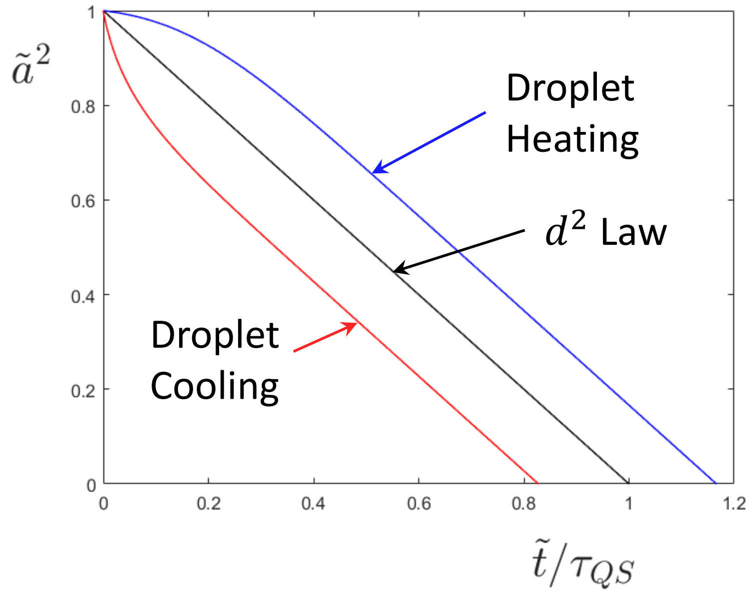
$\tilde{\theta}$ for $\tilde{r} \leq \tilde{a}$

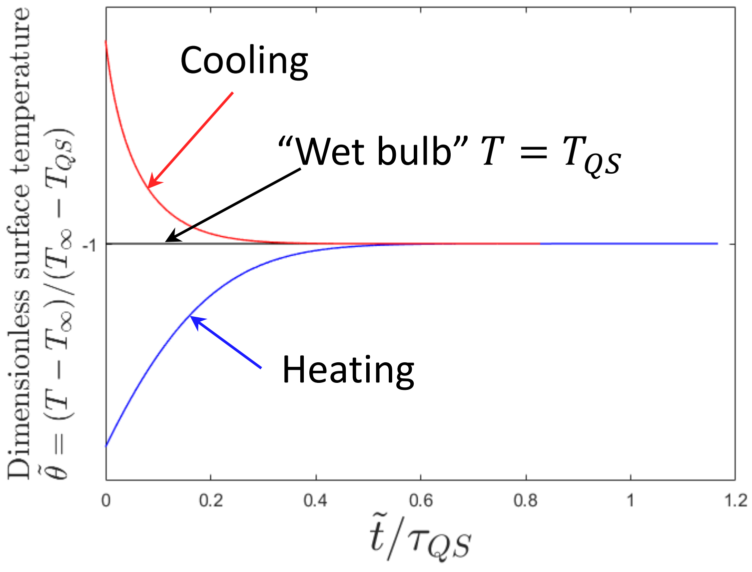
Droplet radius vs time $\tilde{a}(\tilde{t})$

1D moving mesh



4. Current Droplet Evaporation Understanding – Quasi-steady Solution & Liquid Phase Transients





Full Quasi-Steady (QS) → $\frac{\partial}{\partial t} = 0$

Analytical solution;

$$\frac{d\,\tilde{a}^2}{d\tilde{t}} = -2\rho_r \ln(1 + B_M)$$

Quasi-steady evaporation time $\tau_{QS} = \frac{1}{2\rho_r \ln(1+B_M)}$

Liquid heating/ cooling introduces well known transients and deviations from d^2 Law

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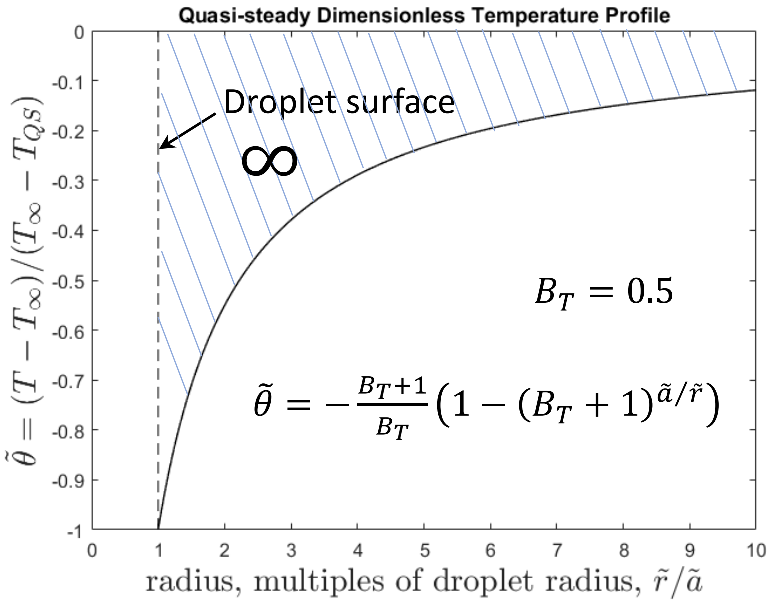
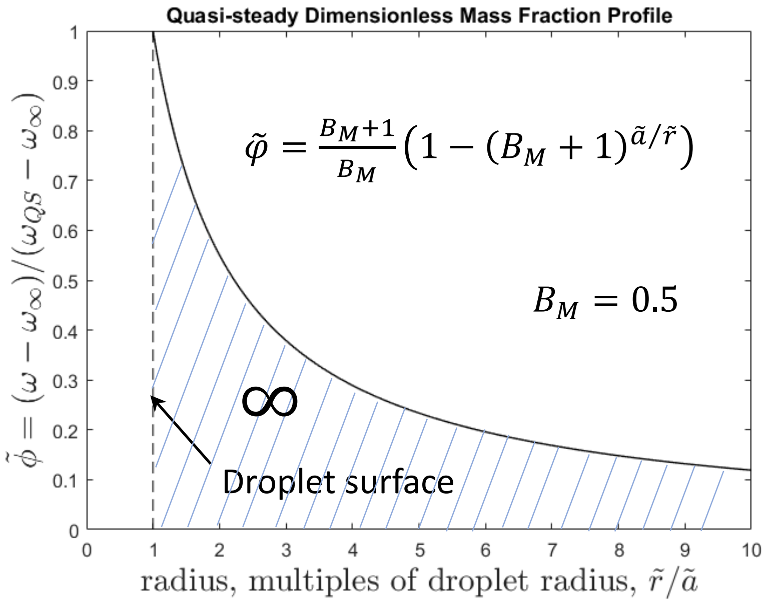
5. Can we take a Steady Gas Phase for Granted?





Steady temperature profile requires infinite energy?

Steady mass fraction profile requires infinite vapour mass?

Is quasi-steady gas phase always valid?

Typical evaporation time $t_{ev} \sim \dfrac{a_i^2\,\rho_l}{2\,\Gamma_\infty \ln(1+B_M)}$

Typical gas-phase response time $t_g \sim \dfrac{a_i^2\,\rho_\infty}{\Gamma_\infty}$

$$\frac{t_g}{t_{ev}} \sim \frac{\rho_\infty}{\rho_l} 2\ln(1+B_M) \sim \frac{\rho_\infty}{\rho_l} \sim 10^{-3} \to 10^{-2}$$

Is this an appropriate typical time for the gas-phase?
At what density ratio does this assumption break-down?

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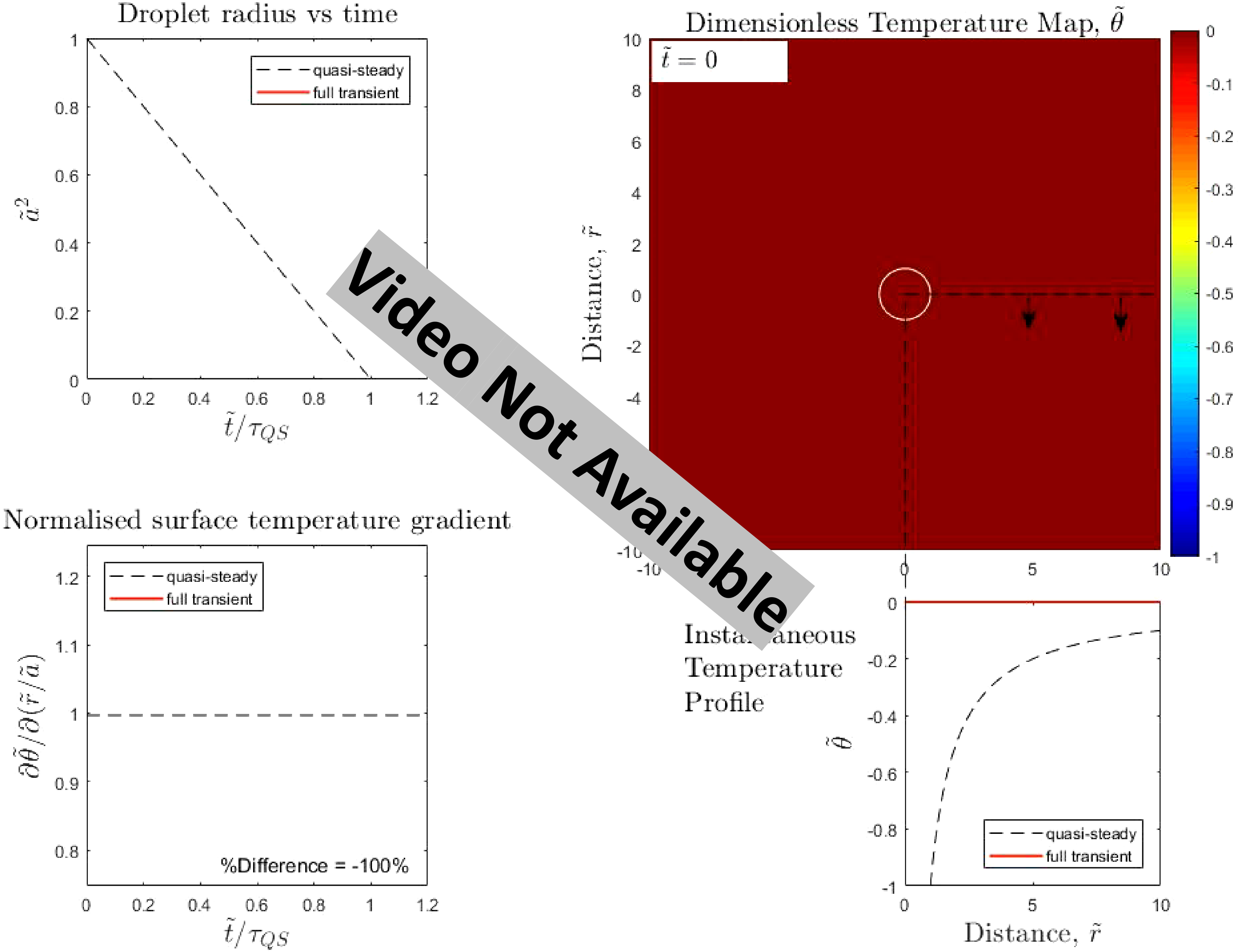
6a. Full Transient Solution: Water droplet in air at 293 K/1 bar / 40% humidity



Inputs:

$Le = 1.26, \; Ja = 0.308$

$\gamma_A = 1.33, \varepsilon = 0.622$,

$c_{pr} = 1.84$, $\rho_r = 0.0012$,

$c_r = 0.446$, $\lambda_r = 0.042$

$\tilde{T}_{ex} = 0.785$, $\delta = 0.993$

Derived constants:

$B_T = 0.0063$

$B_M = 0.0043$

6b. Full Transient Solution: LN_2 in dry air at 300K /1 bar

Inputs:

$Le = 1.02,\ Ja = 0.403$

$\gamma_A = 1.40, \varepsilon = 0.88$,

$c_{pr} = 1.03$, $\rho_r = 0.0014$,

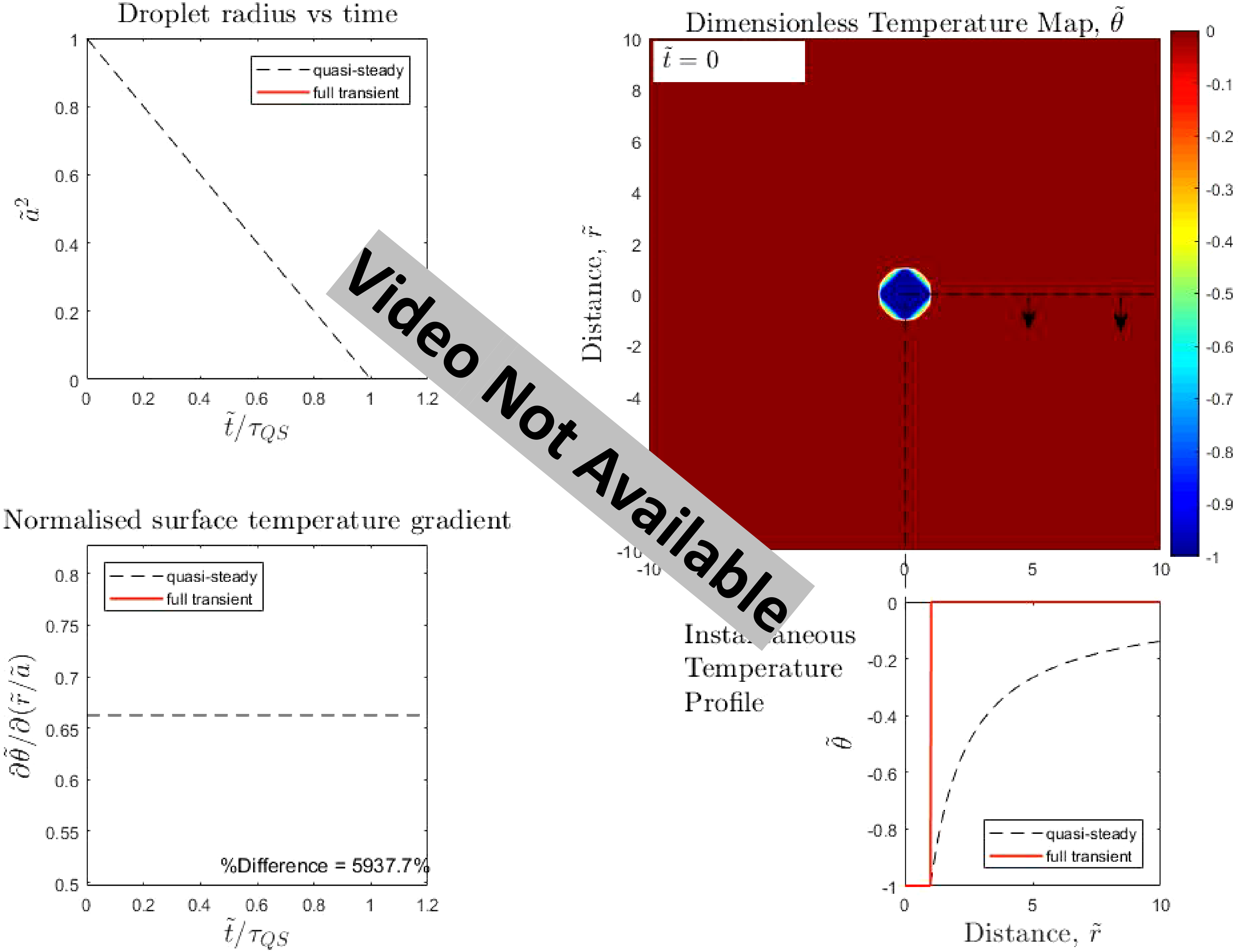
$c_r = 0.518$, $\lambda_r = 0.167$

$\tilde{T}_{ex} = 3.88$, $\delta = 0.233$

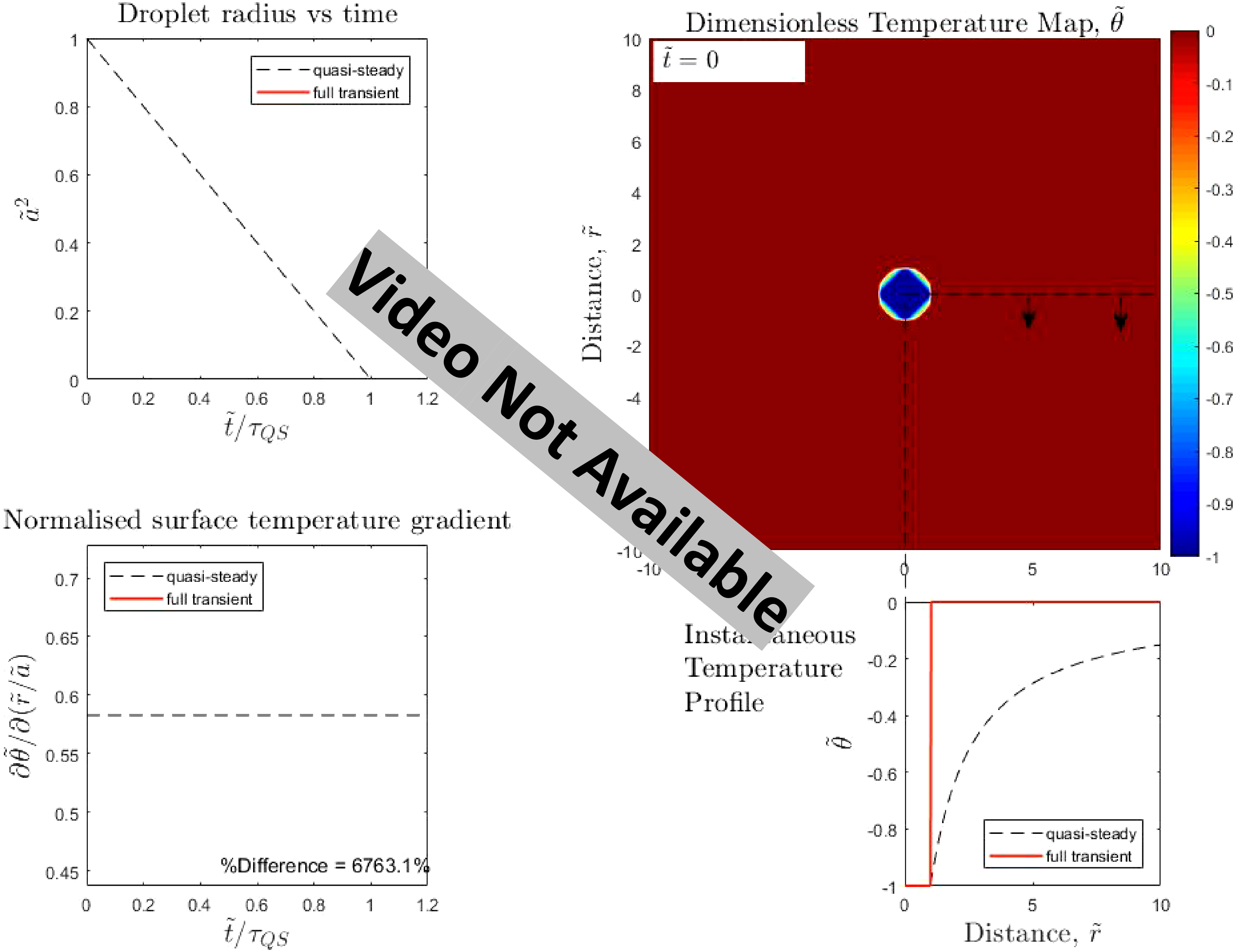
Derived constants:

$B_T = 1.168$

$B_M = 1.162$



6c. Full Transient Solution: LN_2 in dry air at 300K /20 bar



Inputs:

$Le = 1.02,\ Ja = 1.06$

$\gamma_A = 1.40,\ \varepsilon = 0.88$,

$c_{pr} = 1.03$, $\rho_r = 0.0287$,

$c_r = 0.518$, $\lambda_r = 0.167$

$\tilde{T}_{ex} = 2.60$, $\delta = 0.233$

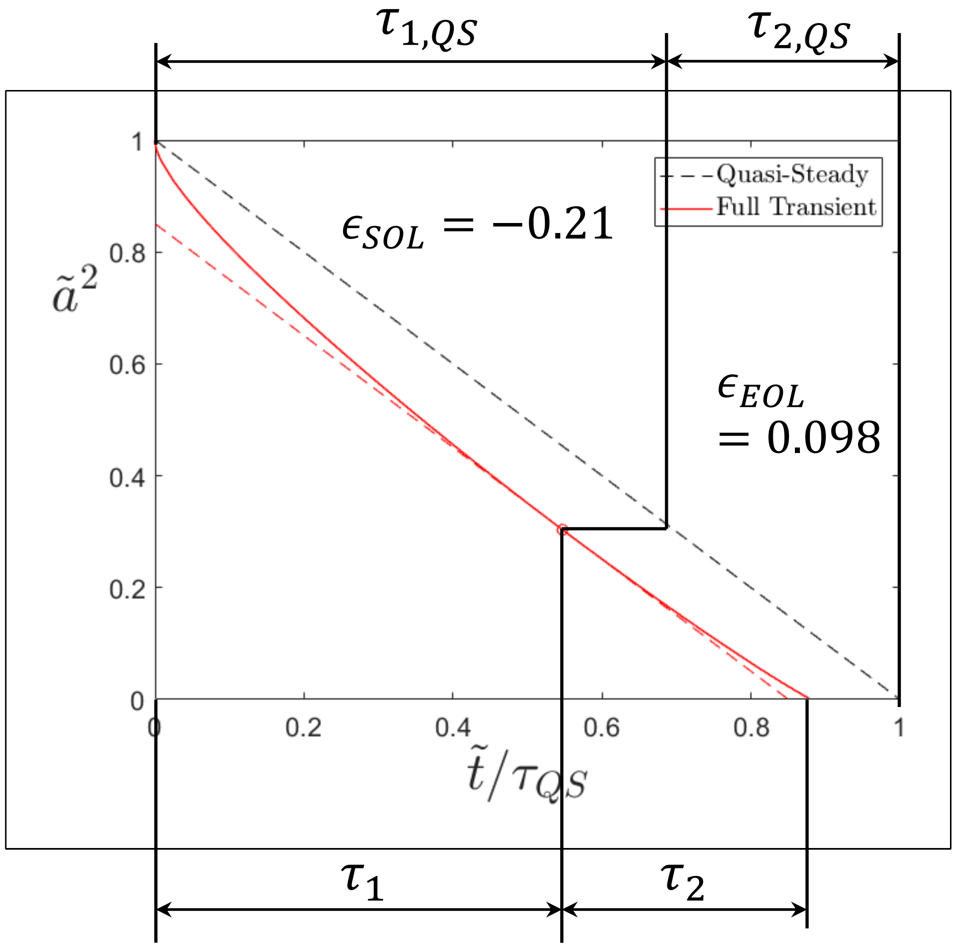
Derived constants:

$B_T = 1.712$

$B_M = 1.702$

7. Characterising the Gas Phase Transients

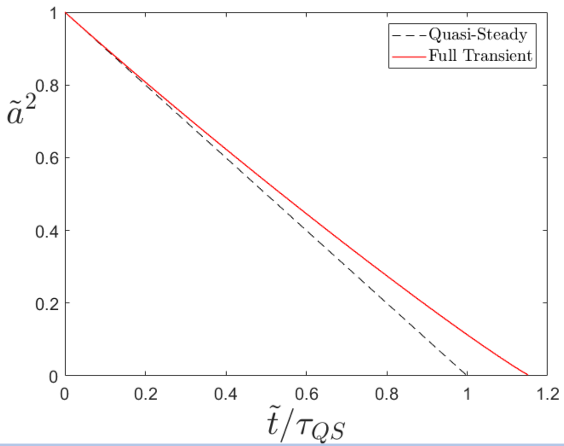
Droplet radius² vs time, N2/Air @ 300K/20bar



Two transient regimes identified	
'Start of life' Transient	'End of life' Transient
• Due to establishing the fields around the droplet • Effect is large if mass/energy required to establish QS fields is comparable to that available within droplet • Initial condition dependent	• Due to **History Dependence** of evaporation process • Early stages of evaporation cool and partially saturate the region around droplet • Its existence is independent of initial conditions
Quantified by: $\epsilon_{SOL} = \frac{\tau_1}{\tau_{1,QS}} - 1$	Quantified by: $\epsilon_{EOL} = \frac{\tau_2}{\tau_{2,QS}} - 1$

Droplet radius² vs time, N2/Air @ 300K/20bar.
Initial gas fields are QS fields

$$\epsilon_{SOL} = 0$$
$$\epsilon_{EOL} = 0.15$$



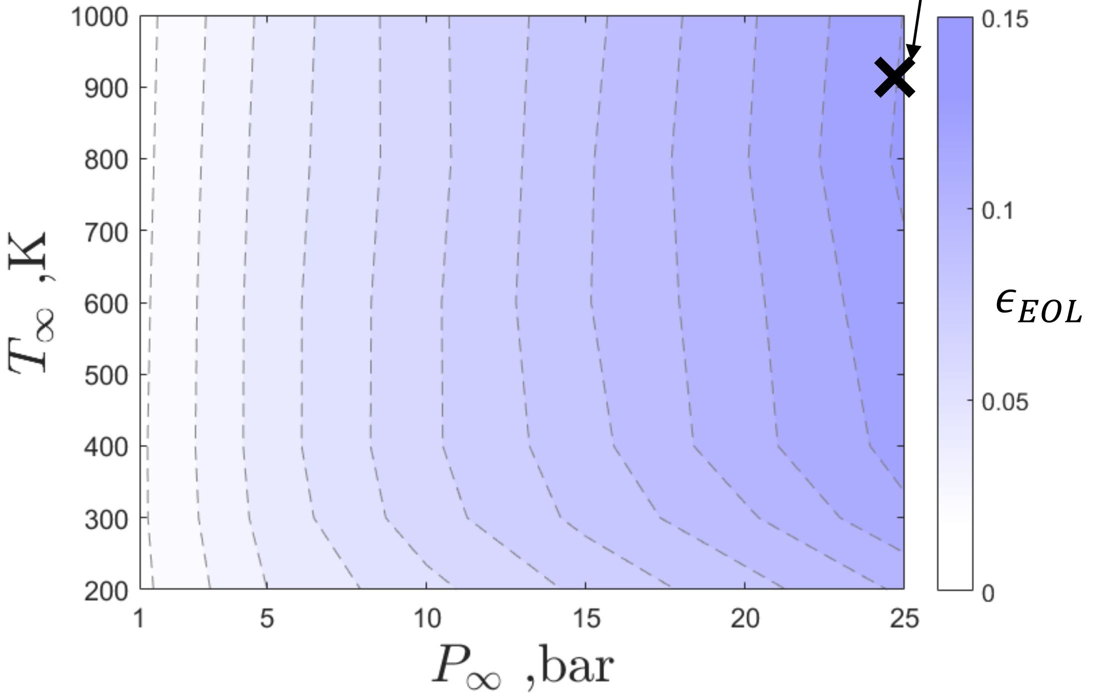
9. Case Study Example – LN_2 Evaporating in Air

For given Fluids, $P_\infty \Uparrow \;\rightarrow\; \rho_r \Uparrow \quad Ja \Uparrow \quad \tilde{T}_{ex} \Downarrow \;\rightarrow$ net increase in transient effects

$T_\infty \Uparrow \;\rightarrow\; \rho_r \Downarrow \quad Ja \; - \quad \tilde{T}_{ex} \Uparrow \;\rightarrow$ only small net effect on transients

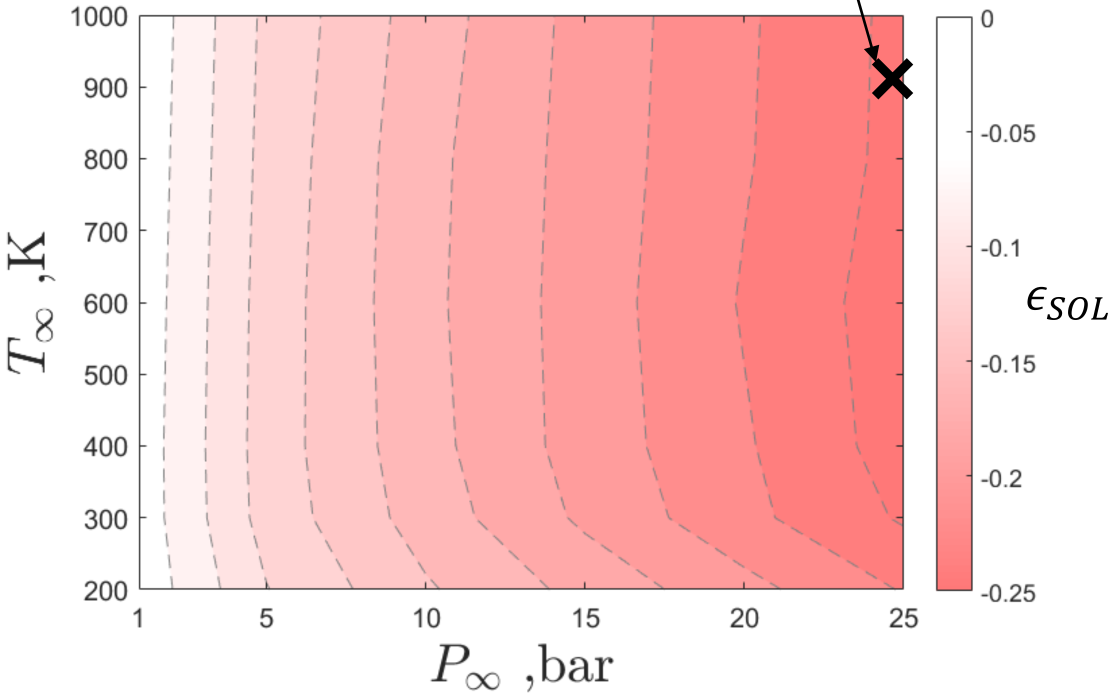
ϵ_{EOL} ***Map***

13% deviation from d² Law



ϵ_{SOL} ***Map***

24% deviation from d² Law



10. Conclusions

1. A new fully transient droplet evaporation model has been developed.

2. The model recovers d^2 law under "normal" conditions

3. The model predicts two transient effects which act in opposing directions;
   a) Evaporation rate is increased during early stages of evaporation as surrounding gas field is established – this is sensitive to initial conditions so experimental validation would be challenging
   b) Evaporation rate is decreased during late stages of evaporation due to a region of low temperature and high vapour concentration around the droplet (self-insulation).

4. The gas phase transient effects manifest under high ρ_r , Ja , and $\tilde{T}_{ex}$.

5. Fluids with low boiling points are more susceptible to simultaneously high ρ_r and $\tilde{T}_{ex}$.

6. For a given fluid combination, the transient effects manifest under high pressures.

7. Neglecting the gas phase transients can account for a ~20% error in evaporation rate predictions. Errors in excess of this value can occur at even higher pressures towards the critical pressure, where the physical assumptions become questionable.

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