

**Droplet evaporation, 0D analysis**  
**Pure solvent**

Data for hexane :

$$\rho = 659.4 \text{ kg} / \text{m}^3$$

$$M = 86.17 \text{ g} / \text{mol} = 0.08617 \text{ kg} / \text{mol}$$

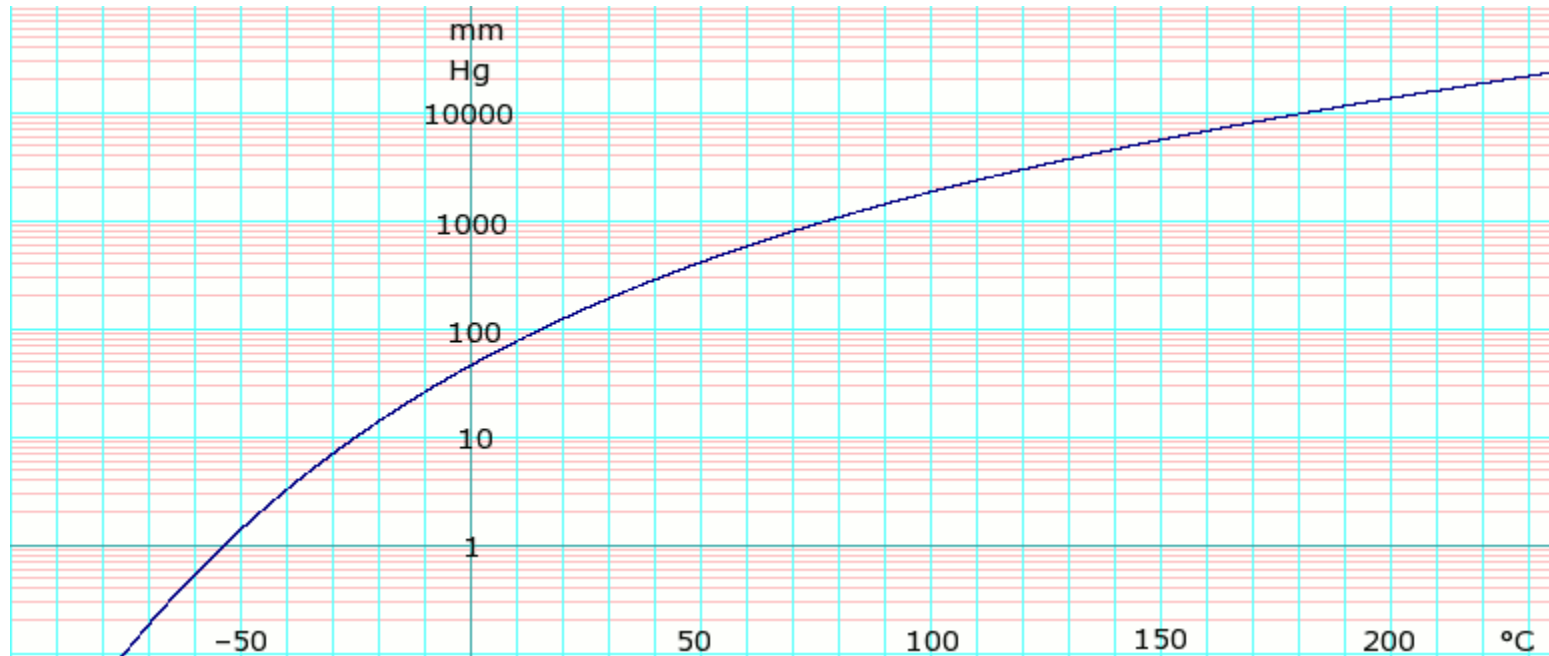
$$V_{m \text{ liquide}} = 1.306.10^{-4} \text{ m}^3 / \text{mol} = 1.515.10^{-3} \text{ m}^3 / \text{kg}$$

$$k_{\text{liquid hexane}} = 0.124 \text{ Wm}^{-1} \text{K}^{-1}$$

$$C_{p \text{ liquid hexane}} = 197.66 \text{ Jmol}^{-1} \text{K}^{-1} = 2293 \text{ Jkg}^{-1} \text{K}^{-1}$$

$$\Delta H_{\text{vap hexane}} = 28.85 \text{ kJ} / \text{mol} = 334 \text{ kJkg}^{-1}$$

$$Bi = \frac{hL}{k} < 0.1 \quad L = 1 \text{ mm}$$



$$\log_{10} P_{\text{vs, mmHg}} = \log_e \left( \frac{760}{101.325} \right) - 13.99935 \log_e (T + 273.15) - \frac{7284.572}{T + 273.15} + 105.9605 + 1.410325 \times 10^{-5} (T + 273.15)^2$$

# Mass transport and heat transfer

The evaporating flux is given by the Hertz-Knudsen Schrage relationship :

$$\overset{\text{kg.s}^{-1}}{\phi_{\text{éaporé}}} = \overset{\text{m}^2}{A_{\text{droplet}}} \frac{2}{2 - \alpha_C} \frac{1}{\sqrt{2\pi M_i R}} \left( \alpha_C \frac{P}{\sqrt{T_{\text{gaz}}}} - \alpha_E \frac{P_{\text{sat}}(T_{\text{liquide}})}{\sqrt{T_{\text{liquide}}}} \right) \cdot \overset{\text{kg.mol}^{-1}}{M_{\text{hexane}}}$$

$$0 \leq \alpha_C \approx \alpha_E \leq 1$$

The differential equation to solve for mass balance is :

$$\frac{dm_{\text{droplet}}}{dt} = -\phi_{\text{éaporé}} \text{ with } A_{\text{droplet}} = 4\pi \left( \frac{3V_{\text{droplet}}}{4\pi} \right)^{2/3}$$

$$\overset{\text{W}}{p} = \overset{\text{kg.s}^{-1}}{\phi_{\text{éaporé}}} \cdot \overset{\text{J.kg}^{-1}}{\Delta H_{\text{vap, hexane}}}$$

The differential equation to solve for heat balance is :

$$m_{\text{droplet}} C_{p_{\text{droplet}}} \frac{dT_{\text{liquide}}}{dt} = -\phi_{\text{éaporé}} \cdot \Delta H_{\text{vap}} - A_e \sigma \varepsilon (T_{\text{liquide}}^4 - T_{\text{gaz}}^4)$$

If the droplets are contained in a fixed volume where the gas temperature is fixed :

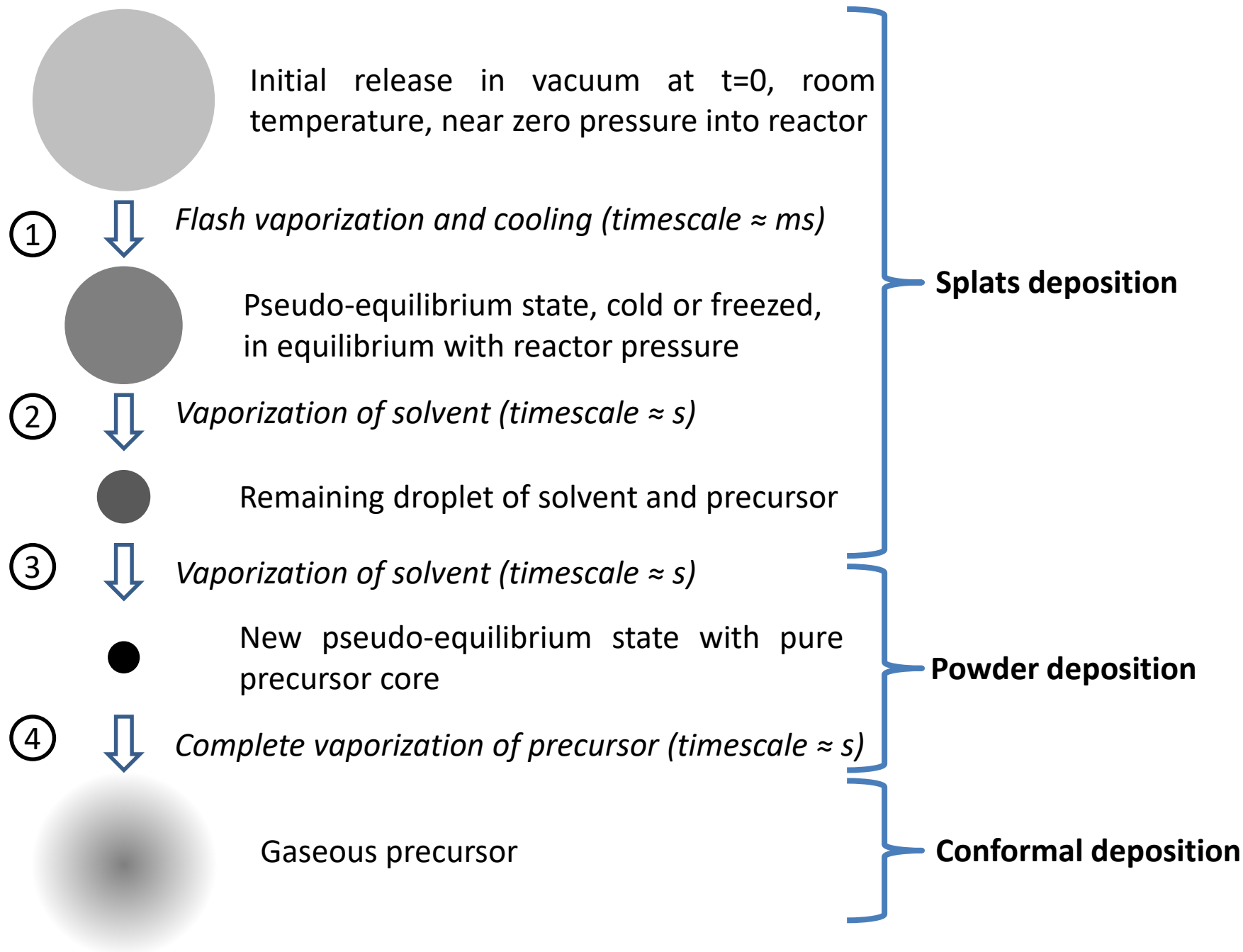
$$\frac{V_{\text{container}}}{RT_{\text{gas}}} \frac{dP_{\text{gas}}}{dt} = \frac{N_{\text{droplets}} \phi_{\text{évaporé}}}{M_{\text{hexane}}} - \frac{Q_{\text{pump}} P_{\text{gas}}}{RT_{\text{gas}}} \quad N_{\text{droplets}} = \frac{m_{\text{hexane,ini}}}{\frac{4}{3} \pi r_{\text{droplets,ini}}^3 \rho_{\text{hexane}}}$$

So you have to solve :

$$\frac{dP_{\text{gas}}}{dt} = \frac{RT_{\text{gas}} N_{\text{droplets}} \phi_{\text{évaporé}}}{V_{\text{container}} M_{\text{hexane}}} - \frac{Q_{\text{pump}} P_{\text{gas}}}{V_{\text{container}}}$$

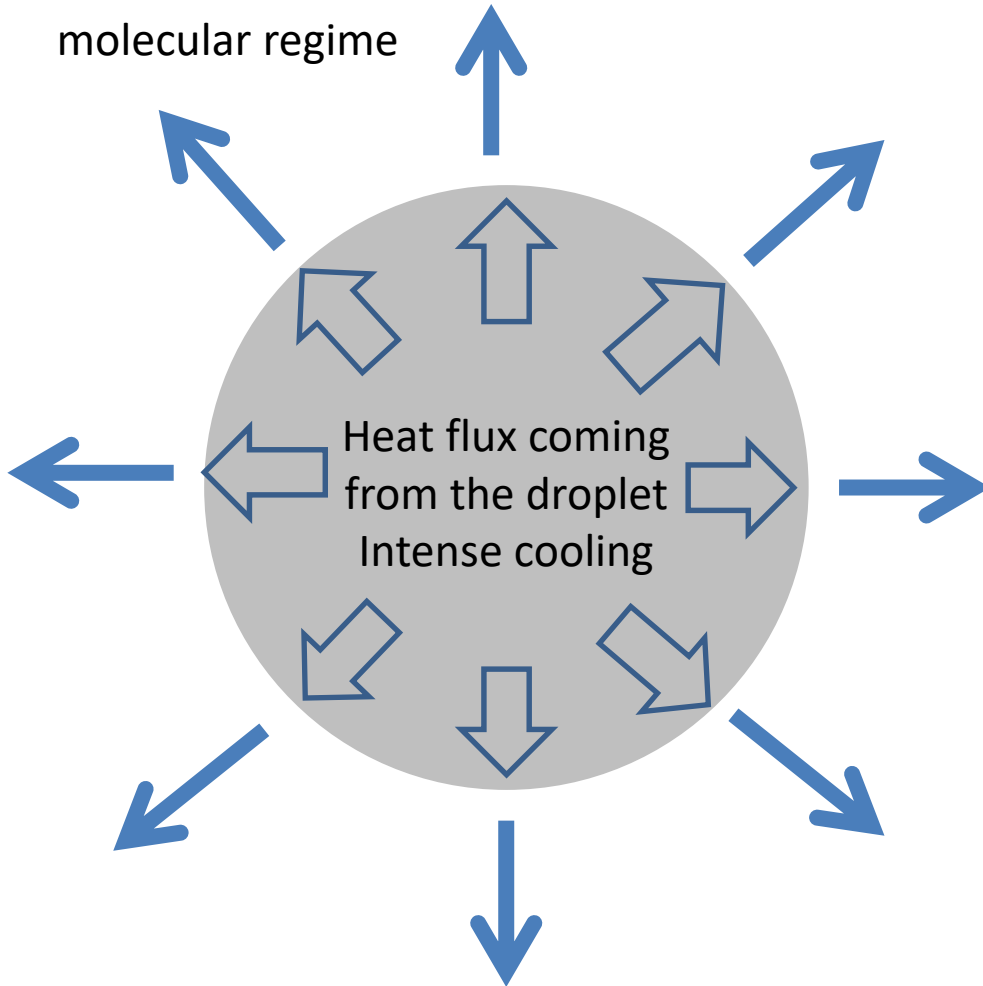
$$\frac{dm_{\text{droplet}}}{dt} = -\phi_{\text{évaporé}}$$

$$\frac{dT_{\text{liquide}}}{dt} = \frac{-\phi_{\text{évaporé}} \cdot \Delta H_{\text{vap,hexane}} - A_e \sigma \varepsilon (T_{\text{liquide}}^4 - T_{\text{gaz}}^4)}{V_{\text{droplet}} \rho_{\text{hexane}} C_p}$$



## Flash vaporization step

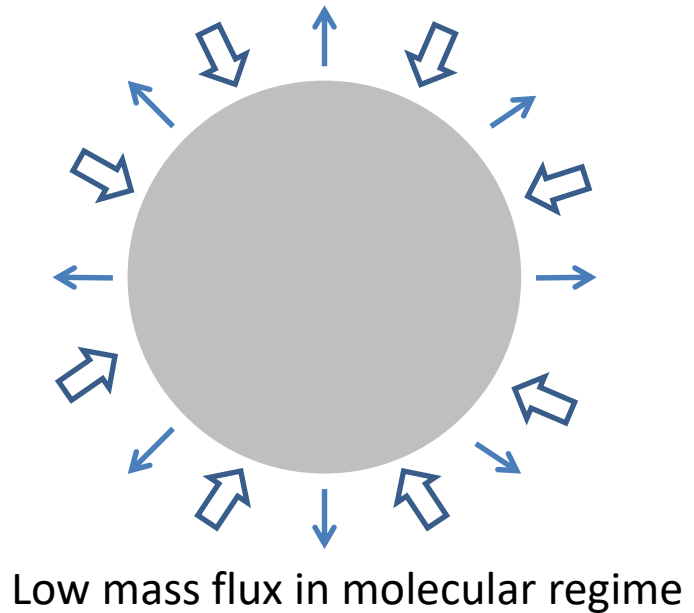
Intense mass flux in  
molecular regime



*During the flash vaporization, the kinetic is limited by a Hertz-Knudsen flux.*

## Pseudo-equilibrium vaporization steps

Low heat flux coming from radiation

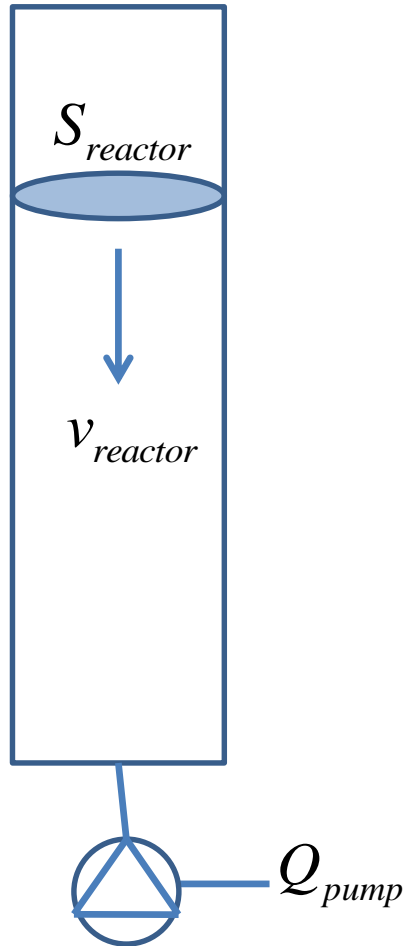


*During the pseudo-equilibrium vaporization, the flux is limited by radiative thermal balance.*

# **Tracking the droplets**

If the pumping rate is constant and the reactor plug-flow type, the vertical velocity of gas is constant (but not the pressure) :

$$v_{reactor} = Q_{pump} / S_{reactor}$$



The force balance on the droplet in Stokes regime is :

$$\frac{dz_{droplet}}{dt} = v_{droplet}$$

$$\frac{dv_{droplet}}{dt} = \frac{\frac{3\pi\eta_{gas}d_{droplet}}{C_c} (v_{droplet} - v_{reactor}) (1 + 0.15 Re_{droplet}^{0.687})}{m_{droplet}} - g$$

$$Re_{droplet} = \frac{\rho_{gas} (v_{droplet} - v_{reactor}) d_{droplet}}{\eta_{gas}} \quad \rho_{gas} = \frac{P_{gas} M_{gas}}{RT_{reactor}}$$

$$C_c = 1 + \frac{2l_{pm}}{d_{droplet}} \left( 1.257 + 0.4 \exp^{-0.55 \frac{d_{droplet}}{l_{pm}}} \right)$$

$$l_{pm} = \frac{1}{\sqrt{2}\pi\sigma_{sol}^2 c}$$

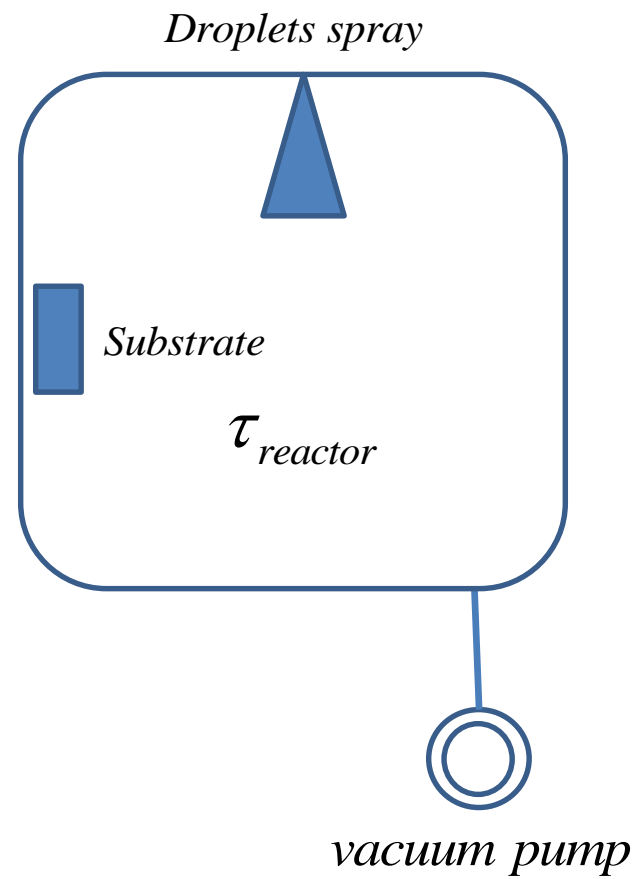
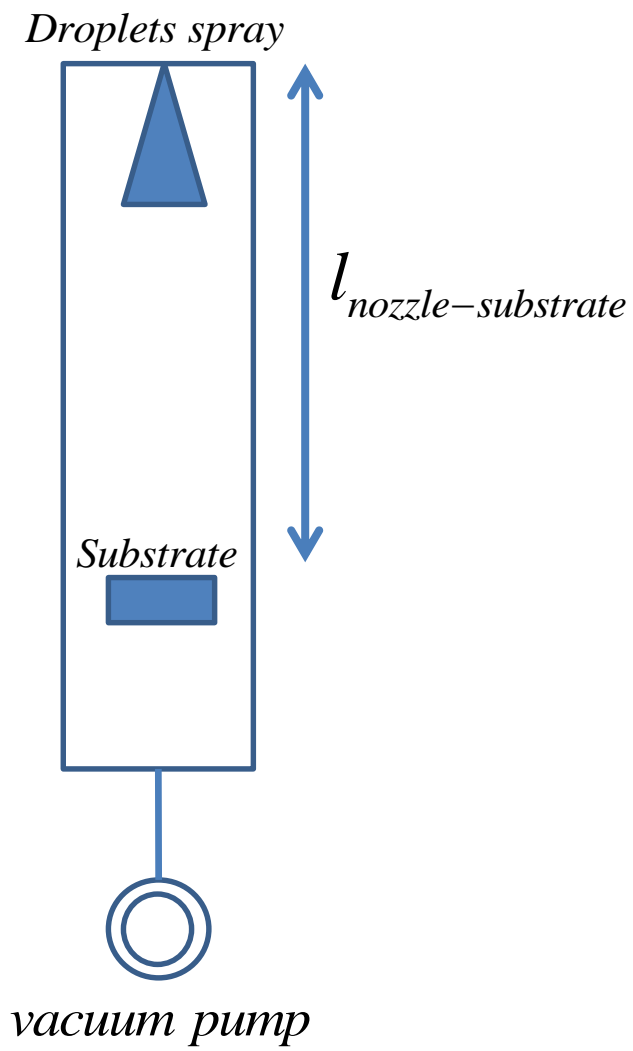


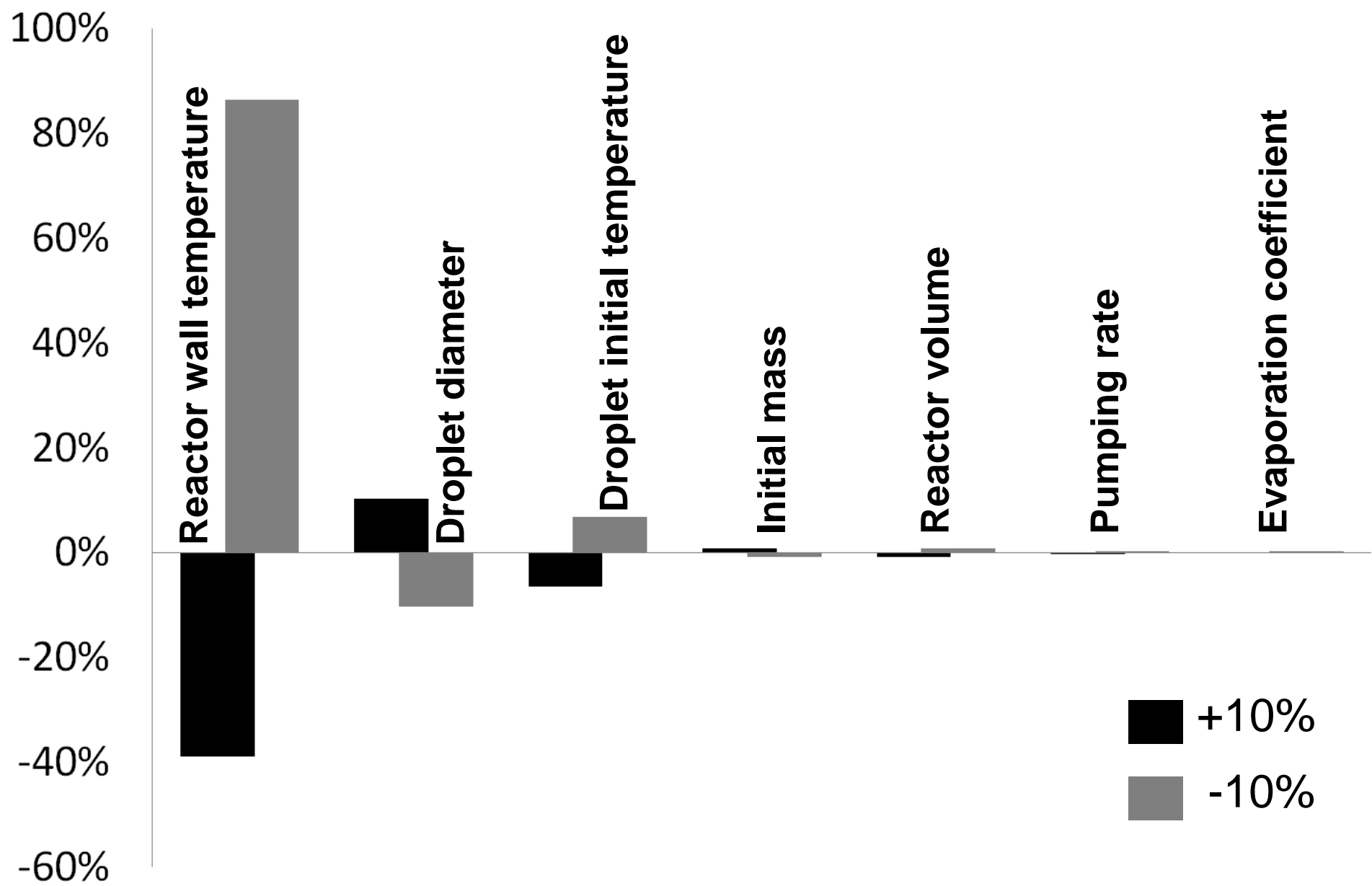
The gaz viscosity is approximated as the one of solvent at reactor temperature :

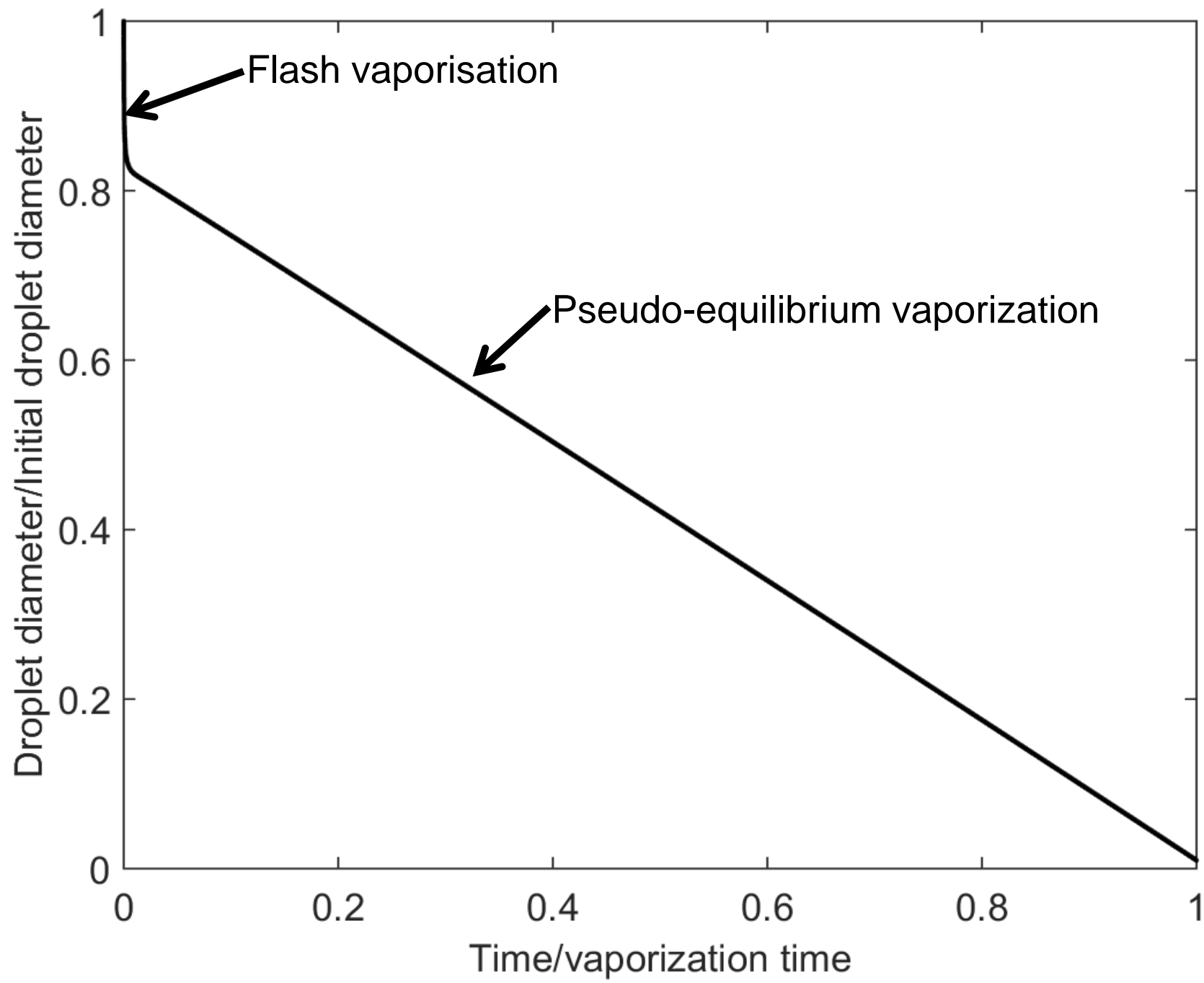
$$\eta_{gas} \approx \eta_{sol} = 2,6693.10^{-6} \frac{\sqrt{M_{sol} T_{reactor}}}{\sigma_{sol}^2 \Omega_{\eta}}$$

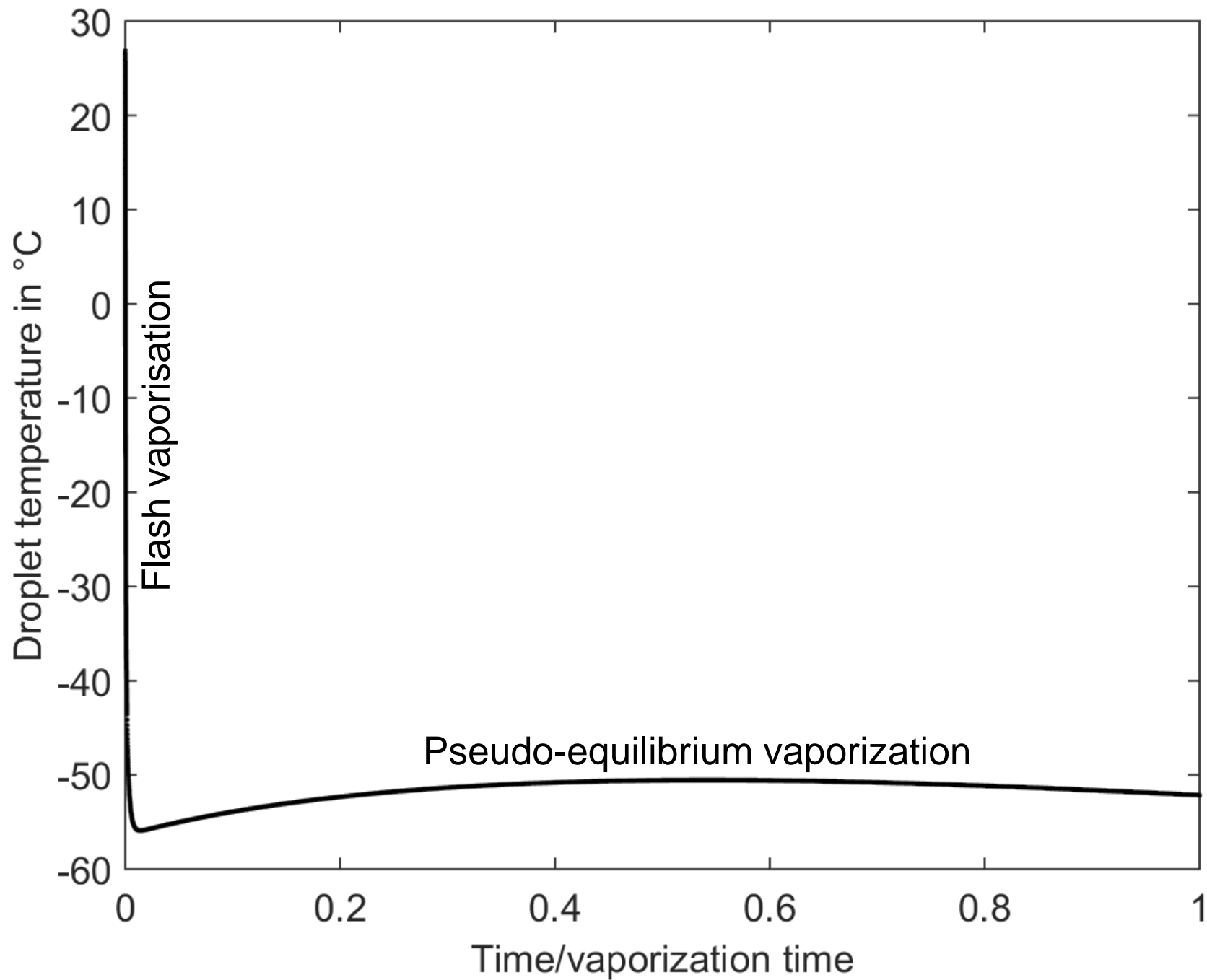
$$T^* = \frac{k_b T_{reactor}}{\mathcal{E}_{sol}}$$

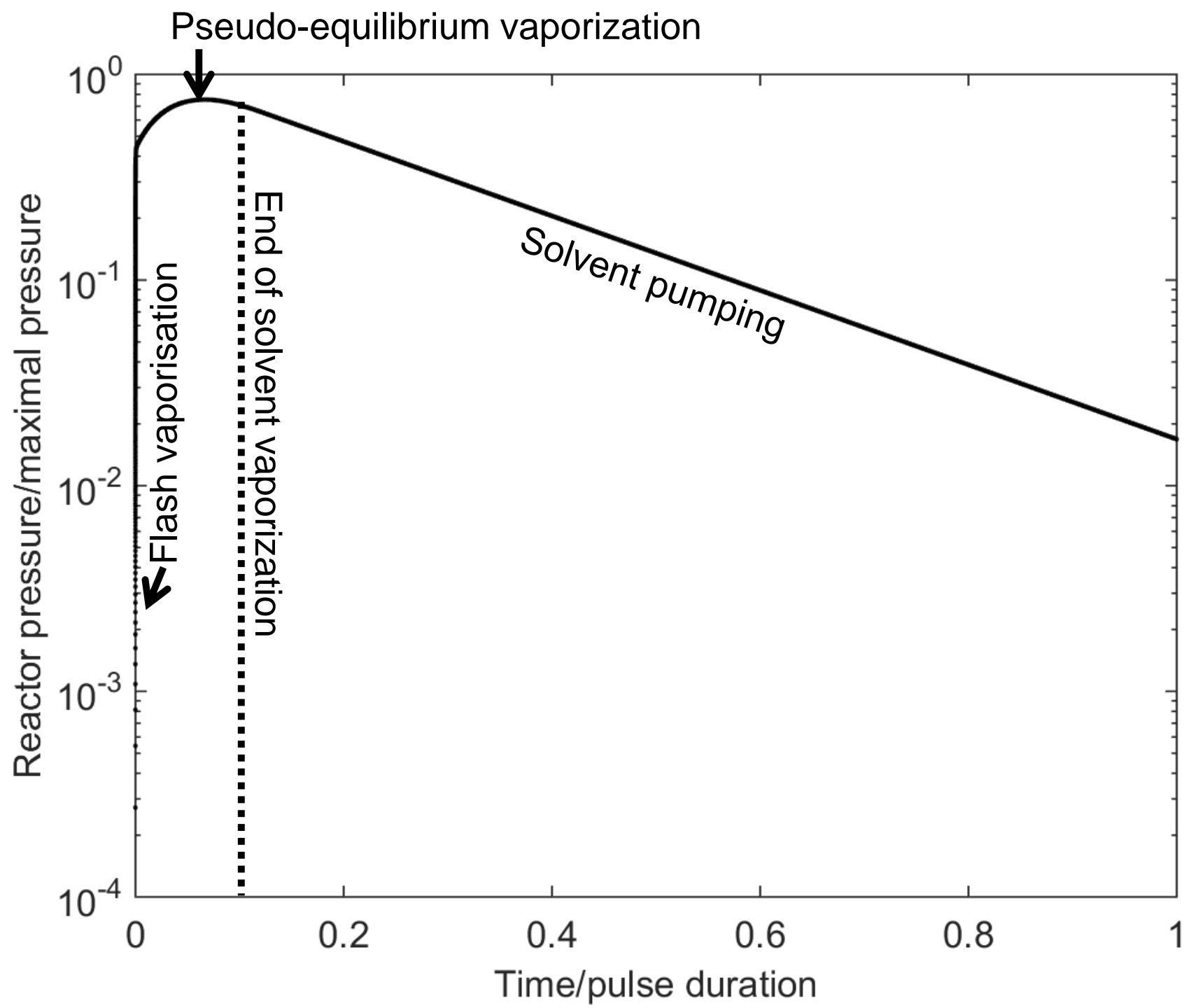
$$\Omega_{\eta} = \frac{1.16145}{T^{*0.14874}} + \frac{0.52487}{\exp(0.7732T^*)} + \frac{2.16178}{\exp(2.43787T^*)}$$

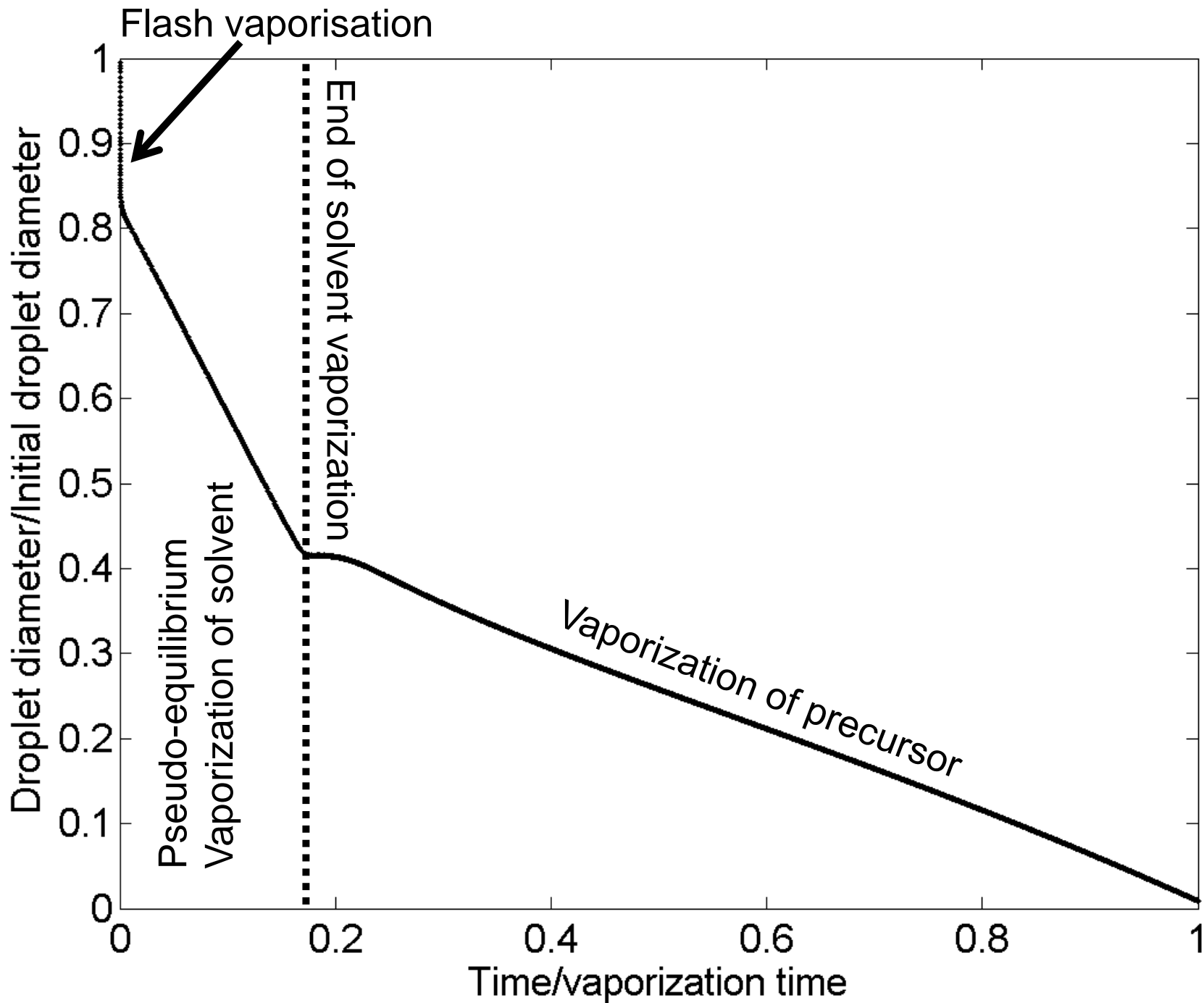


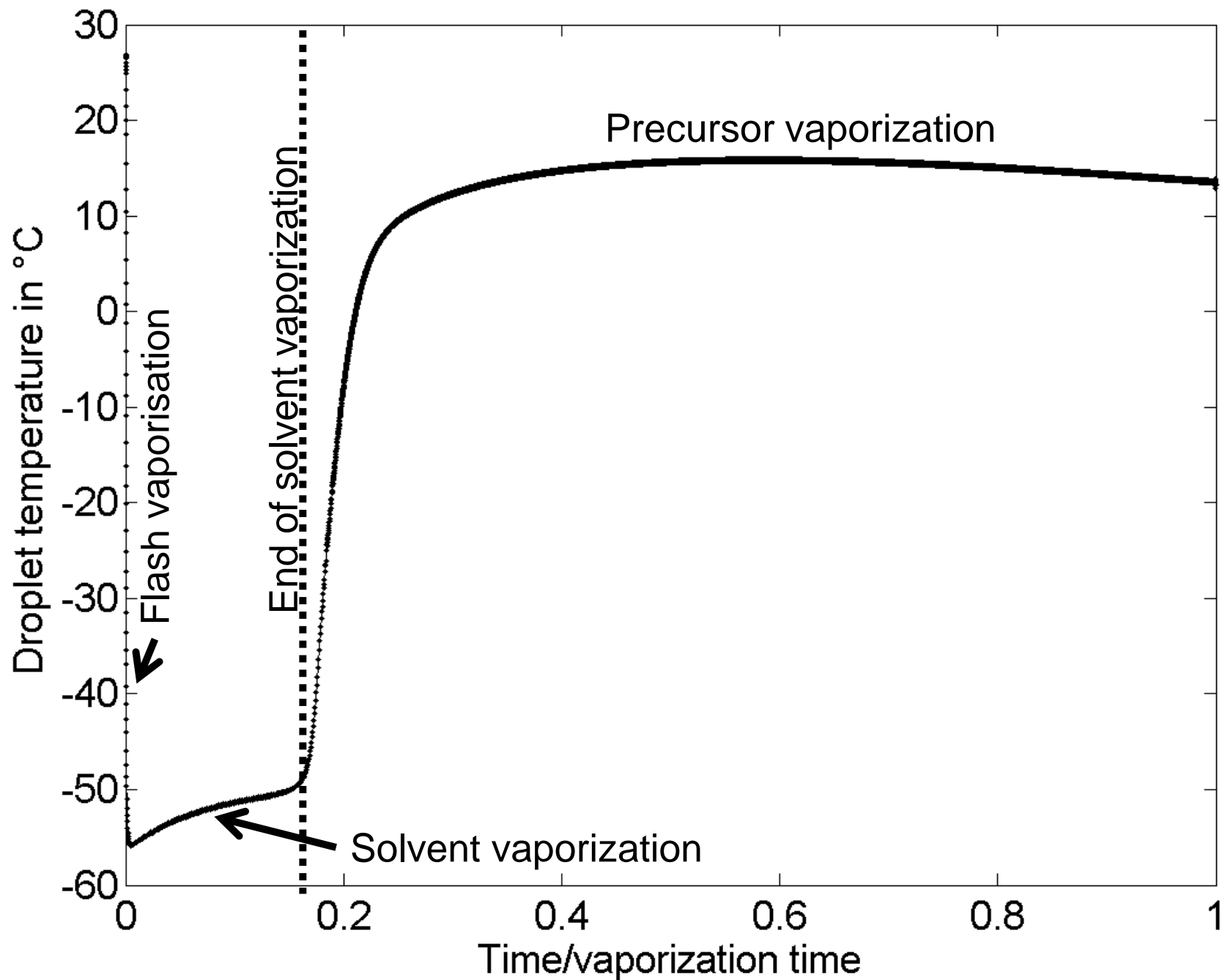




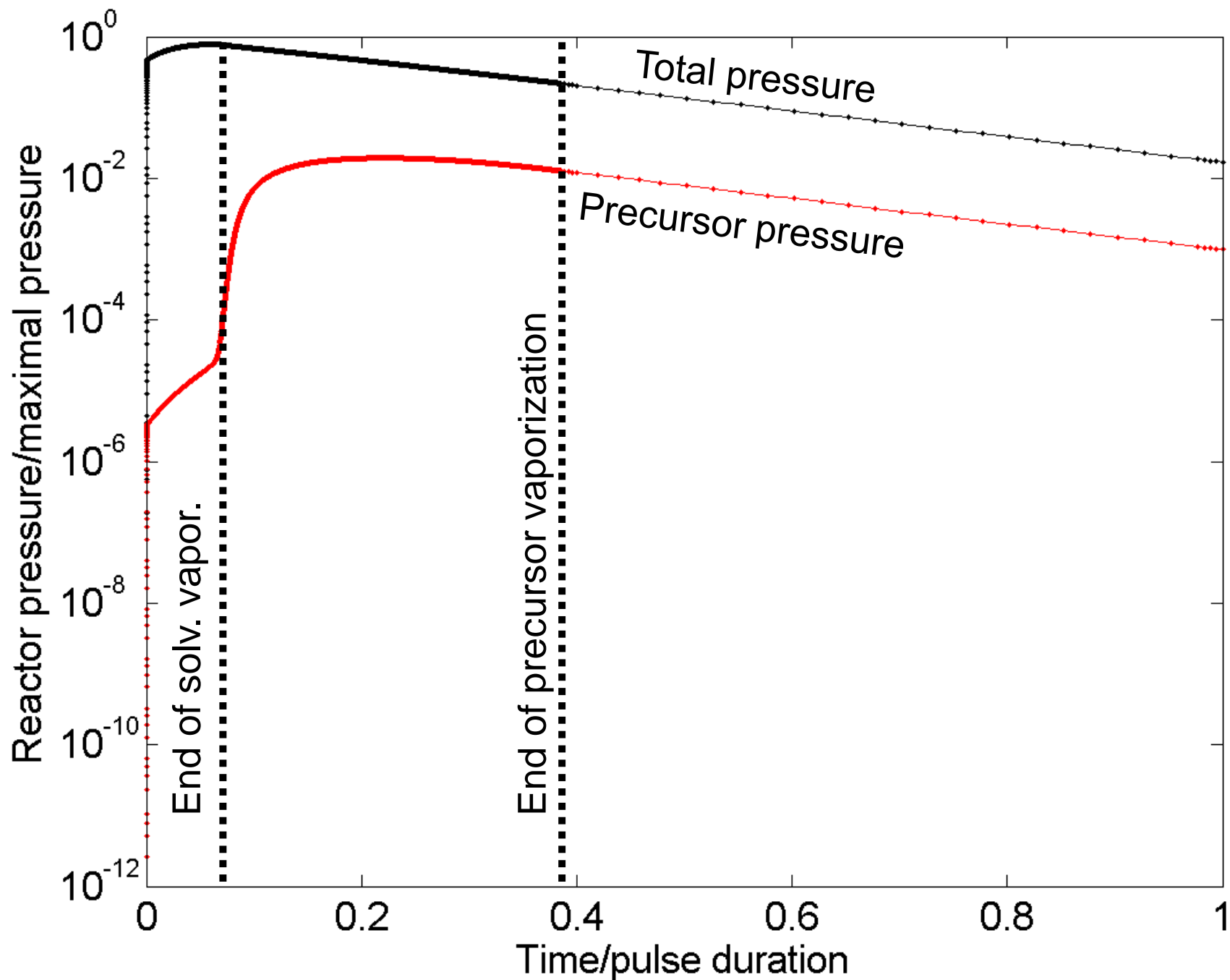


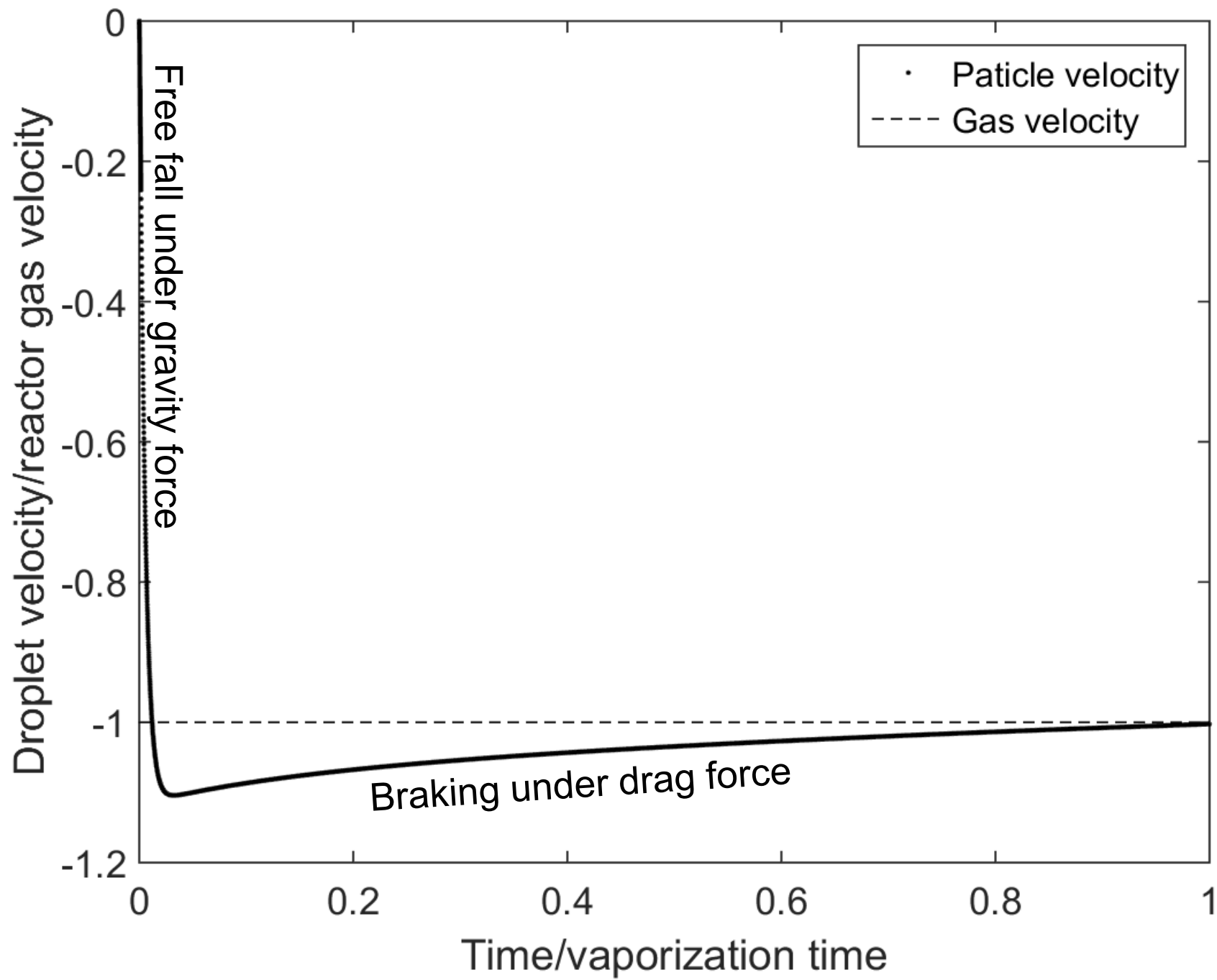


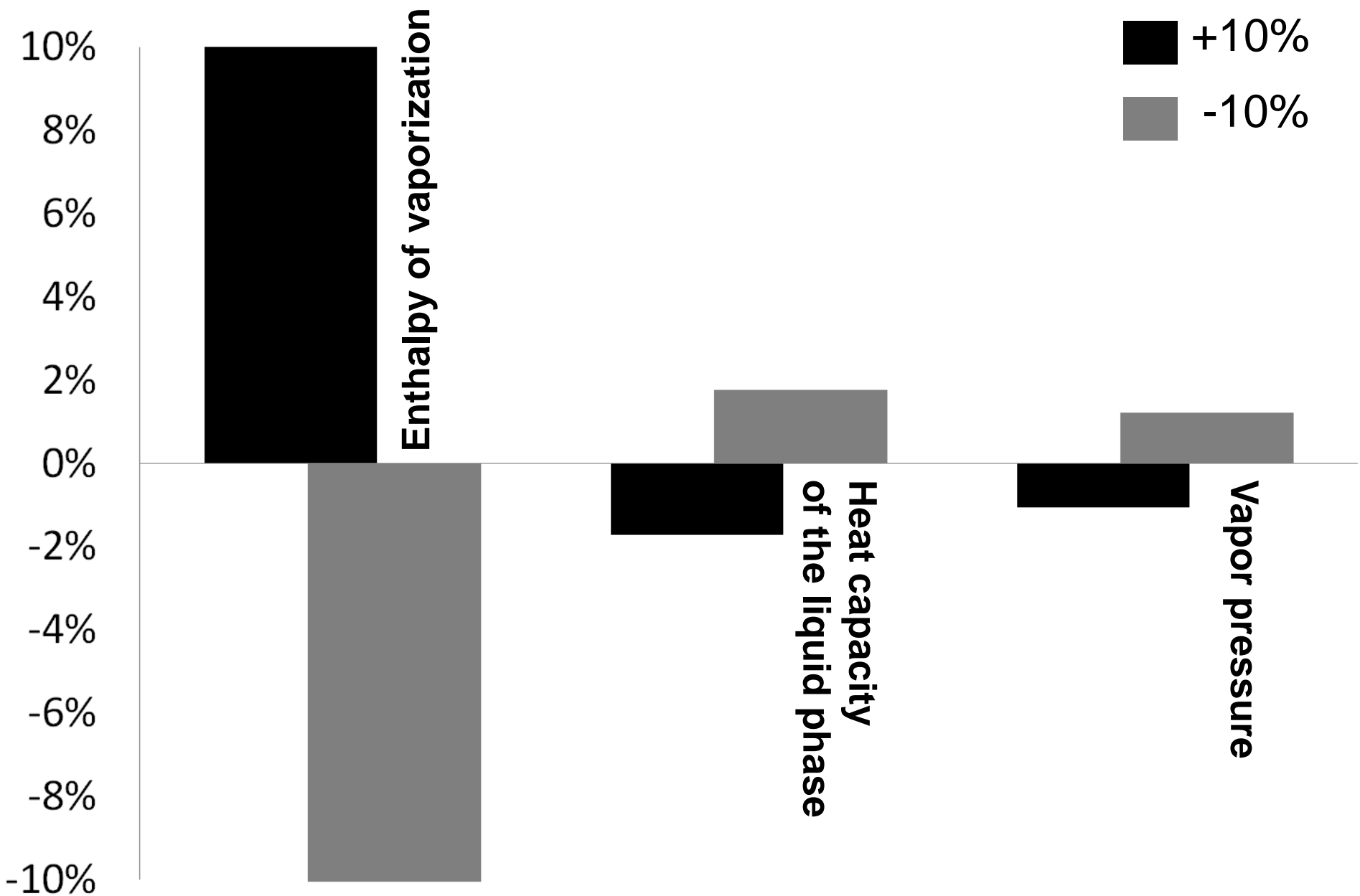


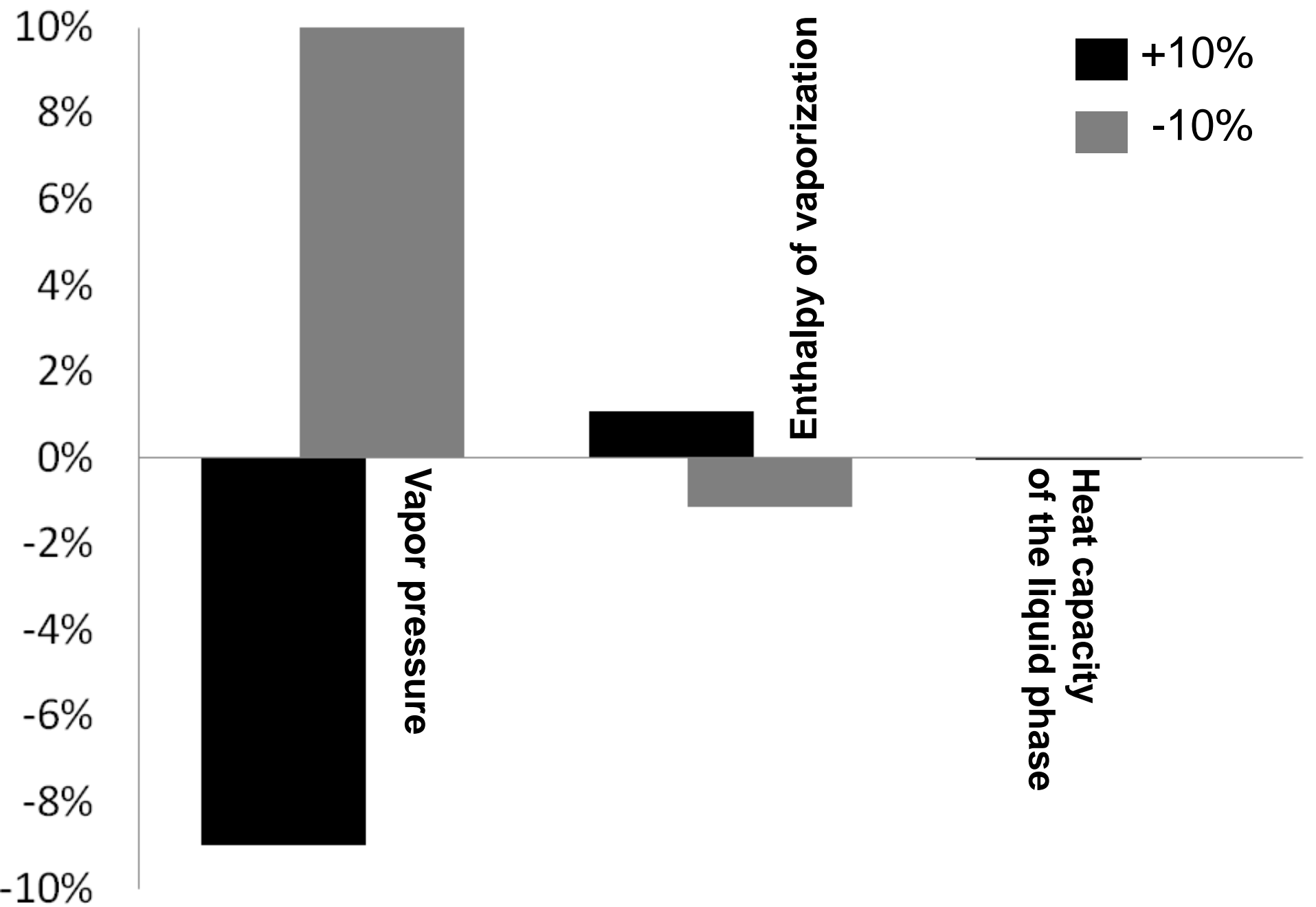


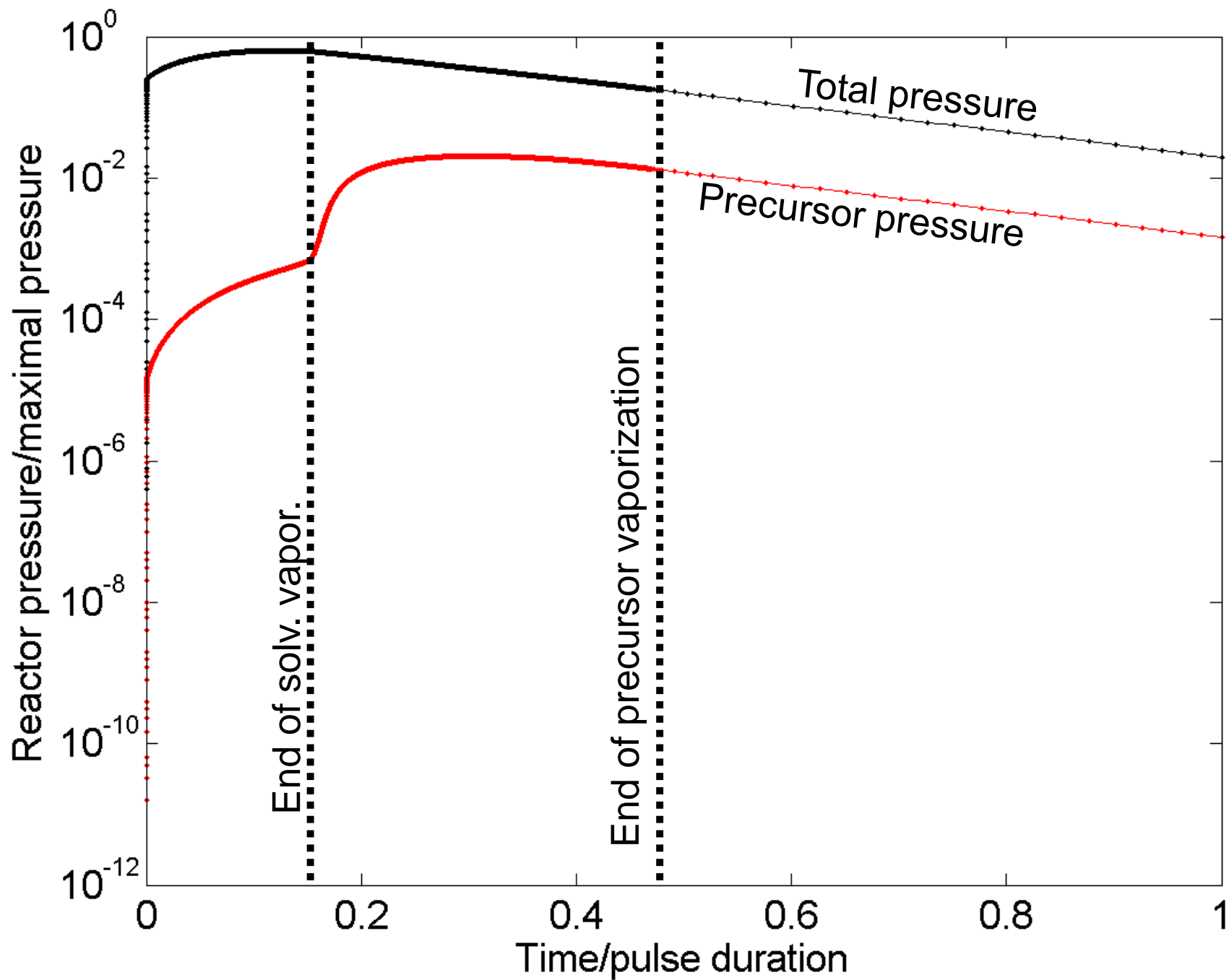


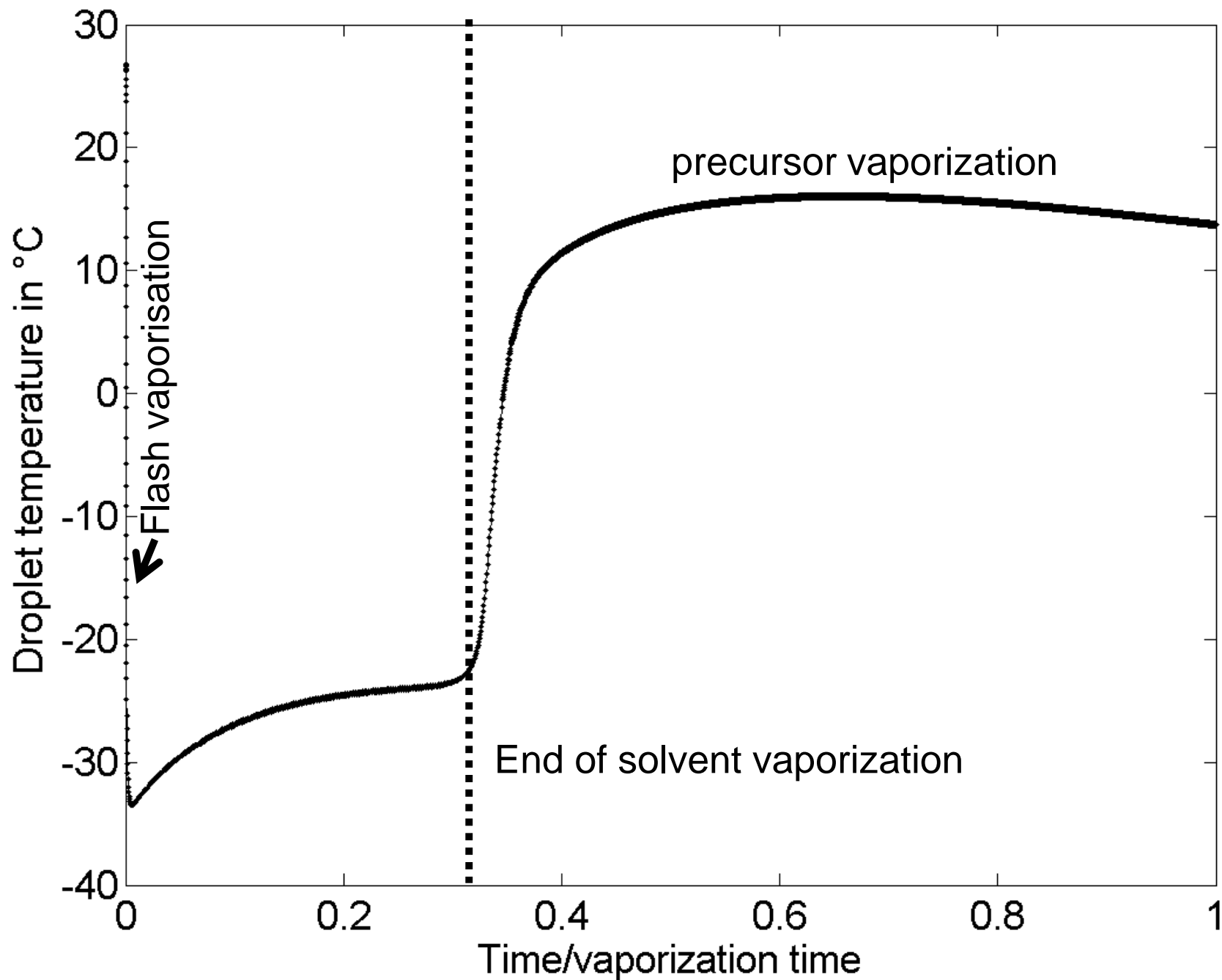




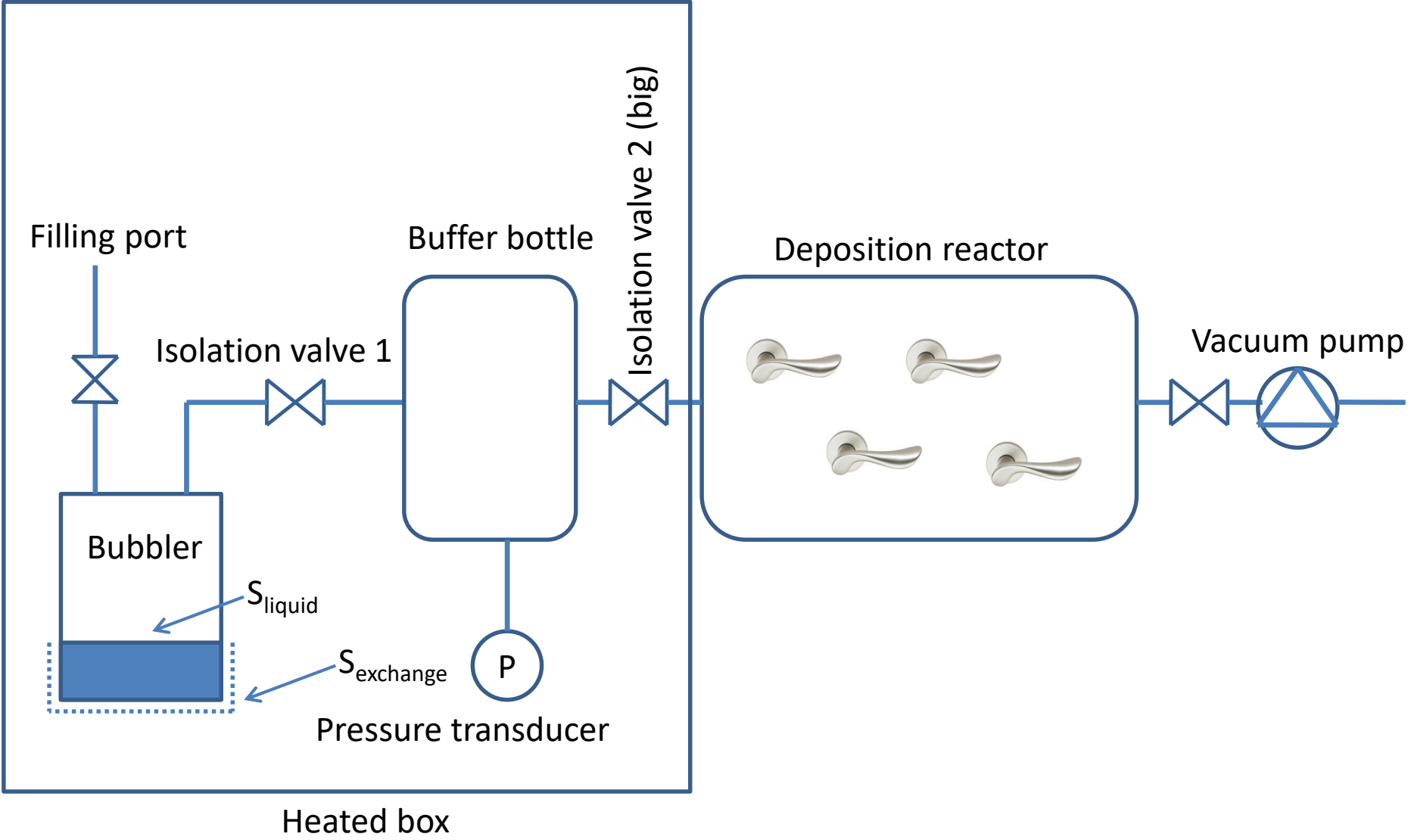








**Buffer bottle process, 0D analysis**  
**Pure precursor**





Maximal pressure you can reach :

$$P_{\max} = \frac{V_{\text{buffer bottle}} + V_{\text{reactor}}}{V_{\text{buffer bottle}}} P_{\text{buffer bottle}}$$

Flux of evaporation from bubbler (liquid surface) :

$$\overset{\text{kg.s}^{-1}}{\phi_{\text{vaporated}}} = \overset{\text{m}^2}{S_{\text{liquid}}} \frac{2}{2 - (0.798)\alpha_C} \frac{1}{\sqrt{2\pi M_i R}} \left( \alpha_C \frac{P}{\sqrt{T_{\text{heating box}}}} - \alpha_E \frac{P_{\text{sat}}(T_{\text{bubbler}})}{\sqrt{T_{\text{bubbler}}}} \right) \cdot \overset{\text{kg.mol}^{-1}}{M_{\text{hexane}}}$$

$$0 \leq \alpha_C \approx \alpha_E \leq 1 \quad 10^{-4} \text{ for precursor is possible}$$

Flux of evaporation from heat balance :

$$\overset{\text{W}}{p} = \overset{\text{kg.s}^{-1}}{\phi_{\text{éaporé}}} \cdot \overset{\text{J.kg}^{-1}}{\Delta H_{\text{vap, precursor}}}$$

$$\overset{\text{W}}{p} = S_{\text{exchange}} \cdot h \left( T_{\text{liquid}} - T_{\text{heating box}} \right)$$

The differential equation to solve for heat balance is :

$$V_{liquid} \rho_{precursor} C_p \frac{dT_{bubbler}}{dt} = -\phi_{vaporated} \cdot \Delta H_{vap, precursor} - S_{exchange} \cdot h (T_{liquid} - T_{heating\ box})$$

The differential equation to solve for pressure in buffer bottle :

$$\frac{dP_{bottle+bubbler}}{dt} = \frac{RT_{heating\ box} \phi_{vaporated}}{(V_{bubbler} + V_{buffer\ bottle}) M_{precursor}}$$

The differential equation to solve for pressure in reactor :

$$\frac{dP_{reactor}}{dt} = -\frac{Q_{pump} P_{reactor}}{(V_{buffer\ bottle} + V_{reactor})}$$