DROPLET NUCLEATION IN TURBULENT STEAM JETS

A. Gallegati, F. Battista, P. Gualtieri, C.M. Casciola

Department of Mechanical and Aerospace Engineering

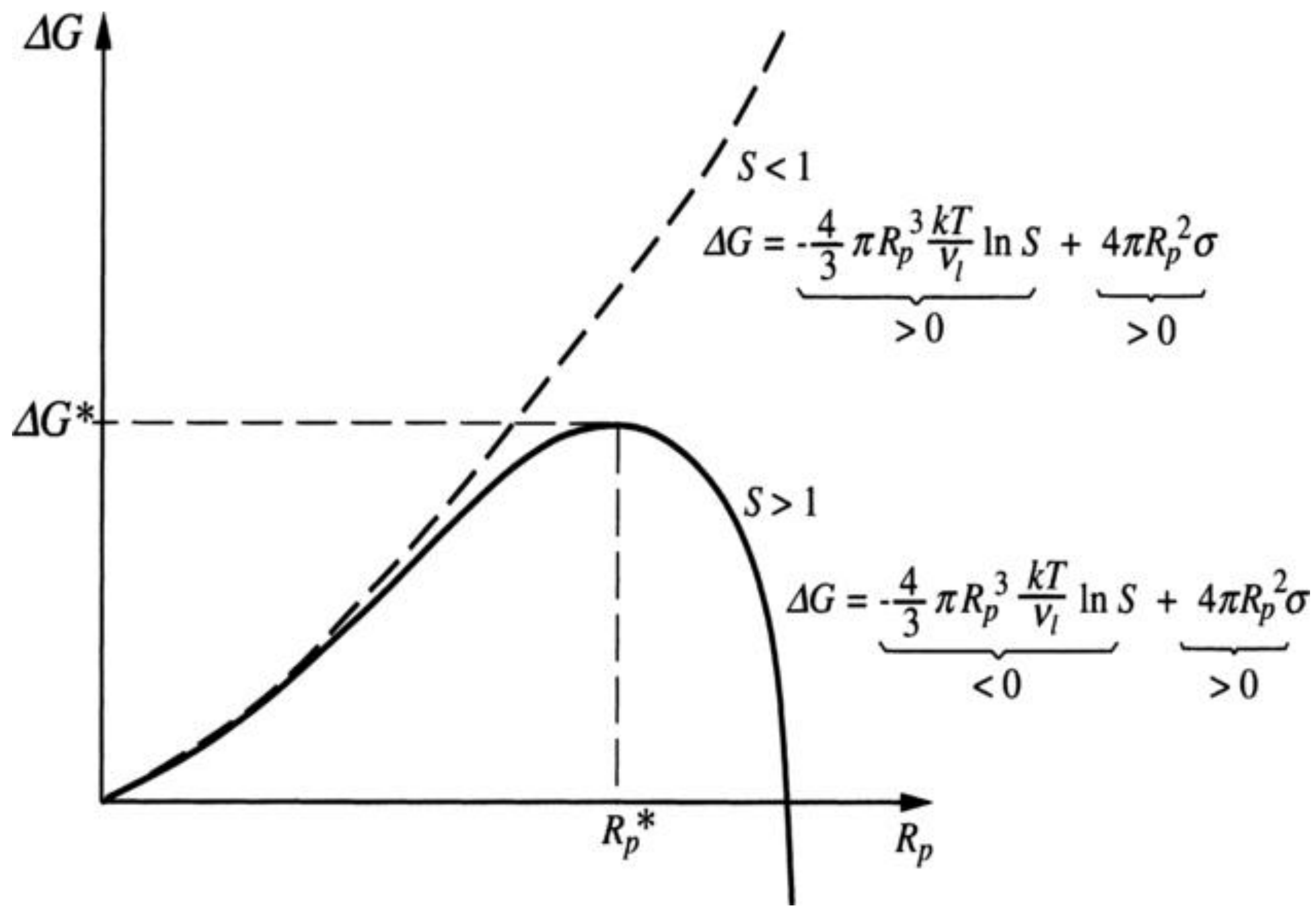
SAPIENZA UNIVERSITÀ DI ROMA

Steam jets & Droplets Nucleation

- Droplets Nucleation
  1) homo/heterogeneous
  2) homo/heteromolecular
- Turbulent flows

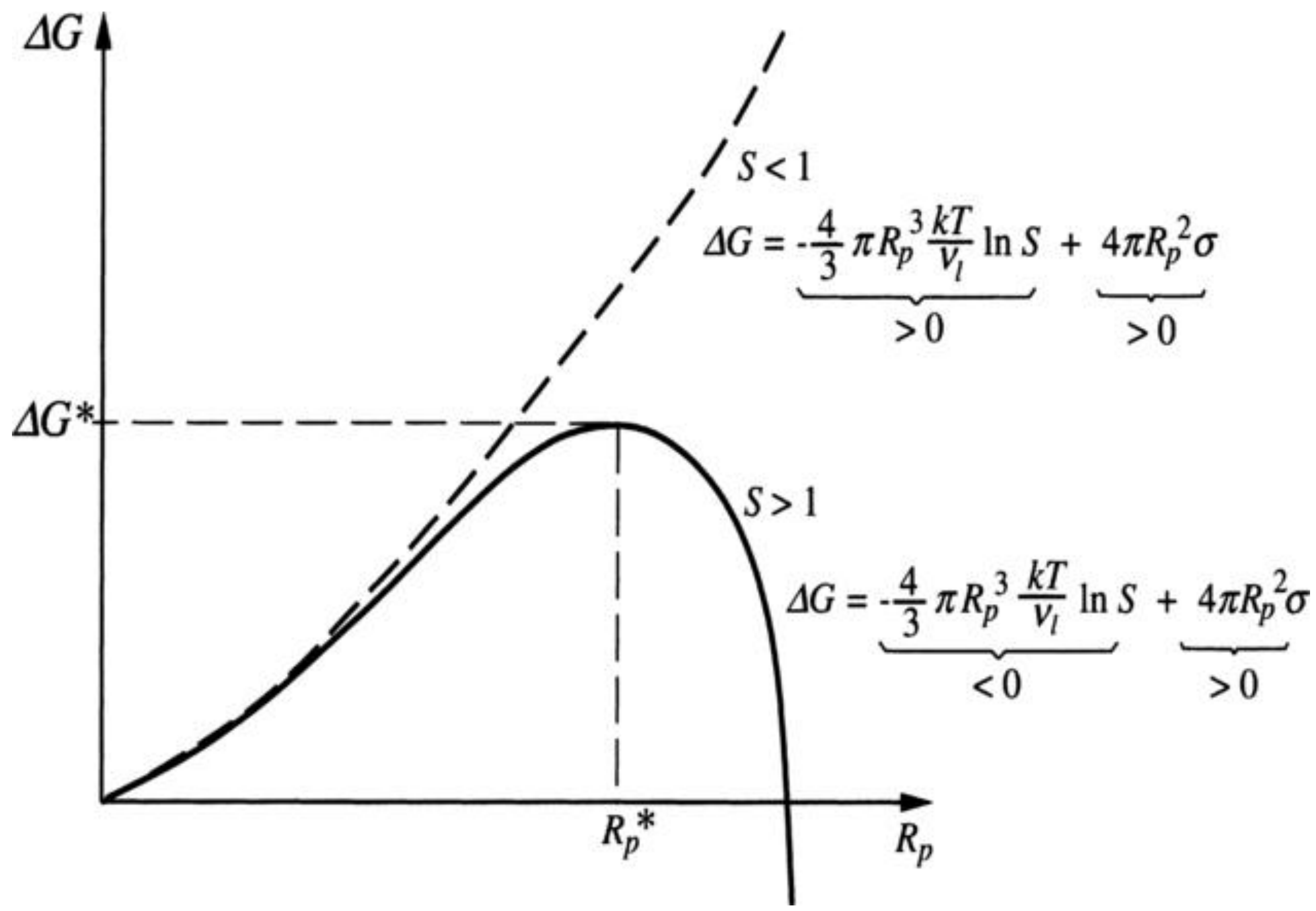
Molecules cluster Free Energy

$$\Delta G\left(r_p\right) = 4\pi r_p^2\,\sigma - \frac{4}{3}\pi r_p^3\,\frac{\rho_p k_B \theta \ln S}{m}\;; \qquad S = \frac{X}{X_s(\theta)}$$



Classical Nucleation Theory rate

$$\frac{\mathrm{d}}{\mathrm{d}r_p}\Big[\Delta G\Big]_{r_p^*} = 0 \quad \Longrightarrow \quad J = \frac{(\rho Y)^2}{\rho_p}\sqrt{\frac{2\sigma}{\pi m^3}}\,\exp\left[-\frac{\Delta G\left(r_p^*\right)}{k_B\theta}\right]$$



Homogeneous droplets nucleation

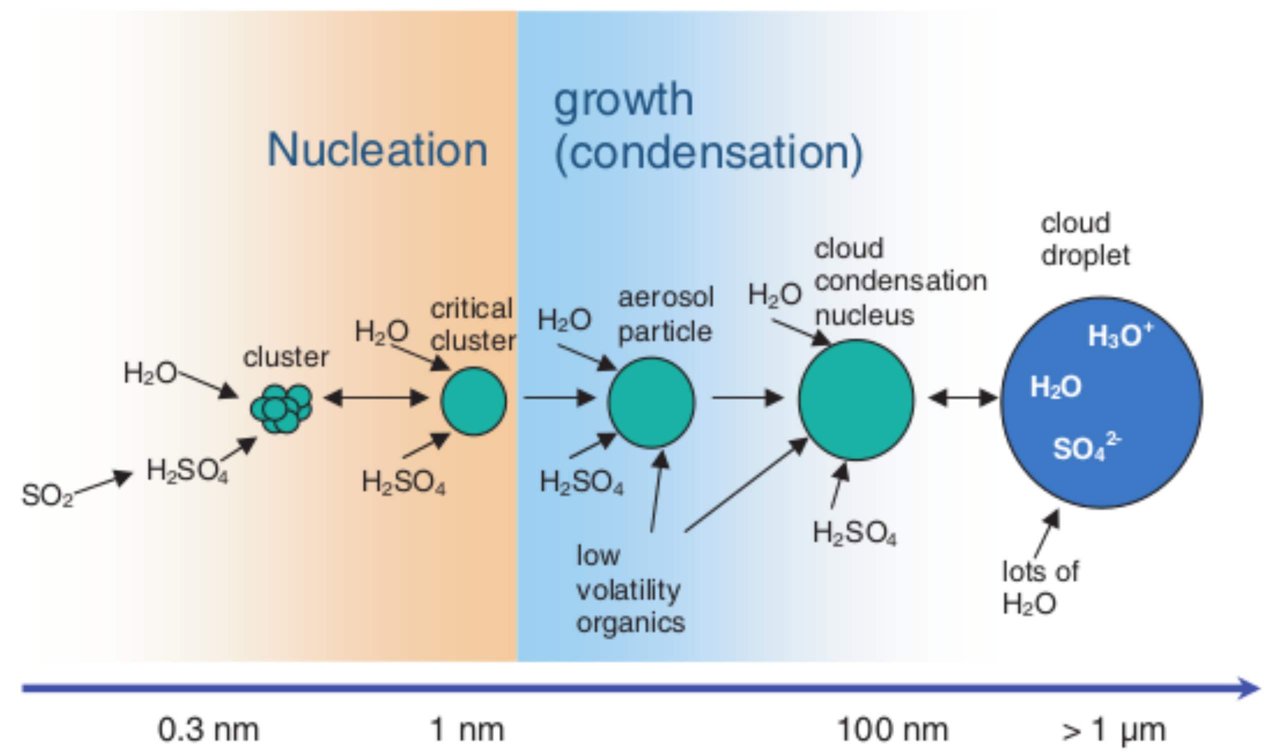
CNT homogeneous rate [Becker, R. & Döring, W. 1935, Ann. Phys.]

$$J(Y,\theta) = \frac{(\rho Y)^2}{\rho_p}\sqrt{\frac{2\sigma}{\pi m^3}}\;\exp\left[-\frac{16\pi}{3}\left(\frac{\sigma}{k_B\theta}\right)^3\left(\frac{m}{\rho_p \ln S}\right)^2\right]$$

$$r_p^* = \frac{2\sigma m}{\rho_p\, k_B \theta\, \ln S}$$

Droplet nucleation - **Poisson process**

(local thermodynamical equilibrium hp.)

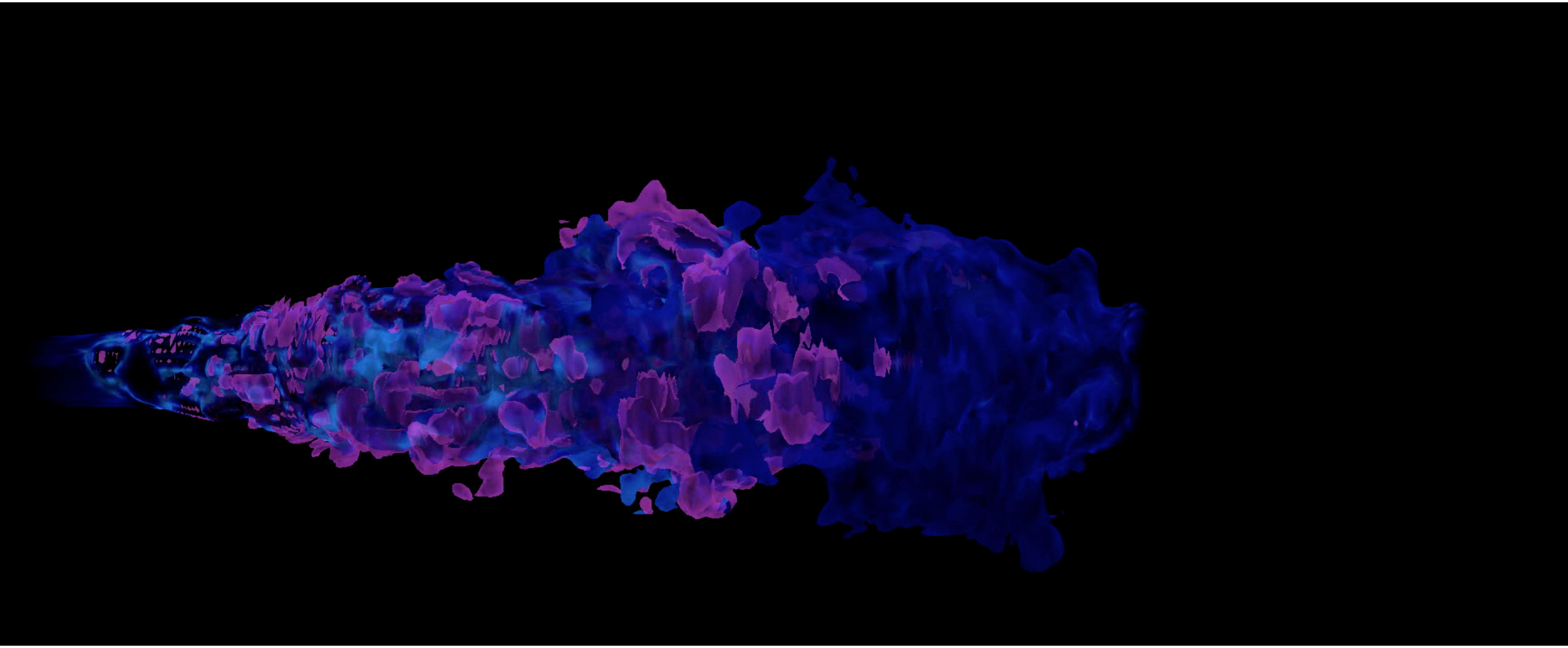


Dibutyl phthalate - DBP

1. **stable** organic compound with **low toxicity**
2. **very low vapour pressure** at ambient temperature
3. USA released 70000 lb in the atmosphere in 1994
   (38 % as **fugitive emissions** - EPA)

- **Experiments** [Lesniewski, T.K. & Friedlander, S.K. 1998, Proc. Royal Soc. A]
- **RANS** [Di Veroli, G.Y. & Rigopoulos, S. 2011, Phys. Fluids]
- **LES** [Pesmazoglou, I., et al. 2014, Chem. Eng. Sci.]
- **DNS** [Fager, A. J. et al. 2012, Phys. Fluids] – **“ a posteriori nucleation ”**
- **What next ?** Complete interphase coupling (mass, momentum and energy)

Droplets nucleation in a turbulent steam jet



$$\theta_{jet} = 413[\mathrm{K}]\,; \quad \theta_{amb} = 299[\mathrm{K}]\,; \quad p_0 = 1[\mathrm{atm}]$$

Navier Stokes complete system

[Okong'o, N.A. & Bellan, J. 2004, J. Fluid Mech.] **low-Mach formulation**

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = -\sum_{p=1}^{N_p} \dot{m}_p g_p(t) \quad \text{where:}\ \ g_p(t) = g_p(\boldsymbol{x} - \boldsymbol{x}_p(t))$$

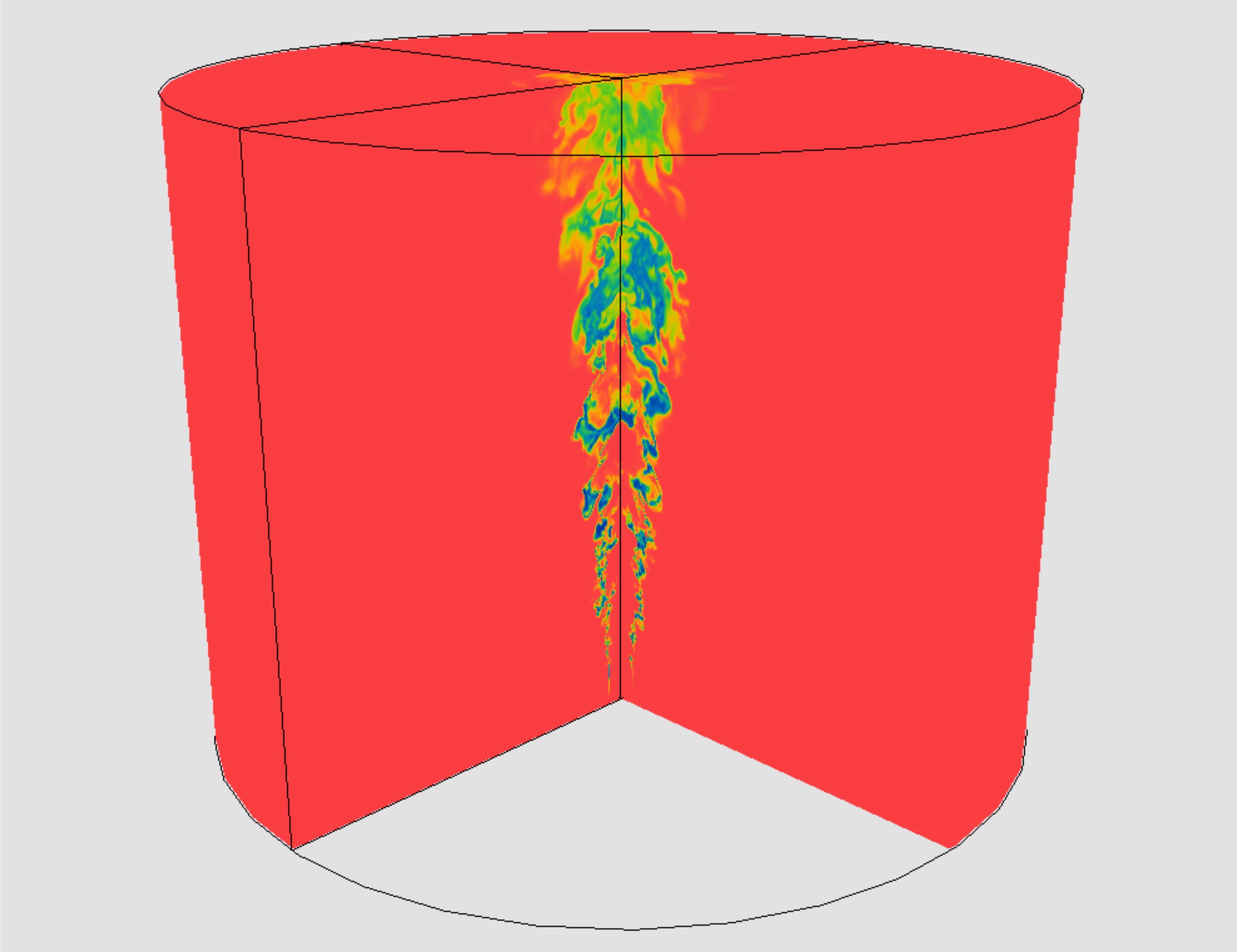
$$\rho \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) = -\frac{1}{\gamma_0} \nabla p + \frac{1}{\mathrm{Re}} \nabla \cdot \boldsymbol{\Sigma} - \sum_{p=1}^{N_p} \left(\boldsymbol{D}_p + \dot{m}_p \boldsymbol{v}_p \right) g_p(t - \epsilon_R)$$

$$\rho c_p \left(\frac{\partial \theta}{\partial t} + \boldsymbol{u} \cdot \nabla \theta \right) = \frac{1}{\mathrm{Re}\,\mathrm{Pr}} \nabla^2 \theta - \frac{(c_p^v - c_p^g)}{\mathrm{Re}\,\mathrm{Sc}} \nabla \cdot (\rho \theta \, \nabla Y) - \sum_{p=1}^{N_p} \left(\dot{Q}_p + \dot{m}_p h_s^v \right) g_p(t - \epsilon_R)$$

$$\rho \left(\frac{\partial Y}{\partial t} + \boldsymbol{u} \cdot \nabla Y \right) = \frac{1}{\mathrm{Re}\,\mathrm{Sc}} \nabla \cdot (\rho \nabla Y) - \sum_{p=1}^{N_p} \dot{m}_p g_p(t - \epsilon_R)$$

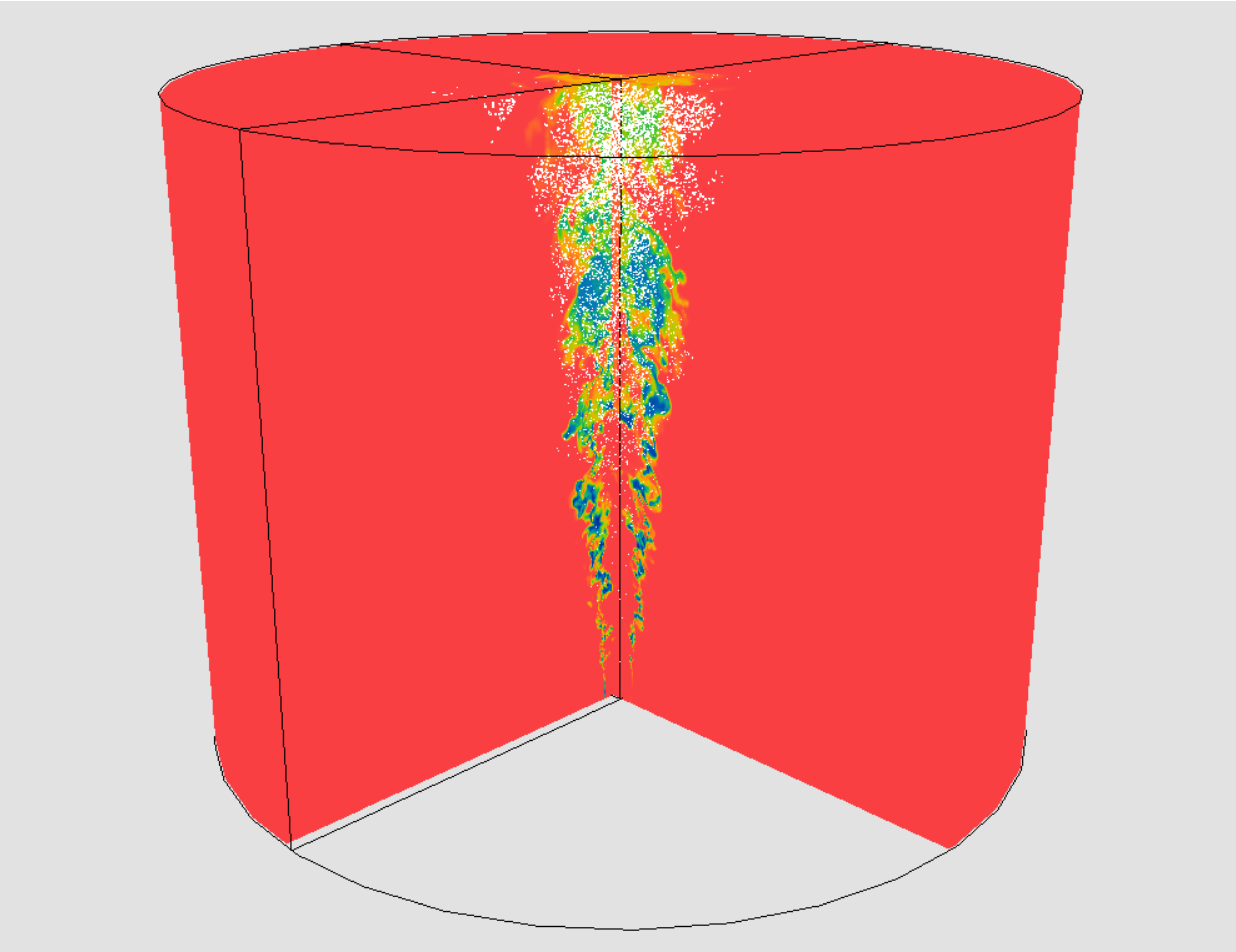
droplets back-reaction regularised according to [Gualtieri, P. et al. 2015, J. Fluid Mech.]

The three-dimensional domain



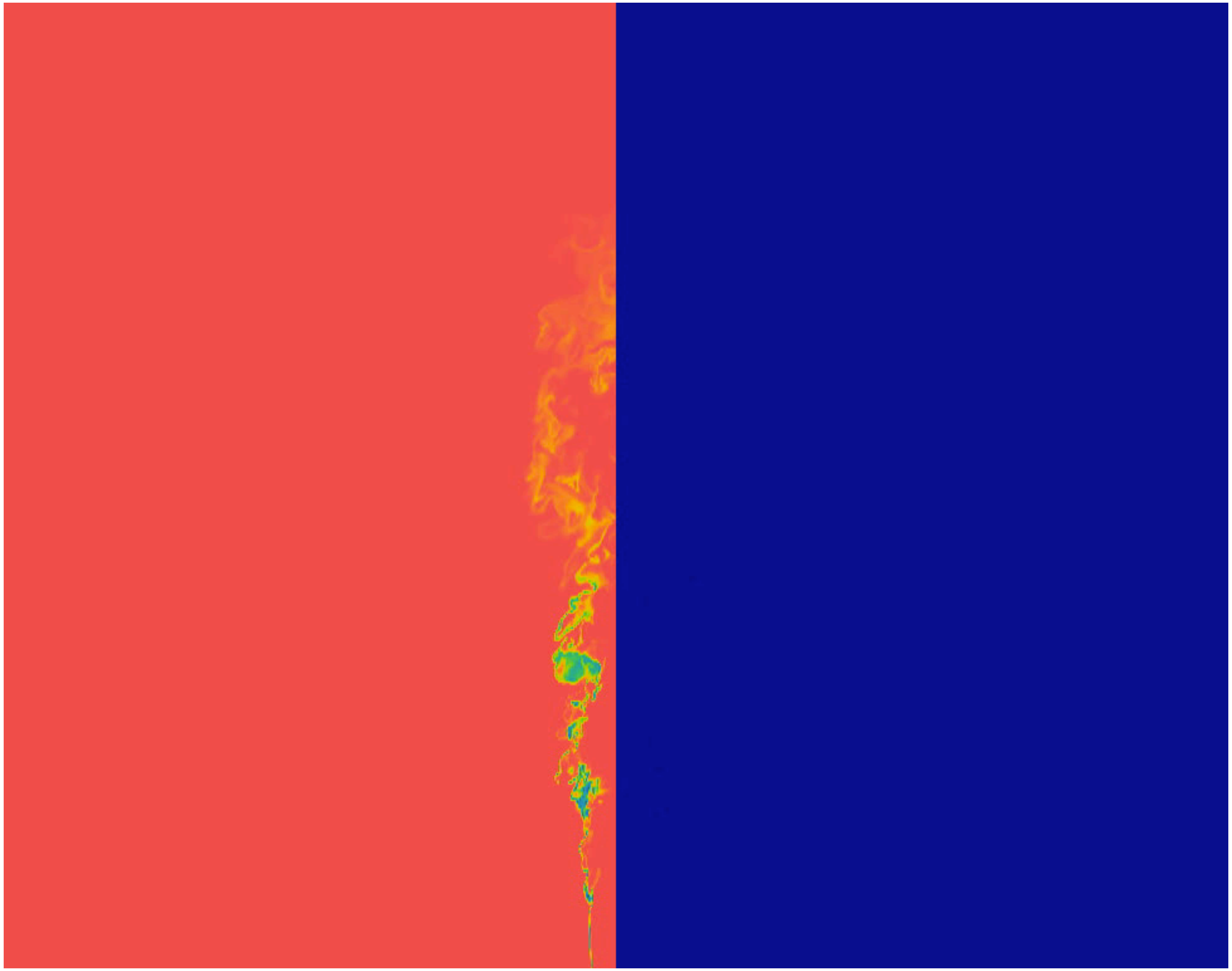
	N_θ	N_r	N_z
Pipe	128	65	128
Jet	128	190	700

Slice of the three-dimensional domain



$$\mathrm{Re} = 3000\,; \quad \text{pipe diameter} = 2.35[\mathrm{mm}]$$

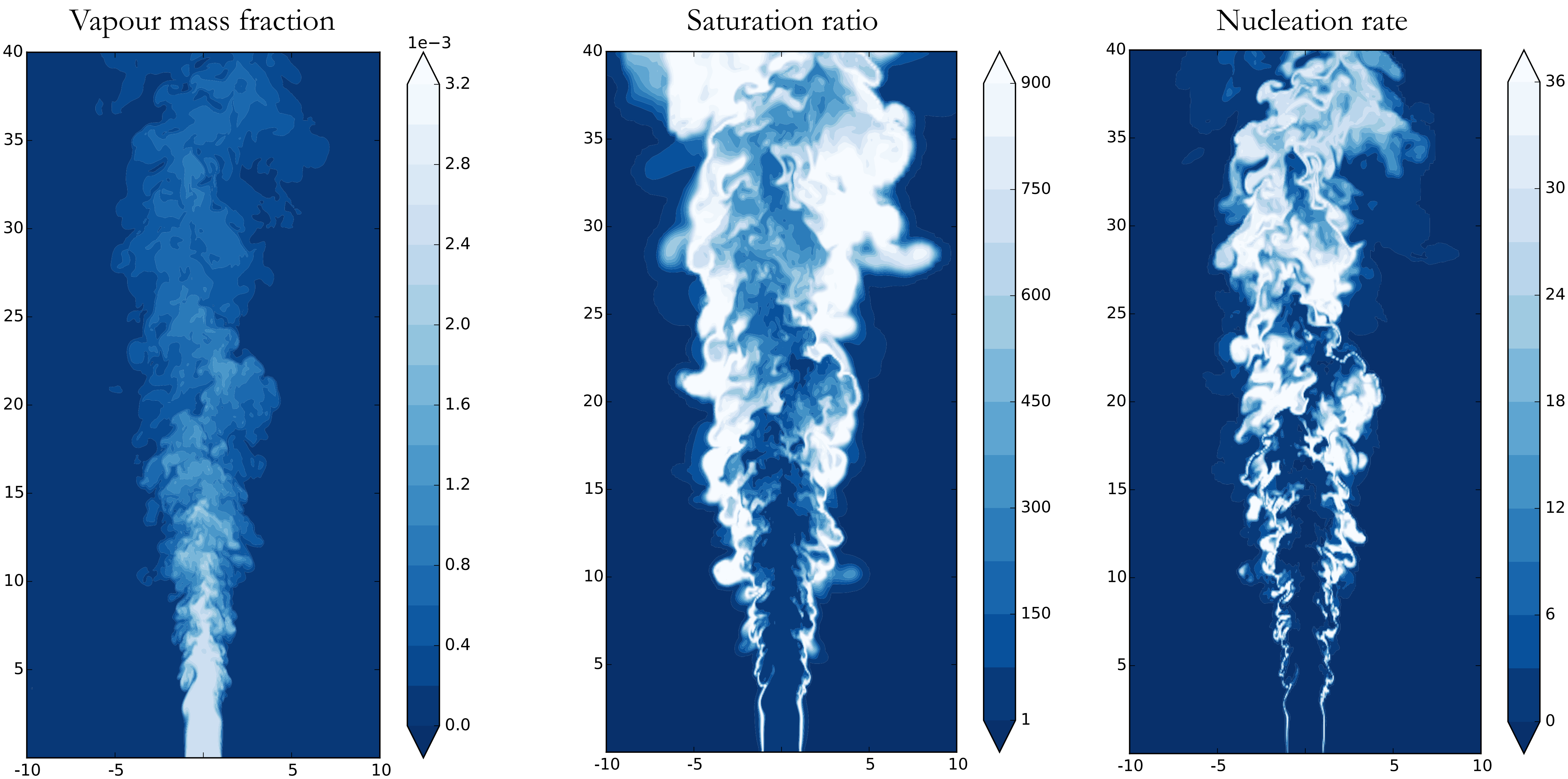
Droplets back-reaction



Nucleation rate
(carrier flow)

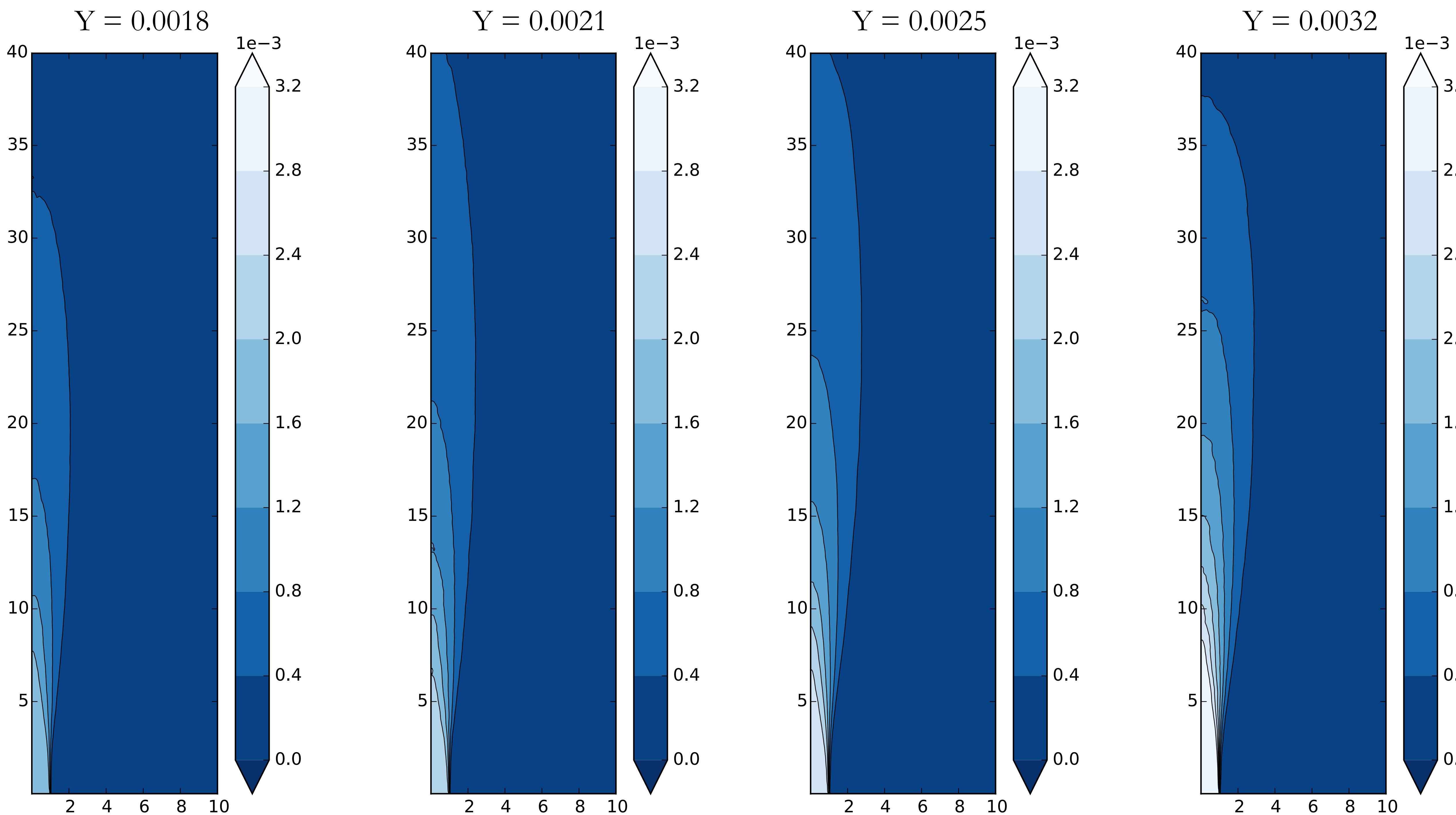
Vapour sink
(droplets feedback)

Turbulent fluctuations & Nucleation rate



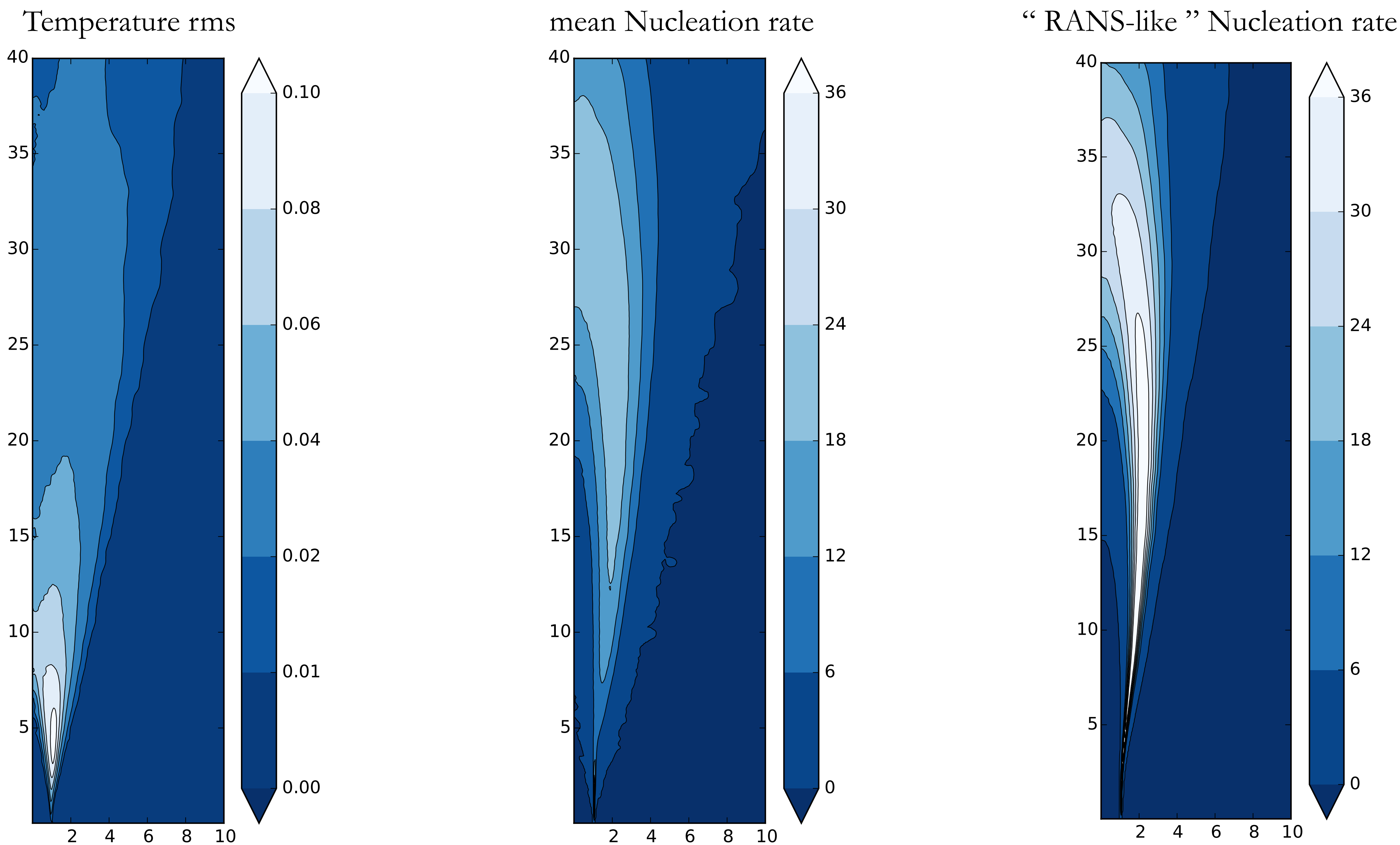
Nucleation rate is **highly intermittent** due to turbulent mixing

Vapour mass fraction injected - mean fields



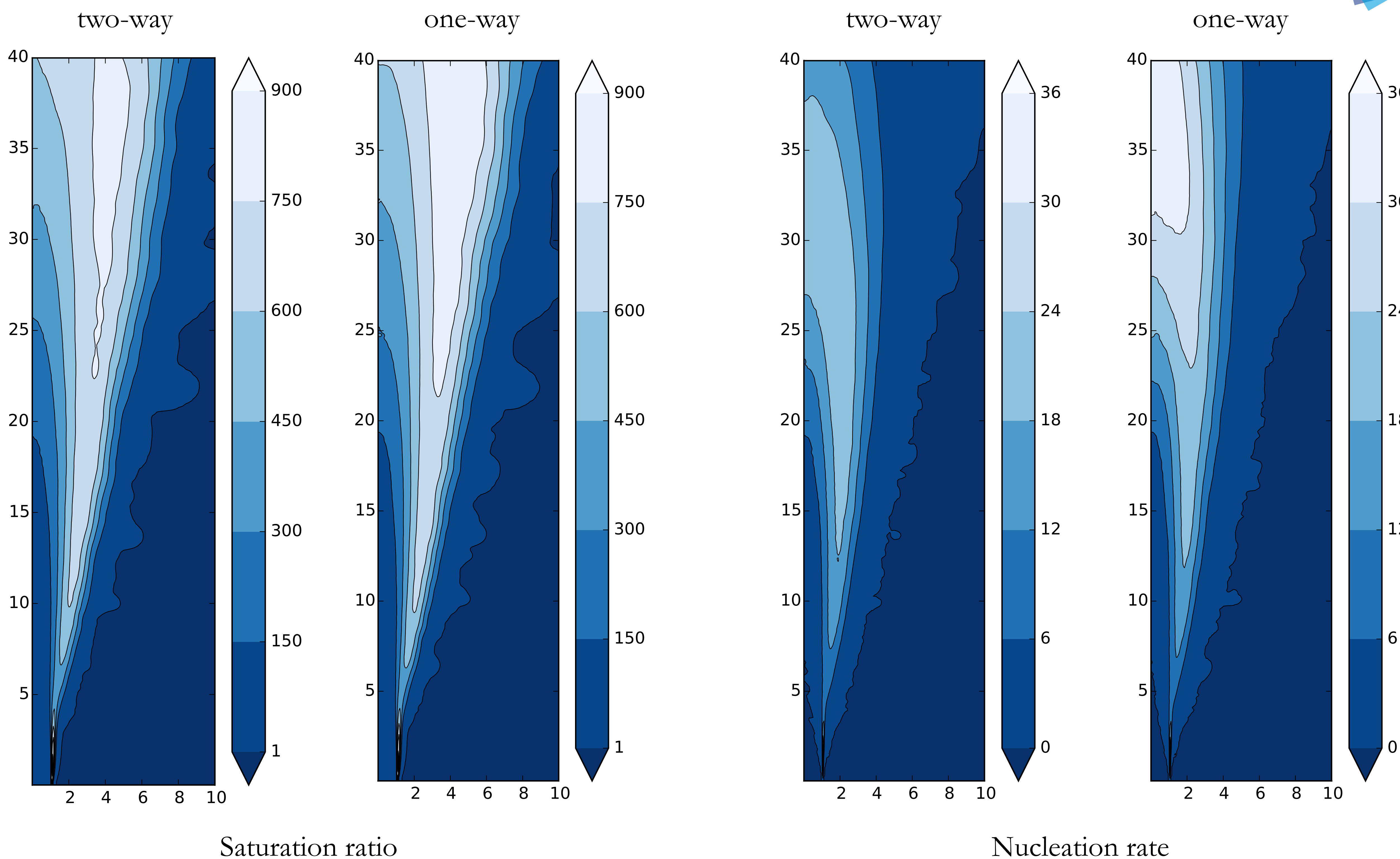
Vapour mass fraction as in Lesniewski & Friedlander 1998, Proc. Royal Soc. A

Turbulent fluctuations & mean Nucleation rate



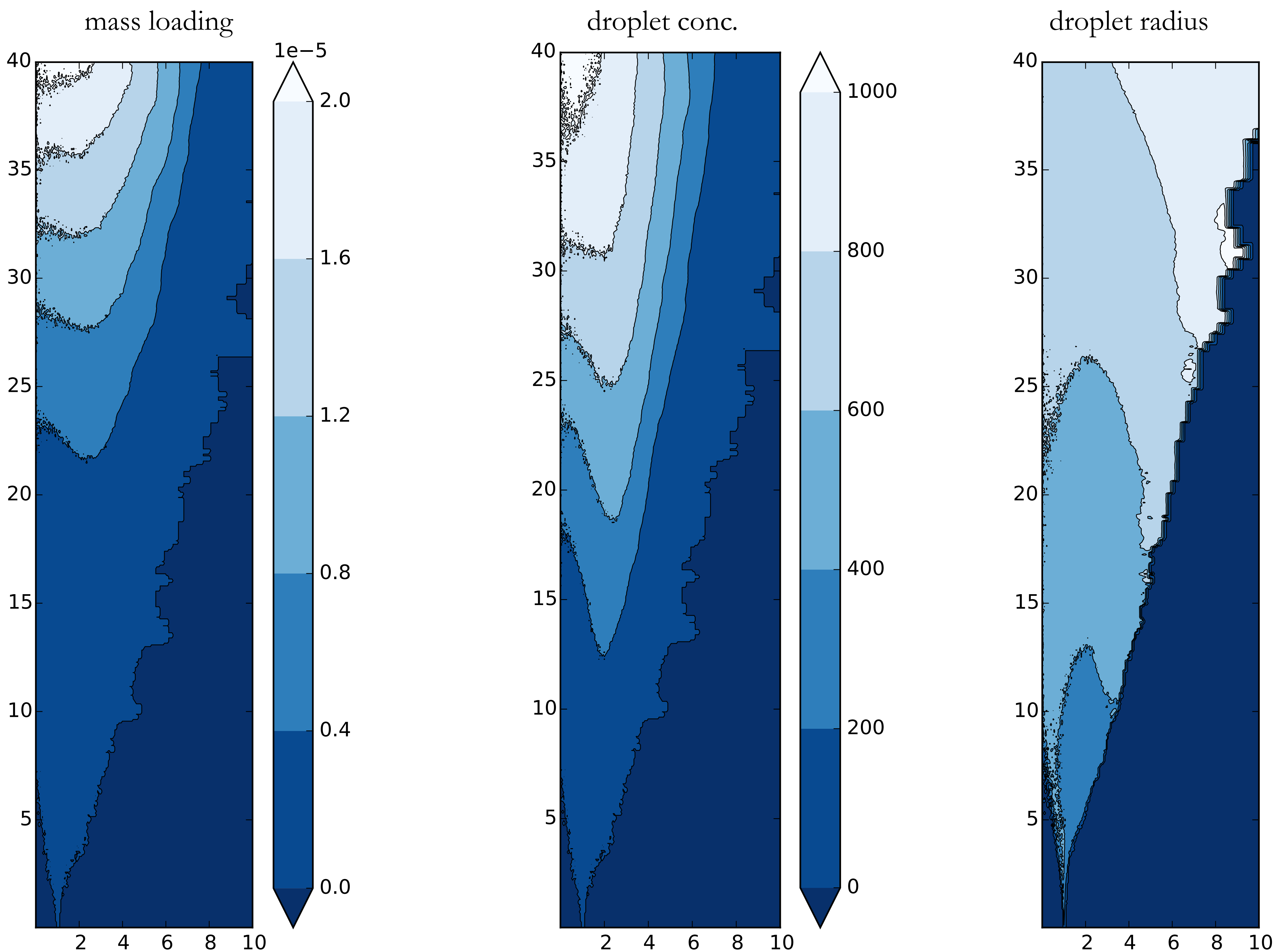
- Nucleation rate **highly non linear** function of local thermodynamic state
- Crucial effect of turbulent fluctuation in determining mean Nucleation process

Two-way coupling effects on Nucleation rate

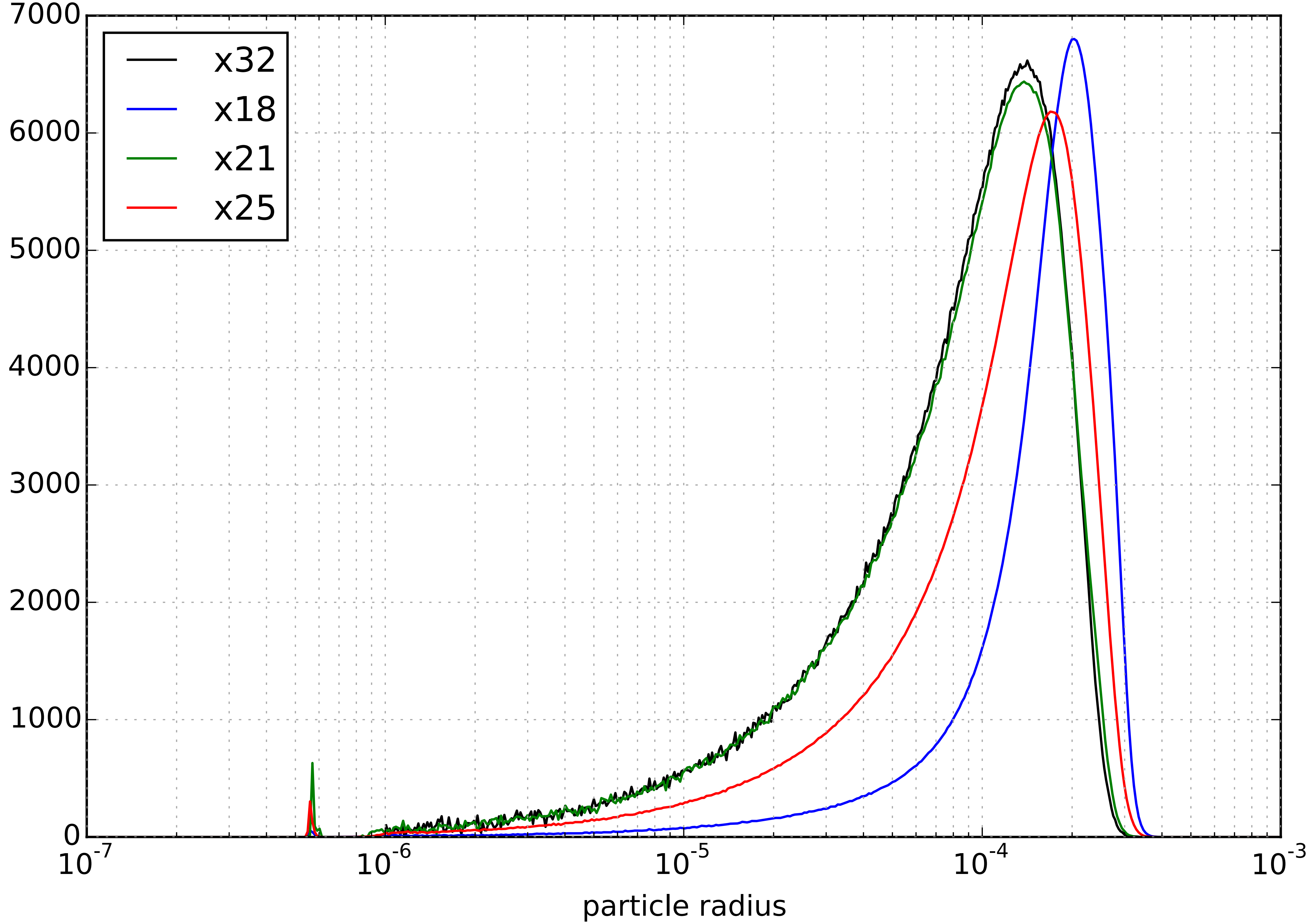


Particles feedback affects the Saturation ratio & the consequent Nucleation rate

Mass load - droplets mean size & concentration



Droplets size distribution



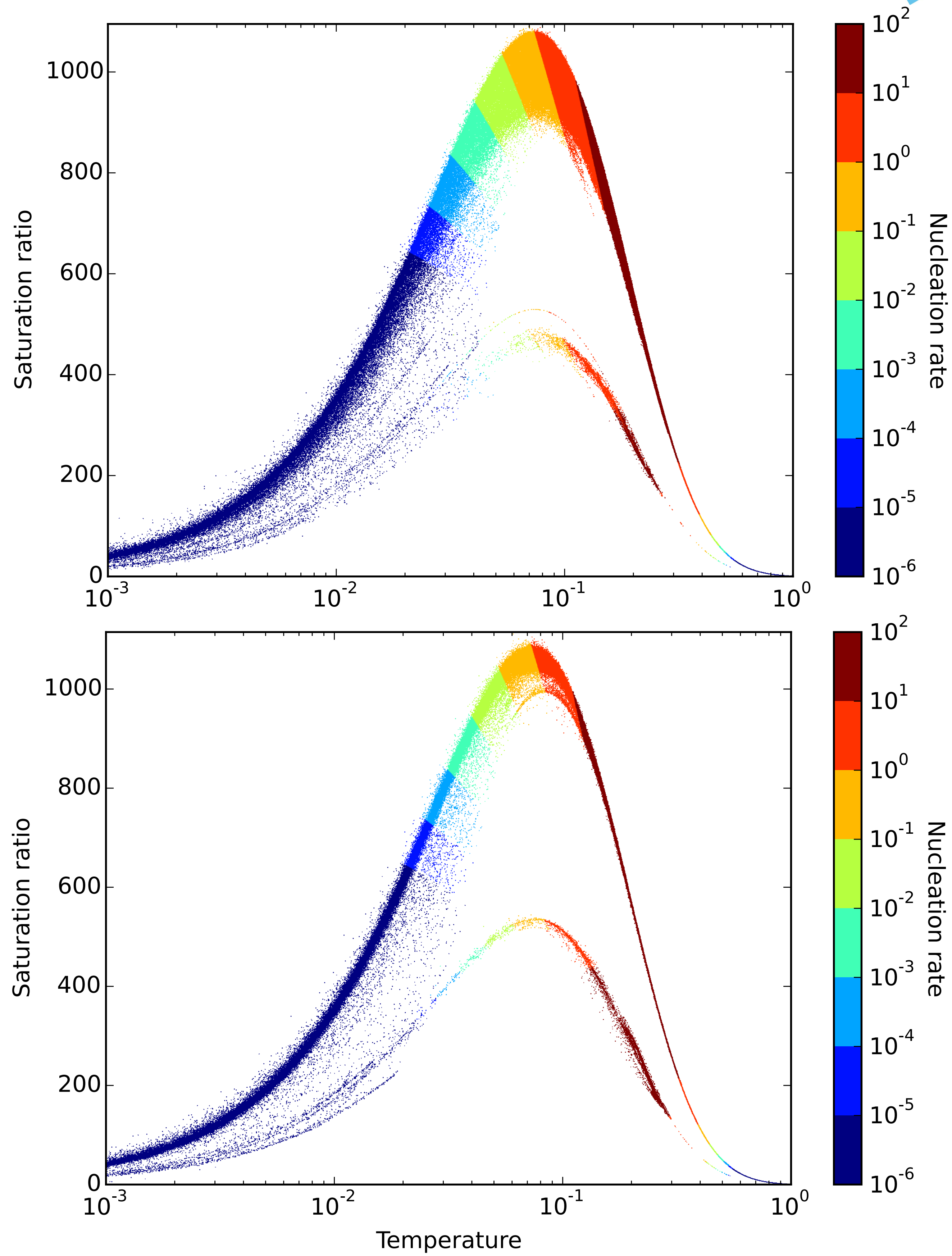
Conclusions & next steps

<u>Crucial for Nucleation process</u>

✓ Relevance of turbulent fluctuations

✓ Relevance two-way coupling

- looking for correlations
- simulating longer domain
- evaluating the effects of :
  1) Nucleation
  2) Condensation
  3) Mixing
- enhancing mass transfer model



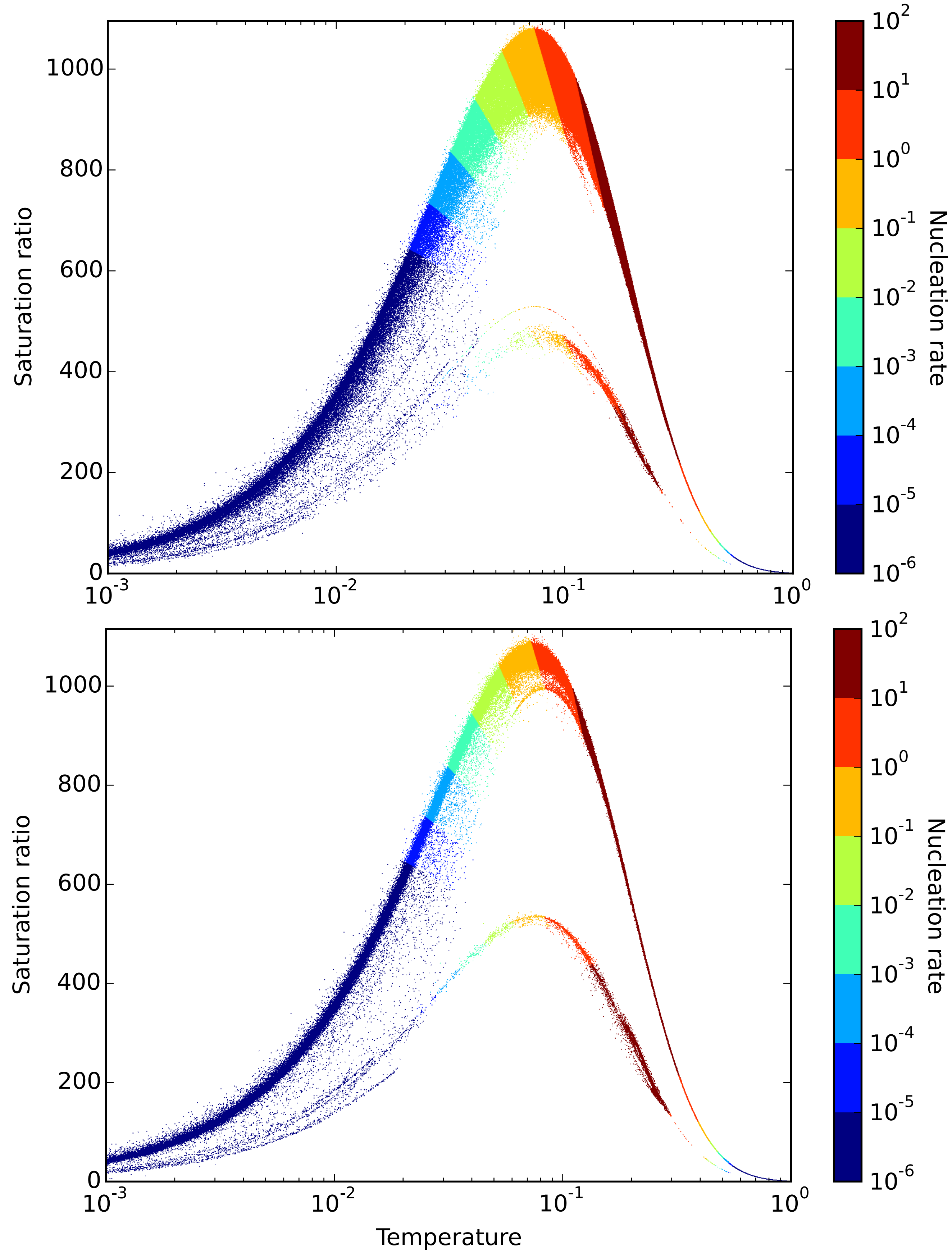
Conclusions & next steps

Crucial for Nucleation process

✓ Relevance of turbulent fluctuations

✓ Relevance two-way coupling

- looking for correlations
- simulating longer domain
- evaluating the effects of :
  1) Nucleation
  2) Condensation
  3) Mixing
- enhancing mass transfer model



Droplets dynamics & Source terms

$$\frac{dr_p}{dt} = \frac{1}{4\pi r_p^2(t)\rho_p}\dot{m}_p$$

$$\dot{m}_p = 2\pi r_p(t)\frac{\mathrm{Sh}}{\mathrm{Re\,Sc}}(\tilde{Y} - Y_{eq}^s)$$

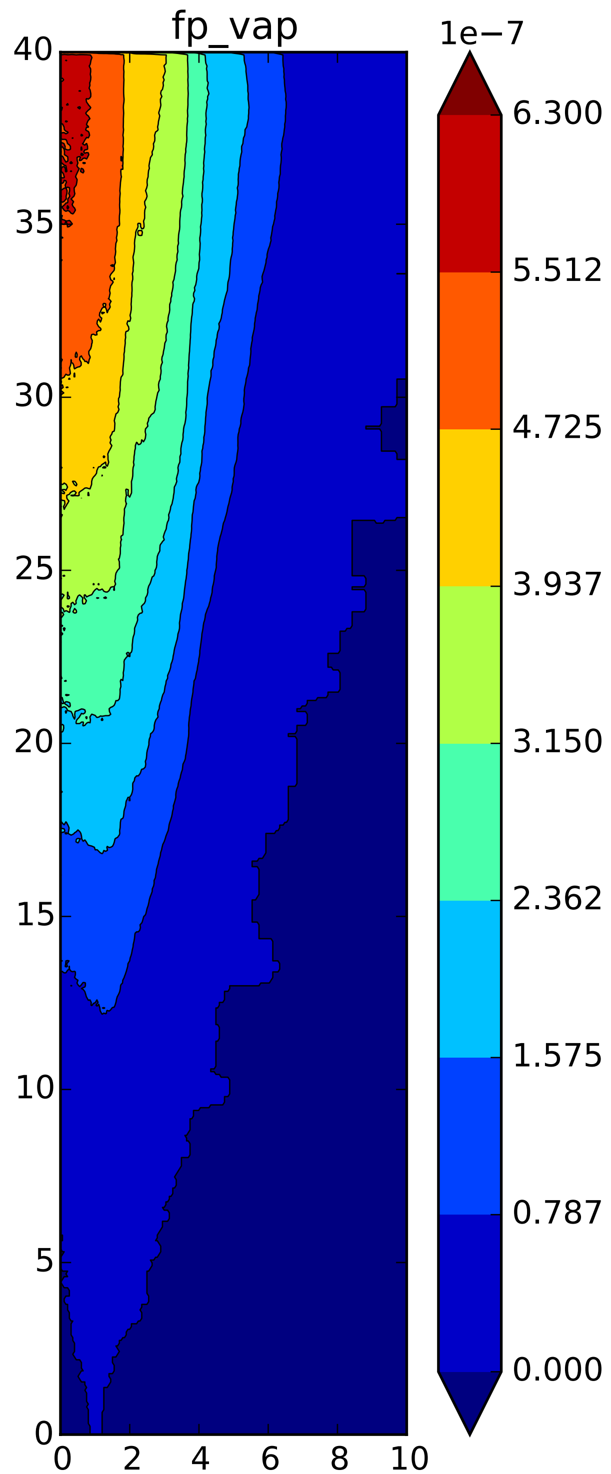
$$\frac{d\boldsymbol{v}_p}{dt} = \frac{1}{m_p}\mathbf{D}_p(t)$$

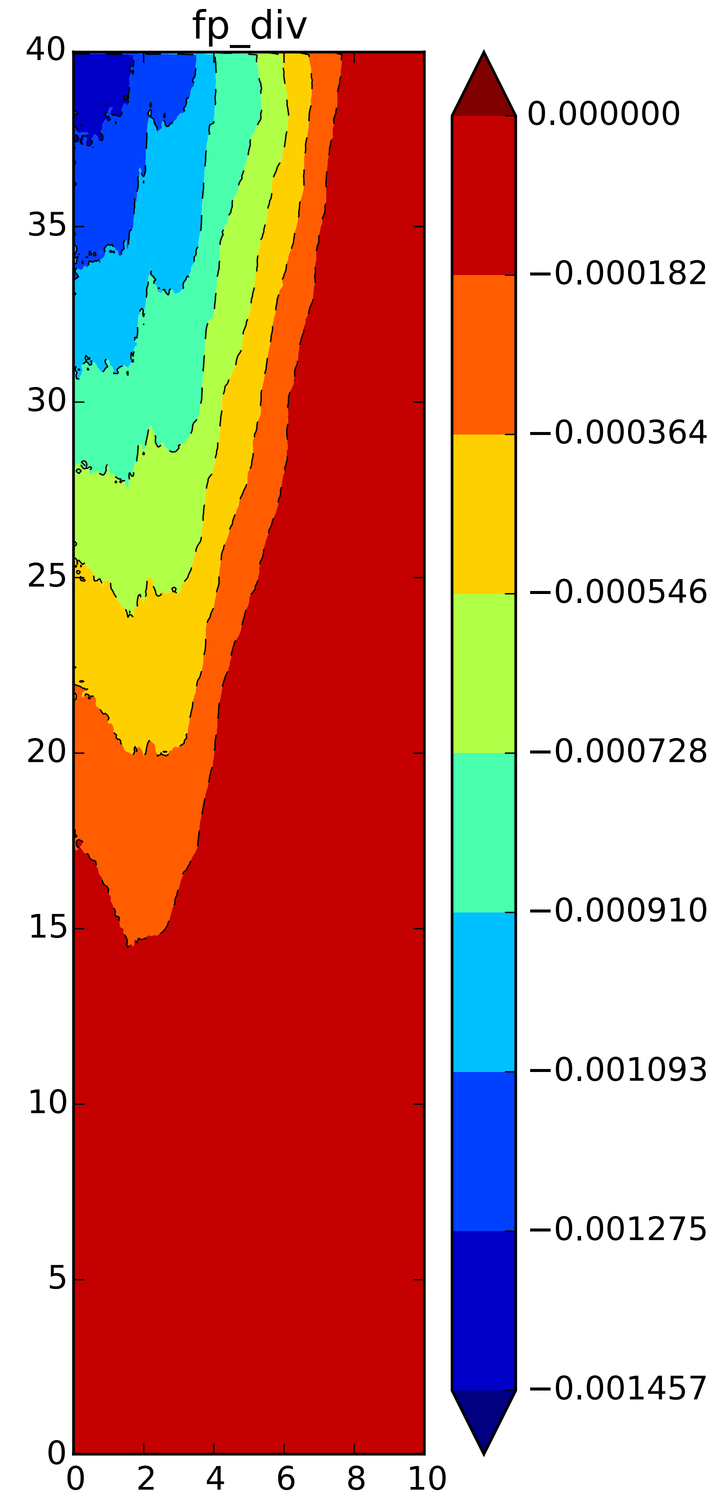
$$\boldsymbol{D}_p = 6\pi r_p(t)\frac{1}{Re}(\tilde{\boldsymbol{u}} - \boldsymbol{v}_p)$$

$$\frac{d\theta_p}{dt} = \frac{1}{m_p c_l}\left(\dot{Q}_p + \dot{m}_p L_v\right)$$

$$\dot{Q}_p = 2\pi r_p(t)\frac{Nu}{RePr}(\tilde{\theta} - \theta_p)$$

Droplets back-reaction





ERPP method - a simplified example

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta - \frac{k_f}{\rho_f} \nabla^2 \theta = 0$$

$$\theta|_{\partial \Omega_p(t)} = \theta_p(\mathbf{x})|_{\partial \Omega_p(t)}$$

$$\theta(\mathbf{x}, 0) = \theta_0(\mathbf{x})$$

$$\begin{cases} \dfrac{\partial \overline{\theta}}{\partial t} + F(\theta) - \dfrac{k_f}{\rho_f} \nabla^2 \overline{\theta} = 0 \\ \\ \overline{\theta}(\mathbf{x}, 0) = \overline{\theta}_0(\mathbf{x}) \end{cases}$$

$$\begin{cases} \dfrac{\partial \tilde{\theta}}{\partial t} - \dfrac{k_f}{\rho_f} \nabla^2 \tilde{\theta} = 0 \qquad \Longrightarrow \quad \mathcal{L}\tilde{\theta} = 0 \\ \\ \tilde{\theta}|_{\partial \Omega_p(t)} = \theta_p(\mathbf{x})|_{\partial \Omega_p(t)} - \overline{\theta}|_{\partial \Omega_p(t)} \\ \tilde{\theta}(\mathbf{x}, 0) = 0 \end{cases}$$

Temperature field decomposition – background & disturbance

Green's theorem – Boundary integral representation

Adjoint operator [Stakgold, 1987]:

$$\begin{cases} \mathcal{L}\tilde{\theta} = 0 \\ \mathcal{L}^+ g^+ = \delta(\xi - \mathbf{x})\delta(\tau - t) \end{cases}$$

$$g(\mathbf{x} - \xi, t - \tau) = g^+(\xi - \mathbf{x}, \tau - t)$$

Reciprocity Thm. [Lanczos, 1961]:

$$\tilde{\theta}(\mathbf{x}, t) = < \tilde{\theta}, \mathcal{L}^+ g^+ > - < g^+, \mathcal{L}\tilde{\theta} > =$$

$$= \int_0^t \mathrm{d}\tau \oint_{\partial\Omega_p(\tau)} \mathrm{d}\xi^2 \left[g^+ \frac{k_f}{\rho_f} \nabla\tilde{\theta}(\xi, \tau) - \tilde{\theta}(\xi, \tau) \frac{k_f}{\rho_f} \nabla g^+ \right] \cdot \hat{\mathbf{n}} \simeq$$

$$\simeq \int_0^t g(\mathbf{x} - \mathbf{x_p}, t - \tau) \dot{Q}_p(\tau) \mathrm{d}t$$

$$\frac{\partial\tilde{\theta}}{\partial t} - \frac{k_f}{\rho_f} \nabla^2 \tilde{\theta} = \int_0^t \dot{Q}_p(\tau) \left[\frac{\partial g}{\partial t} - \frac{k_f}{\rho_f} \nabla^2 g \right] \mathrm{d}t = \dot{Q}_p(t) \delta(\mathbf{x} - \mathbf{x_p})$$