Modeling bubble nucleation and growth by pore network model
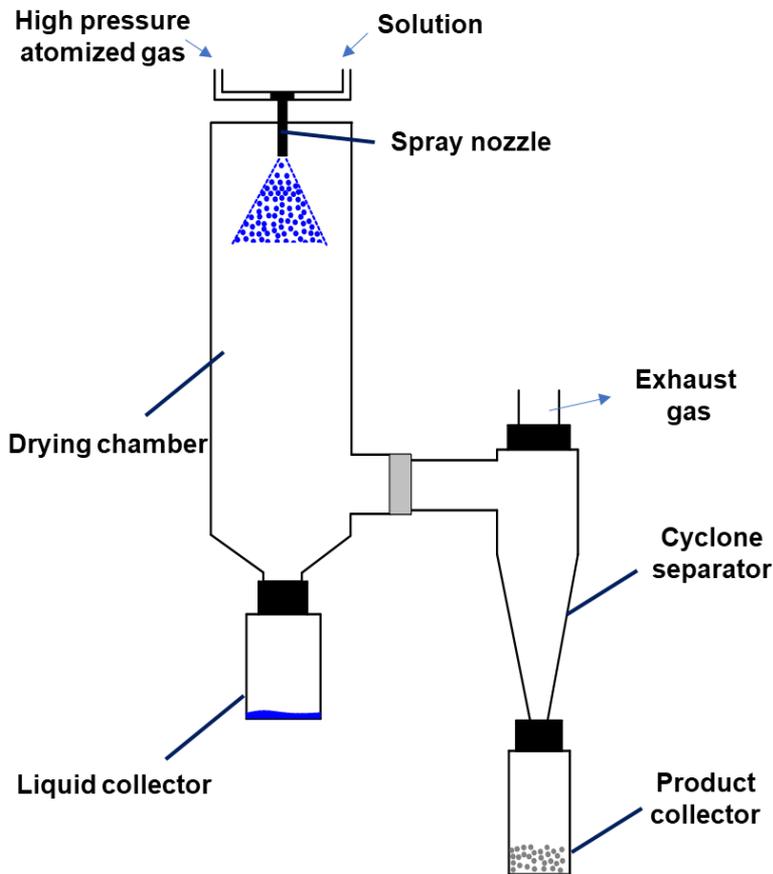
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IFPRI Annual General Meeting, June 15-19, 2024, Toronto
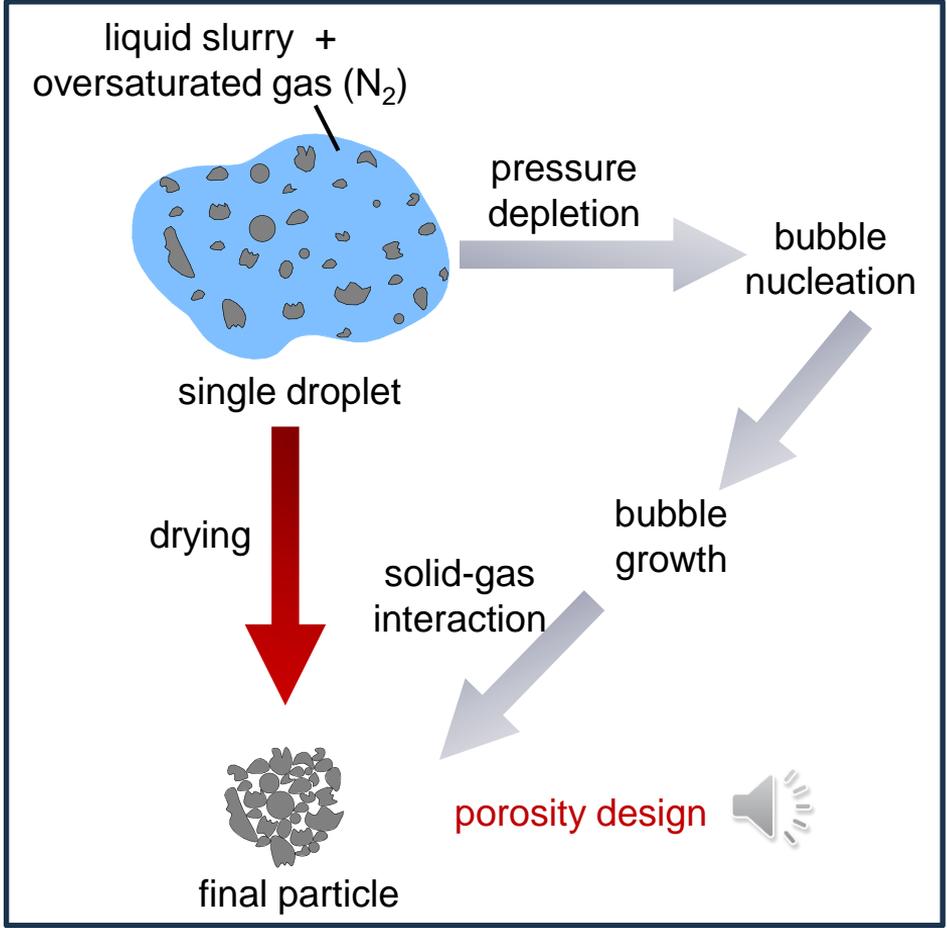
Thermal Process Engineering, Otto von Guericke University Magdeburg

Research motivation

Foam spray drying

High pressure atomized gas

Solution

Spray nozzle

Drying chamber

Exhaust gas

Cyclone separator

Liquid collector

Product collector

liquid slurry + oversaturated gas (N_2)

single droplet

pressure depletion

bubble nucleation

bubble growth

solid-gas interaction

drying

final particle

porosity design

Our tasks in the project

☐ Deliver high-resolution single droplet model of foam spray drying using **pore network model**

- bubble nucleation and growth

- diffusion of gas molecules in the liquid phase and their transport from liquid into bubbles

- couple bubble nucleation and growth with the drying process

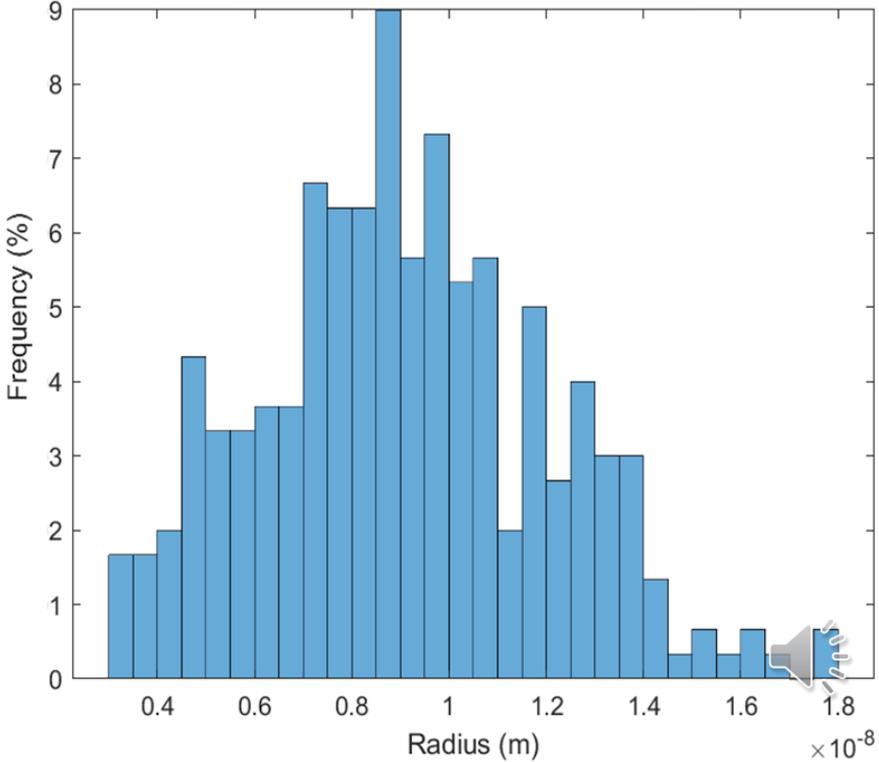- consider the gas-solid interaction leading to the structural changes
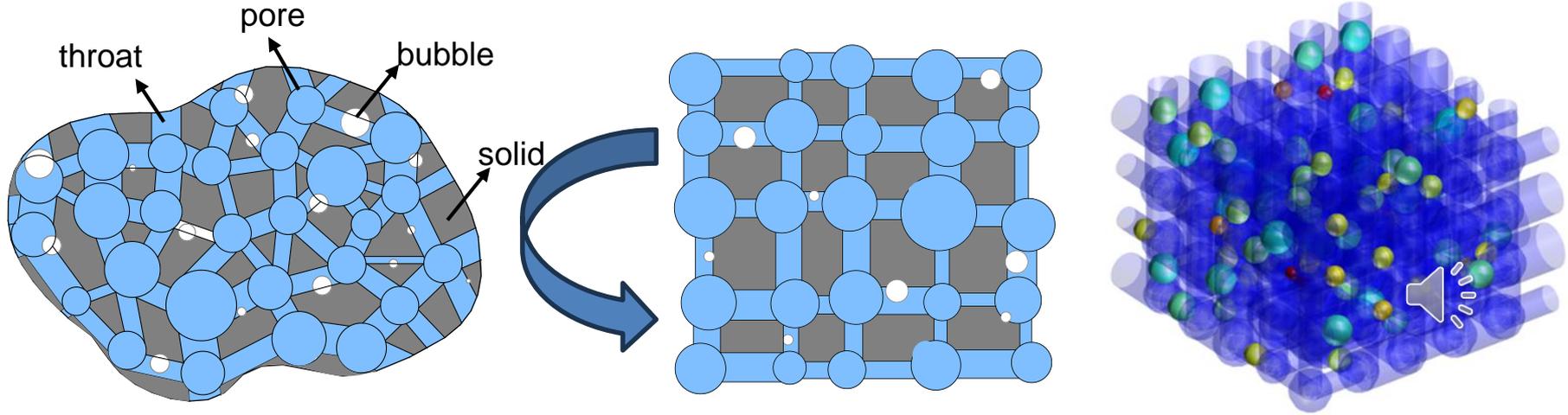
Heterogenous nucleation

❑ Steady-state condition maintained at high pressure, e.g., 200 bar
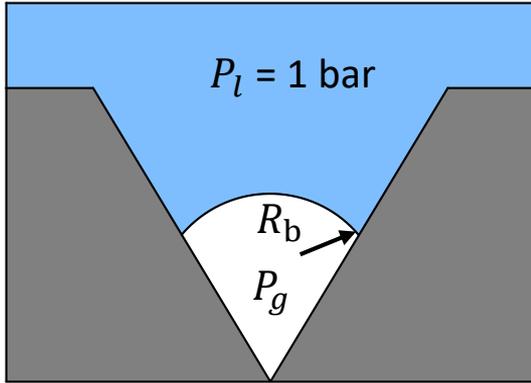
P_l = 200 bar

R_c

P_g
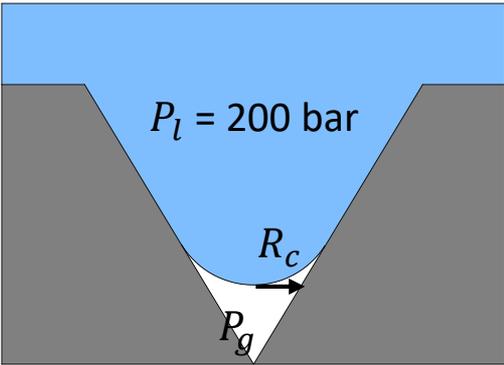
bubble nucleation sites exist at the nano-size crevices

balance equation: $P_g = P_l - P_c$

Heterogenous nucleation

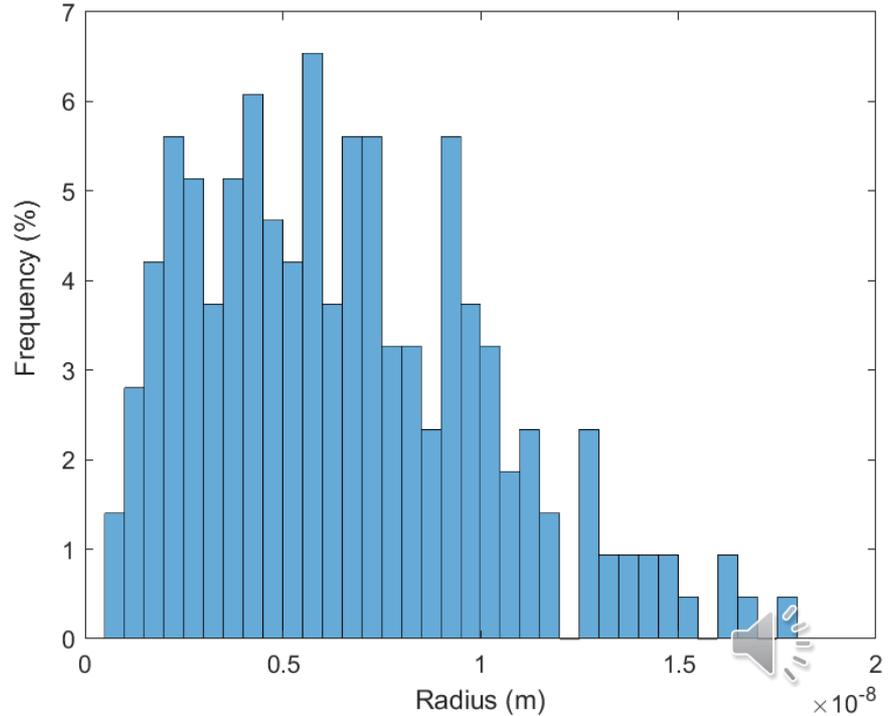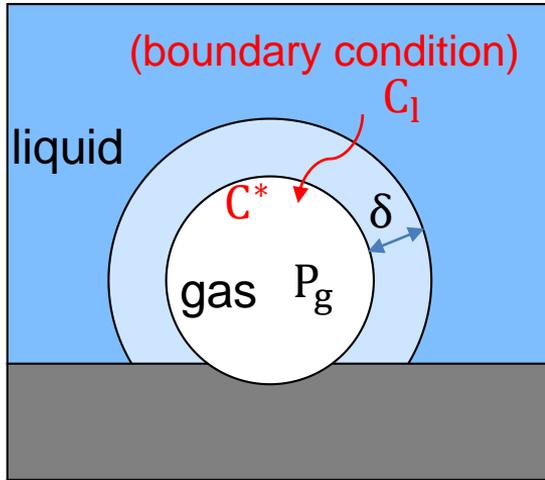❑ Pressure depletion, e.g., from 200 bar to 1 bar: bubble nucleation

bubble radius in nucleation

P_l = 1 bar

R_b

P_g

balance equation: $\quad P_g = P_l + P_c$

some bubble sites could not be activated since the balance equation cannot be satisfied.

Bubble growth: diffusion process

(boundary condition)
C_l

liquid

C^*

δ

gas P_g

A: surface area of bubble
sh: Sherwood number
D: liquid phase diffusivity of gas
δ: thickness of the boundary layer
C_l: bulk concentration
C^*: interface concentration
H: Henry's law solubility constant

Update bubble size/gas concentration

$$P_g V = nRT, \; P_g = P_l + \frac{2\sigma}{R_b}$$
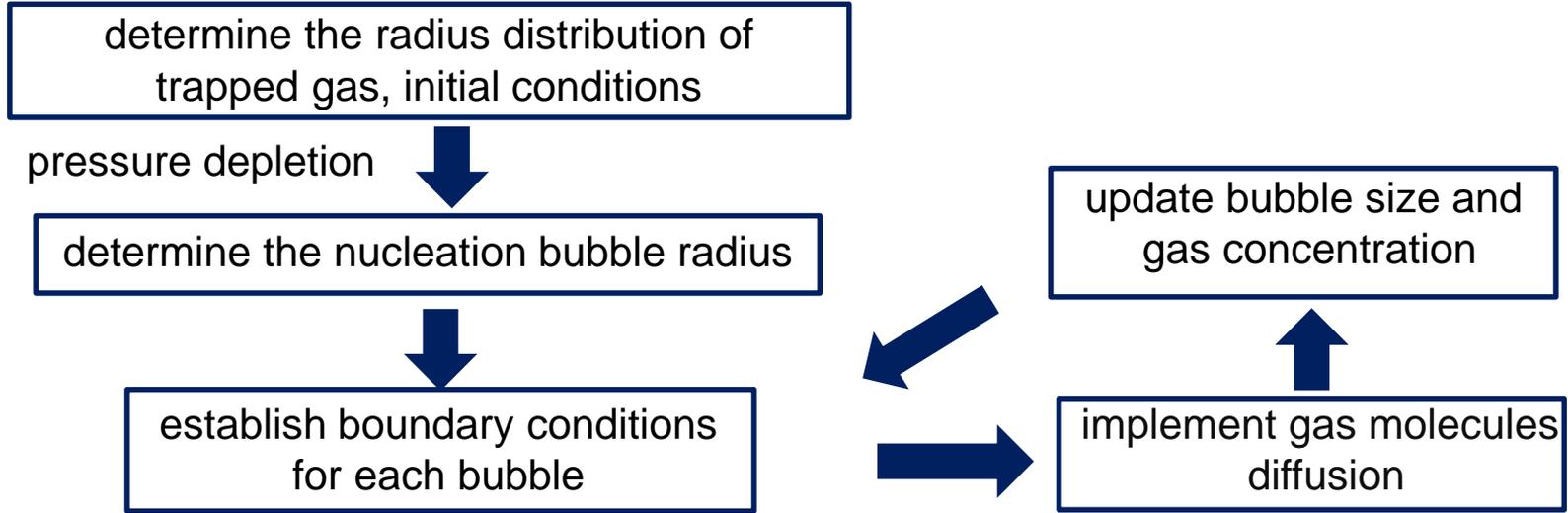
diffusion process of the gas molecular:

$$\frac{dn}{dt} = \frac{A \cdot D \cdot (C_l - C^*)}{\delta} = \frac{A \cdot \text{sh} \cdot D \cdot (C_l - C^*)}{2R_b}, \quad C^* = \frac{P_g}{H}$$

If $C^* > C_l$ bubble size shrinking   If $C^* < C_l$ bubble size growing

Bubble nucleation and growth algorithm

determine the radius distribution of trapped gas, initial conditions

pressure depletion

determine the nucleation bubble radius

establish boundary conditions for each bubble

implement gas molecules diffusion

update bubble size and gas concentration
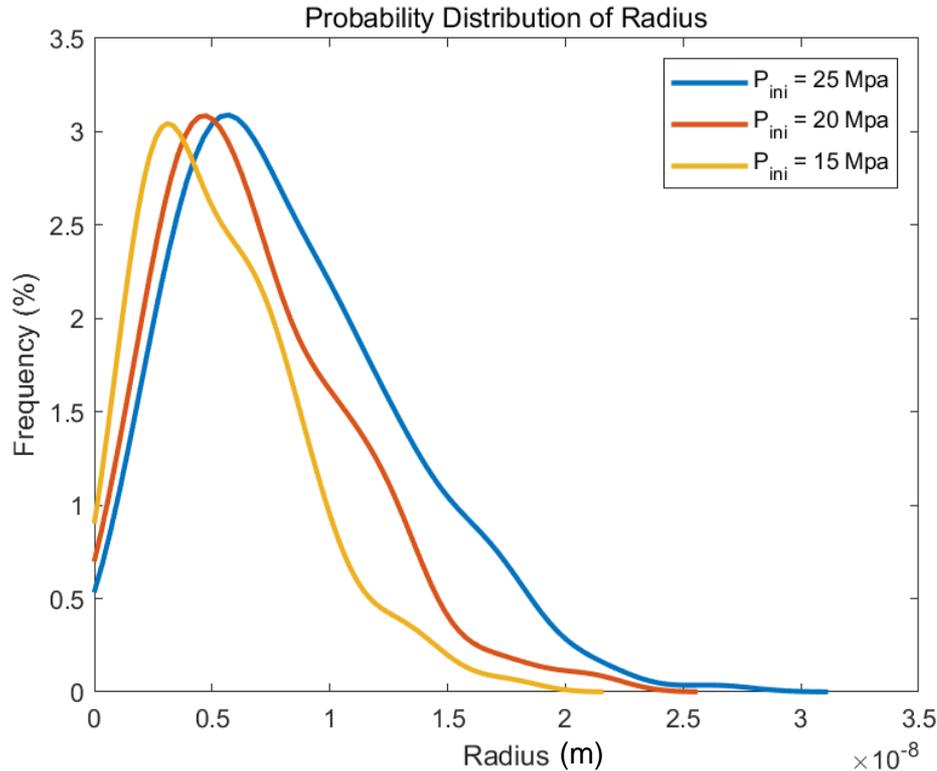
Initial liquid pressure (MPa)	Initial concentration C (mol/m^3)	Ultimate liquid pressure (MPa)	Diffusion coefficient D (m^2/s)
20	100	0.1	2×10^{-9}

Bubble size and gas pressure evolution

Pg (MPa)

0.1   0.105   0.11   0.115   0.12   0.125

0.1 ms

9.9 ms

liquid pressure drops from
20 MPa to 0.1 MPa
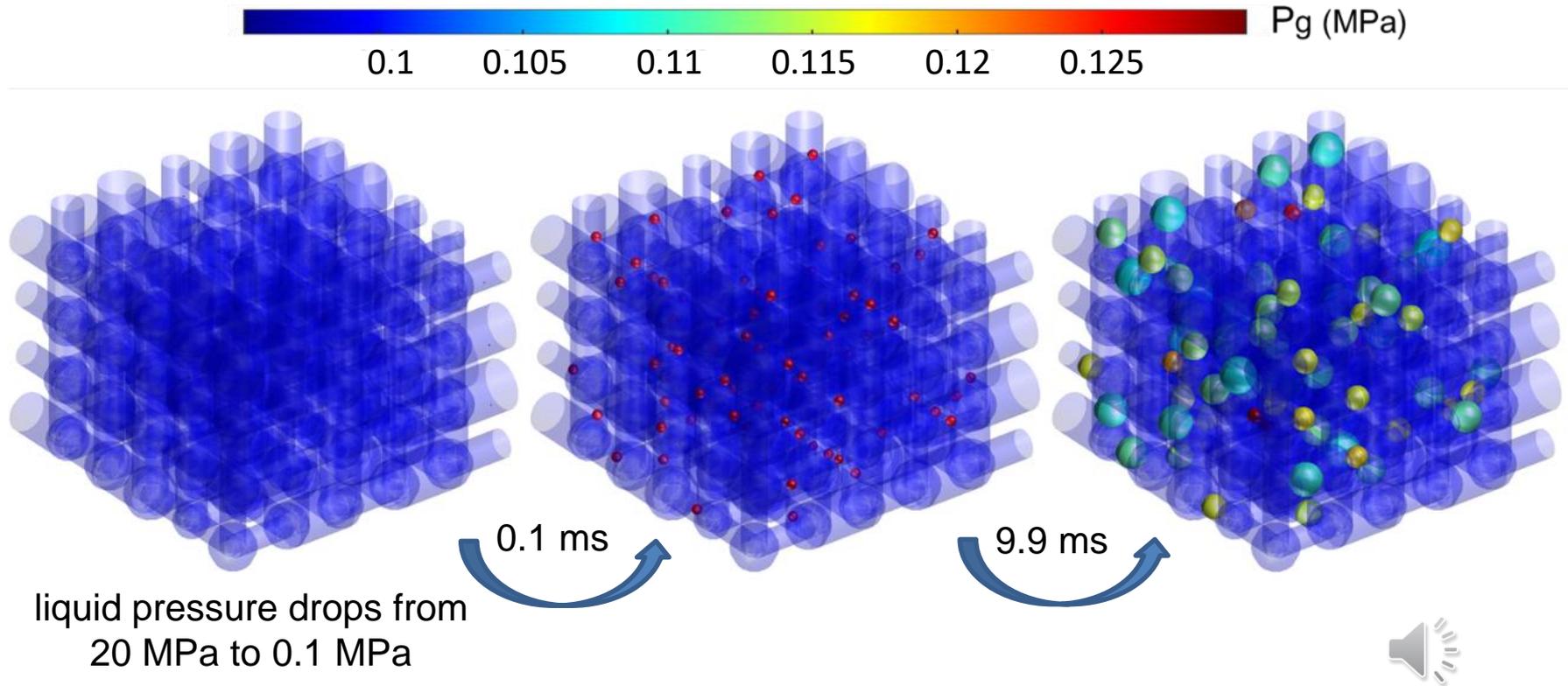
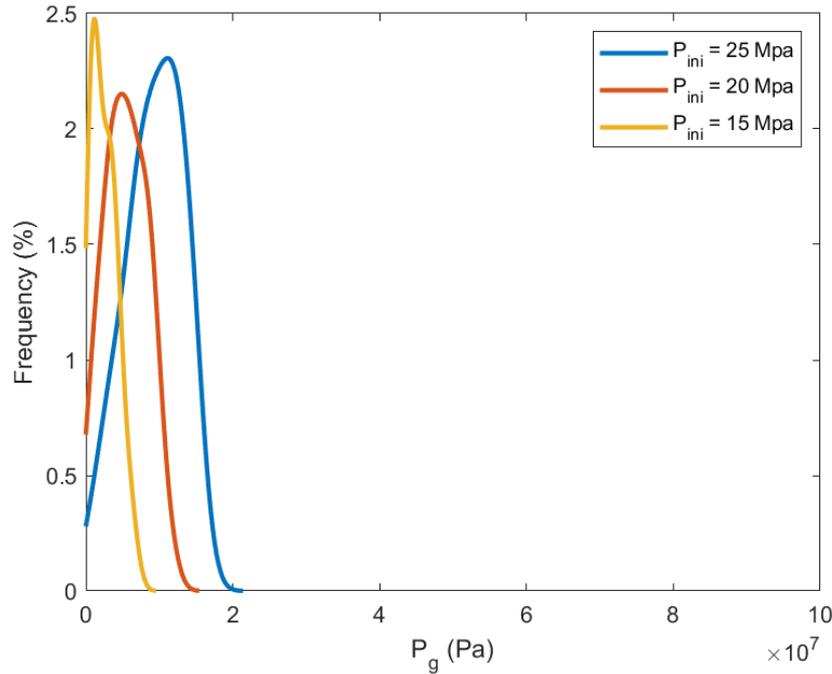# Influence of initial operation pressure on nucleation

bubble radius distribution at nucleation
after pressure depletion

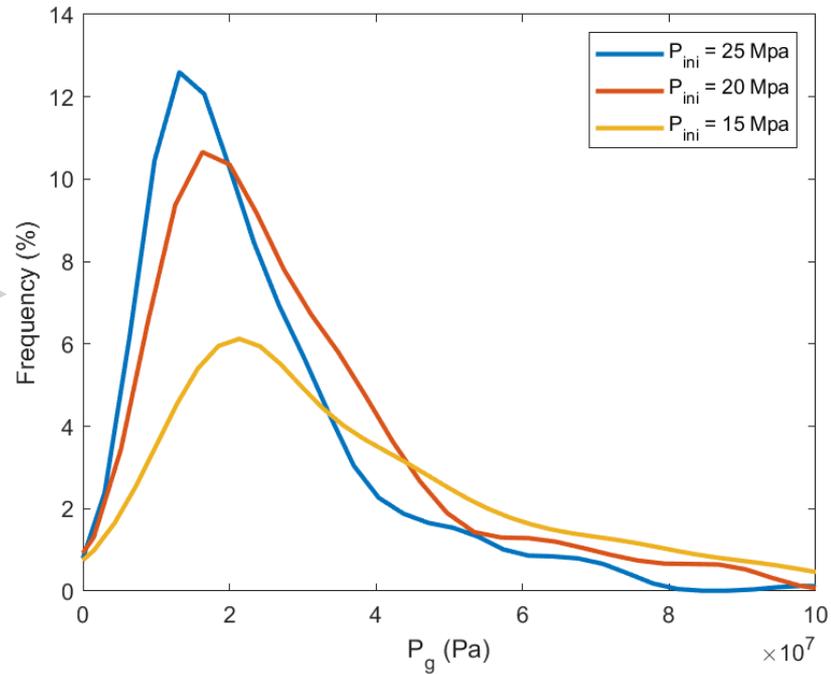percentage of activated bubbles
compared to initial crevice sites

P_{ini} = 25 MPa	P_{ini} = 20 MPa	P_{ini} = 15 MPa
87%	73%	41%

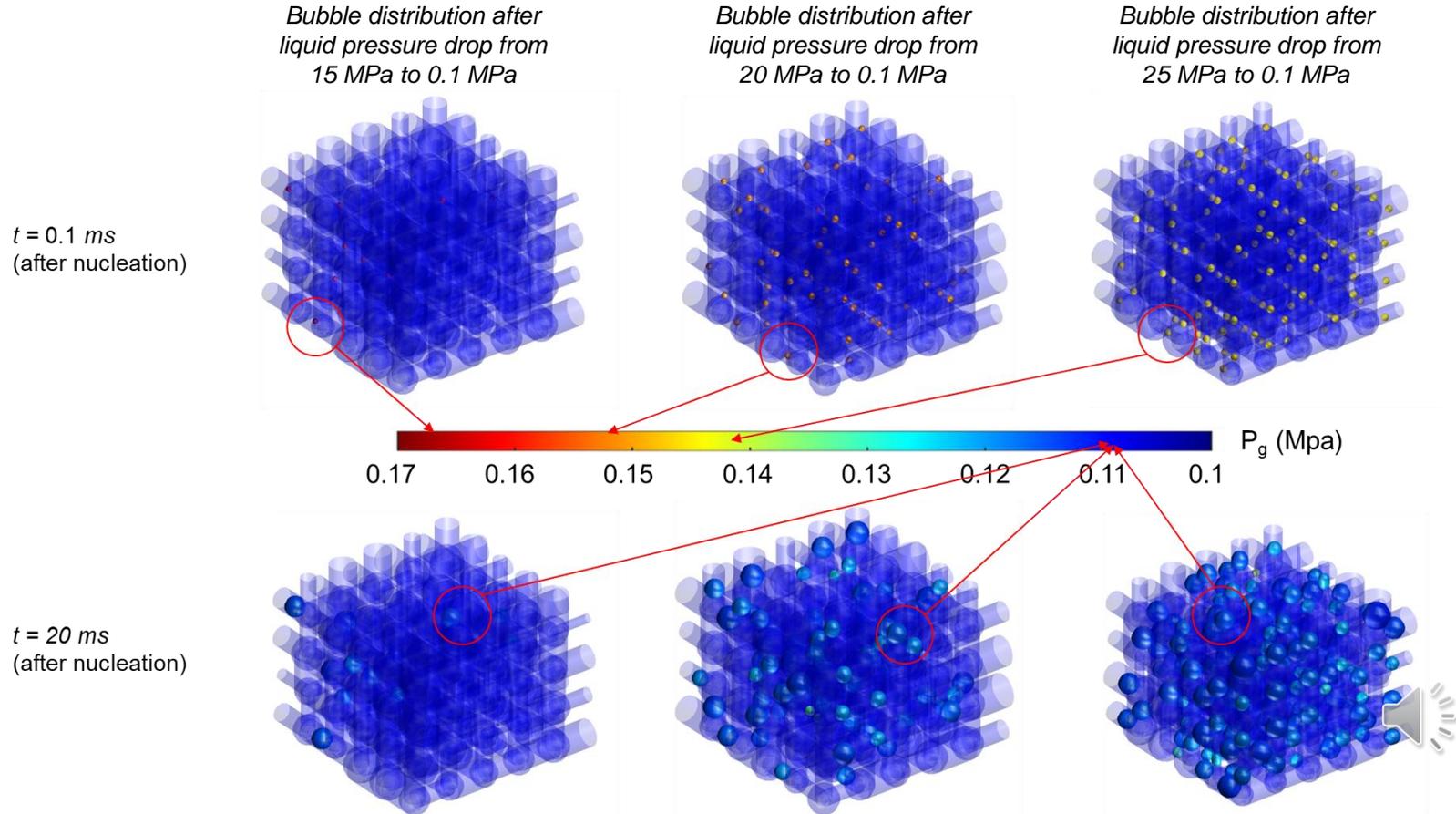# Bubble gas pressure changes before and after nucleation

initial bubble gas pressure under operating pressure

bubble gas pressure at nucleation after pressure depletion

Bubble size and pressure evolution after nucleation

Bubble distribution after liquid pressure drop from 15 MPa to 0.1 MPa

Bubble distribution after liquid pressure drop from 20 MPa to 0.1 MPa

Bubble distribution after liquid pressure drop from 25 MPa to 0.1 MPa

t = 0.1 ms (after nucleation)

P_g (Mpa)

0.17   0.16   0.15   0.14   0.13   0.12   0.11   0.1

t = 20 ms (after nucleation)

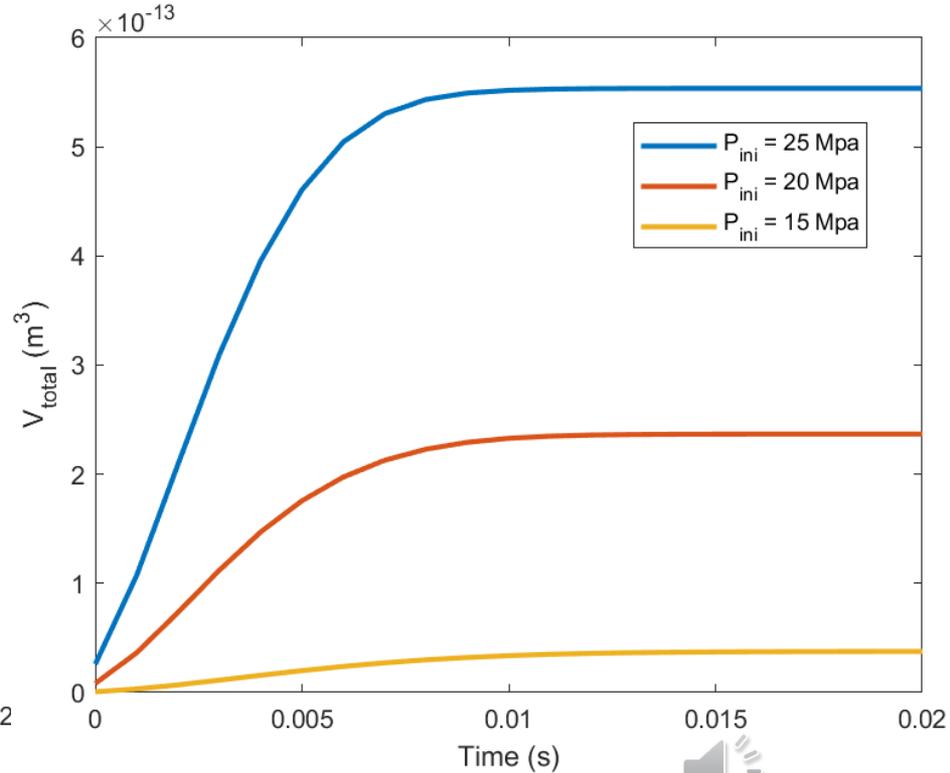# Bubble size distribution after nucleation

t = 0.1 ms
(after nucleation)

t = 20 ms
(after nucleation)
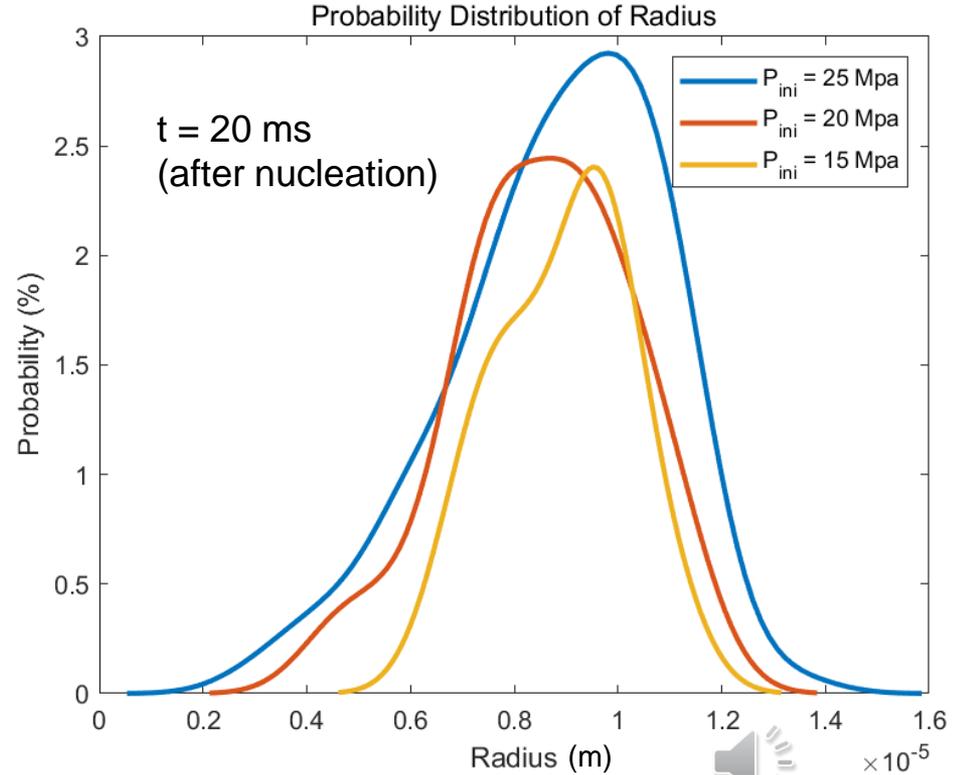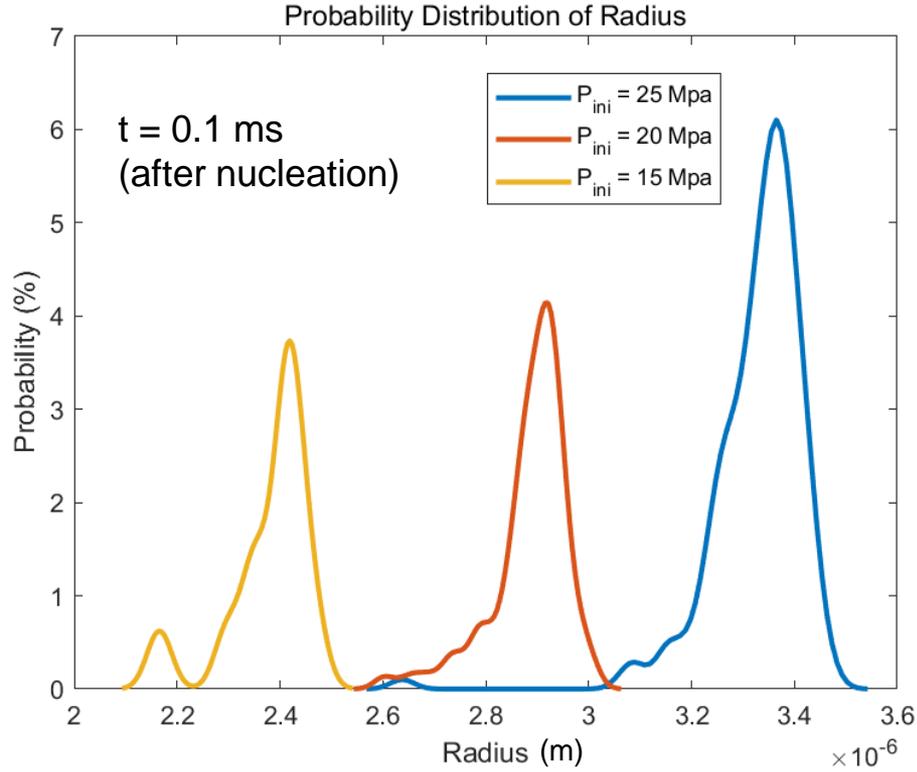
Gas concentration in the liquid and total bubble volume
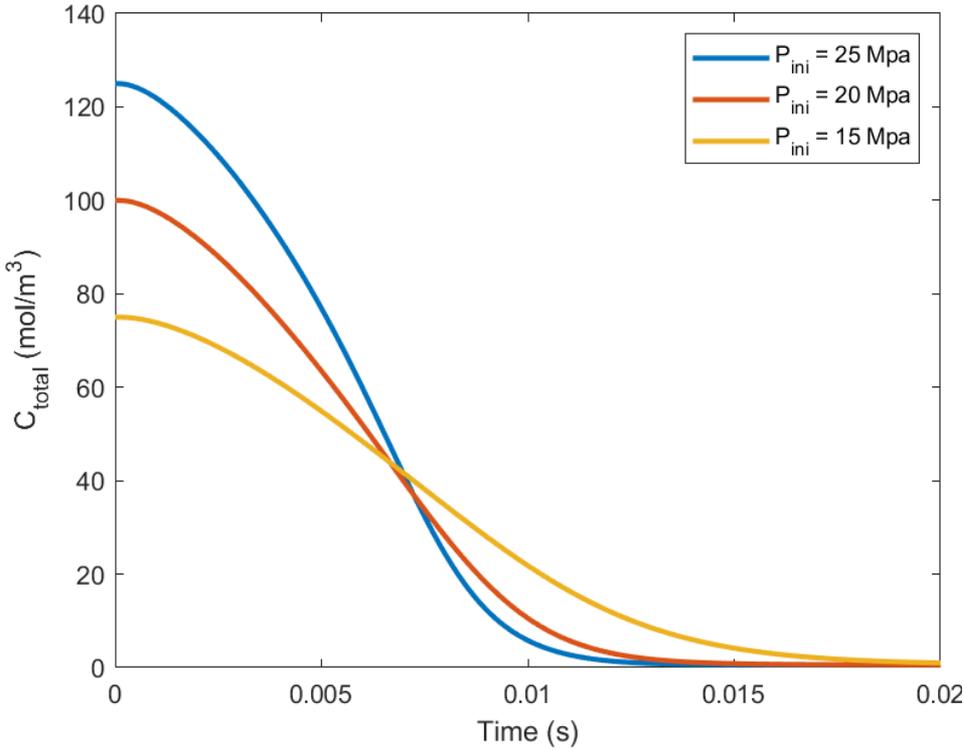
gas concentration change over time after pressure depletion

total bubble volume change

Summary and outlooks

- A 3D dynamic pore network model (PNM) is developed to simulate bubble nucleation and growth.

- The distributions of bubble size and gas pressure in the bubbles are obtained from the PNM simulations.

- Changes in nucleation ratio over total nucleation sites, bubble size, bubble pressure, concentration of gas in bulk liquid, and total bubble volume at different operating gas pressures are analyzed.

On-going work

❖ Integrate the drying process into the developed PNM model.

❖ Take into account the fluid viscous effect.

❖ Introduce the solid-gas interaction.

Thank you!