

CCSI²

Carbon Capture Simulation for Industry Impact

Modeling Aerosol Growth in Amine Scrubbing for Carbon Capture

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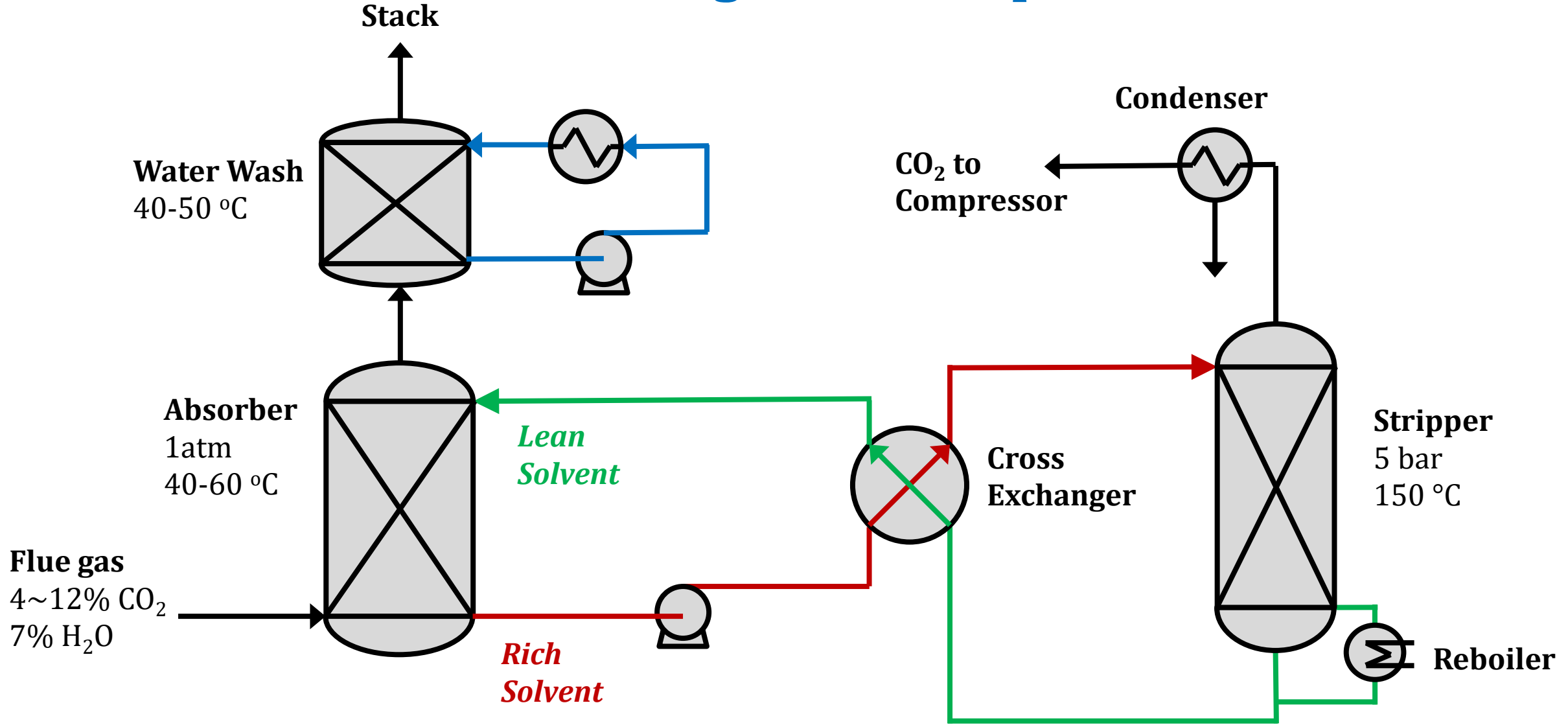
Gary T. Rochelle, University of Texas at Austin



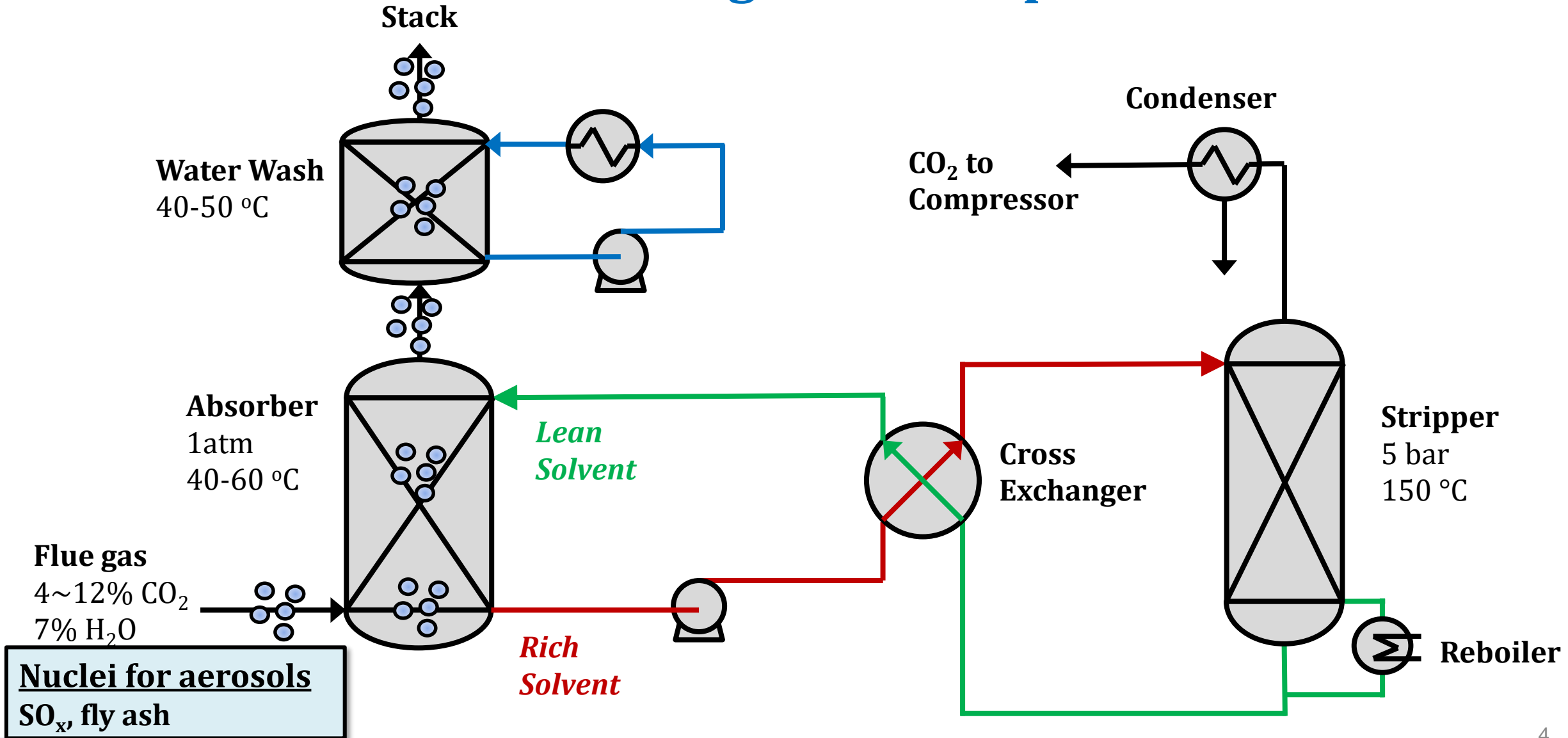
Executive Summary

- **Research Objective:** understand growth mechanisms and develop strategies to remove aerosols by quantitative and accurate modeling
- **Growth mechanisms:**
 - as part. conc increases, aerosol growth decreases due to amine driving force depletion
 - the **limiting** driving force of aerosol growth is amine
 - high amine volatility increases growth
- **Strategies to remove aerosols:**
 - reduce aerosol nuclei below 10^6 part./cm³
 - choose solvents with **moderate** volatility, avoid solvents with low volatility
 - expand WW and pre-humidify dry bed

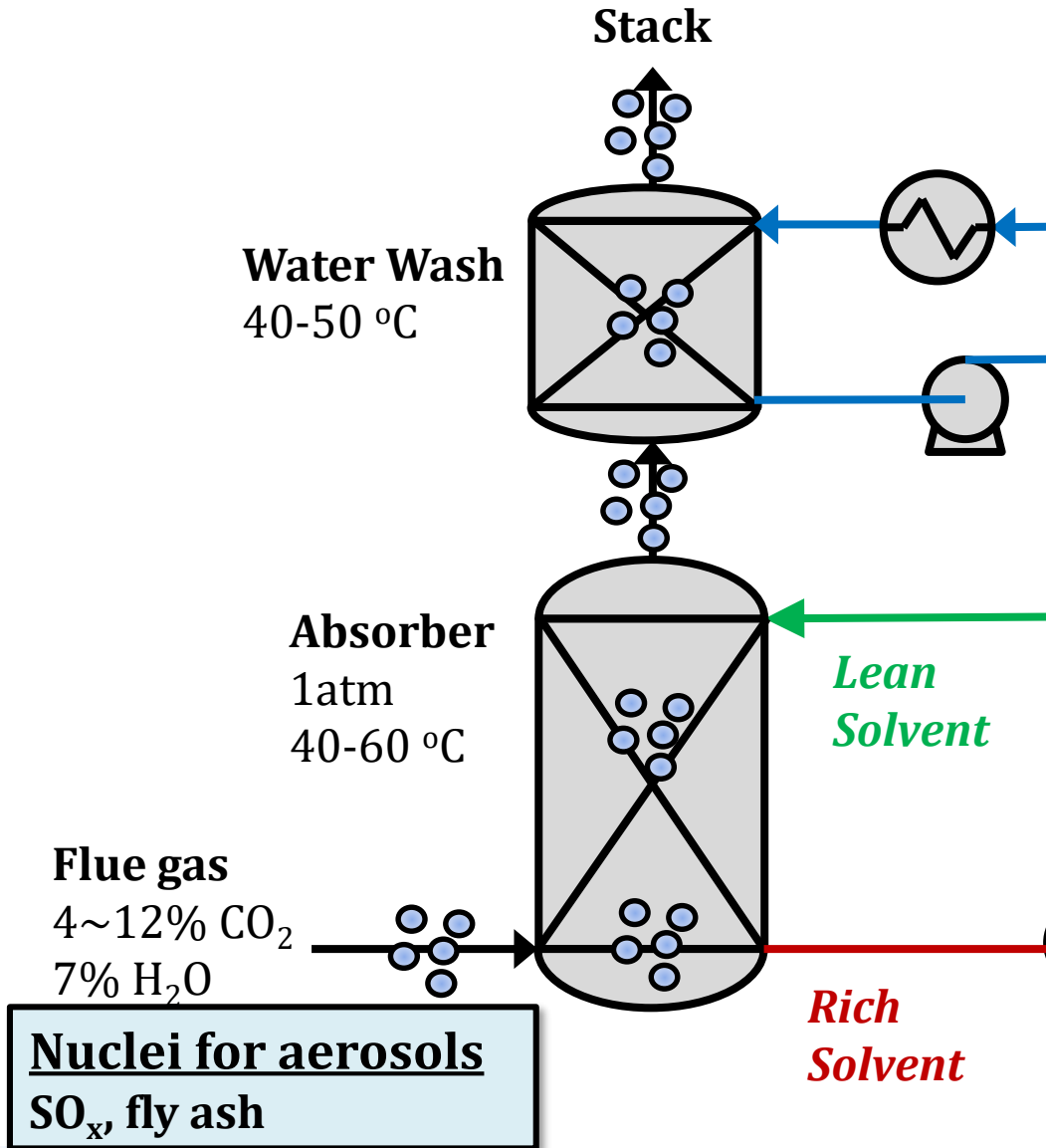
Amine Scrubbing Carbon Capture



Amine Scrubbing Carbon Capture



Amine Scrubbing Carbon Capture



Bad

- if aerosol is not captured: emissions result in solvent loss & environmental impact

Good

- if aerosol grows enough: will be captured. > 3 μm, captured by impaction

This work

- How much aerosol grows
- How we can manage aerosol growth

PZ Makes Aerosol

- April 2017 UT-SRP pilot plant with 5 m PZ and 52 ppm SO₃



Growth Mechanisms Are NOT Well-understood

- **Limiting driving force for growth**
- **Solvent selection**
- **Operating conditions**
- **Effective process configurations**

Industrial Configurations for Emissions Control

Configurations demonstrated in field

- Acid Wash by *Aker Solutions*^{1,2}
- Two-stage Water Wash by *Linde-BASF*³
- Dry Bed by *BASF-Linde-RWE Power*^{4,5}

In this study

- Aerosol with a wide range of particle number conc
- Amine with different volatility
- Dry Bed, Intercoolers, Multi-stage Water Wash

*J. Knudsen, et al., 2013*¹
*O. Bade, et al., 2014*²
*T. Stoffregen, et al., 2014*³
*P. Moser, et al., 2013*⁴
*P. Moser, et al., 2014*⁵

Sequential Aerosol Growth Model

PZ Model by *Fulk*¹, *Kang*², and *Zhang*

- Steady-state absorber and water wash simulations in Aspen Plus, and aerosol calculations in gPROMS
- Proposed gas phase amine **driving force depletion**

MEA Model by *Majeed*³

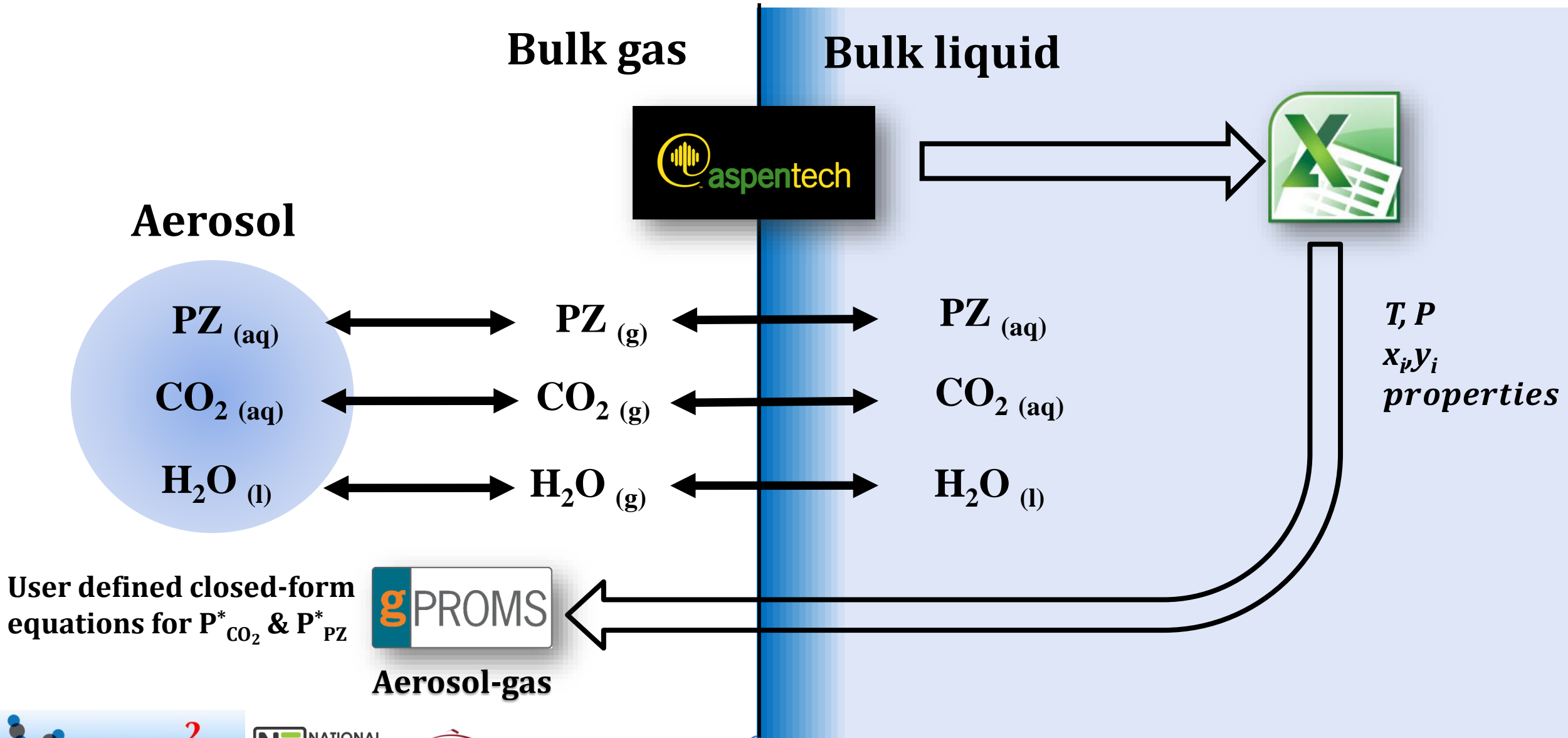
- Steady-state absorber simulations in NTNU in-house simulator, and aerosol calculations in MATLAB
- Also proved gas phase MEA depletion

*Fulk, et al., 2016*¹

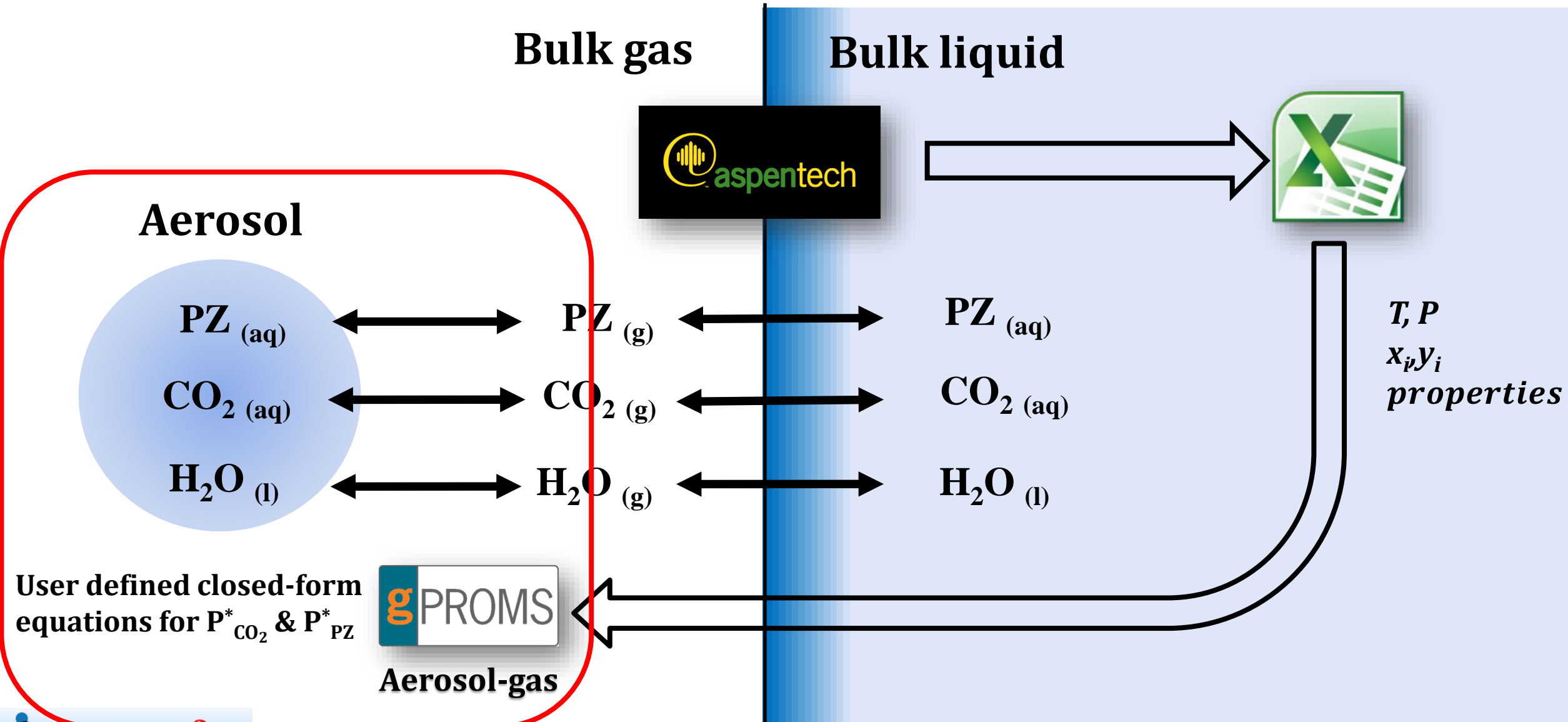
*Kang, et al., 2017*²

*Majeed, et al., 2017*³

Sequential Aerosol Growth Model



Sequential Aerosol Growth Model

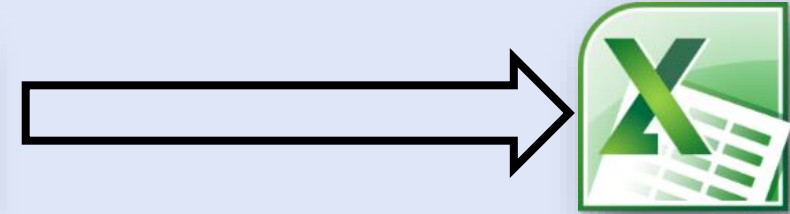
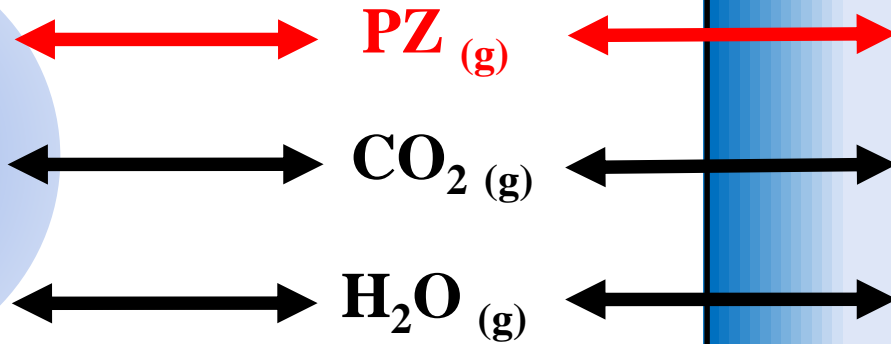
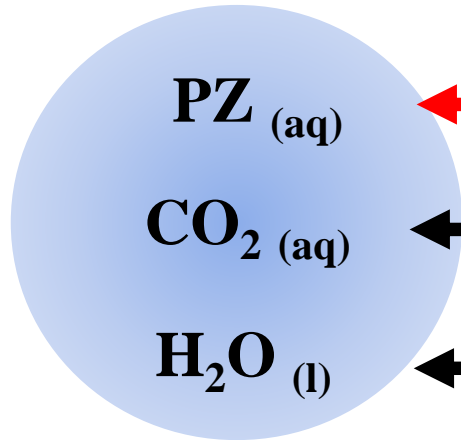


Model Assumptions

PZ mass transfer decreases gas phase PZ
 CO_2 , H_2O , N_2 , T , P still remain constant

Bulk liquid

Aerosol



T, P
 x_i, y_i
properties



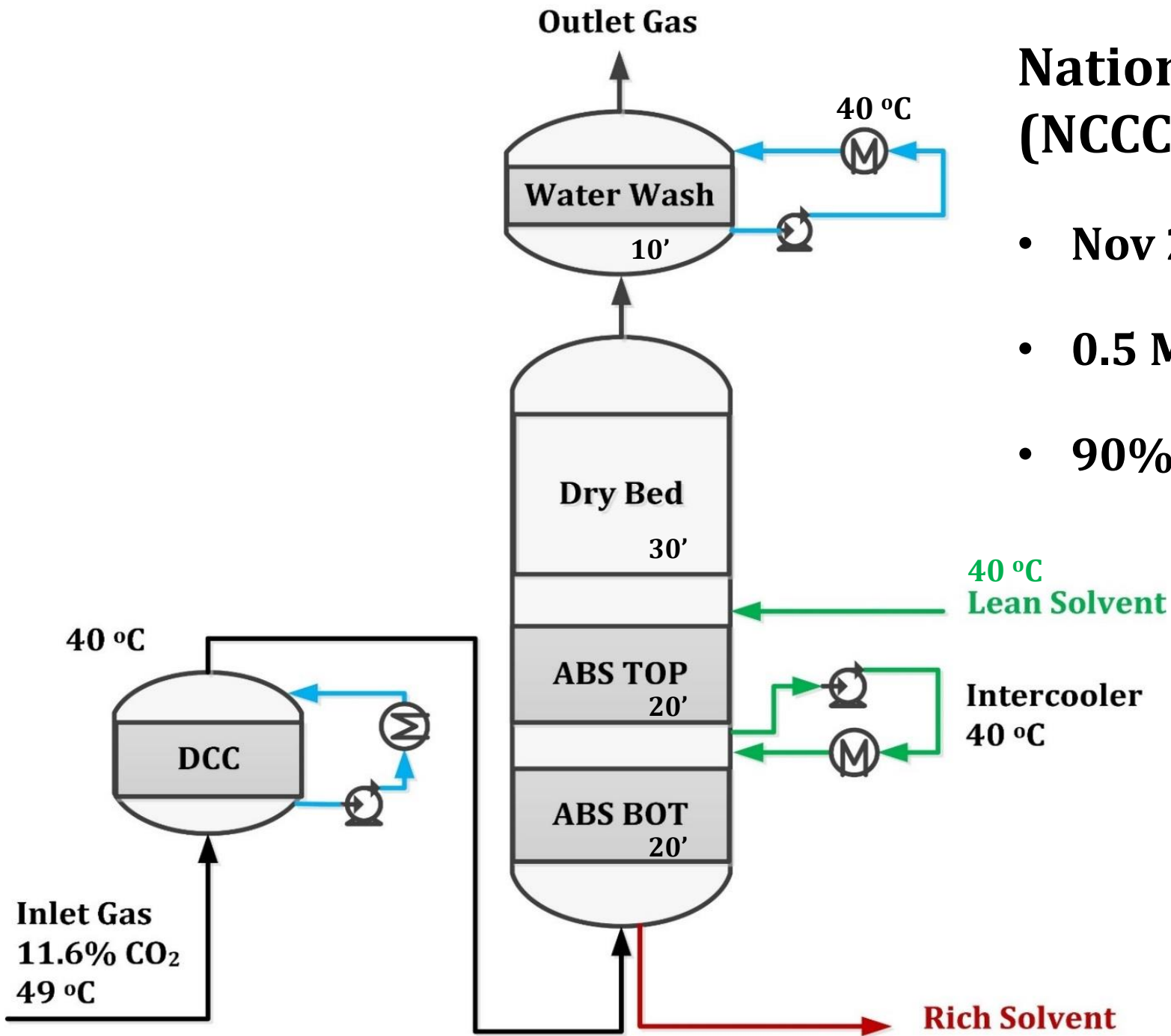
Aerosol-gas

Preliminary Modeling Results

Aerosol Growth at Realistic Plant Conditions

National Carbon Capture Center (NCCC) Absorber

- Nov 2017 NCCC Campaign
- 0.5 MWe Pilot Solvent Test Unit
- 90% removal



Rate-based Absorber Modeling

- **Independence Model**
 - **Developed in Aspen Plus® RateSep™,¹**
 - **Rigorous e-NRTL thermodynamic framework**
 - **Rigorous kinetics with reactions in boundary layer**
- **Solvent**
 - **5 m PZ: fast absorption rate, low viscosity, good energy performance**
 - **Lean Loading at 0.22 (mol CO₂/mol alk)**

P. Frailie, 2014¹

Assumptions for Aerosols

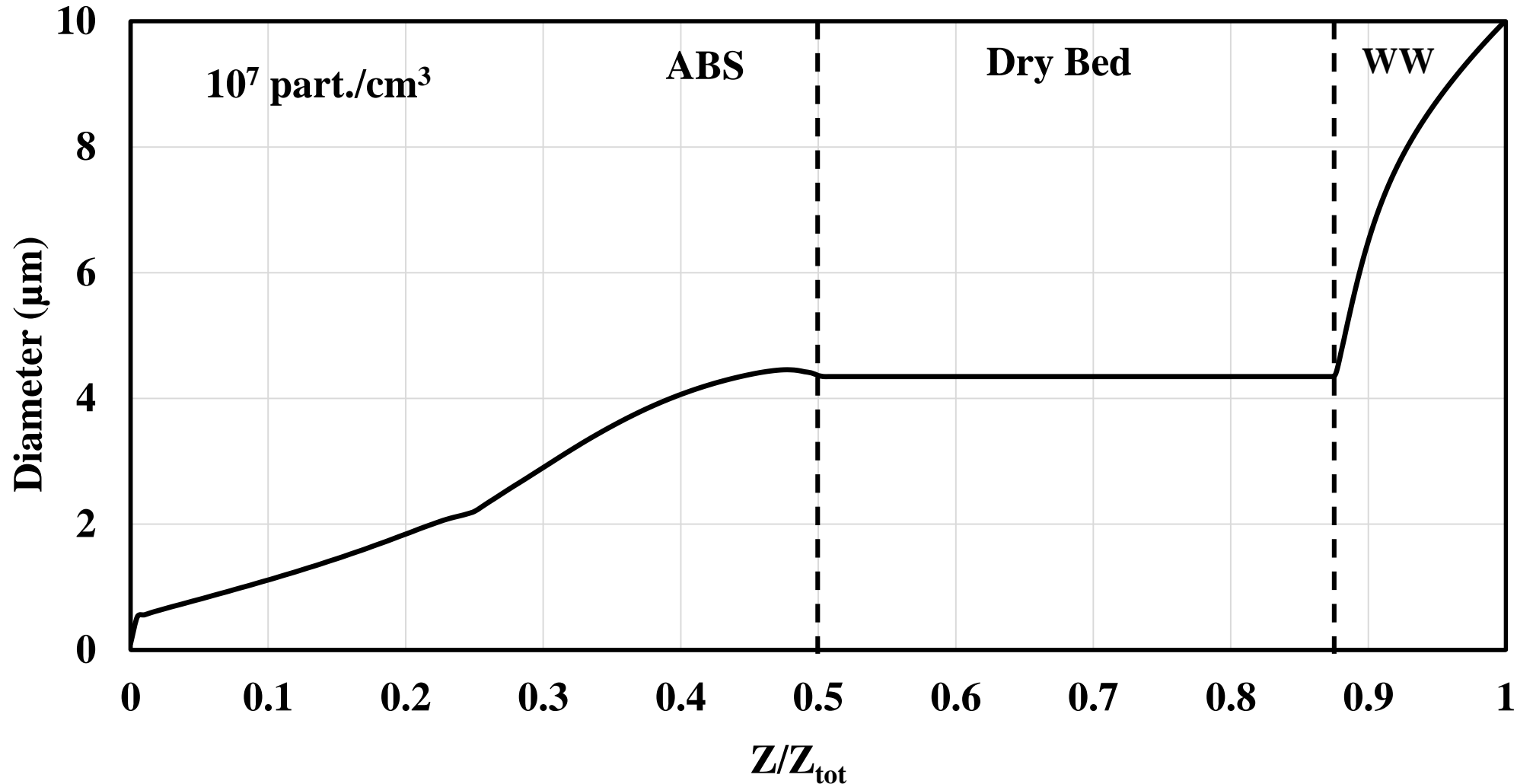
- Well-mixed
- Particle conc at 10^7 part./cm³
 - < 10^6 : emits < 1ppm amine
 - > 10^8 : starts coagulation
 - ~ 10^7 : most often observed at site
- Initial conditions
 - 0.1 μm , 5 m PZ, 0.36 CO₂ loading

PZ (aq)

CO₂ (aq)

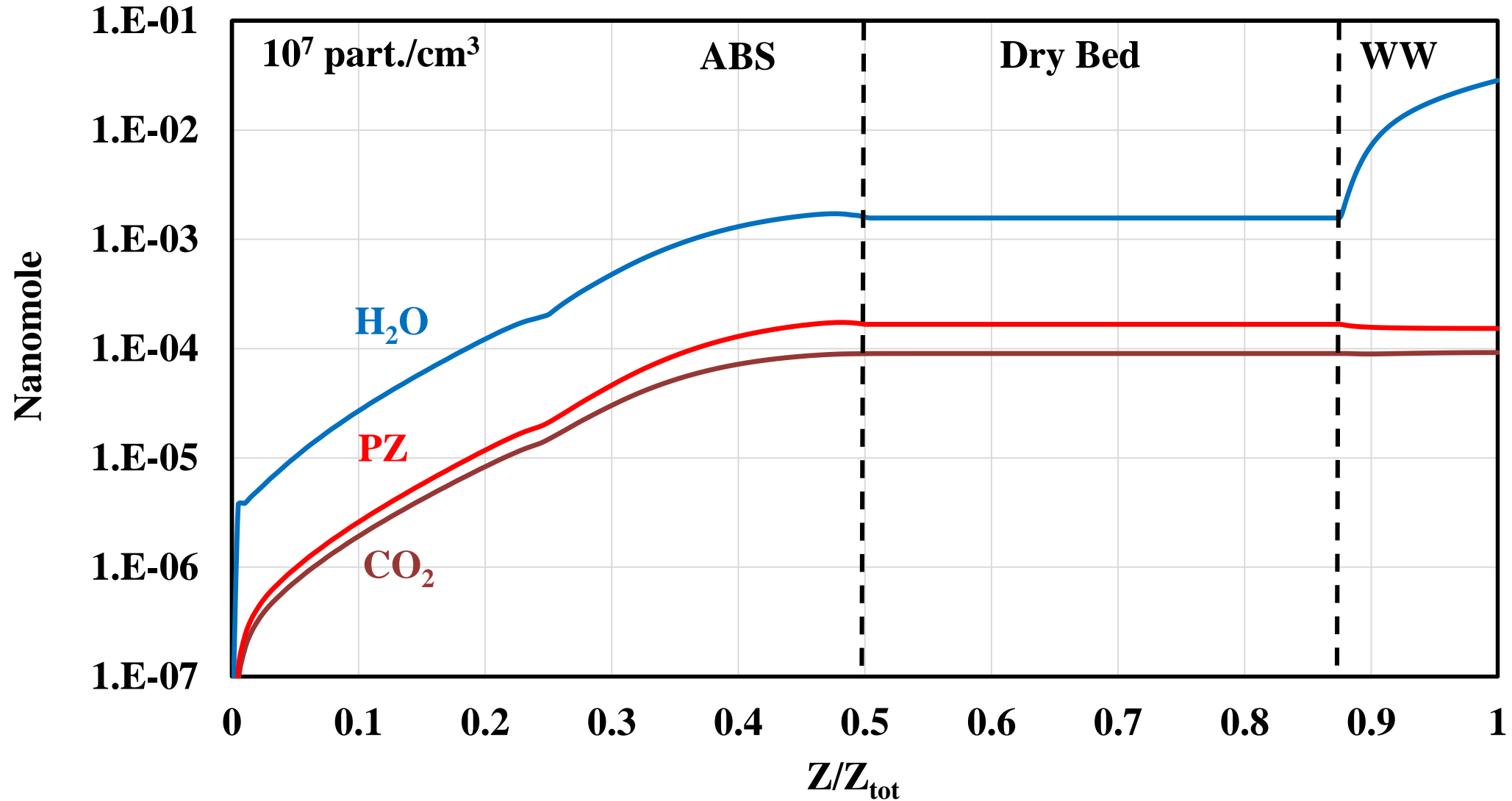
H₂O (l)

General aerosol growth profile



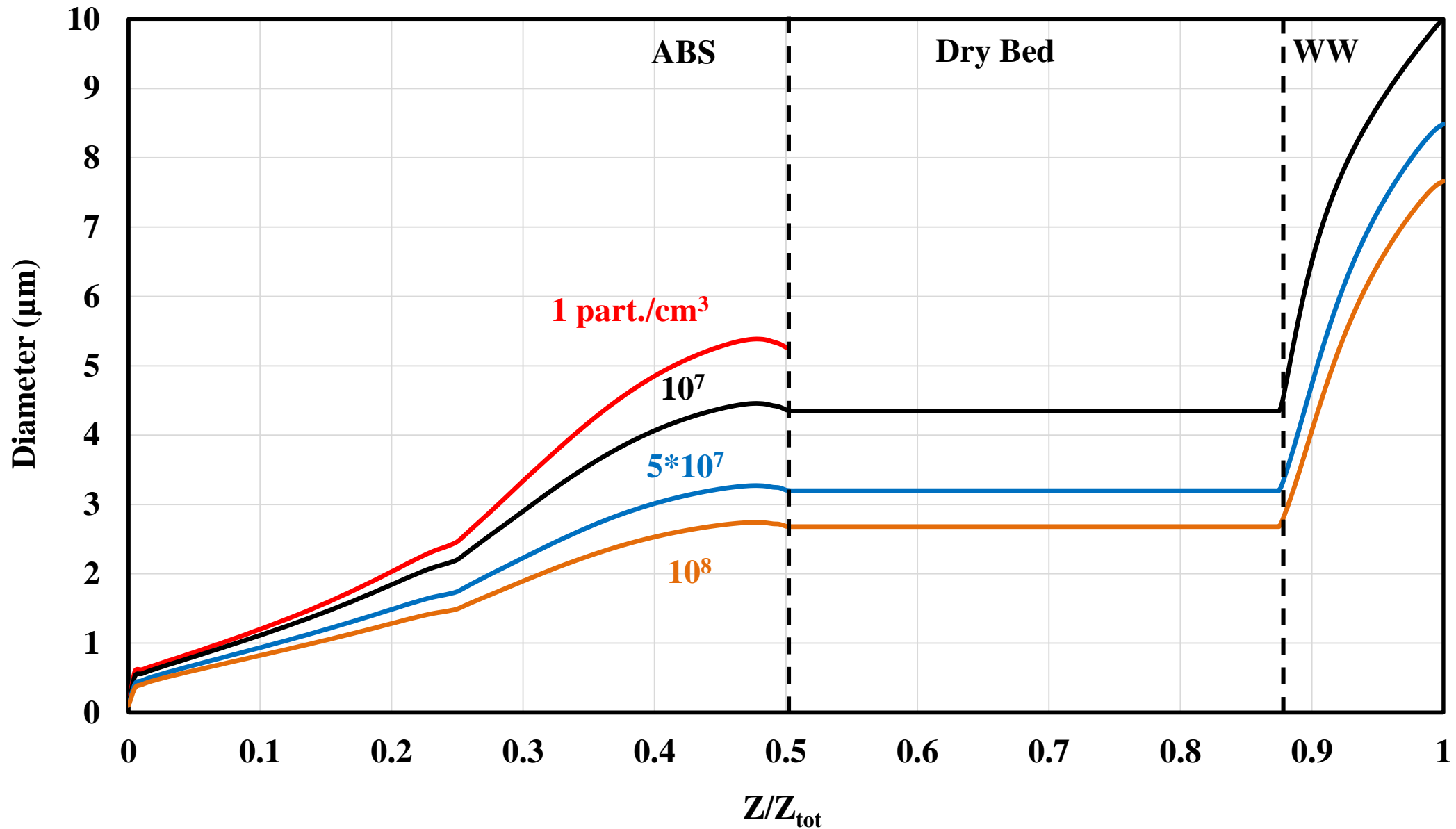
- Aerosols grow from $0.1\mu\text{m}$ to 4.4 in ABS, and 10 in WW (collectable)
- Aerosol initial diameter is not critical

Component pickup in aerosol

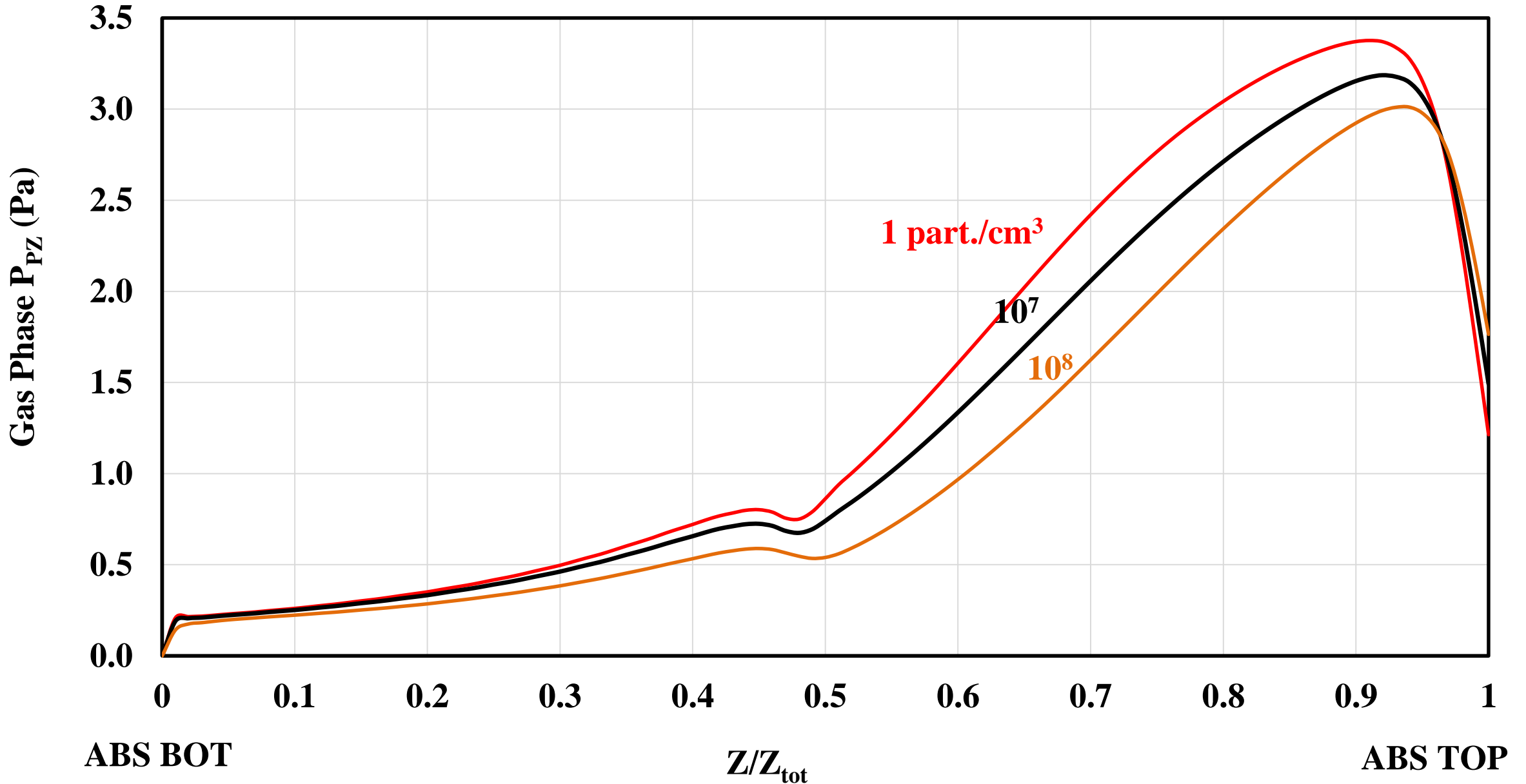


- Aerosols grow in WW by picking up water

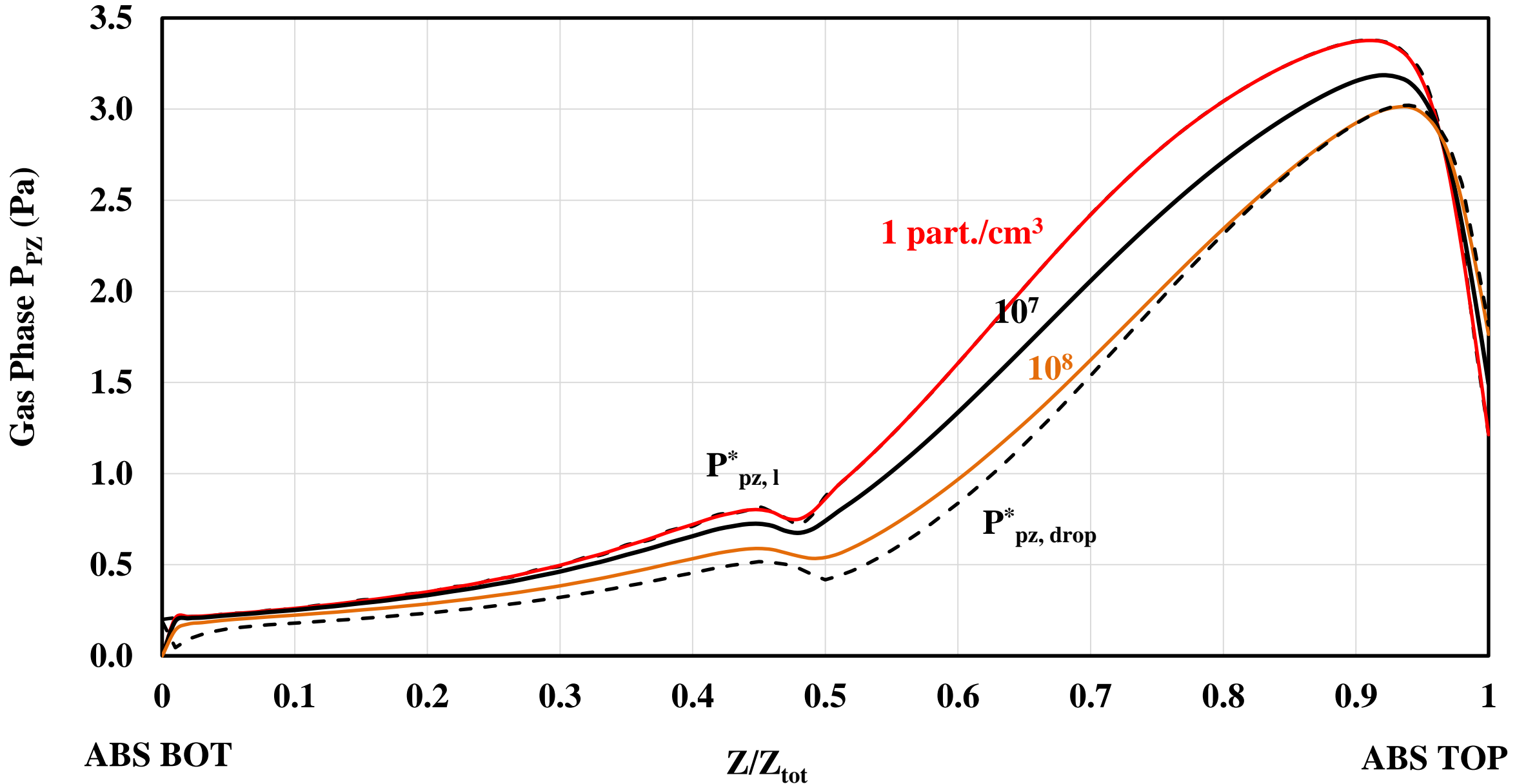
High part. conc reduces aerosol growth



PZ driving force depletion in gas phase

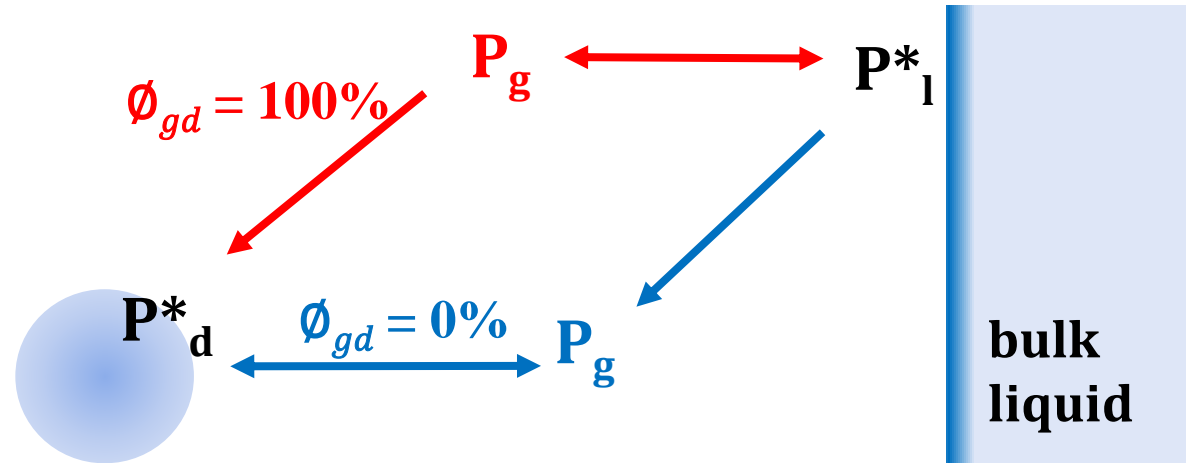


PZ driving force depletion in gas phase



Relative driving force ratio between g-d

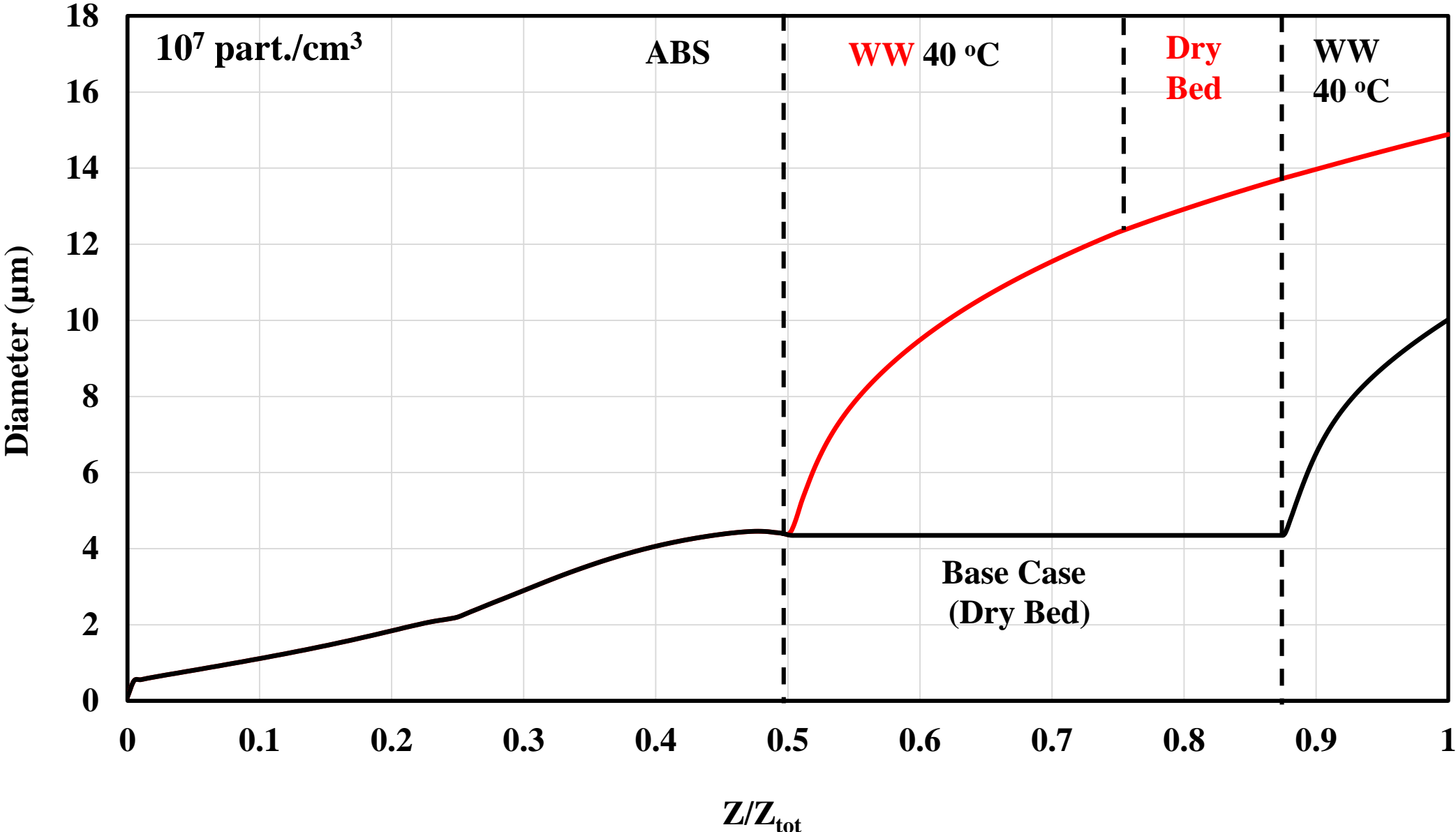
$$\phi_{gd} = \frac{\Delta P_{gd}}{\Delta P_{ld}}$$



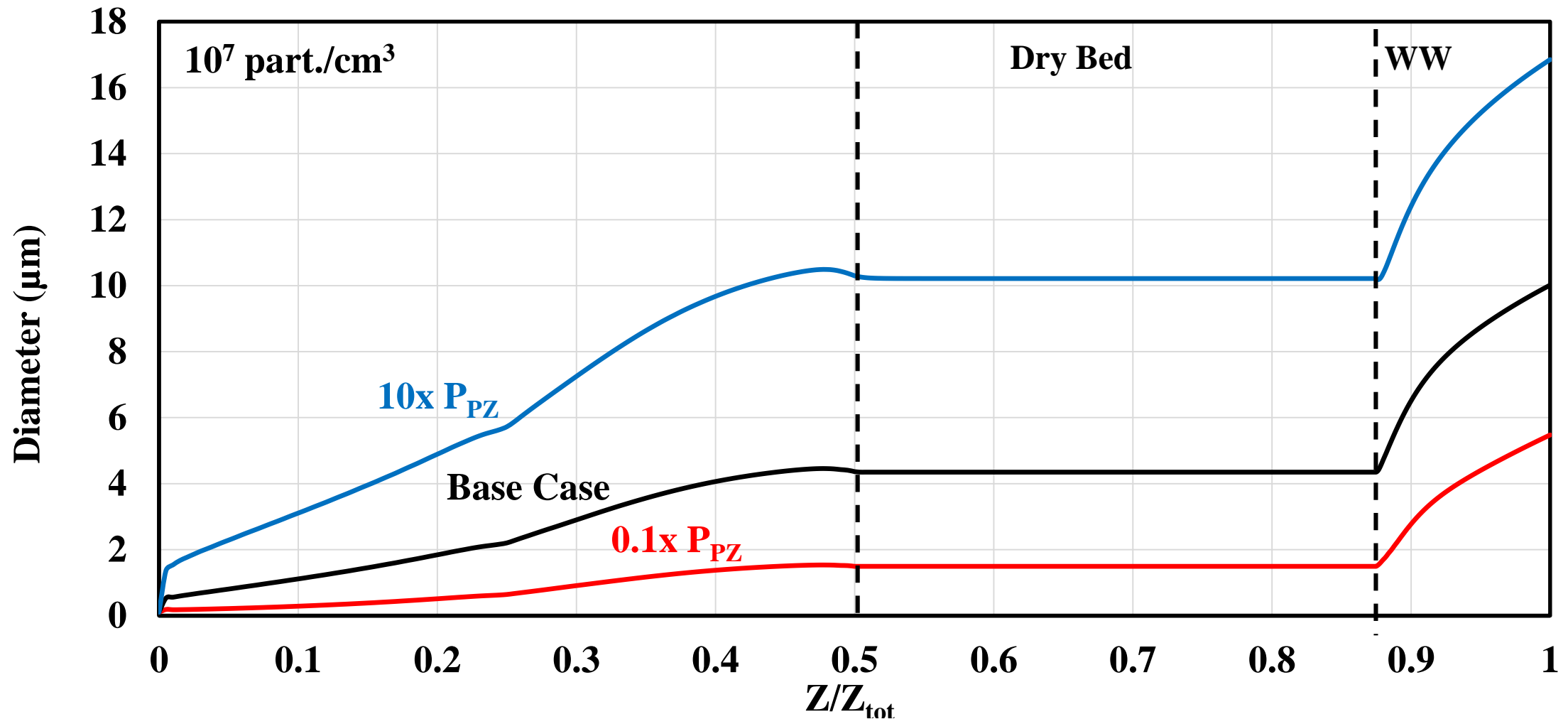
	1 part./cm ³	10 ⁷	10 ⁸
Avg $\phi_{gd, \mathbf{PZ}}$	100%	72%	32%
Avg $\phi_{gd, \mathbf{water}}$	0%	0%	0%

- The limiting driving force of growth is **PZ**
- As part. conc increases, limiting driving force (PZ) shifts from g-d to l-g
- Aerosol is always in **equilibrium** with water in gas

Dry bed needs to be pre-humidified to grow aerosols



Increase and decrease PZ volatility by 10x



- Choose solvents with moderate volatility, like PZ (collectable)
- Avoid solvents with low volatility (non-collectable)

Conclusions - growth mechanisms

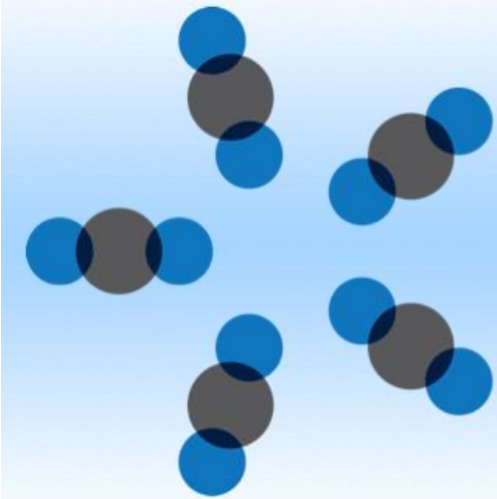
- As part. conc increases, aerosol growth decreases due to amine driving force depletion. The limiting driving force **shifts** from g-d to l-g
- In NCCC with 5 m PZ
 - 10^7 part./cm³ are collectable
 - **w/o** water wash, 10^8 part./cm³ are non-collectable
- In water wash, aerosol grows by picking up **water**
- Higher amine volatility increases growth

Recommendations

- **Nuclei**
 - Reduce aerosol nuclei below 10^6 part./cm³
- **Solvent selection**
 - Choose solvents with **moderate** volatility, like PZ
 - Avoid solvents with low volatility
- **Process configurations**
 - Expand WW
 - Pre-humidify dry bed

Possible Future Work

- Test a wide variety of amines/blends
- Particle size/residence time distribution



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