

Reducing Ultra-High-Purity (UHP) Gas Consumption By Characterization of Trace Contaminant Kinetic and Transport Behavior in UHP Fab Environments

Customized Project; Sponsored by Intel

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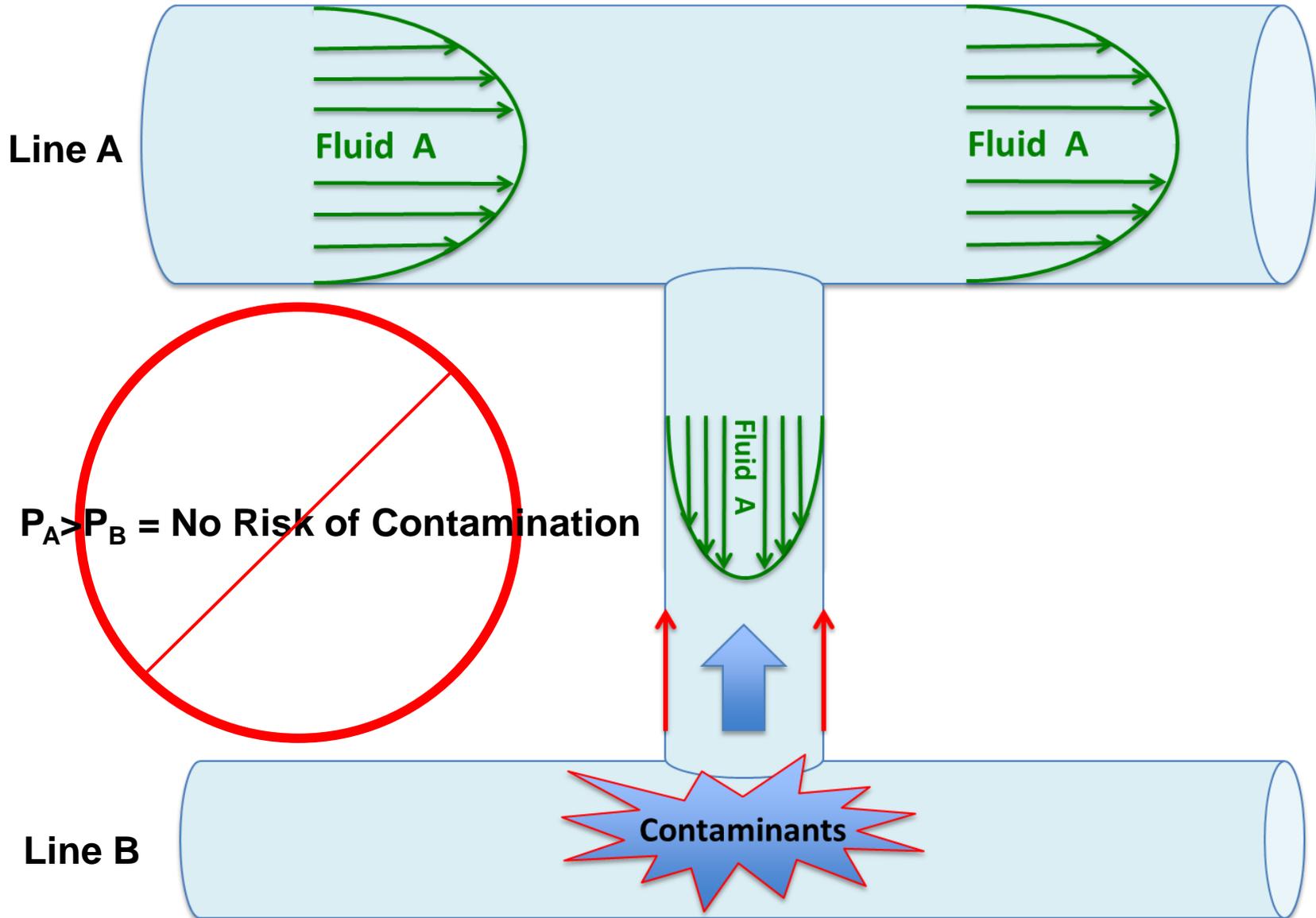
PI:

- Farhang Shadman, Chemical and Environmental Engineering, UA

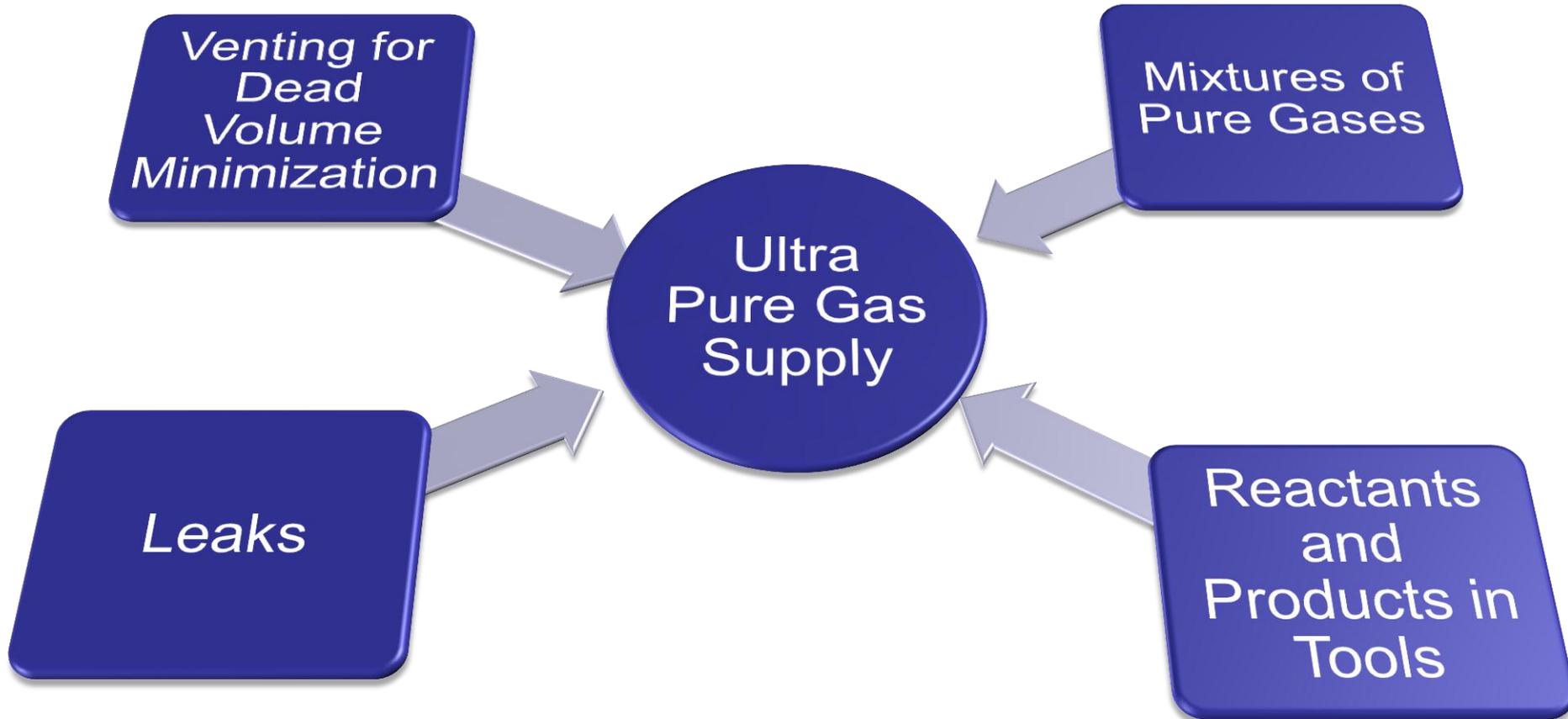
Co-PI:

- Carl Geisert, Sr. Principal Engineer, Intel

Back Diffusion Sources and Mechanisms



Back Diffusion Sources and Mechanisms



Objectives

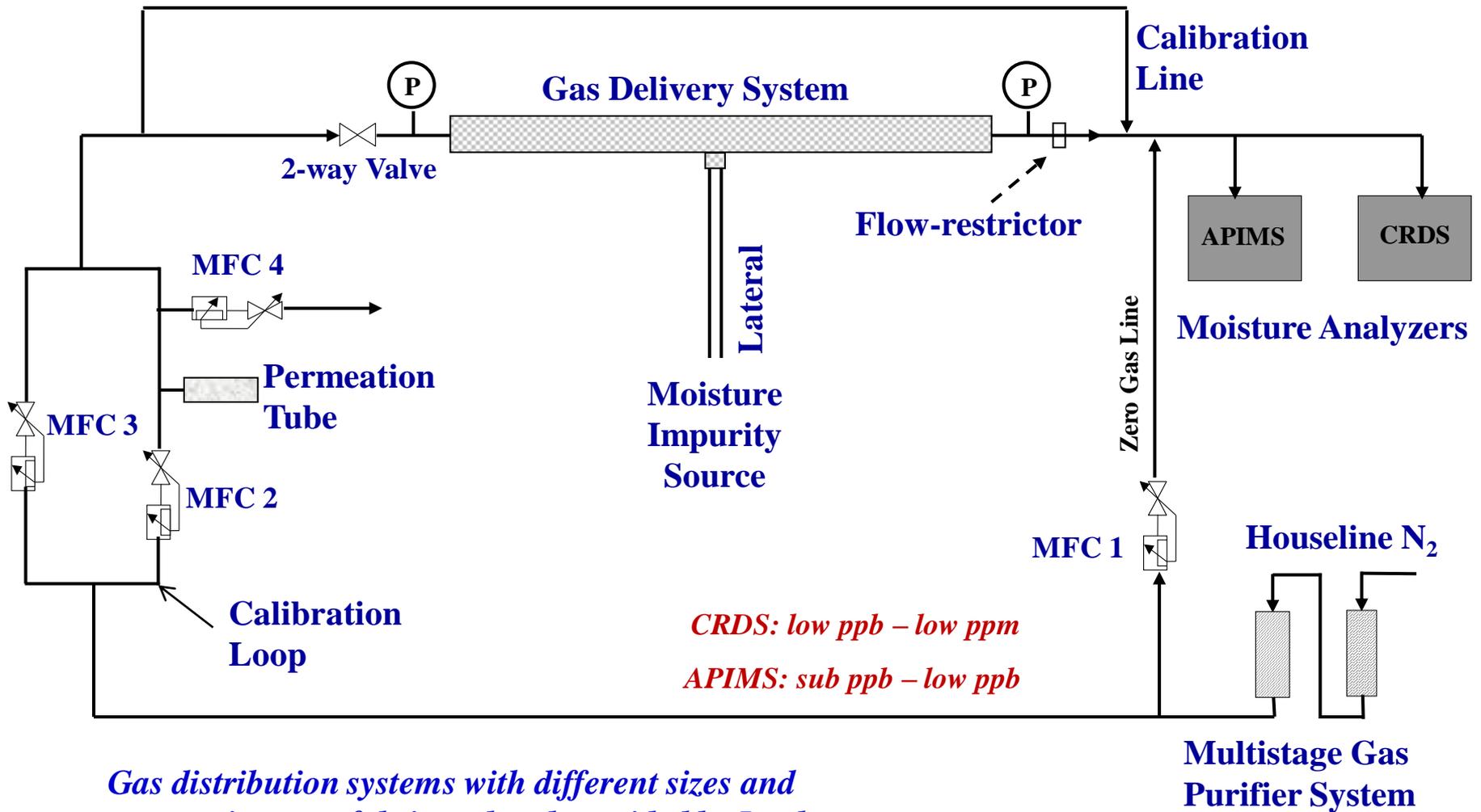
- **Develop operational parameters that will minimize back diffusion of impurities into fluidic distribution systems.**
- **Develop and validate a process simulator that can help industry design and operate systems while minimizing back diffusion, gas usage, and system dead volumes.**
- **Develop a better understanding of back diffusion since little is known or has been published on the subject.**

Motivation and ESH Impact

- **Contamination of gas distribution systems during normal operation results in major wasting of materials, energy, and valuable tool operation time.**

Experimental Testbed

Laterals Added to the Main Line



Gas distribution systems with different sizes and geometries were fabricated and provided by Intel

Back Diffusion Process Simulator

Convective Flux

$$J_c = -U_3 C_g$$

Gas Phase Dispersive Flux

$$J = -D \frac{dC_g}{dz}$$

Surface Diffusive Flux

$$J_s = -D_s \frac{dC_s}{dz} - D_s \frac{k_a}{k_d} \frac{dC_g}{dz}$$

Total Dispersive Mass Flow Rate

$$\pi r^2 J_e = \pi r^2 J + 2\pi r J_s$$

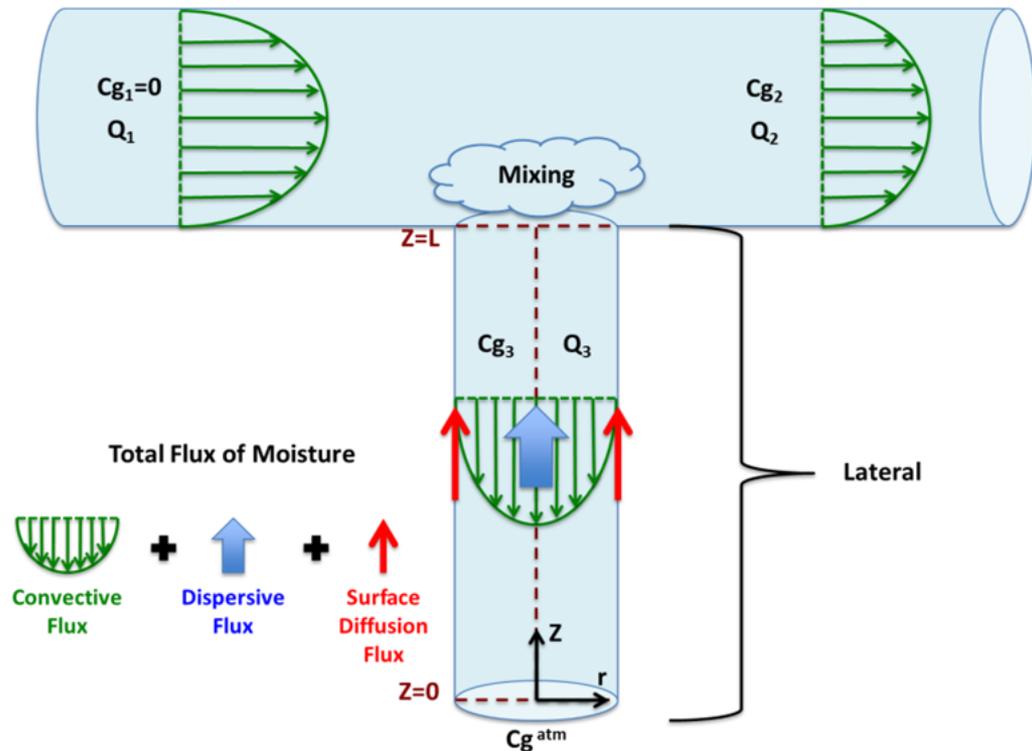
Effective Dispersion Coefficient

$$D_e = D + \frac{2}{r} D_s K_e$$

Governing Equation

$$U_3 \frac{dC_g}{dz} + D_e \frac{d^2 C_g}{dz^2} = 0$$

Convection
Effective Dispersion



Boundary Condition 1

$$z = 0, \quad C_g = C_g^{atm}$$

Boundary Condition 2

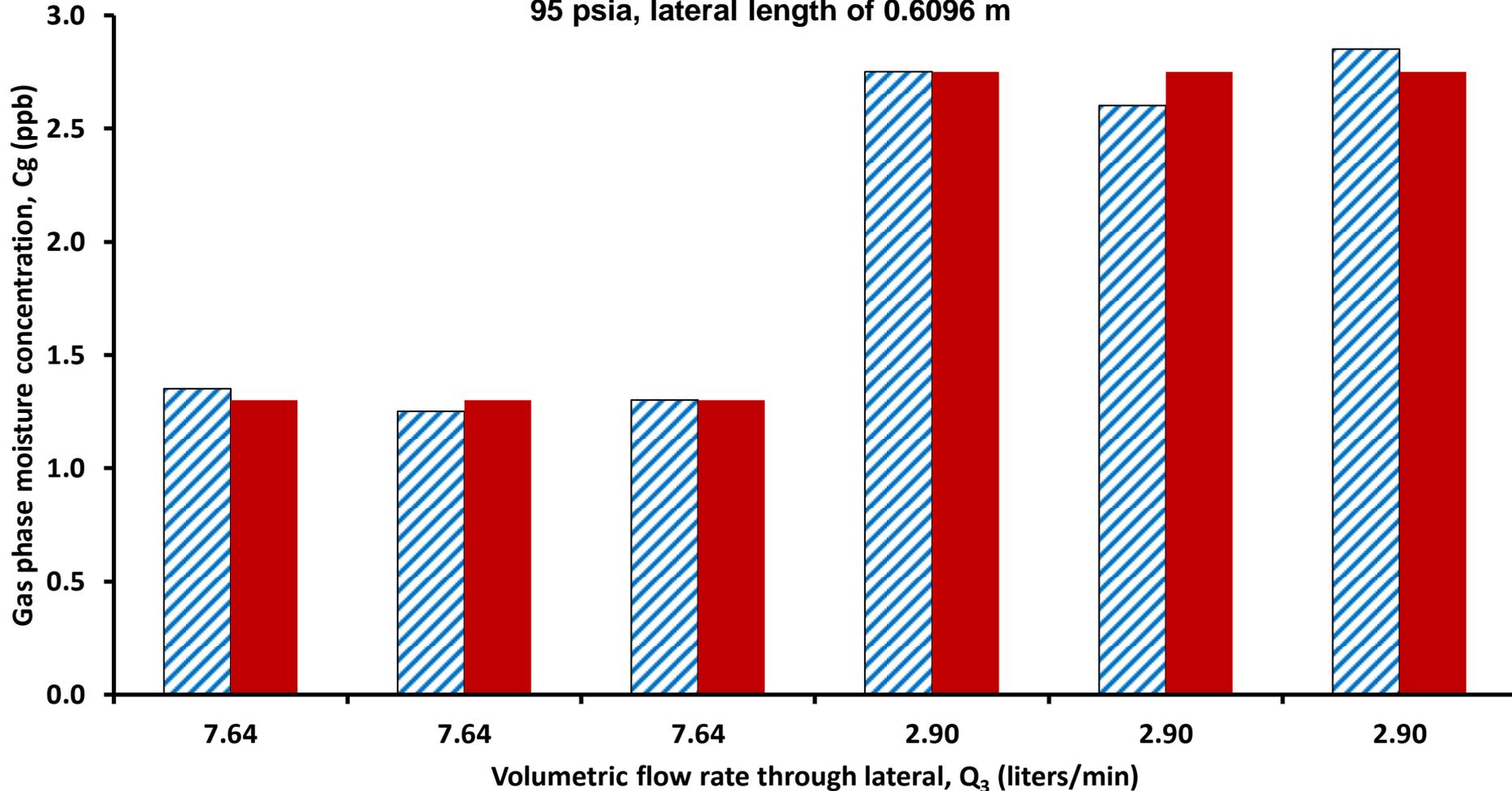
$$z = L, \quad C_g \Big|_{z=L} = \left(\underbrace{-U_3 C_g \Big|_{z=L}}_{\text{Convective Flux}} - \underbrace{D_e \frac{dC_g}{dz} \Big|_{z=L}}_{\text{Effective Dispersive Flux}} \right) \frac{A_{lateral}}{Q_2}$$

Process Simulator Verification

Simulator Prediction

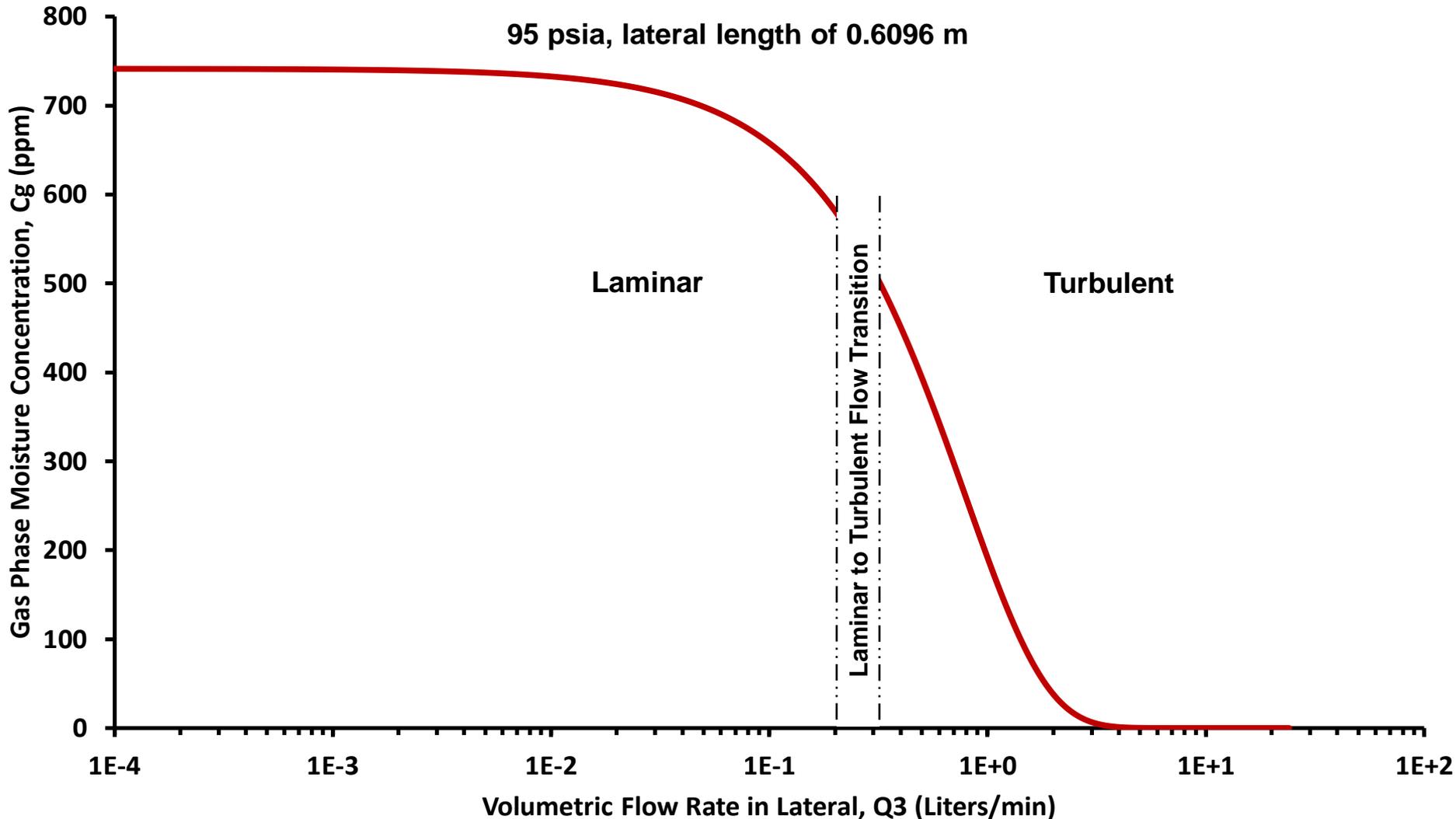
Experimental Results Model Prediction

95 psia, lateral length of 0.6096 m



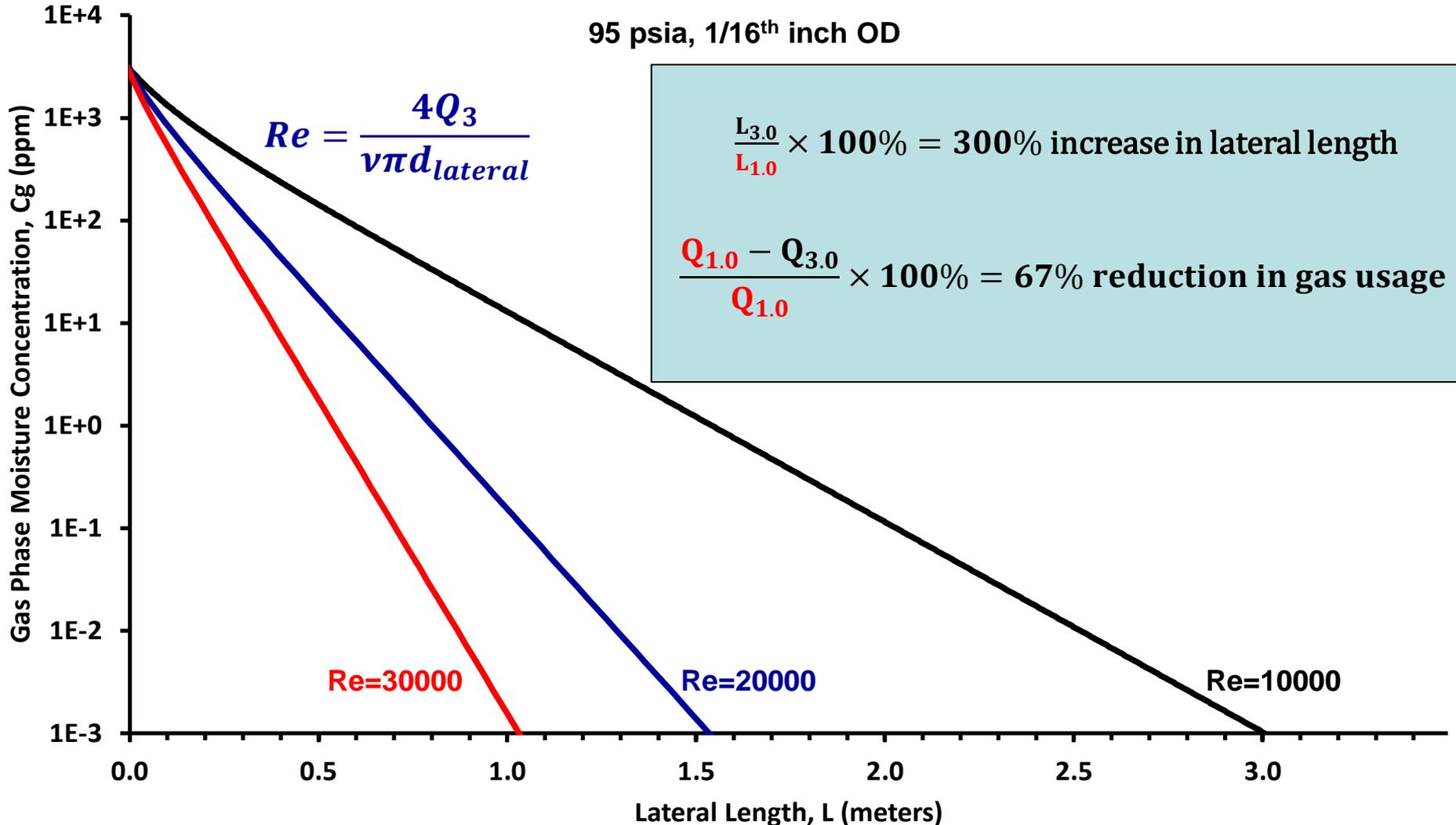
Parametric Studies

Effect of Flow Rate on Gas Phase Moisture



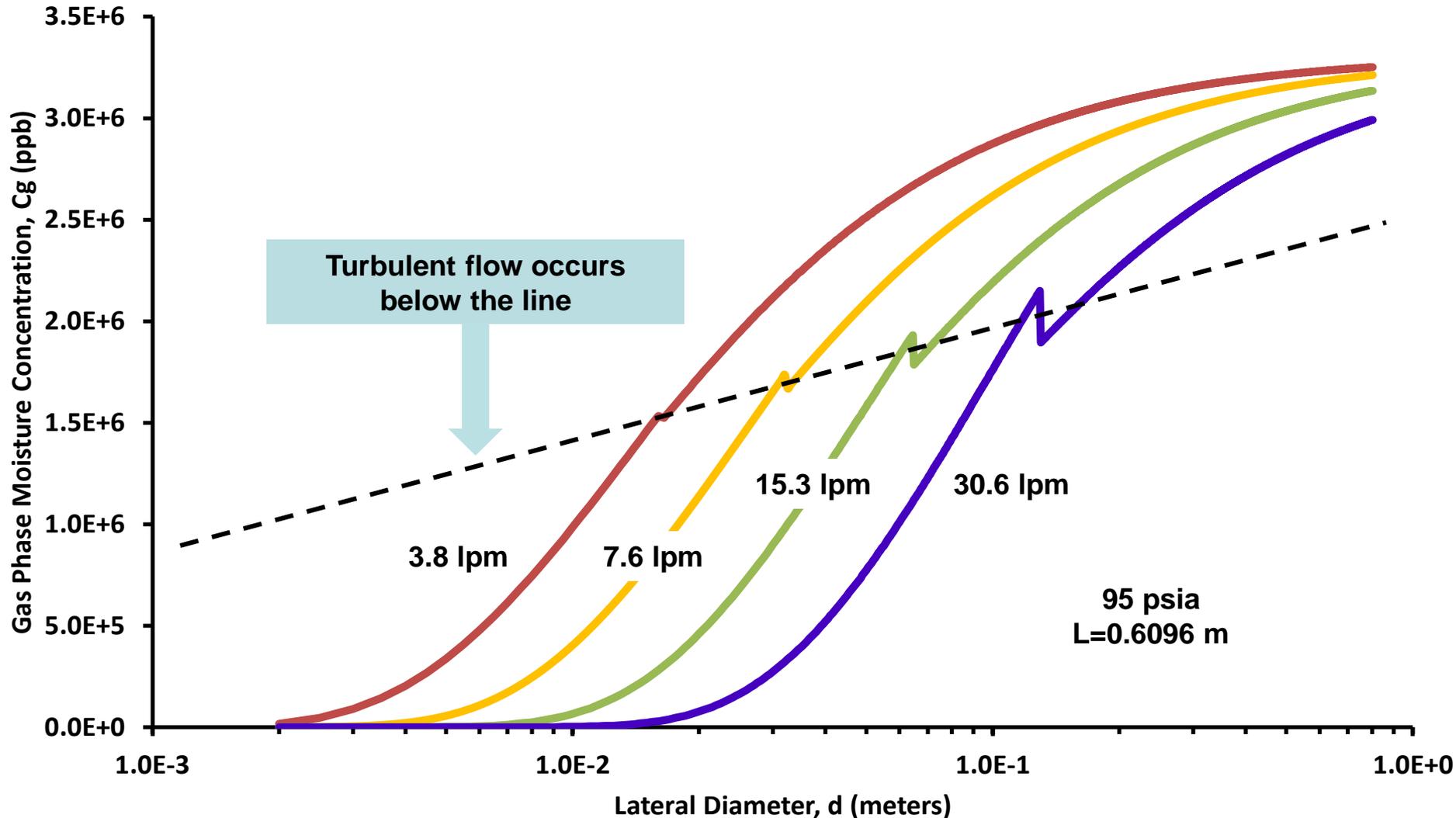
Parametric Studies

Effect of Lateral Length on Gas Phase Moisture



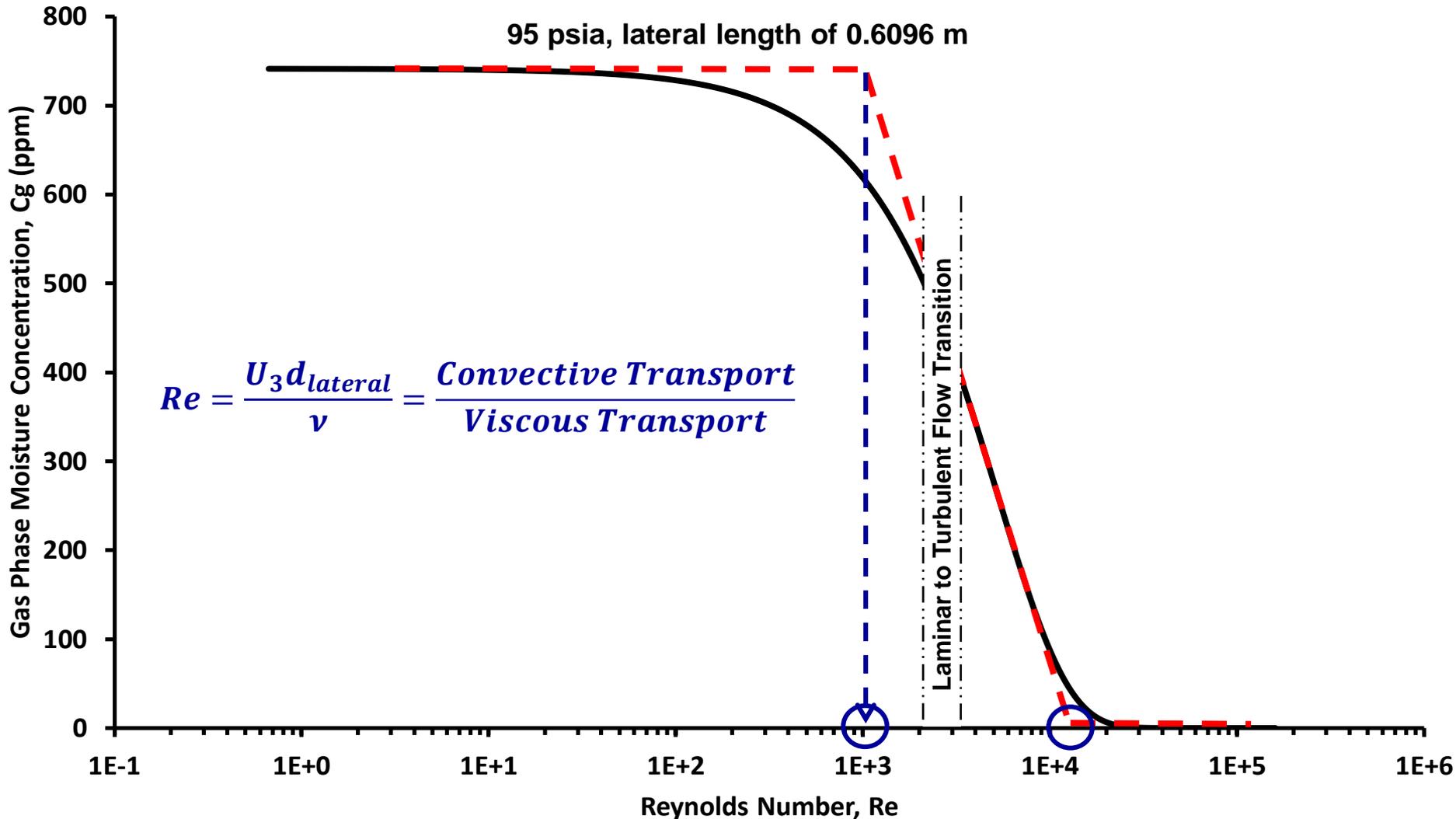
Parametric Studies

Effect of Lateral Diameter on Gas Phase Moisture



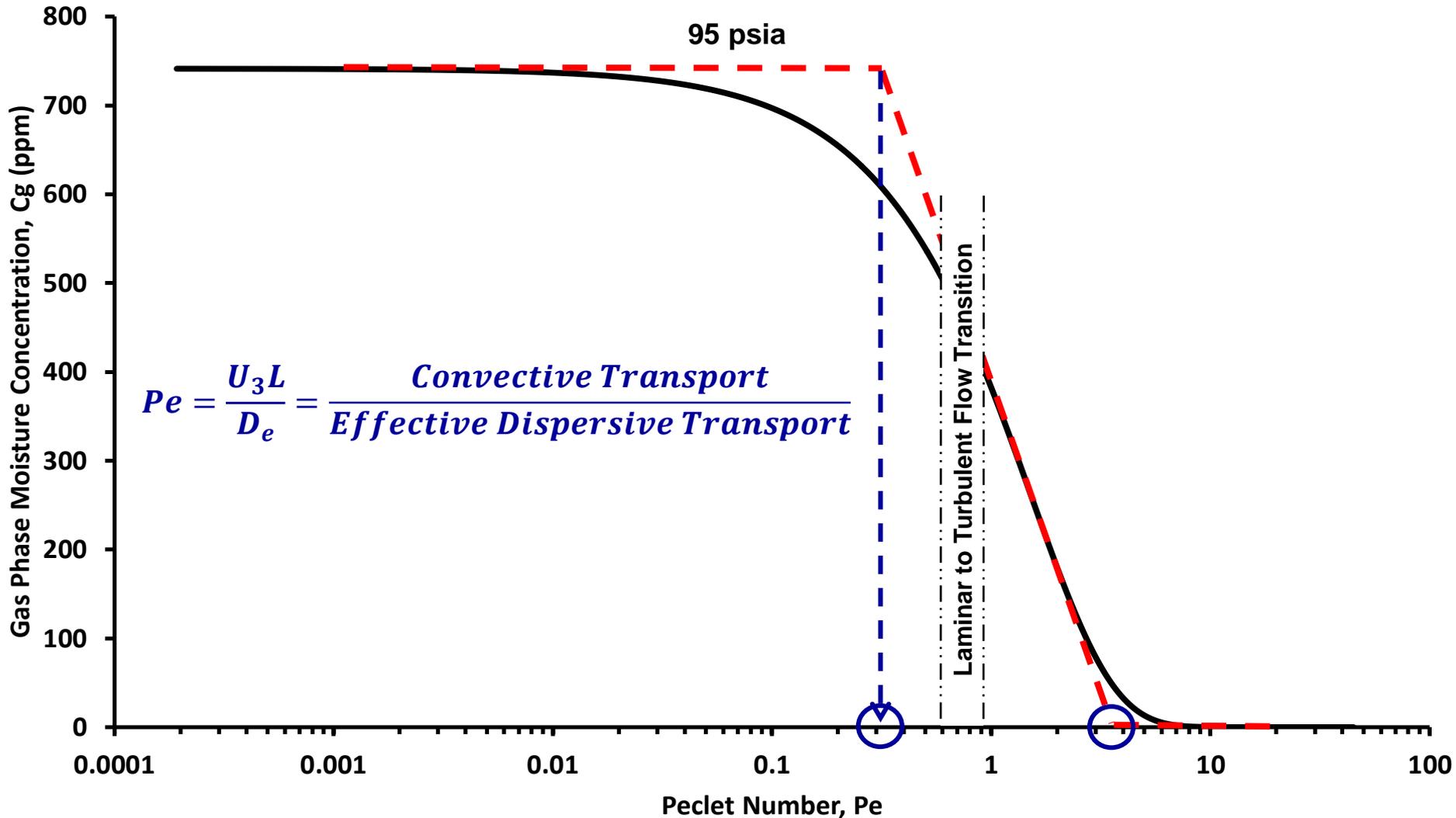
Parametric Studies

Effect of Reynolds Number on Gas Phase Moisture



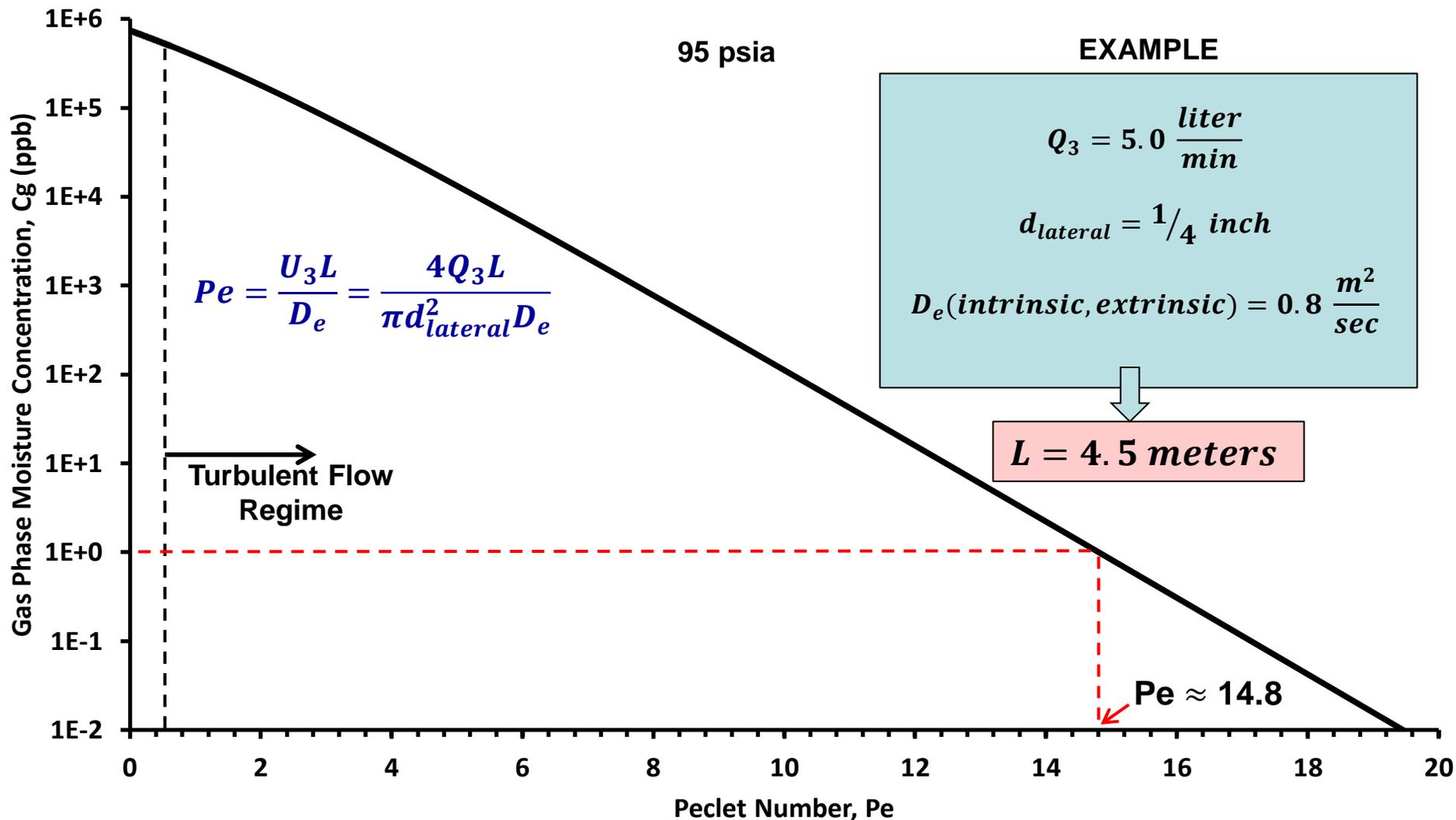
Parametric Studies

Effect of Peclet Number on Gas Phase Moisture



Parametric Studies

Effect of Peclet Number on Gas Phase Moisture



Back Diffusion Process Simulator: Orifice Addition

Convective Flux

$$J_c = -U_3 C_g$$

Gas Phase Dispersive Flux

$$J = -D \frac{dC_g}{dz}$$

Surface Diffusive Flux

$$J_s = -D_s \frac{dC_s}{dz} - D_s \frac{k_a}{k_d} \frac{dC_g}{dz}$$

Total Dispersive Mass Flow Rate

$$\pi r^2 J_e = \pi r^2 J + 2\pi r J_s$$

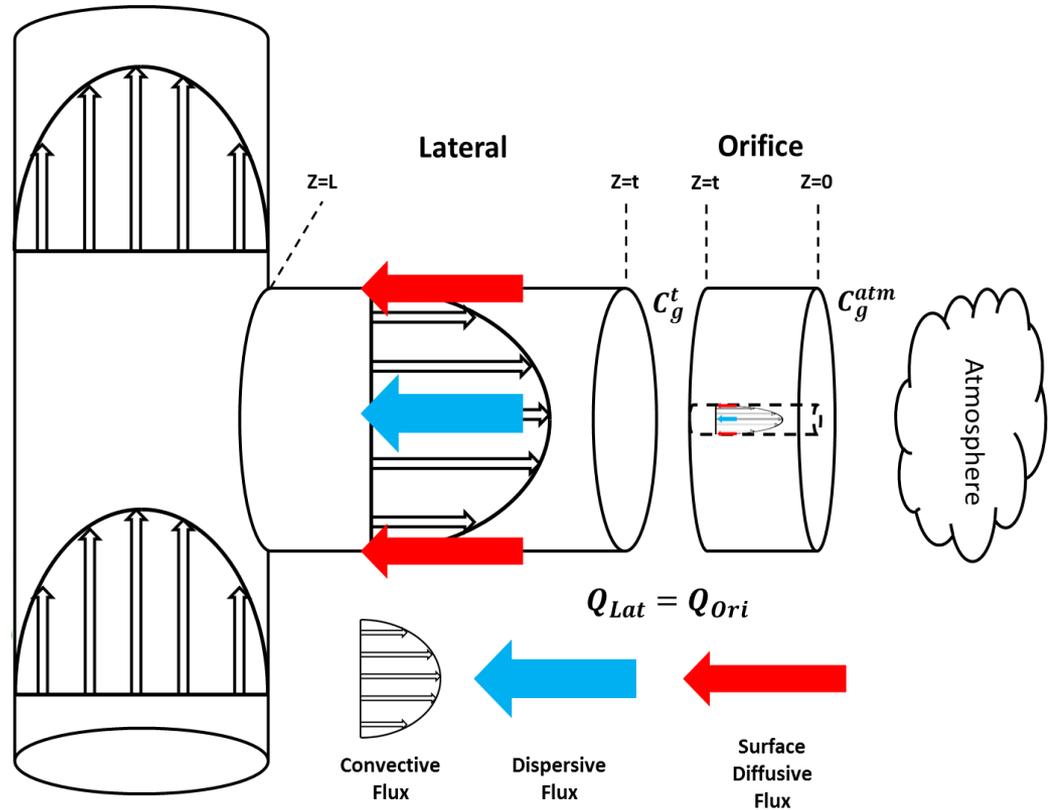
Effective Dispersion Coefficient

$$D_e = D + \frac{2}{r} D_s K_e$$

Governing Equation

$$U_3 \frac{dC_g}{dz} + D_e \frac{d^2 C_g}{dz^2} = 0$$

Convection
Effective Dispersion



Boundary Condition 1

$$z = 0, \quad D_m \left(\frac{C_g^{atm} - C_g}{t} \right) = \frac{Q_3}{A_{ori}} C_g$$

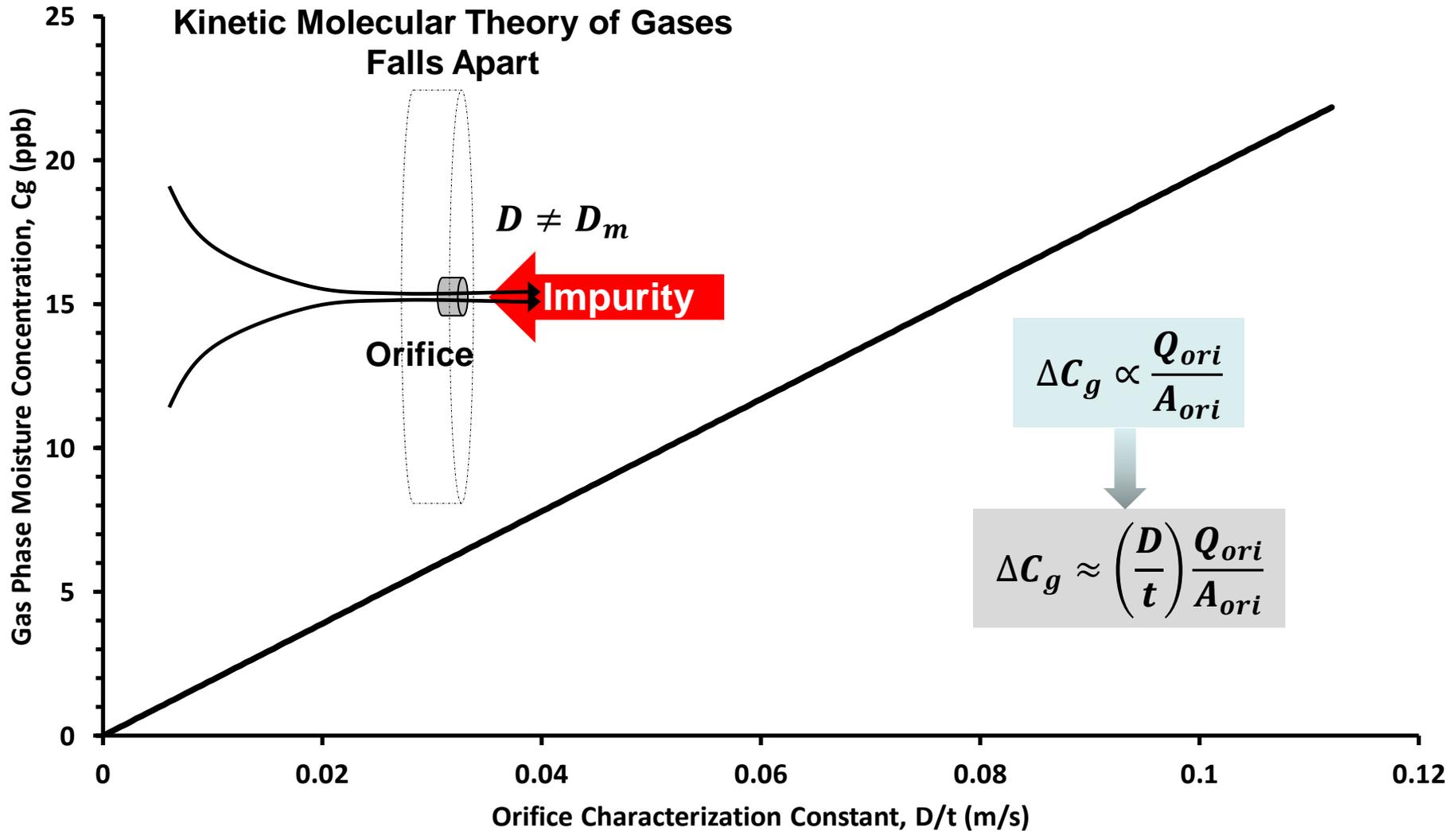
Convective Flux

Boundary Condition 2

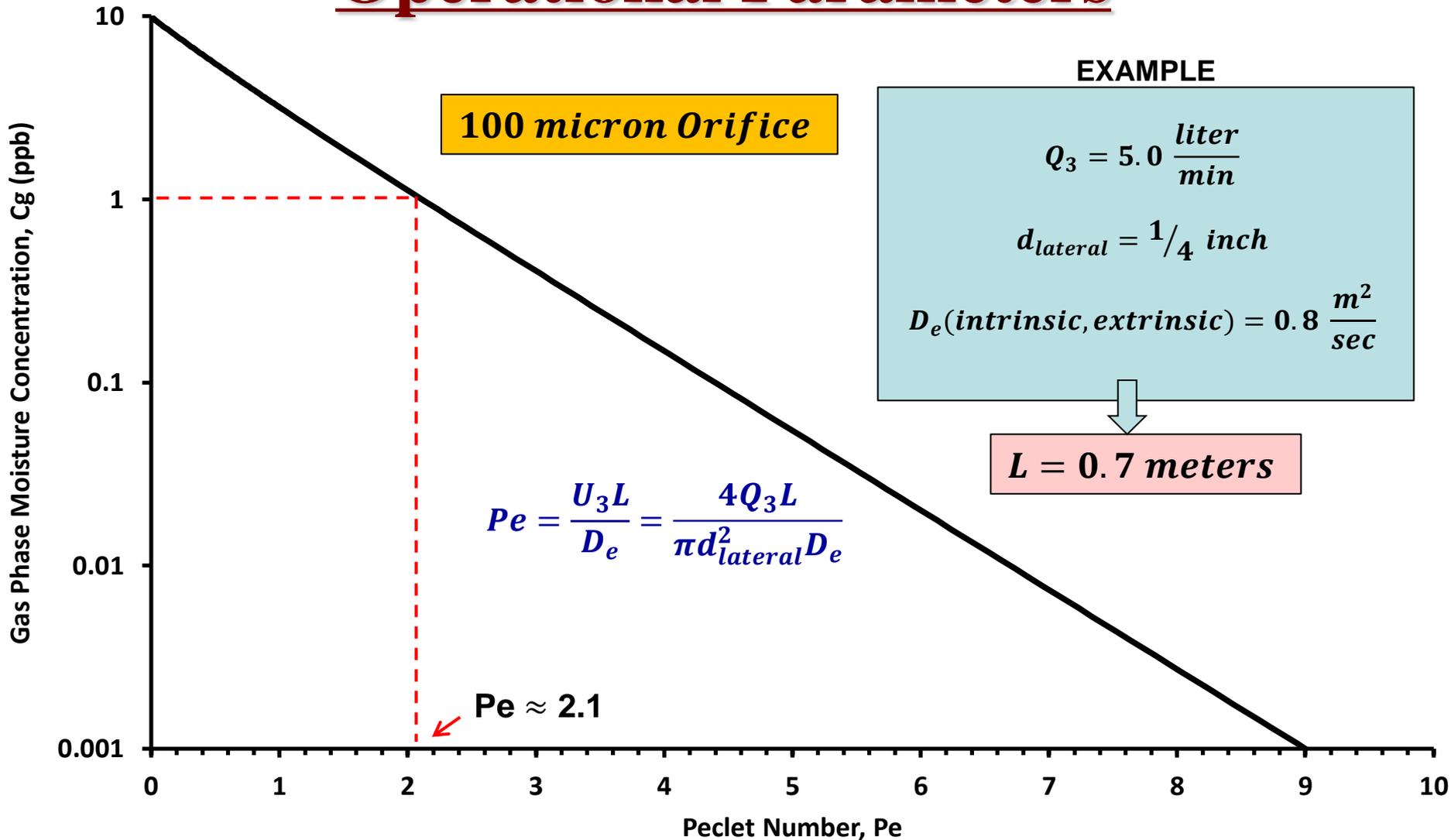
$$z = L, \quad C_g|_{z=L} = \left(-U_3 C_g|_{z=L} - D_e \frac{dC_g}{dz} \Big|_{z=L} \right) \frac{A_{lateral}}{Q_2}$$

Effective Dispersive Flux

Orifice Addition to Simulator



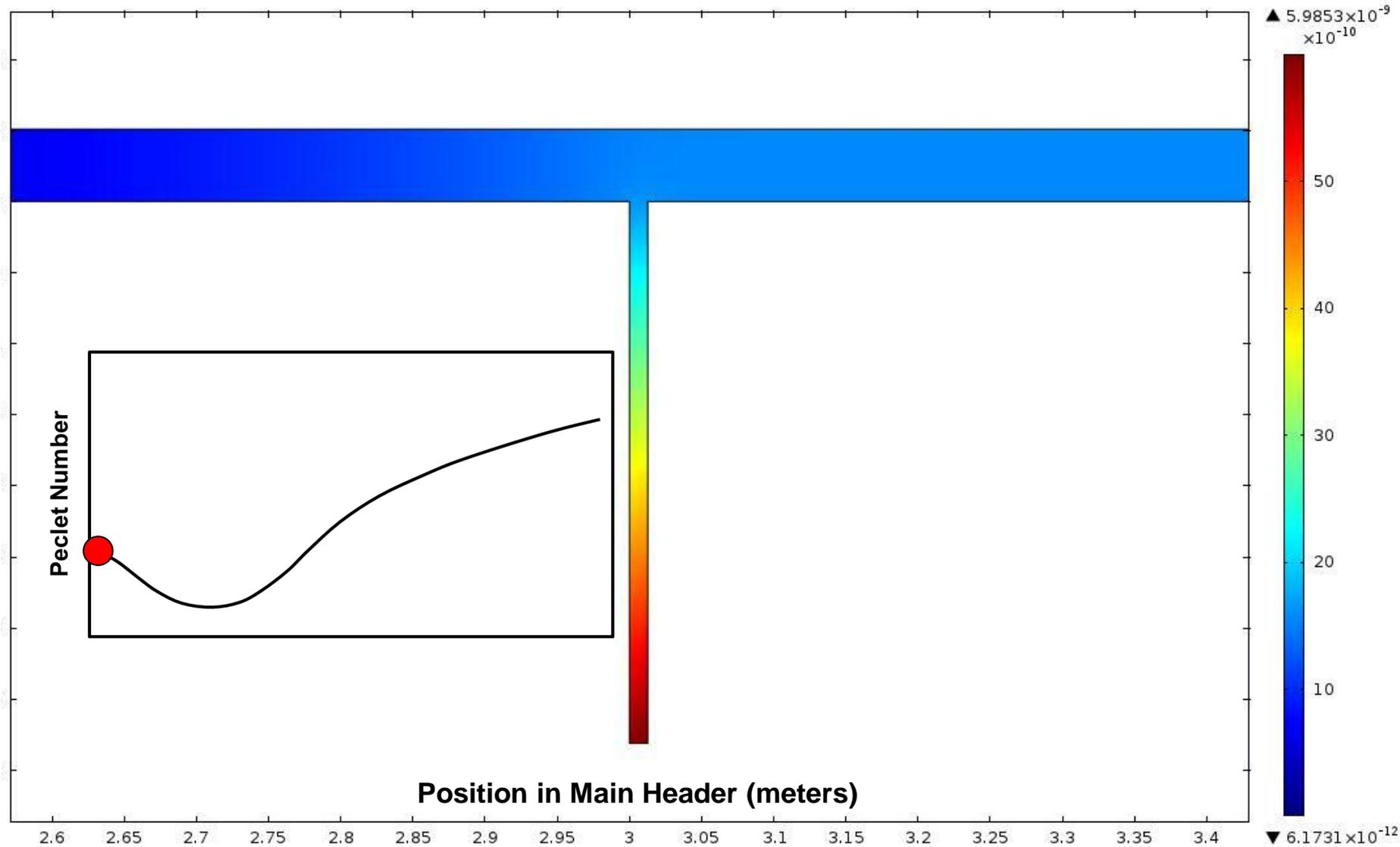
Orifice Impact on Design and Operational Parameters



Simulation: 1

Surface: Concentration (mol/m³)

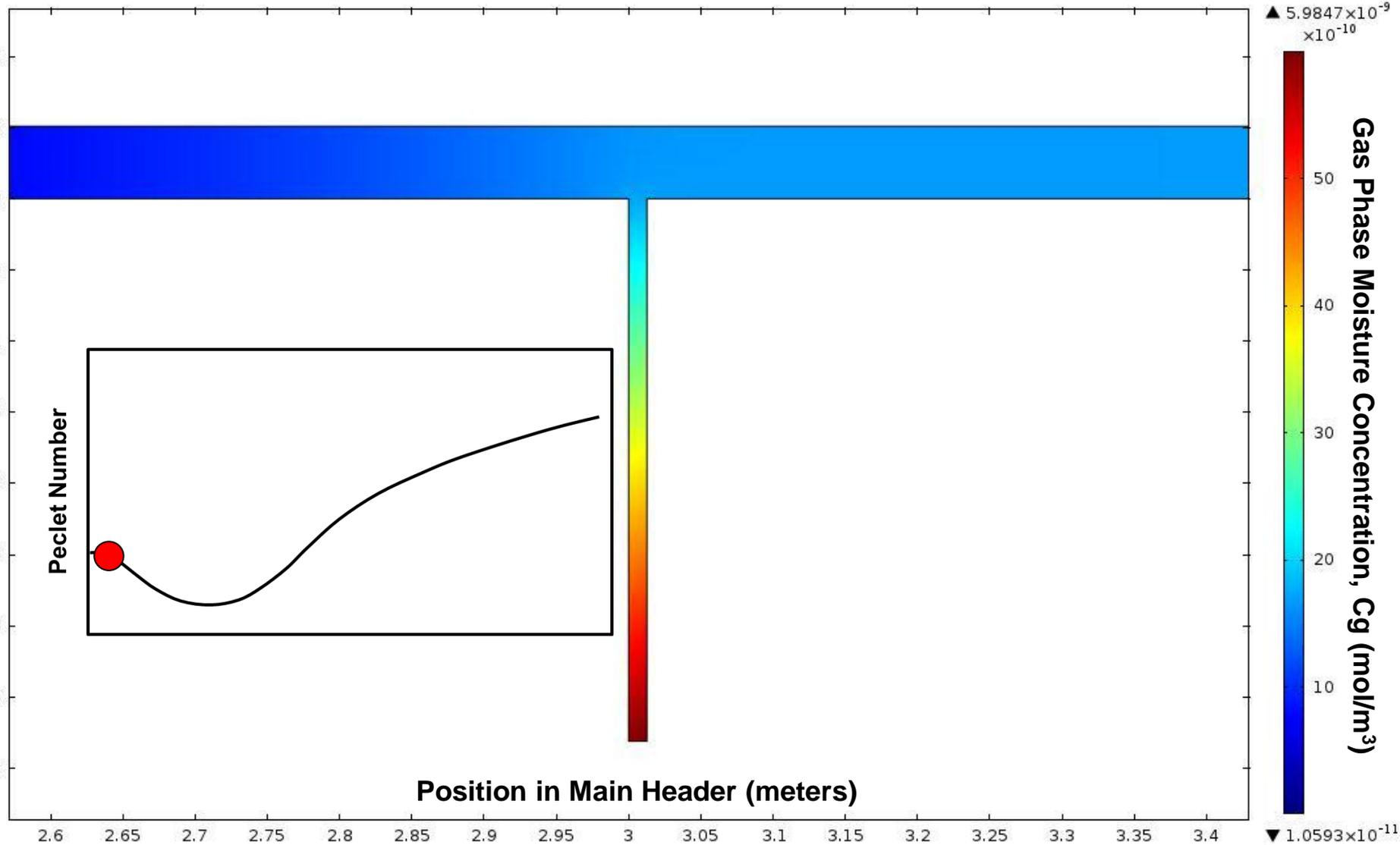
COMSOL
MULTIPHYSICS



Simulation: 2

Surface: Concentration (mol/m³)

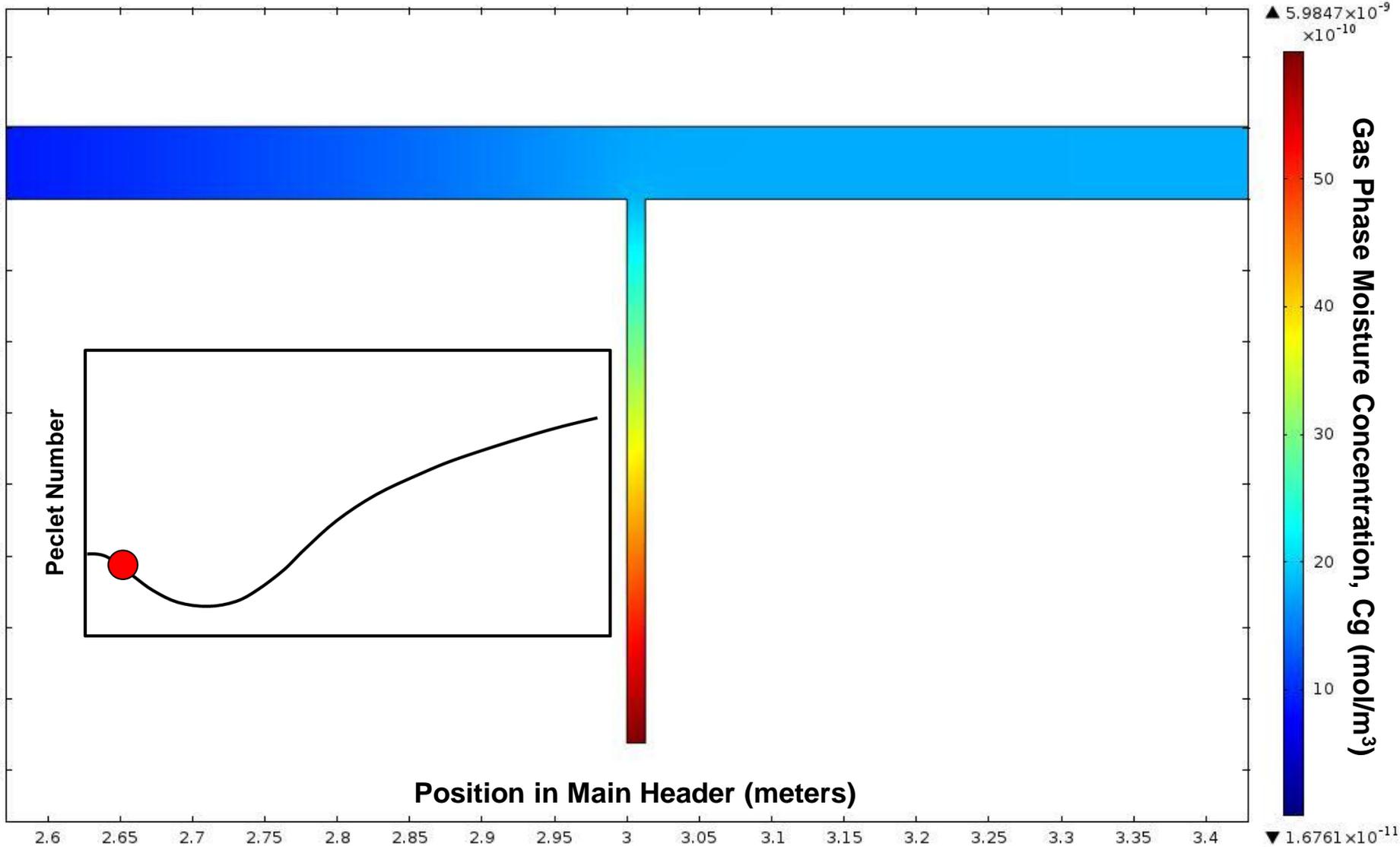
COMSOL
MULTIPHYSICS



Simulation: 3

Surface: Concentration (mol/m³)

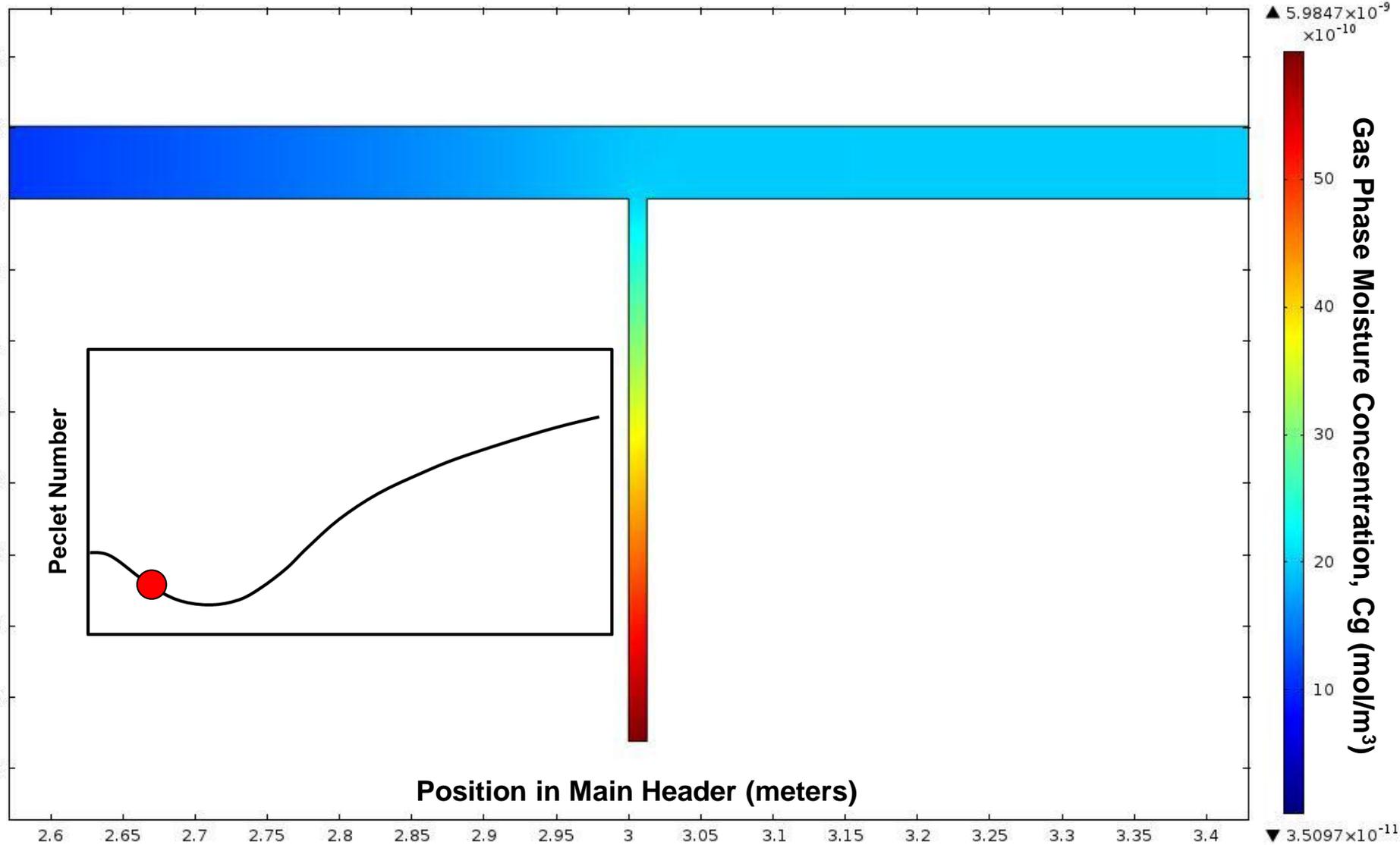
COMSOL
MULTIPHYSICS



Simulation: 4

Surface: Concentration (mol/m³)

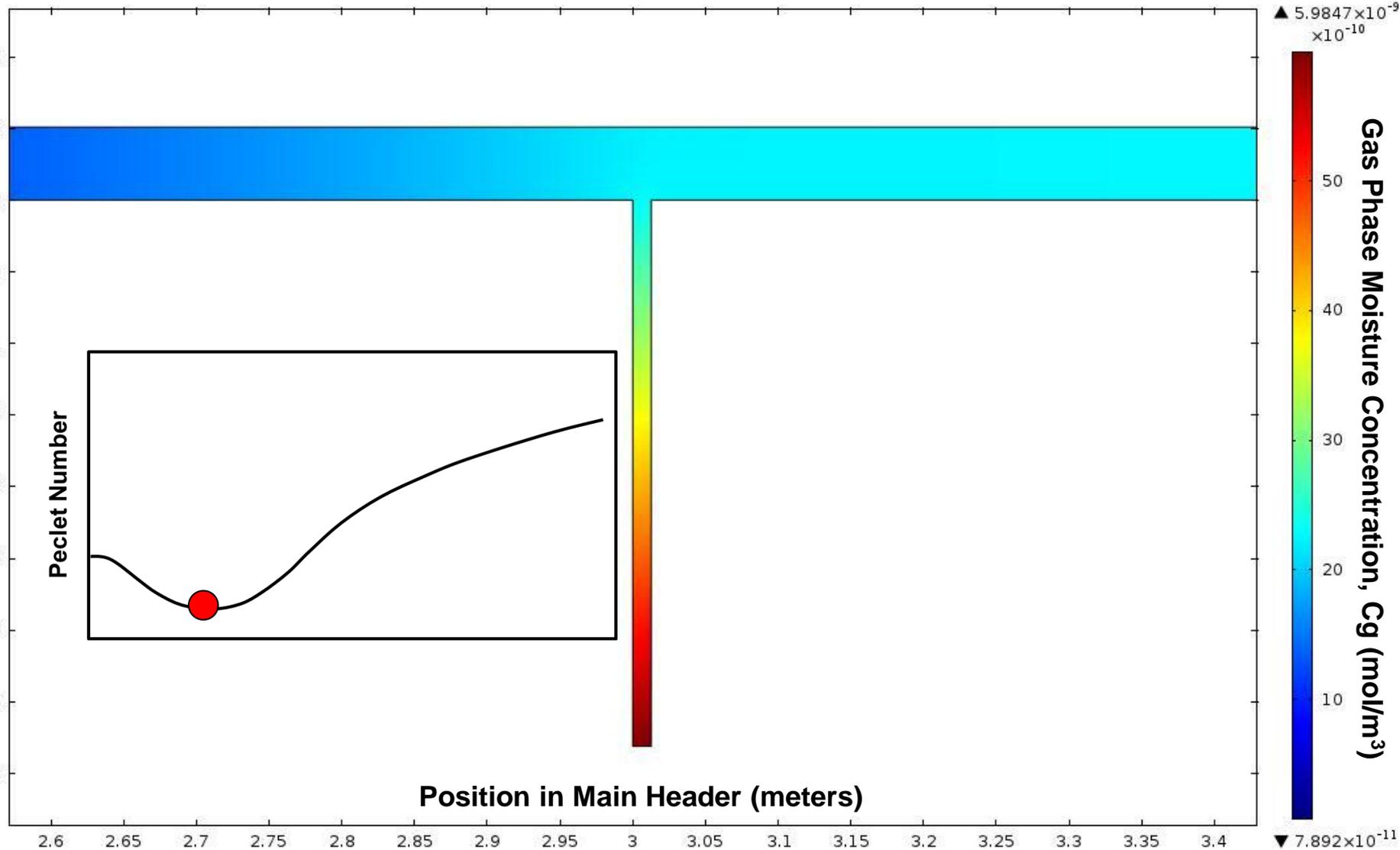
COMSOL
MULTIPHYSICS



Simulation: 5

Surface: Concentration (mol/m³)

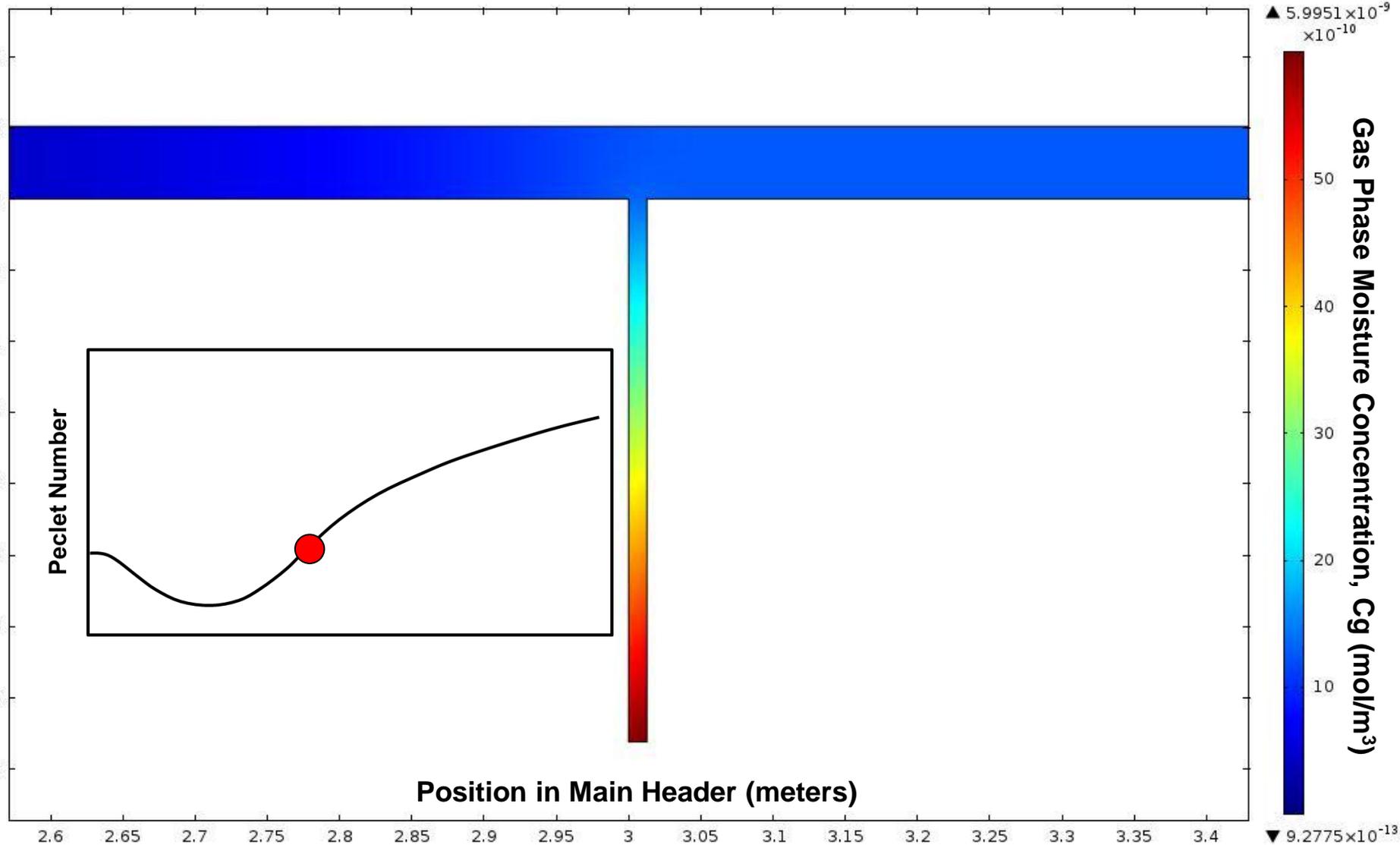
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Simulation: 6

Surface: Concentration (mol/m³)

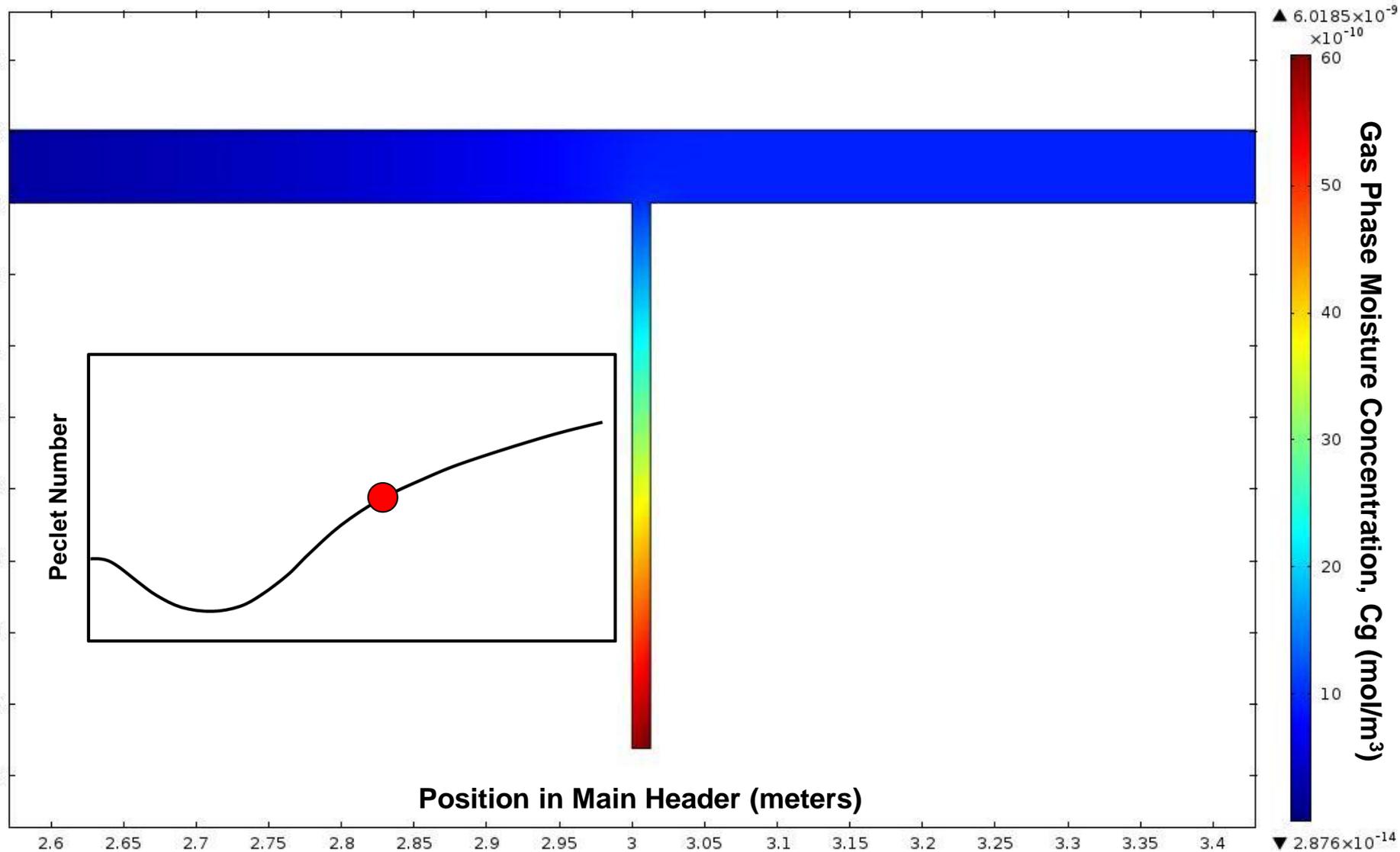
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Simulation: 7

Surface: Concentration (mol/m³)

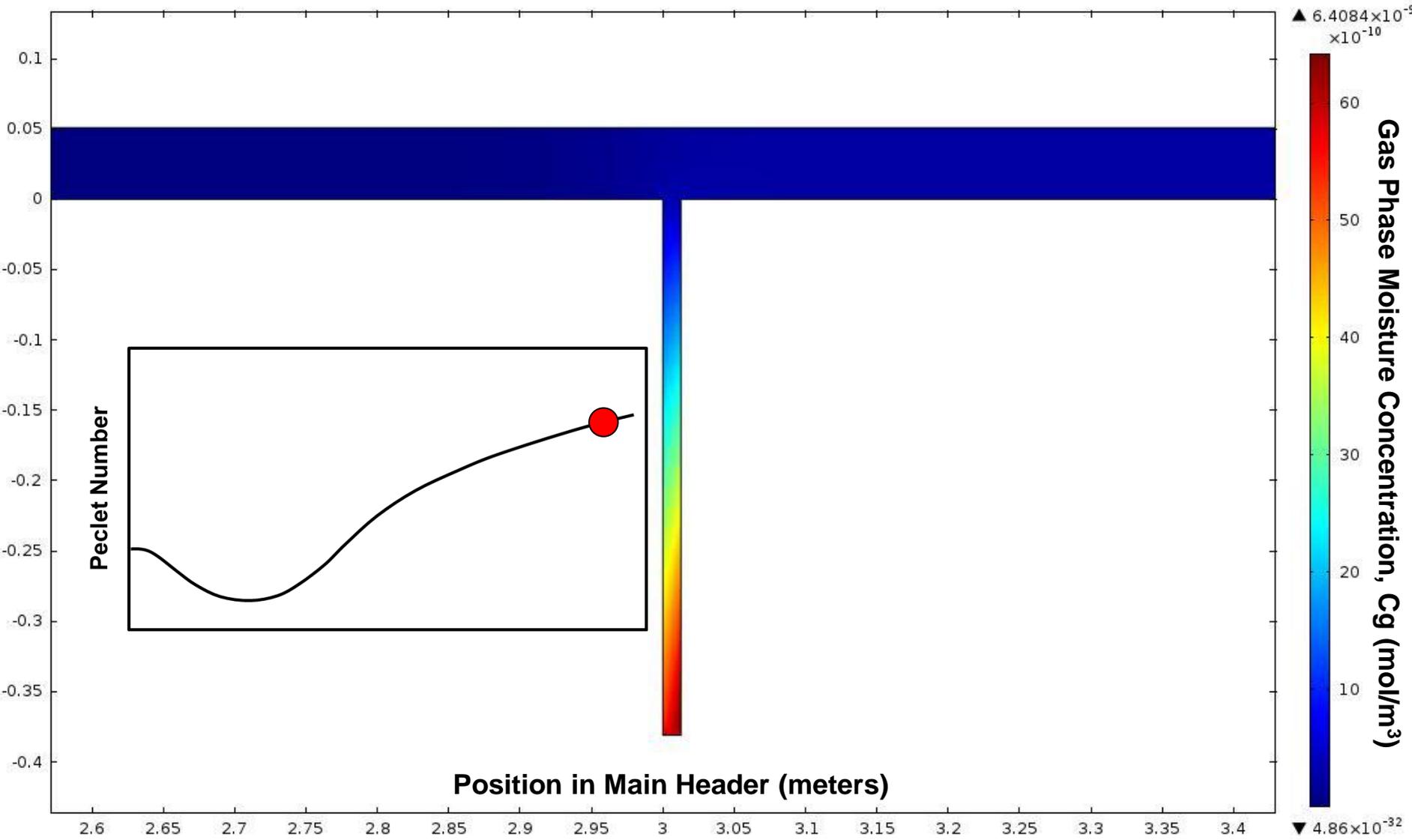
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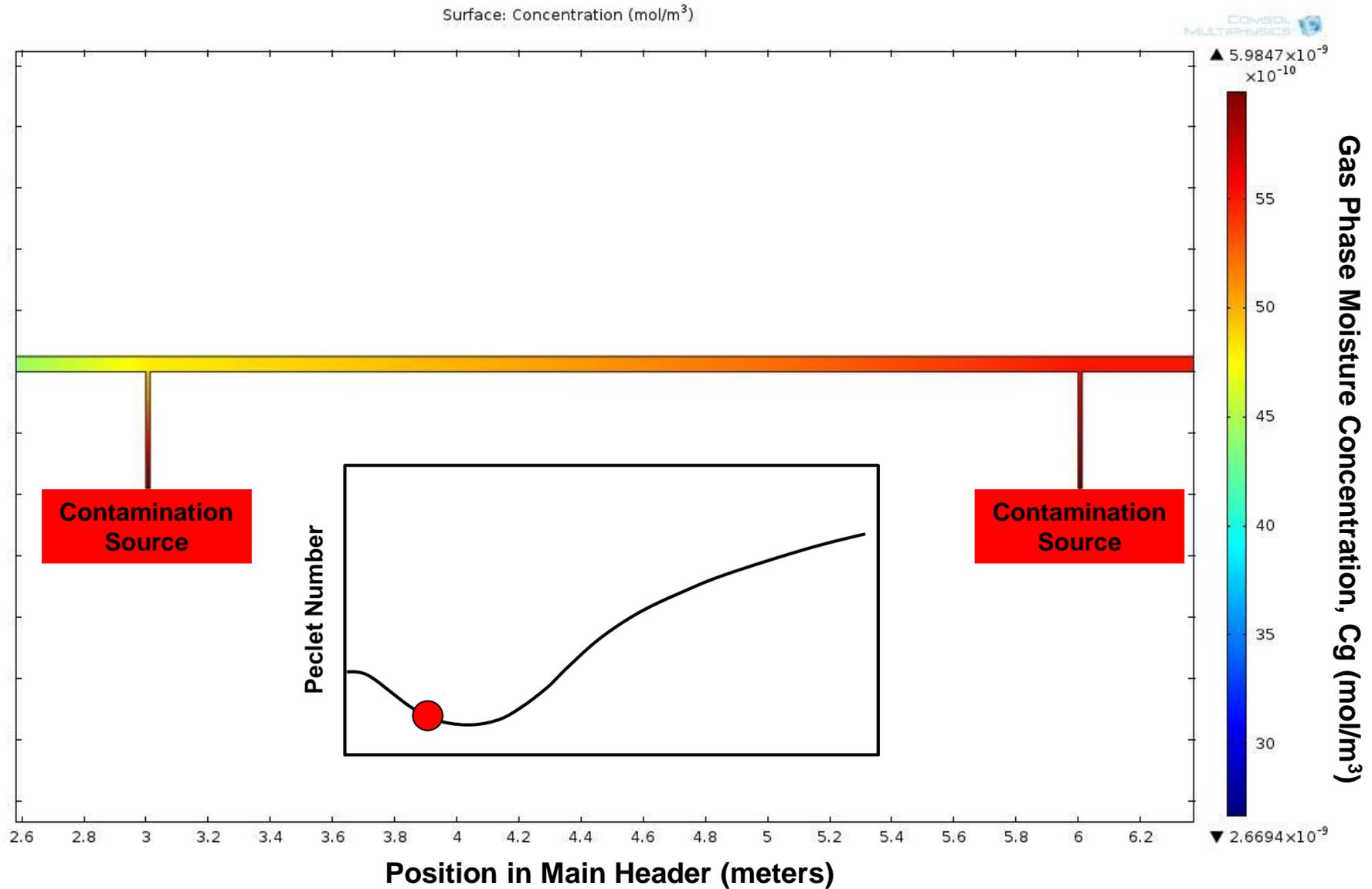
Simulation: 8

Surface: Concentration (mol/m³)

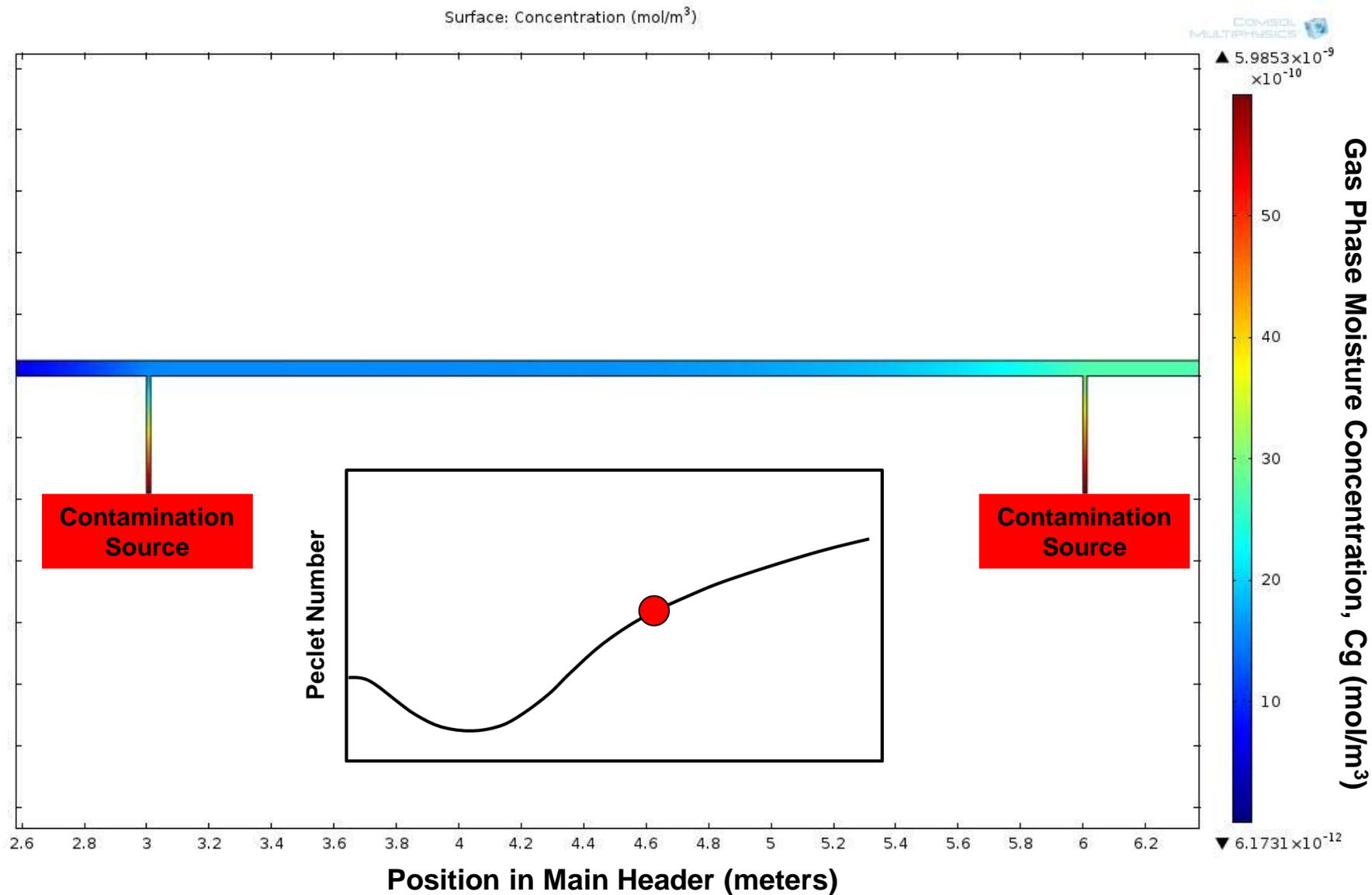
COMSOL
MULTIPHYSICS



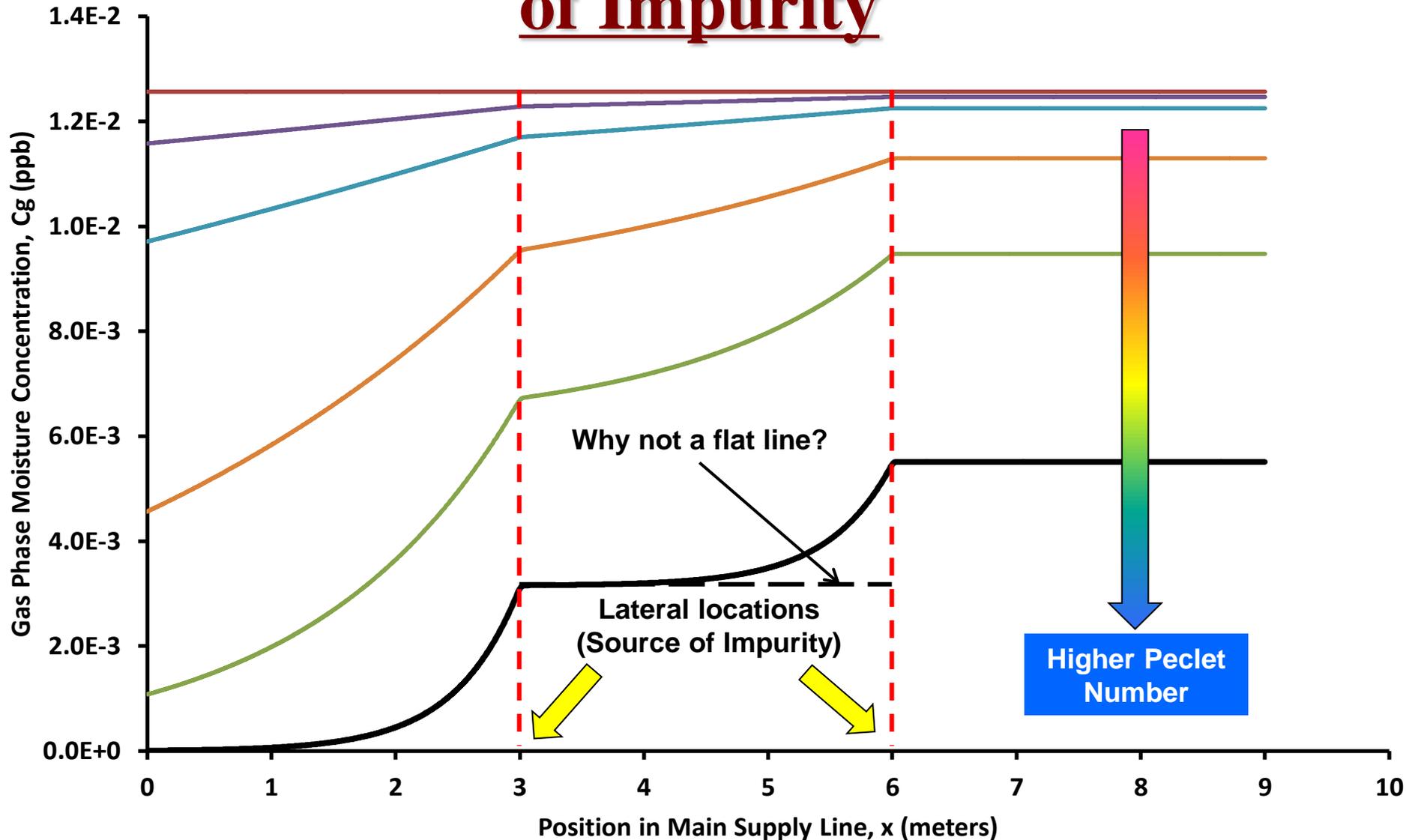
Simulation: 9



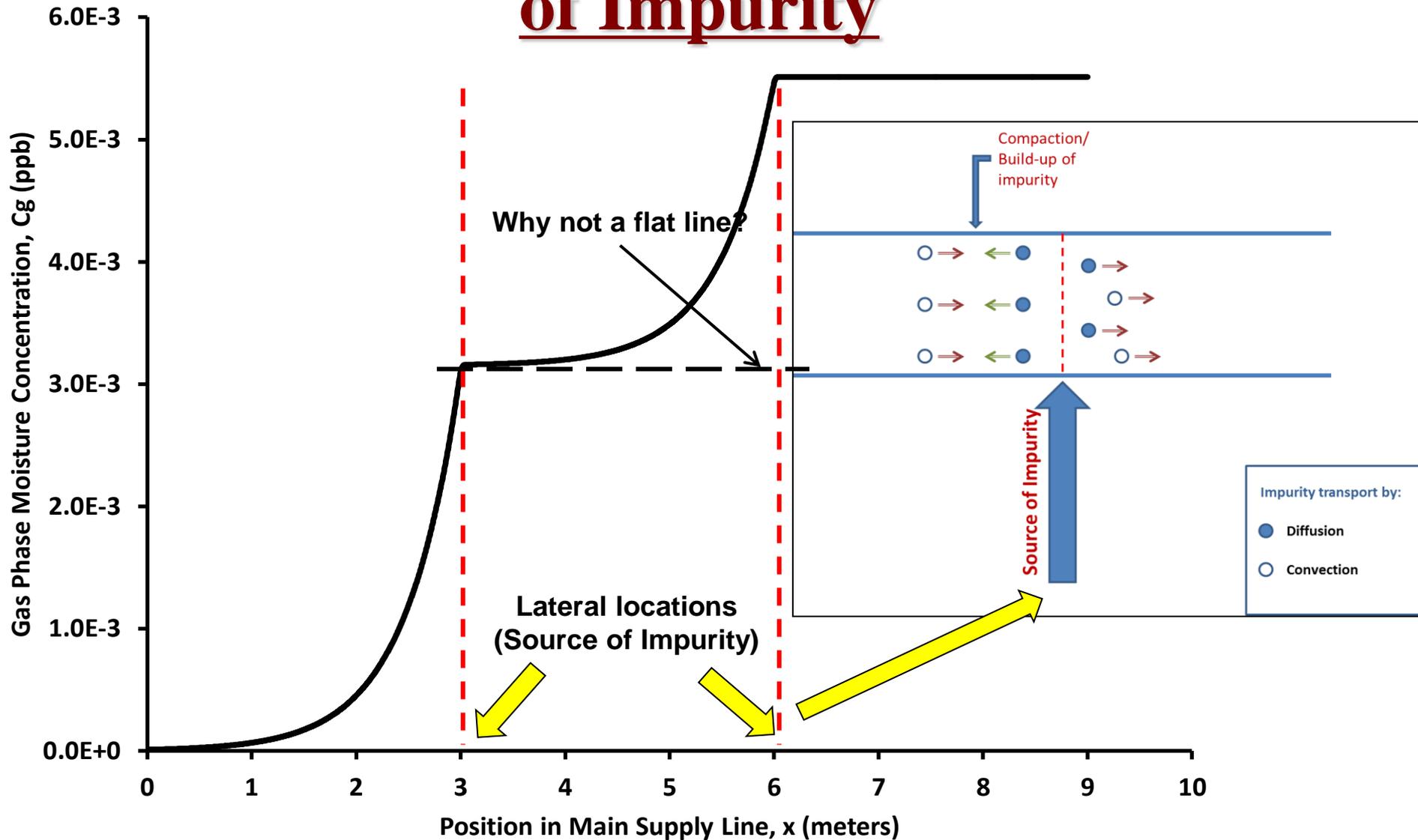
Simulation: 10



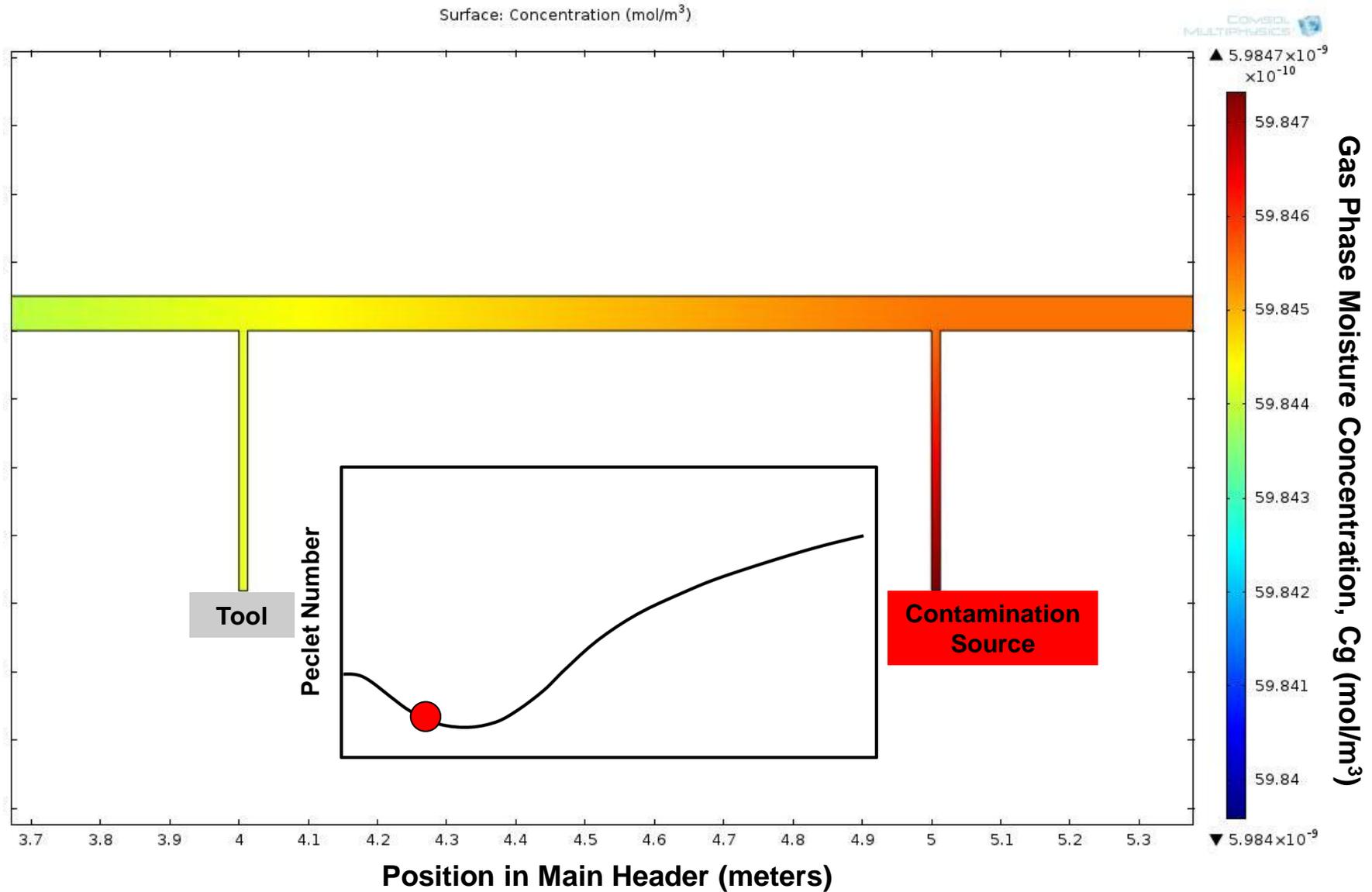
Compounding Effect of Multiple Sources of Impurity



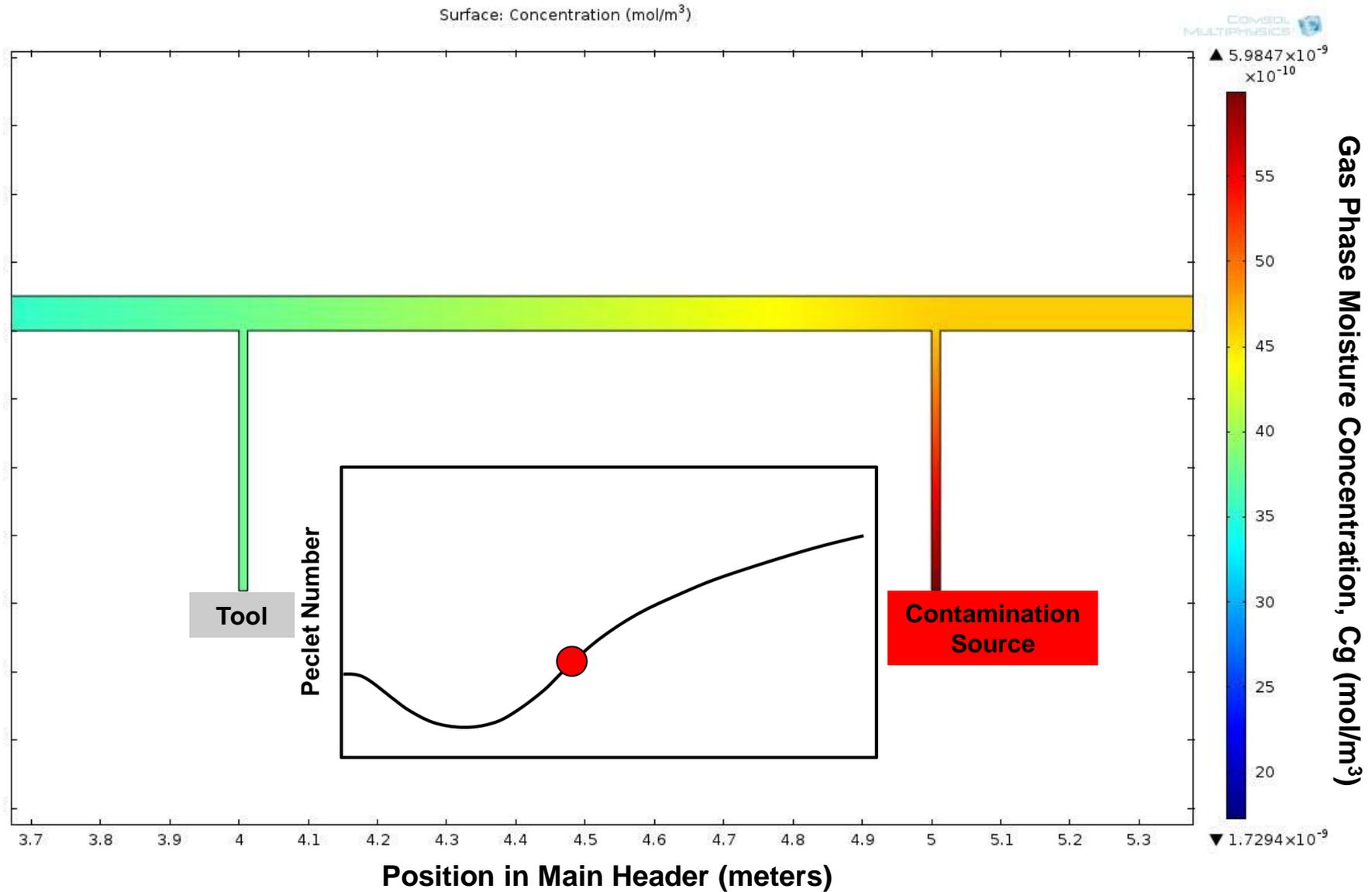
Compounding Effect of Multiple Sources of Impurity



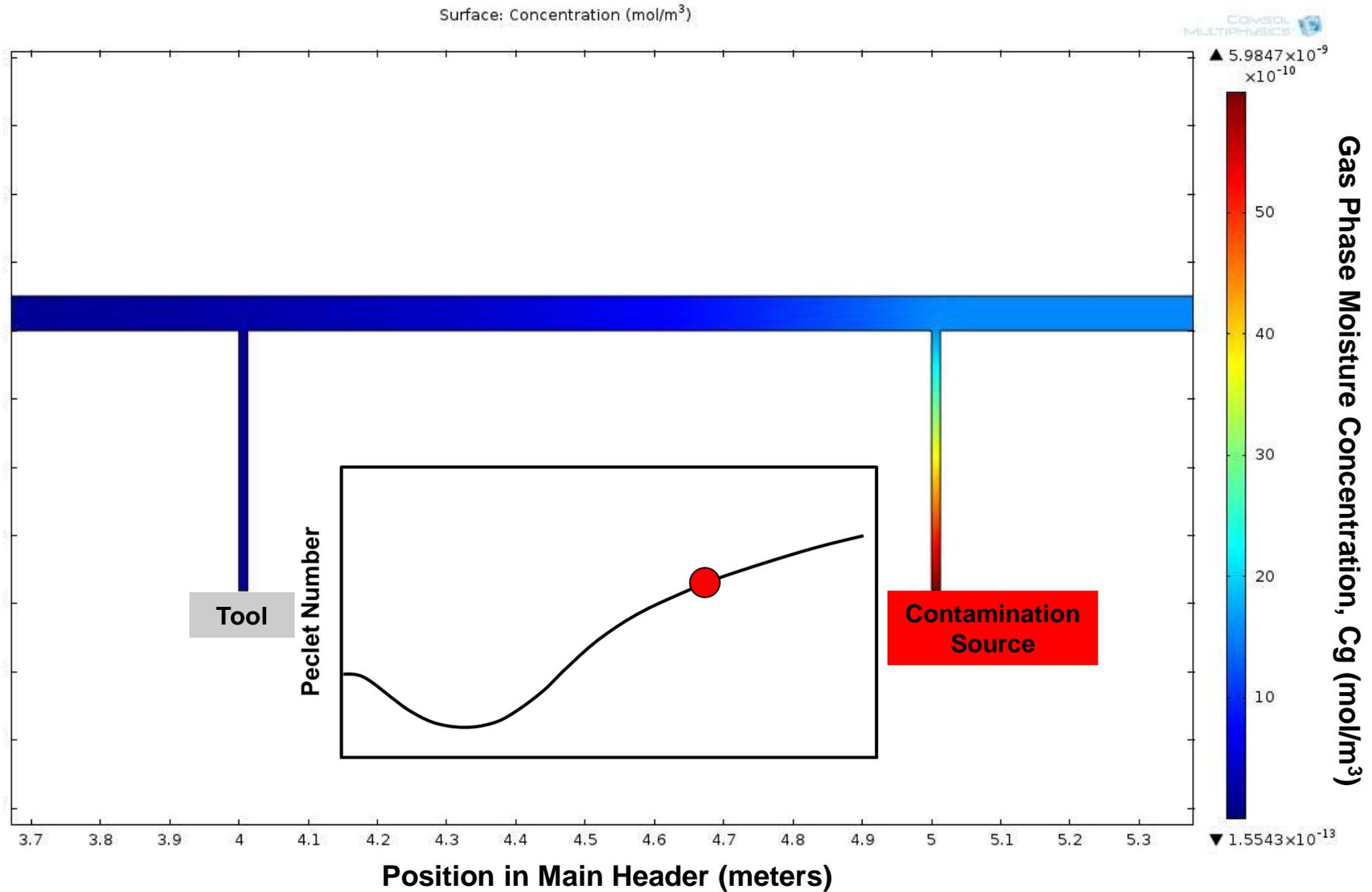
Simulation: 11



Simulation: 12



Simulation: 13



Highlights

- **The experimental approach allowed for the observation of back diffusion in an adjustable and controllable manner.**
- **The process model accurately predicted experimental results and was invaluable in performing parametric studies.**
- **The moisture contamination due to back diffusion was a strong function of lateral diameter, length, and gas flow rate through the lateral.**
- **Characteristic groups were identified that allowed us to present generalized correlations that would help in the design and operation of UHP fluidic systems being exposed to a source of contamination**
- **This methodology was expanded to include an orifice and lateral in series and was effective in determining a design approach that will safeguard against the back diffusion of impurities into both bulk and process gases.**
- **The simulator showed flexibility in regards to being able to predict contaminant transport in systems with multiple sources of contamination as well as predicting the impact of such contamination on neighboring tools.**

Industrial Interactions and Future Plans

- **Continue our work with Intel on novel impurity control strategies to reduce gas usage**
- **Making the process simulator available to industry**
- **Extending the present study to other fluids, contaminants, and components**

Acknowledgements

- **Carl Geisert, Intel**
- **Tiger Optics support team**