Lowering Material and Energy Usage during Dry-down of Ultra-pure Gas Delivery Systems*

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**** Customized project for Intel***

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Outline

- Background
- Research objectives and ESH implications
- Parts need to be cleaned in UHP gas delivery systems
- Potential major contamination sources in UHP gas delivery systems
- Experimental and process models
    1. Pipe wall
    2. Dead leg
    3. Back-diffusion
- Comprehensive model & its application
- Conclusion
- Future work and Acknowledgements

Objectives

- **Develop methods to analyze contamination *introduction* and *removal* in ultra-pure gas delivery systems**

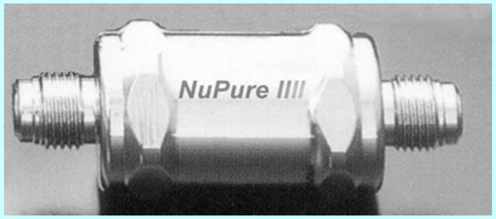
ESH Impacts

- **Contamination of gas distribution systems during operation or at start-up is a major source of wasted time, materials, and energy.**
- **Significant reduction in purging time and gas usage can be accomplished by optimizing purging and cleaning processes, based on the project results.**

What needs to be cleaned?

EPSS Pipes

Valves



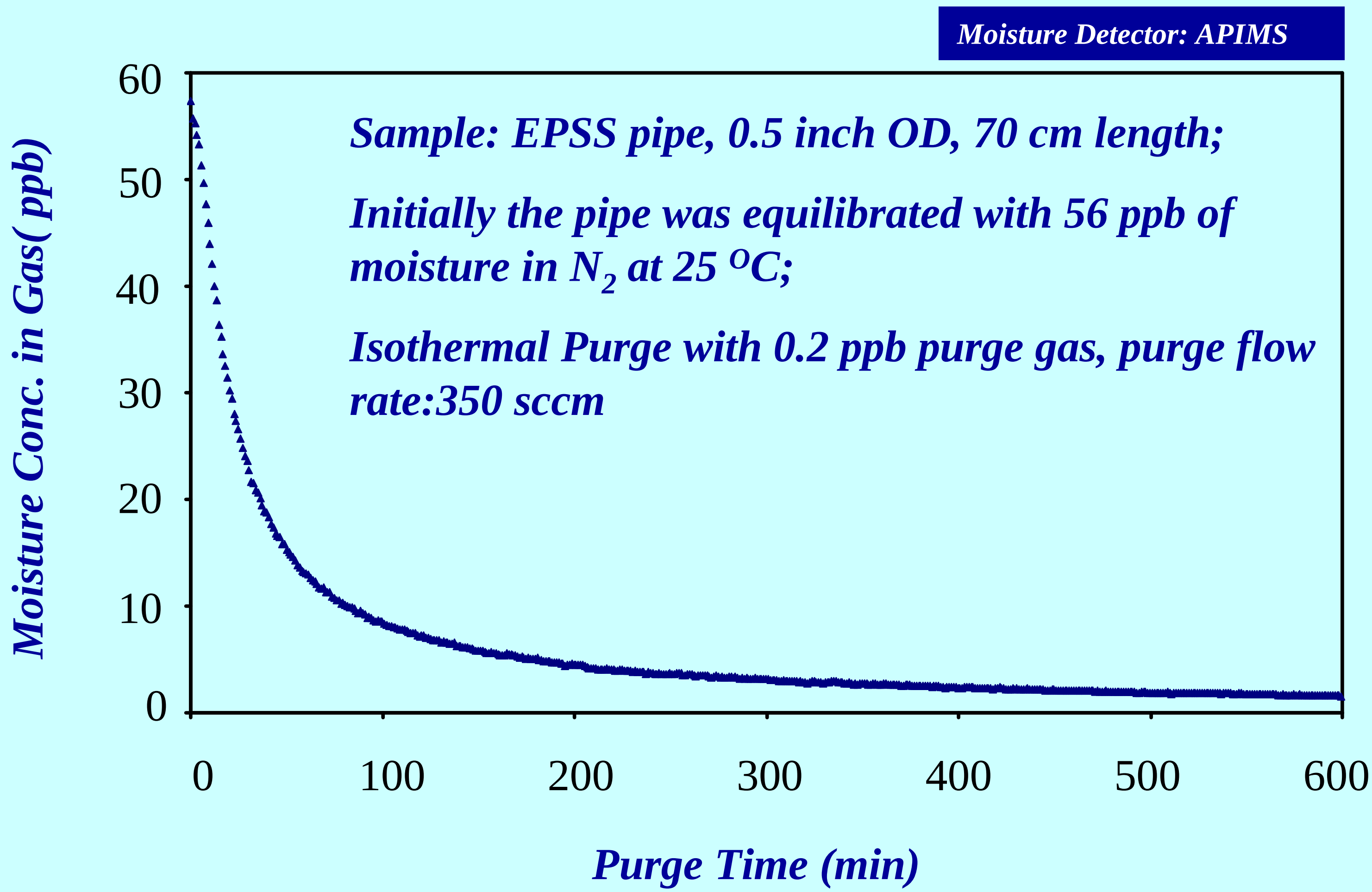
Particle Filters

Mass Flow Controllers, Flow Meters

Regulators

Cleaning/purging processes for these contaminated parts fast or slow?

Moisture Dry-down --- *EPSS* Pipe

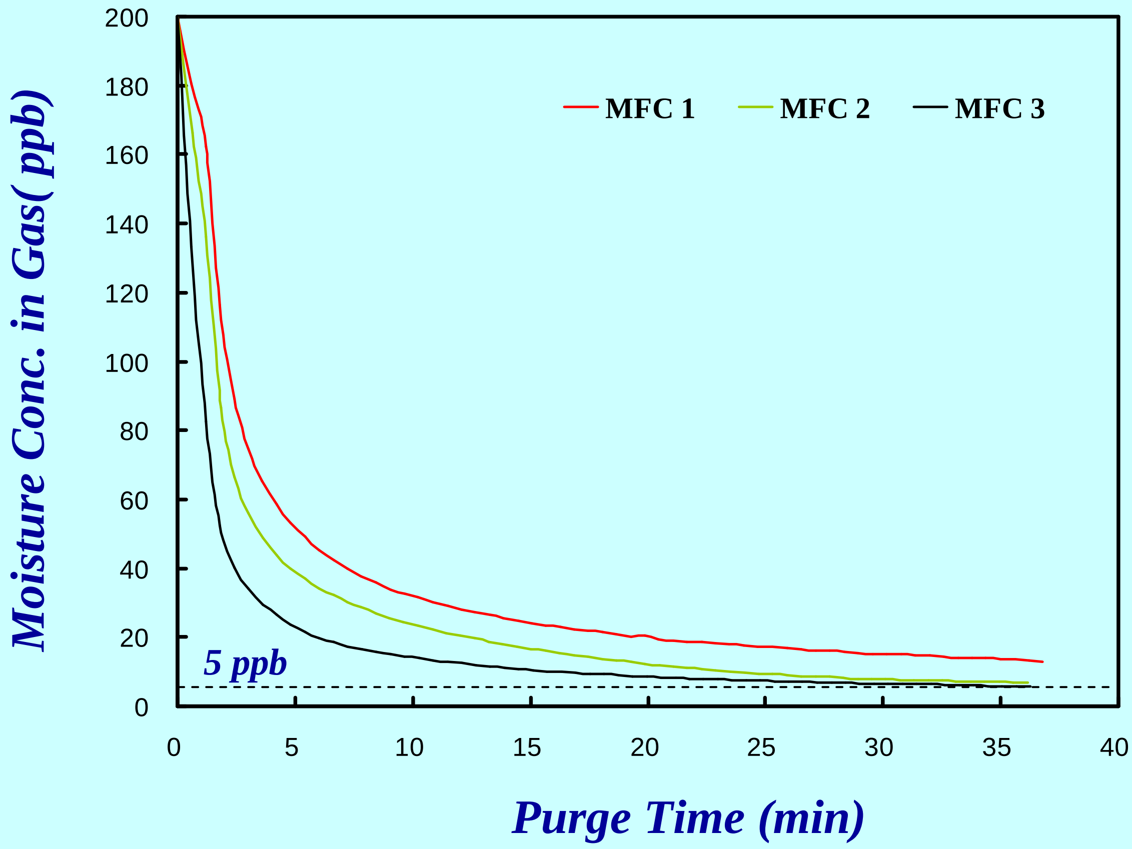


Moisture removal on stainless steel pipe is a slow process.

Moisture Dry-down --- MFC

Initially the MFCs were equilibrated with 200 ppb of moisture in N_2 at 25 ^{O}C;

Isothermal Purge with 0.2 ppb purge gas , purge flow rate: 500 sccm



Moisture Detector: APIMS

Moisture Dry-down --- Other Components

Valves*: please refer to literature

***Filters*:**

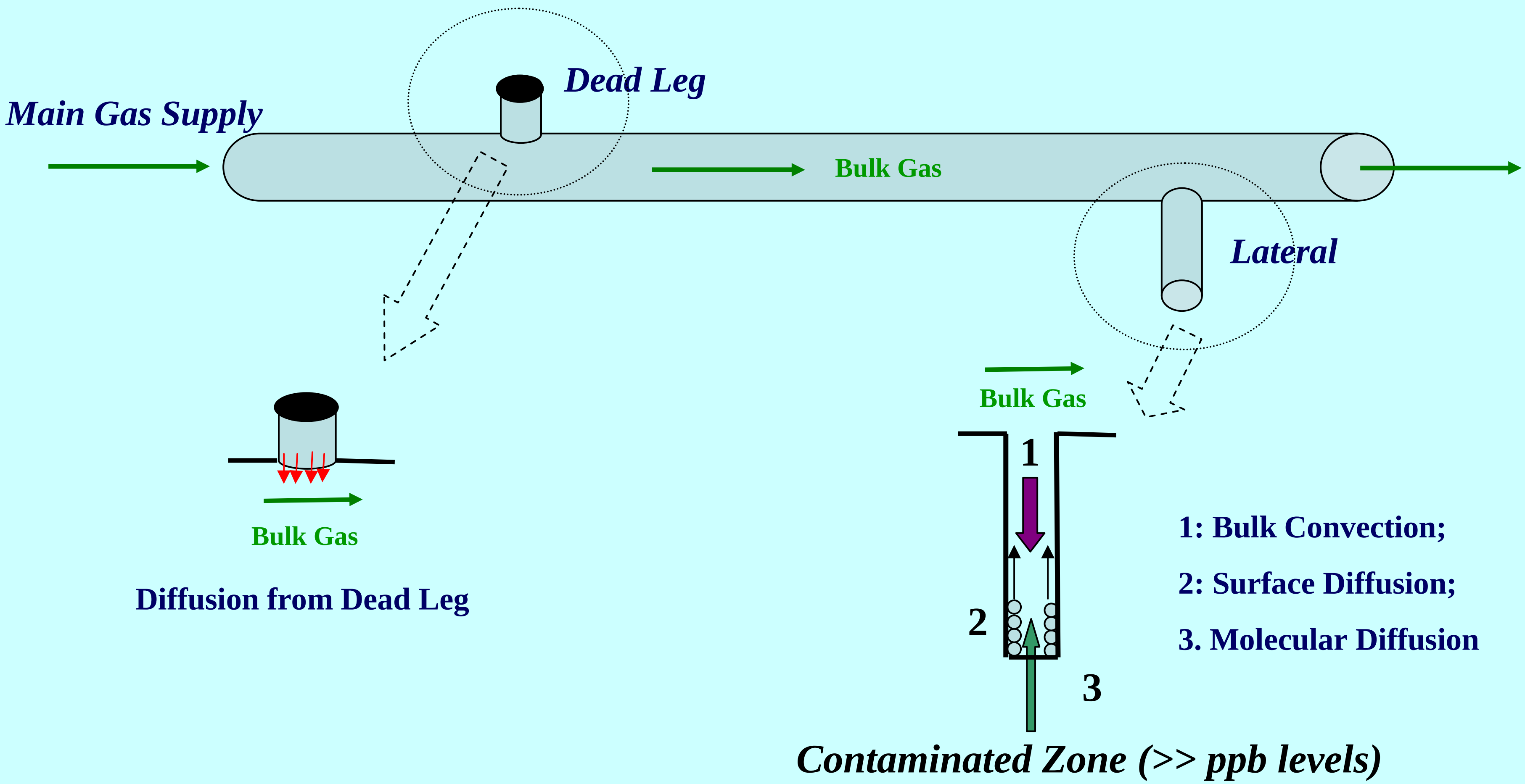
*Moisture Dry-down of Different Types of Filters ***

Filters (Surface area/m^2)	Ceramic (13.65)	Metallic (1.19)	Polymeric A (0.52)	Polymeric B (0.96)	Polymeric C (1.5)
Concentration (ppb)	180 → 20	300 → 20	100 → 20	150 → 20	180 → 20
Time (min)	580	110	12	65	42

** Seksan Dheandhanoo, James H. Yang, and Michael D. Wagner. Modeling the Characteristics of Gas System Dry-down. Solid State Technology, Vol. 44 No. 6 , June 2001, p.125.*

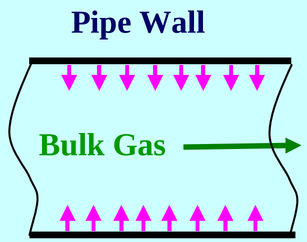
*** Asad M. Haider, Ce Ma, and Farhang Shadman, Interactions of Ceramic. Metallic and Polymeric Filters with Gaseous Contaminants. Proceedings of Institute of Environmental Sciences, 1993, p.158.*

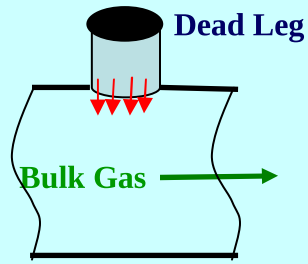
Other Potential Sources of Contamination

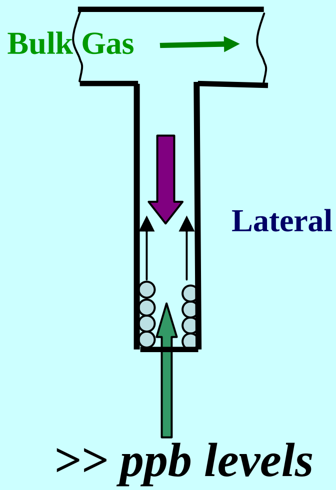


Diffusion from dead legs and back diffusion from ambient or contaminated zones can cause contamination to the whole gas delivery system.

What was mainly considered?







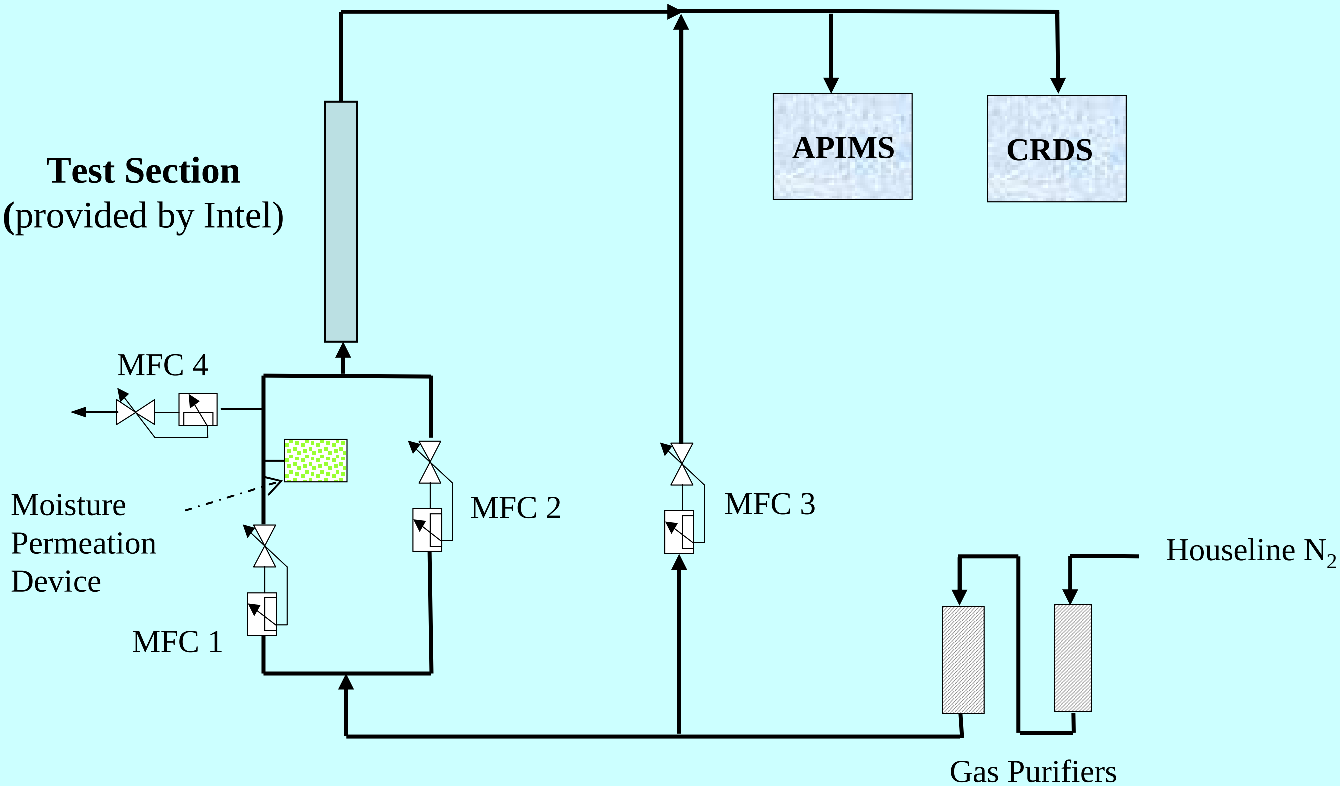
Desorption from Pipe Wall

Diffusion from Dead Leg

Back diffusion from Lateral

Comprehensive Model

Experimental Setup

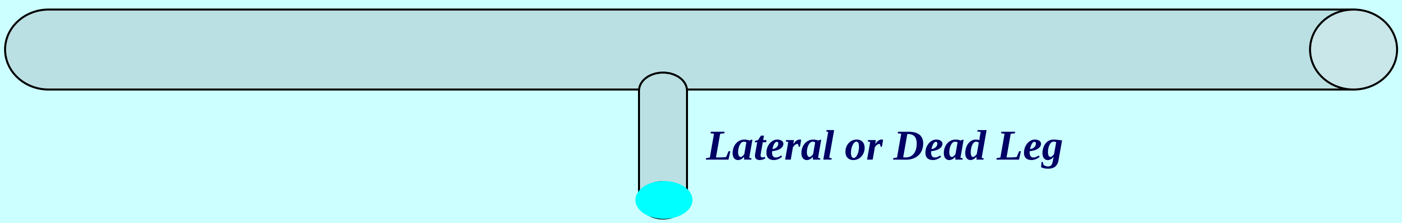


- **Atmospheric Pressure Ionization Mass Spectrometer (APIMS)**
- **Cavity Ring Down Spectroscope (CRDS)**

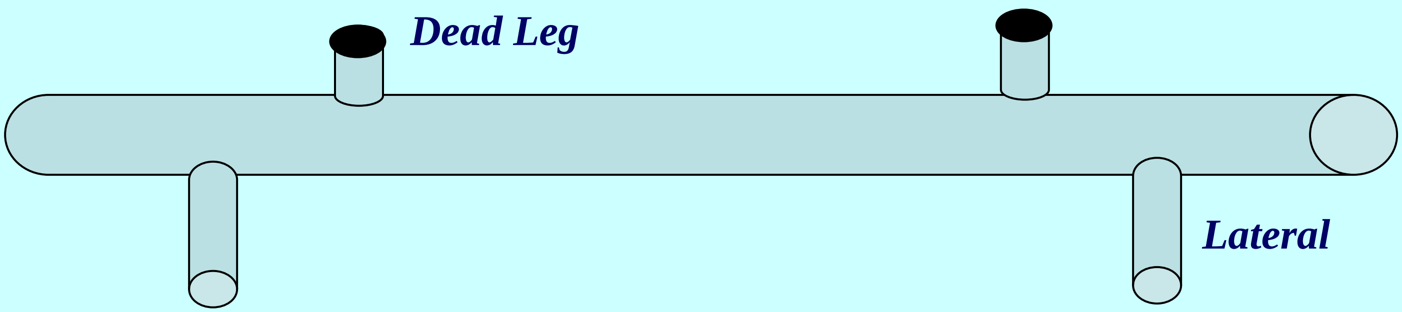
Test Sections (Provided by Intel)

Sample 1: single pipe

Sample 2: main pipe + one dead leg or one lateral

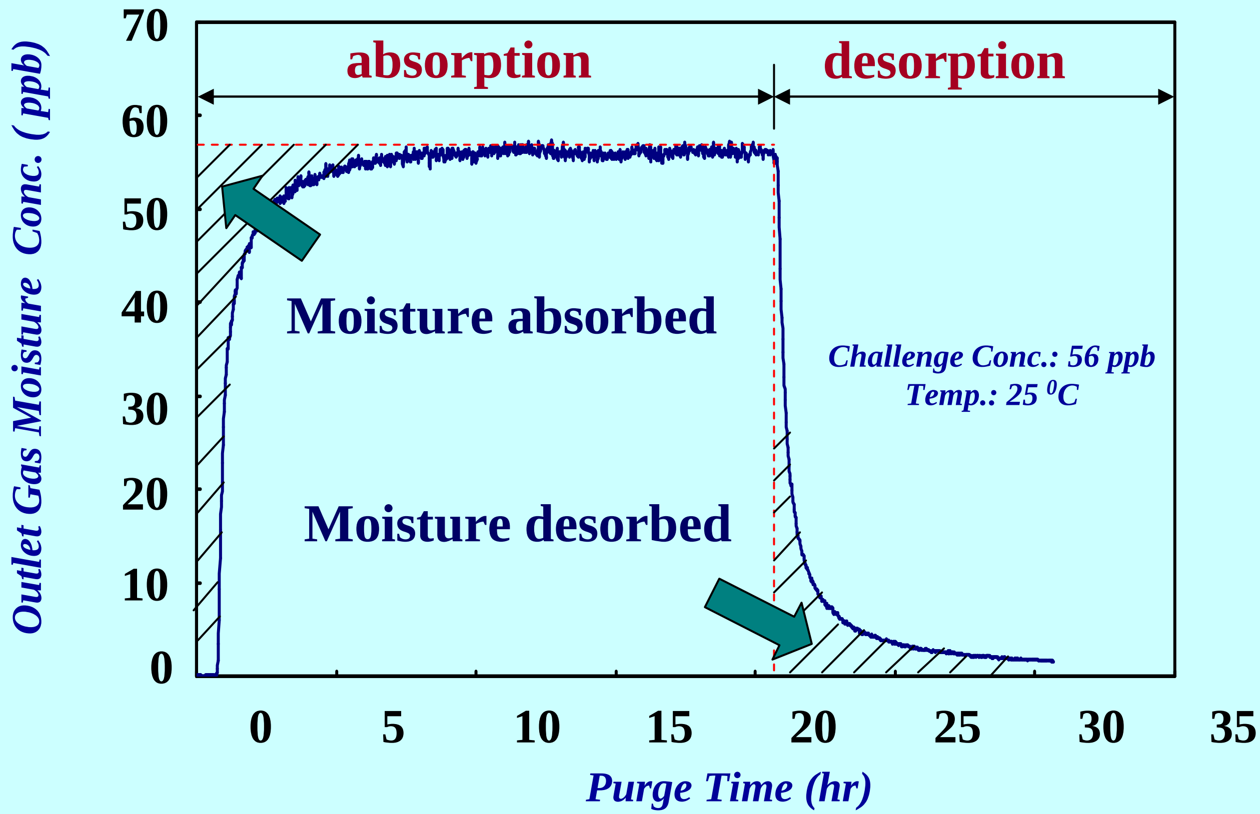


Sample 3: main pipe + several dead legs and laterals



- **The test sections represent some key features of a typical gas delivery system**
- **Fabricated and provided by Intel Arizona**

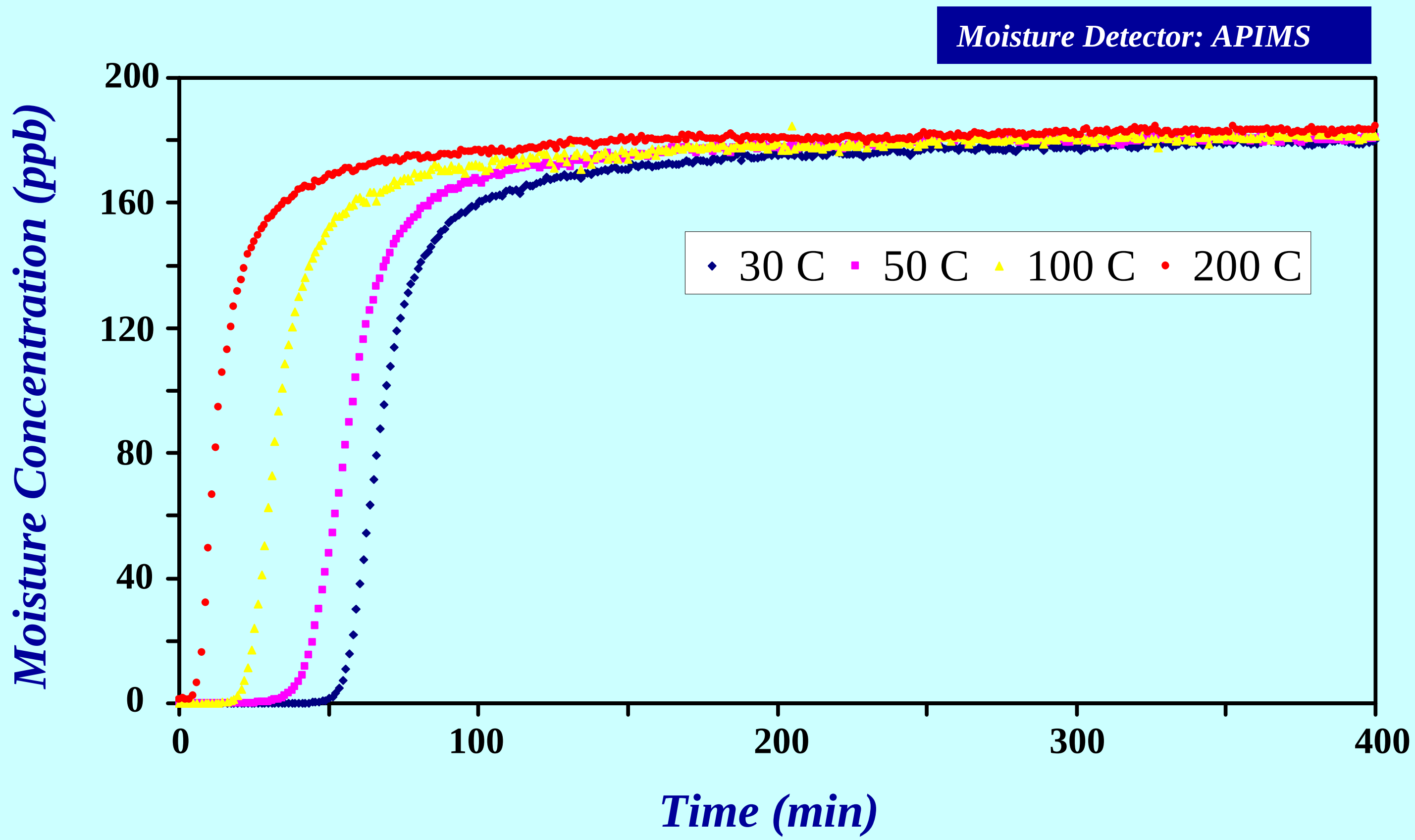
Experimental Procedure



Temporal profile of moisture isothermal absorption/desorption processes

Dynamics of Adsorption

Test Section: EPSS pipe with 1.5 inch OD and 14 inch length. Initially the system was baked at 200 ^{0}C.
Challenge at four different temperatures with moisture concentration at 181 ppb and flow rate: 350 sccm

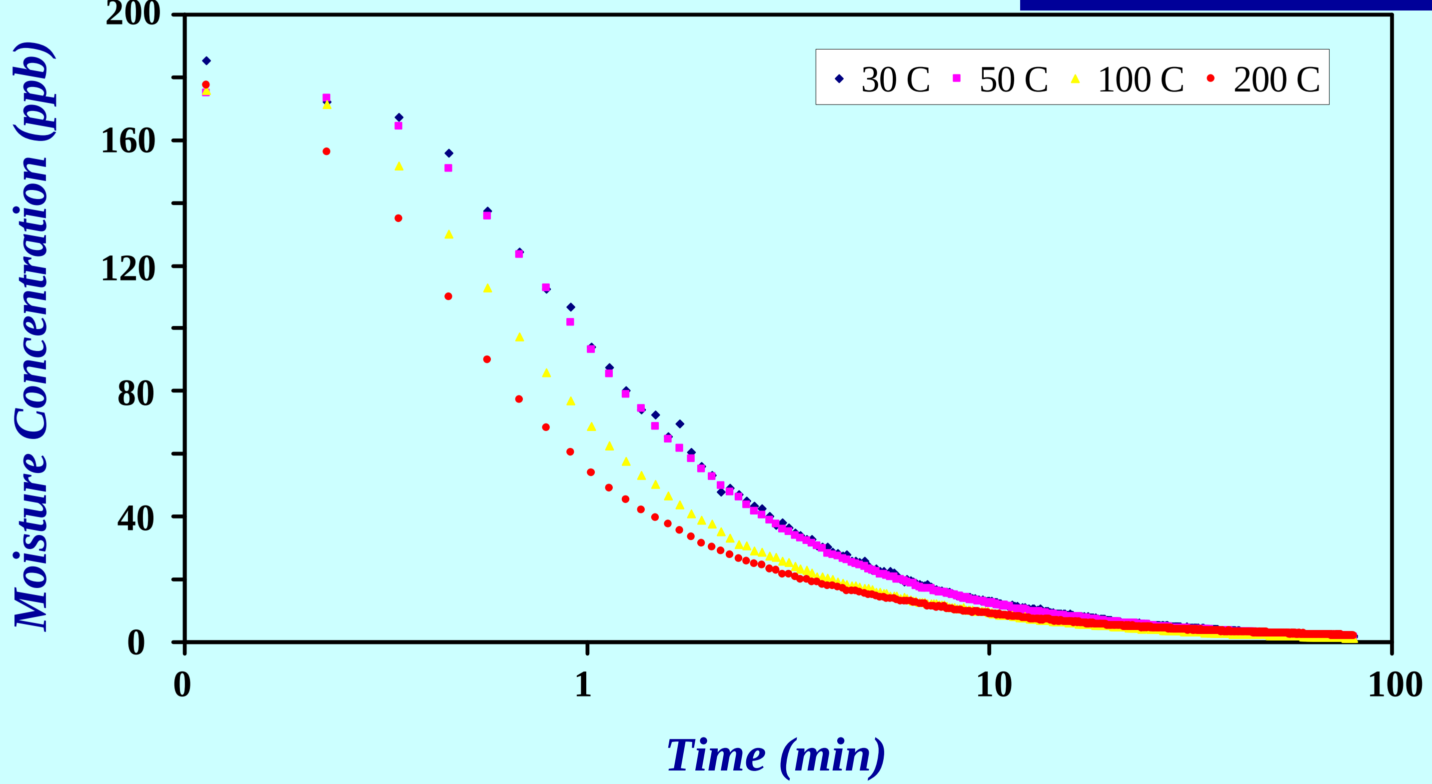


Reduction in adsorption as temperature increases

Dynamics of Desorption

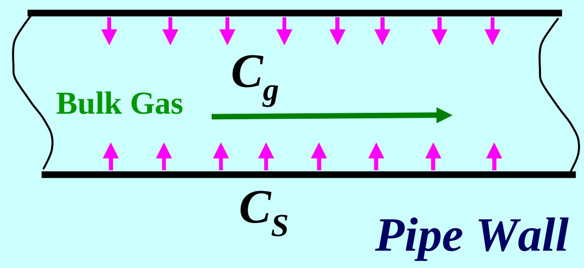
Test Section: EPSS pipe with 1.5 inch OD and 14 inch length. Initially the system was equilibrated with 181 ppb of moisture at four different temperatures, then isothermal purged with 0.2 ppb purge gas and flow rate: 350 sccm

Moisture Detector: APIMS



Desorption is also very sensitive to temperature

Process Model I --- A Single Pipe



Change of moisture concentration on pipe wall:

$$\frac{\partial C_S}{\partial t} = k_{ads} C_g (S_0 - C_S) - k_{des} C_S$$

Change of moisture concentration in gas phase:

$$\frac{\partial C_g}{\partial t} = D_L \frac{\partial^2 C_g}{\partial z^2} - u \frac{\partial C_g}{\partial z} + \frac{A_S}{V} (k_{des} C_S - k_{ads} C_g (S_0 - C_S))$$

C_S: moisture concentration on pipe wall, mol/cm^2; C_g: moisture concentration in gas, mol/cm^3;

k_{ads}: adsorption rate constant, cm^3/mol/s; k_{des}: desorption rate constant, 1/s

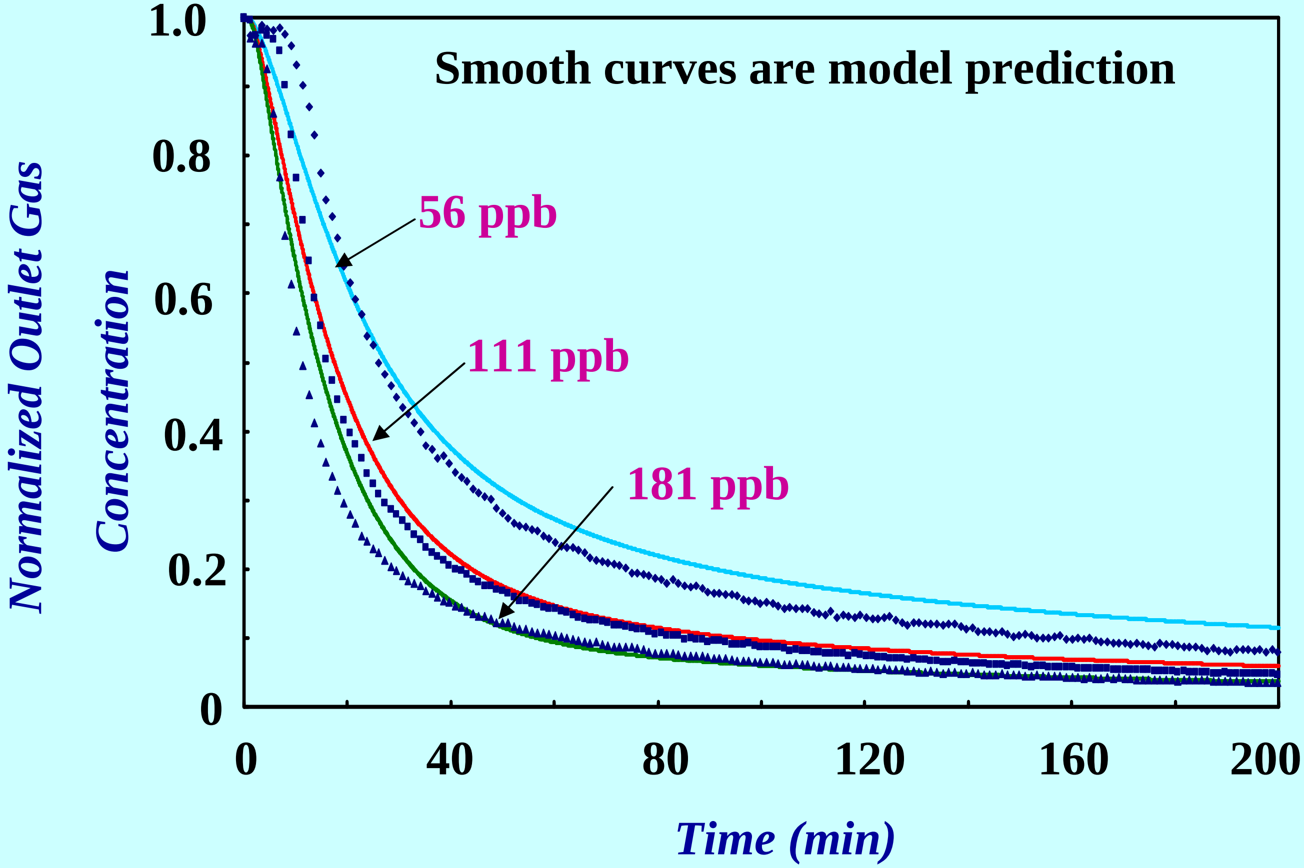
S_0: site density of surface adsorption, mol/cm^2; D_L: dispersion coefficient, cm^2/s;

u: velocity, cm/s; A_S: surface area of pipe wall, cm^2; V: volume of pipe, cm^3

Model Validation and Parametric Estimation

Test Section: EPSS pipe with 1.5 inch OD and 36 inch length. Initially the whole system was equilibrated with different concentrations of moisture at 25 ^{0}C. Isothermal purge with 0.2 ppb purge gas; purge gas flow rate: 350 sccm

Moisture Detector: APIMS and CRDS



k_{ads}: 3.359×10^9 $cm^3/mol/s$;

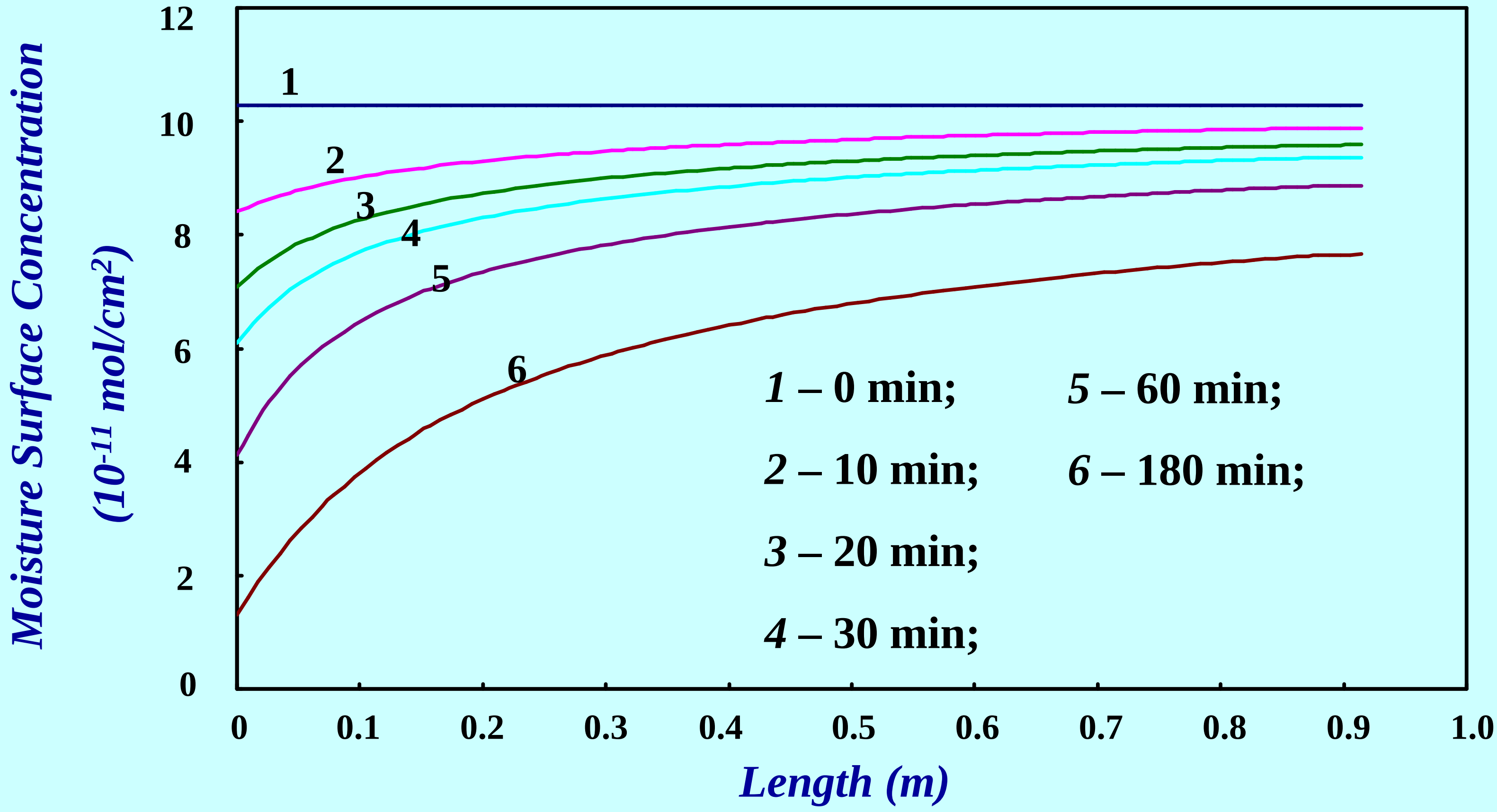
k_{des}: 4×10^{-4} $1/s$;

S_0: 6.29×10^{13} # of sites/cm^2;

Application of Process Model I

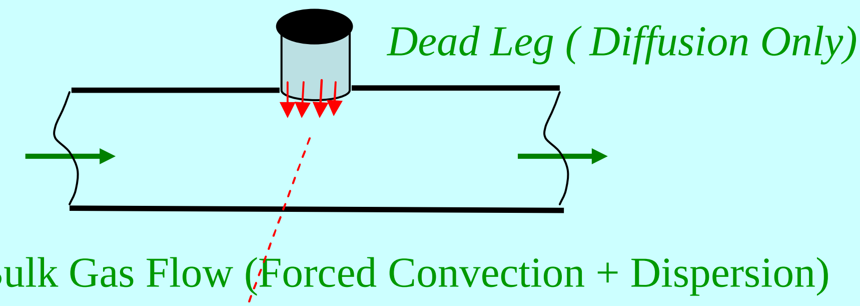
Moisture Distribution along Pipe During Purging Process

Test Section: EPSS pipe with 1.5 inch OD 36 inch length. Initially the whole system was equilibrated with 181 ppb at 25 ^{0}C. Isothermal purge with 0.2 ppb and 350 sccm purge gas



After 3 hrs of purging, roughly only 50% of the total moisture absorbed on pipe wall has been removed

Process Model II – Dead Leg



Moisture concentration in bulk gas:

$$\frac{\partial C_g}{\partial t} = D_L \frac{\partial^2 C_g}{\partial z^2} - u \frac{\partial C_g}{\partial z} + \frac{A_S}{V}(k_{des} C_S - k_{ads} C_g (S_0 - C_S))$$

Moisture concentration in dead leg:

$$\frac{\partial C_{gD}}{\partial t} = D_0 \frac{\partial^2 C_{gD}}{\partial z^2} + \frac{A_{SD}}{V_D}(k_{des} C_{SD} - k_{ads} C_{gD} (S_0 - C_{SD}))$$

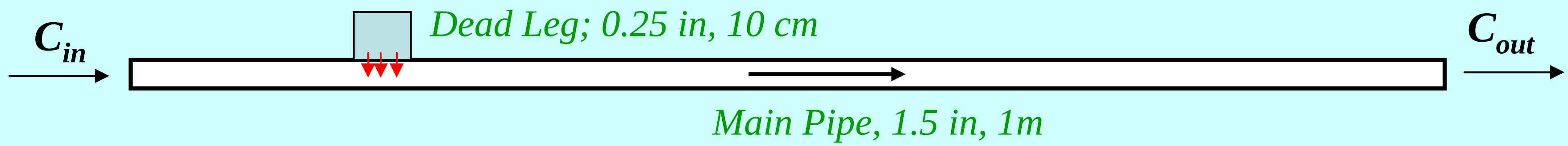
Boundary condition:

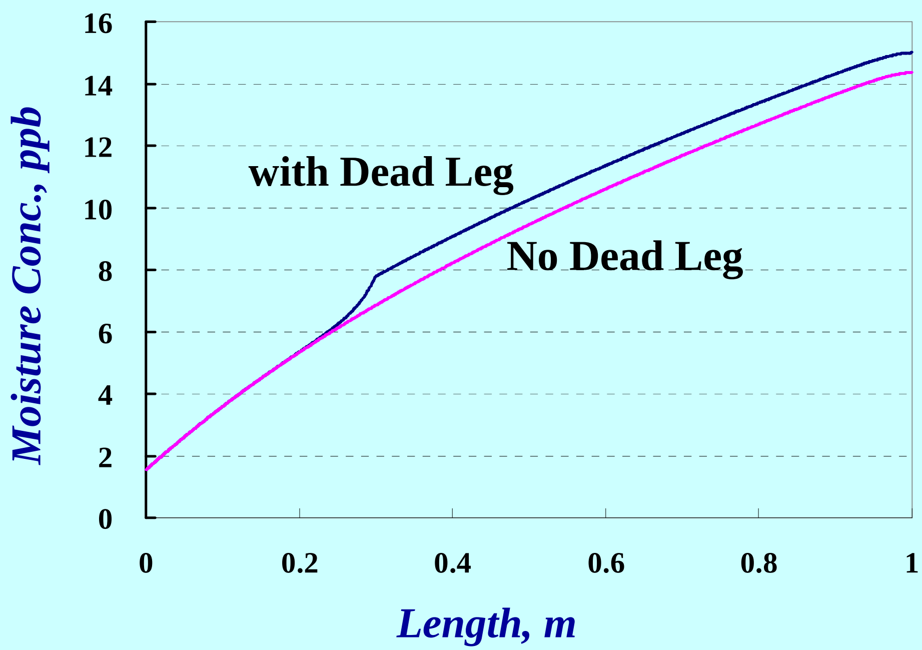
$$(-D_L \frac{\partial C_{g\mathrm{I}}}{\partial x} + u_{\mathrm{I}} \cdot C_{g\mathrm{I}}) + \frac{A_{cD}}{A_{cm}}(-D_0 \frac{\partial C_{gD}}{\partial z}) = -D_L \frac{\partial C_{g\mathrm{II}}}{\partial x} + u_{\mathrm{II}} \cdot C_{g\mathrm{II}}$$

Moisture removal in dead leg is much slower than that in main pipe since only diffusion is involved in mass transport mechanism.

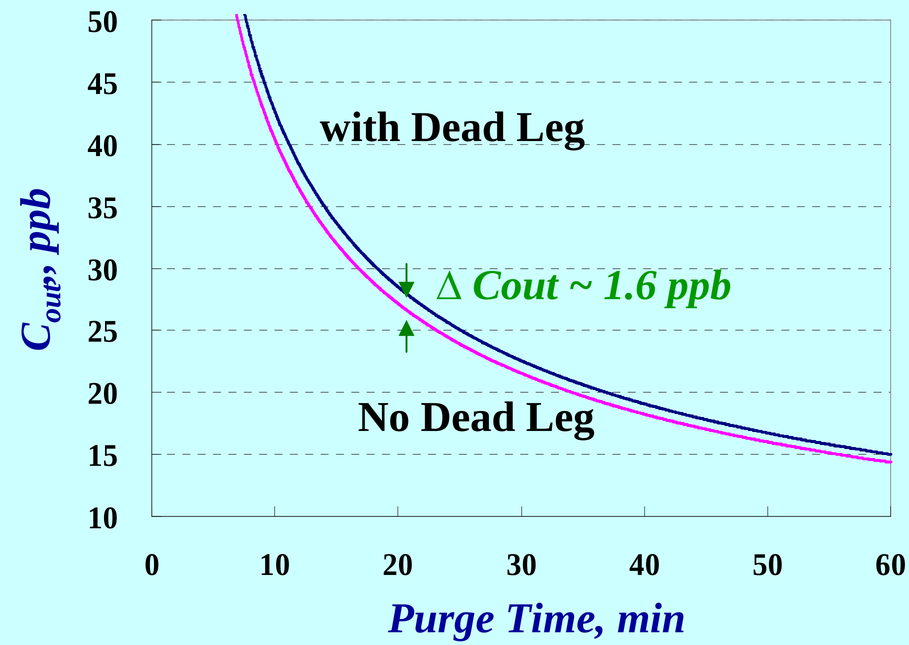
Application of Process Model II- Effects of a Dead Leg

Initially the whole system was equilibrated with 200 ppb of moisture at 25 ^{0}C. Isothermal purge for 1 hr with 0.2 ppb purge gas, and purge gas flow rate: 500 sccm



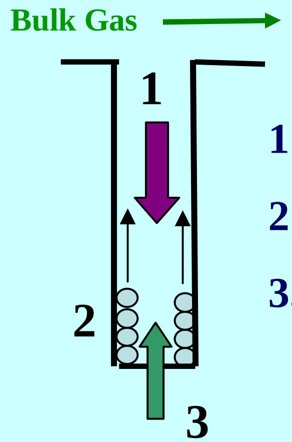


Moisture profile along the main pipe after 1 hr purge



C_{out} vs. purge time

Process Model III - Back Diffusion



1: Bulk Convection;

2: Surface Diffusion;

3. Molecular Diffusion

C_{g0} >> ppb levels

Bulk gas:

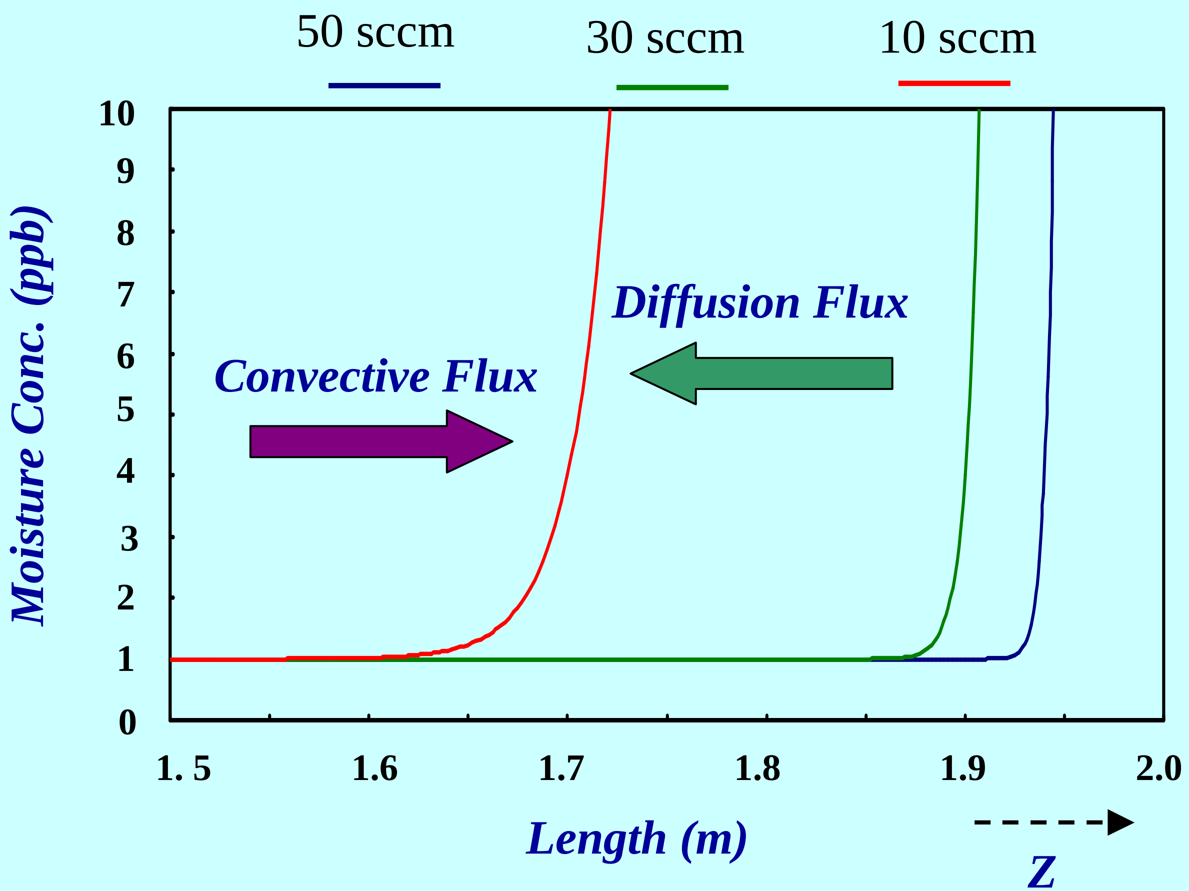
$$D_L \frac{\partial^2 C_g}{\partial z^2} - u \frac{\partial C_g}{\partial z} + \frac{A_S}{V}(k_{des} C_S - k_{ads} C_g (S_0 - C_S)) = 0$$

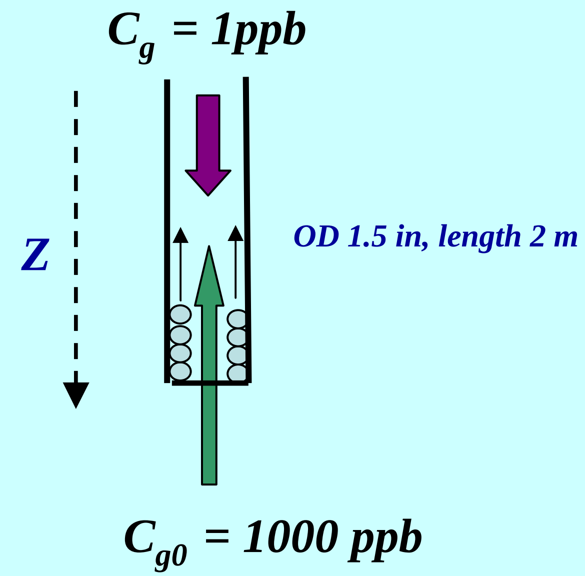
Surface reaction and surface diffusion:

$$D_S \frac{\partial^2 C_S}{\partial z^2} + k_{ads} C_g (S_0 - C_S) - k_{des} C_S = 0$$

D_S: Surface diffusion coefficient, cm^2/s; C_{g0}: ambient moisture concentration , >> 1 ppb;

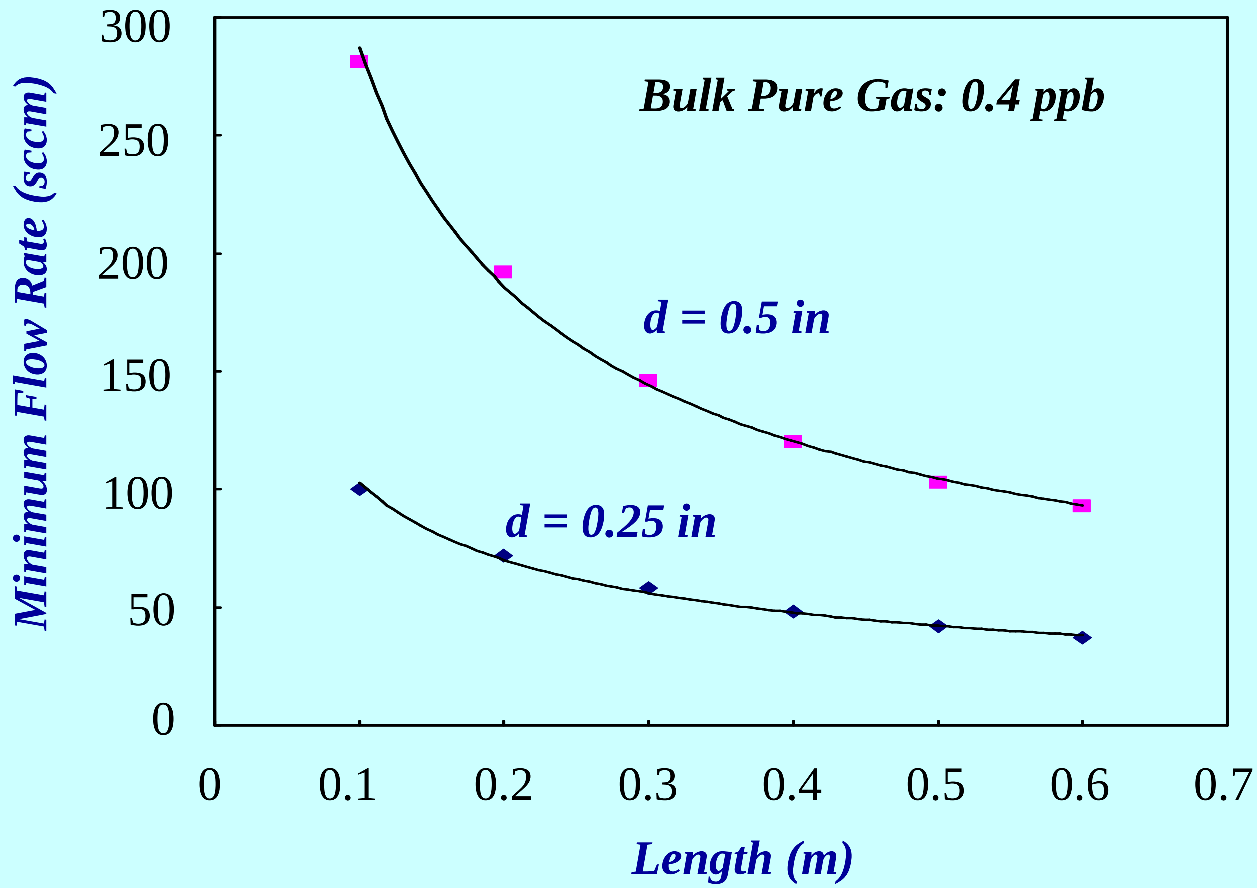
Application of Process Model III – Contaminated Zones of Laterals

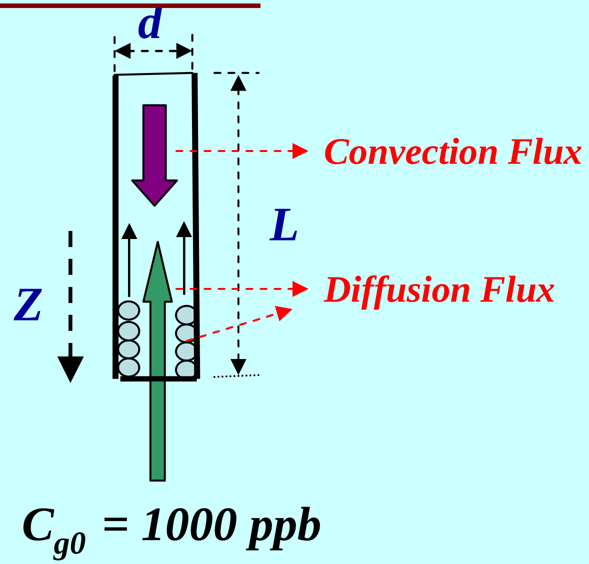




Contaminated area decreases as purge flow rate increases.

Application of Process Model III – Critical Flow to Block Back Diffusion





Critical Flow:

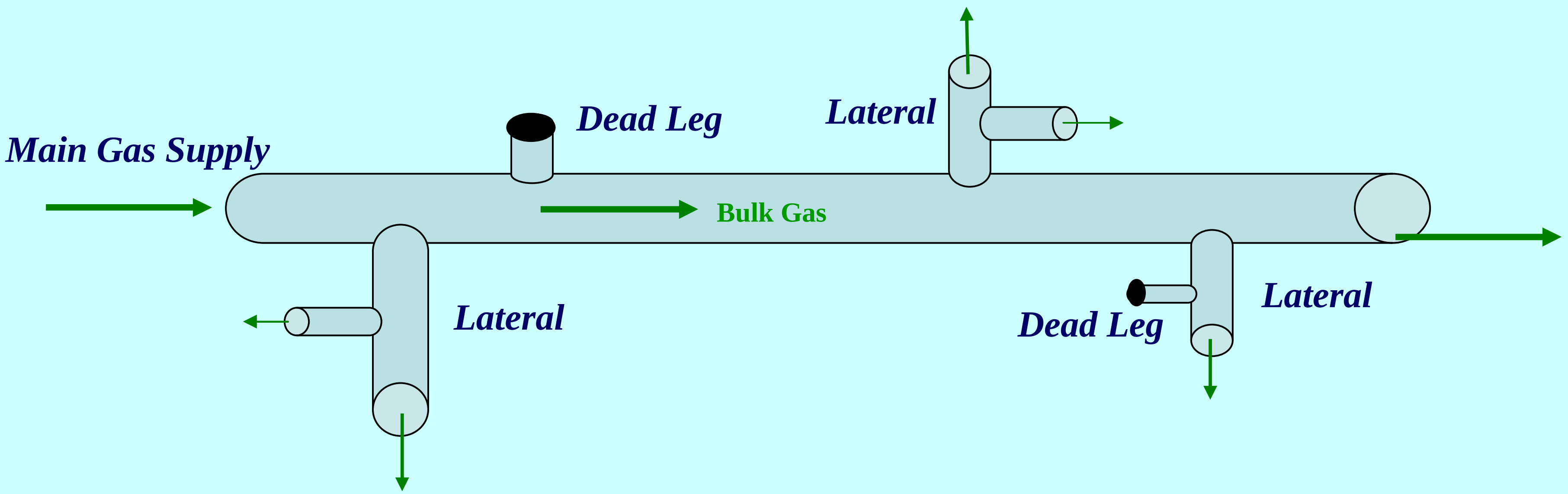
Convection Flux = Diffusion Flux

1. The required minimum flow decreases as the length of lateral increases.

2. Large size lateral needs higher critical flow rate than small size lateral.

Comprehensive Model

Pipe Wall + Dead Legs + Laterals



The comprehensive model can help us to predict:

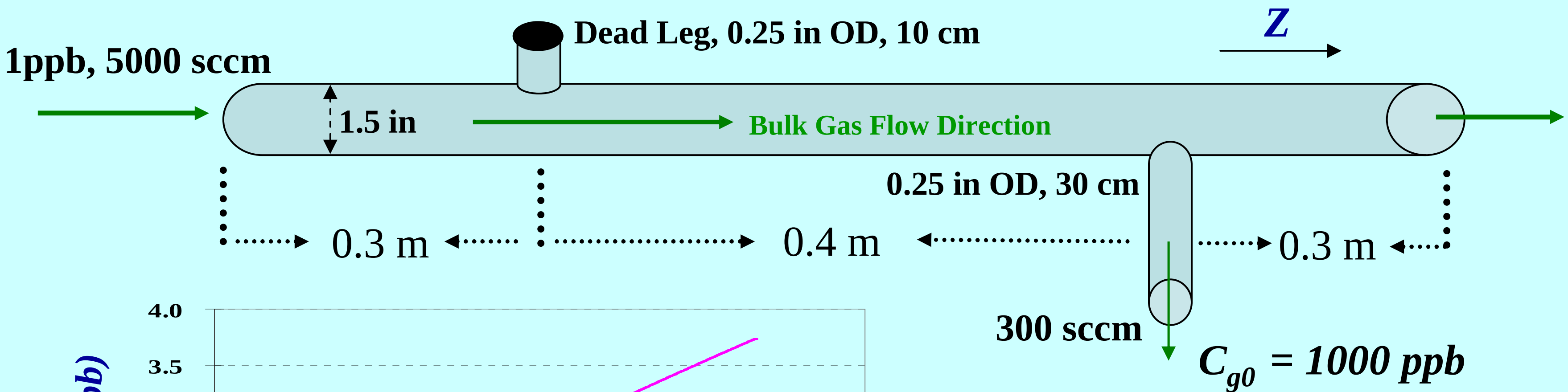
1. The distribution profiles and removal of moisture in main pipe and laterals

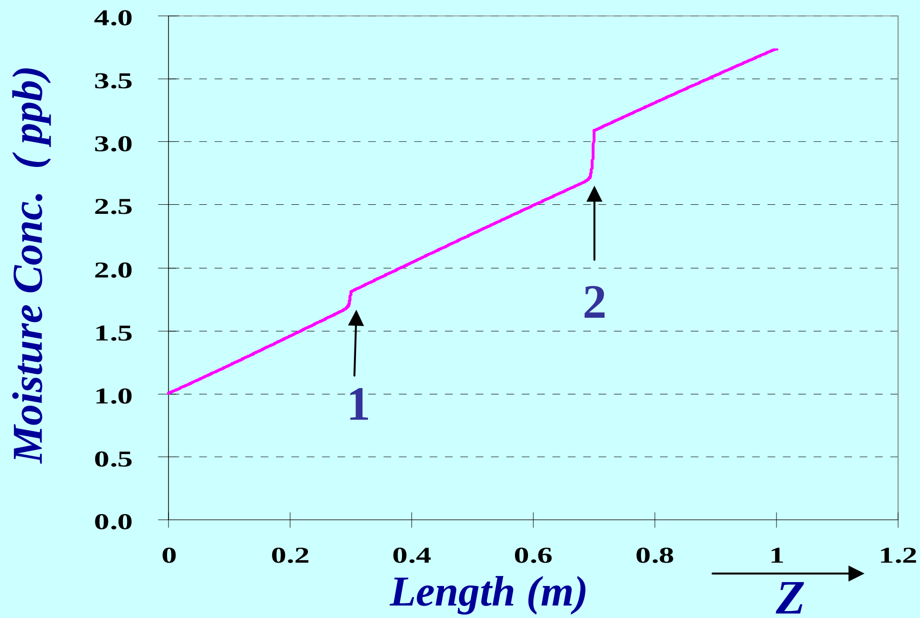
2. The effects of dead legs and back diffusion on moisture concentration in main stream

Model Application- Comprehensive Model

Example 1

Sample: One main pipe with one dead leg and one lateral. Initially the whole system was equilibrated with 200 ppb of moisture at 25 ^{O}C. Isothermal purge for 1 hr with 1 ppb purge gas, and total purge gas flow rate: 5000 sccm





1: due to dead leg

2: due to back diffusion

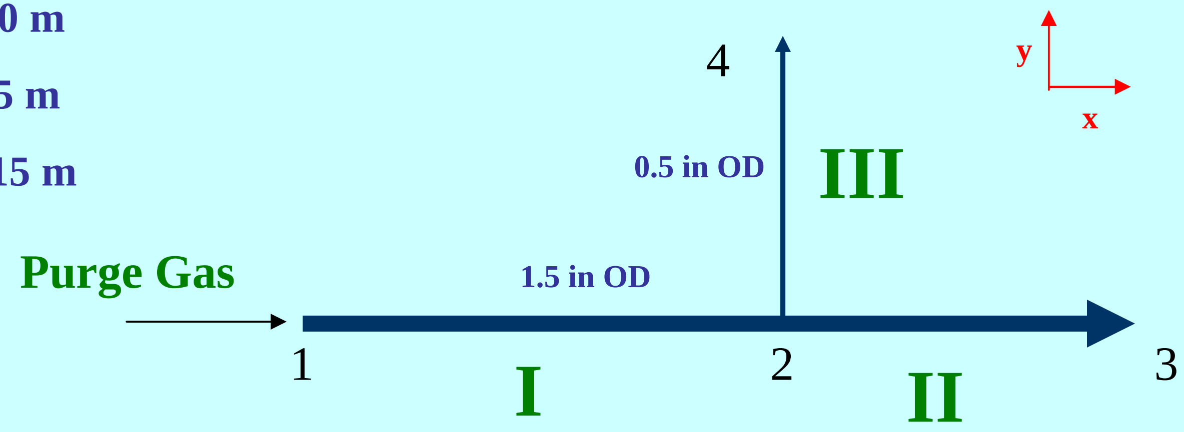
Model Application- Comprehensive Model

Example 2

Segment I: 500 m

Segment II: 15 m

Segment III: 15 m



Assumption: Initially the whole system was equilibrated with 100 ppb of moisture at 25 ^{0}C; then isothermal purge with 1 ppb purge gas, and compare the moisture concentration at 3 and 4.

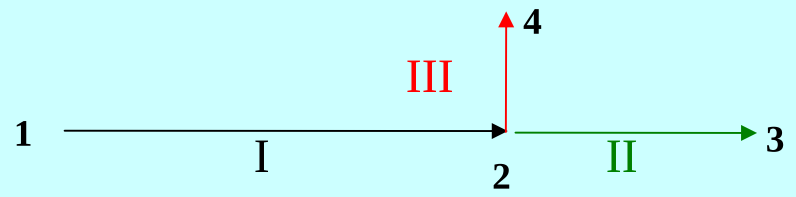
Flow rates for 2 scenarios:

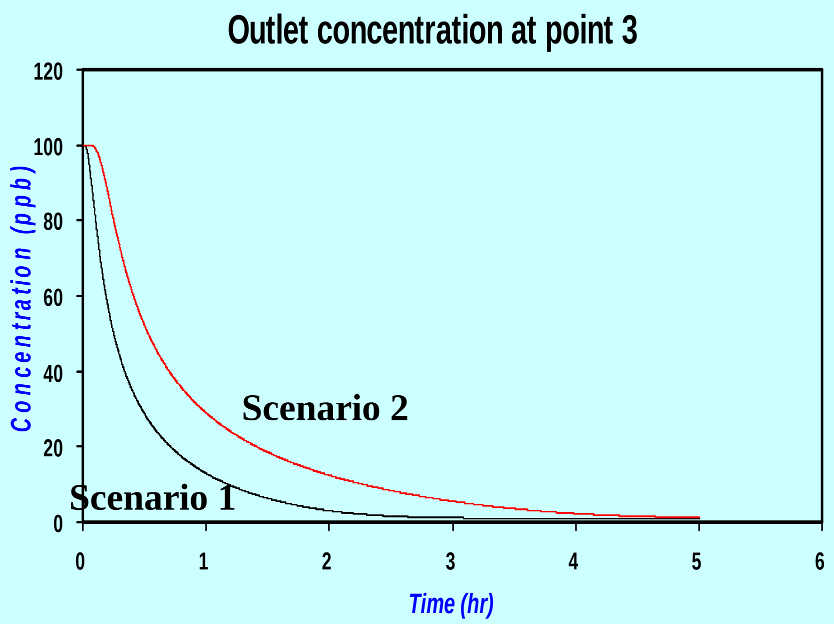
Scenario 1: In Segment I: 1000 scfh;
In Segment II: 990 scfh;
In Segment III: 10 scfh;

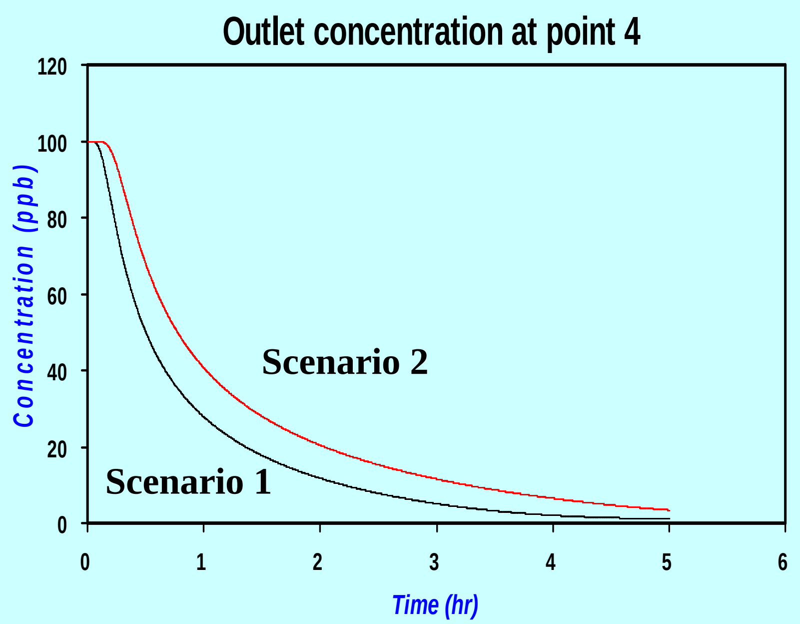
Scenario 2: In Segment I: 500 scfh;
In Segment II: 490 scfh;
In Segment III: 10 scfh;

Model Application - Comprehensive Model

Example 2 (*continued*)



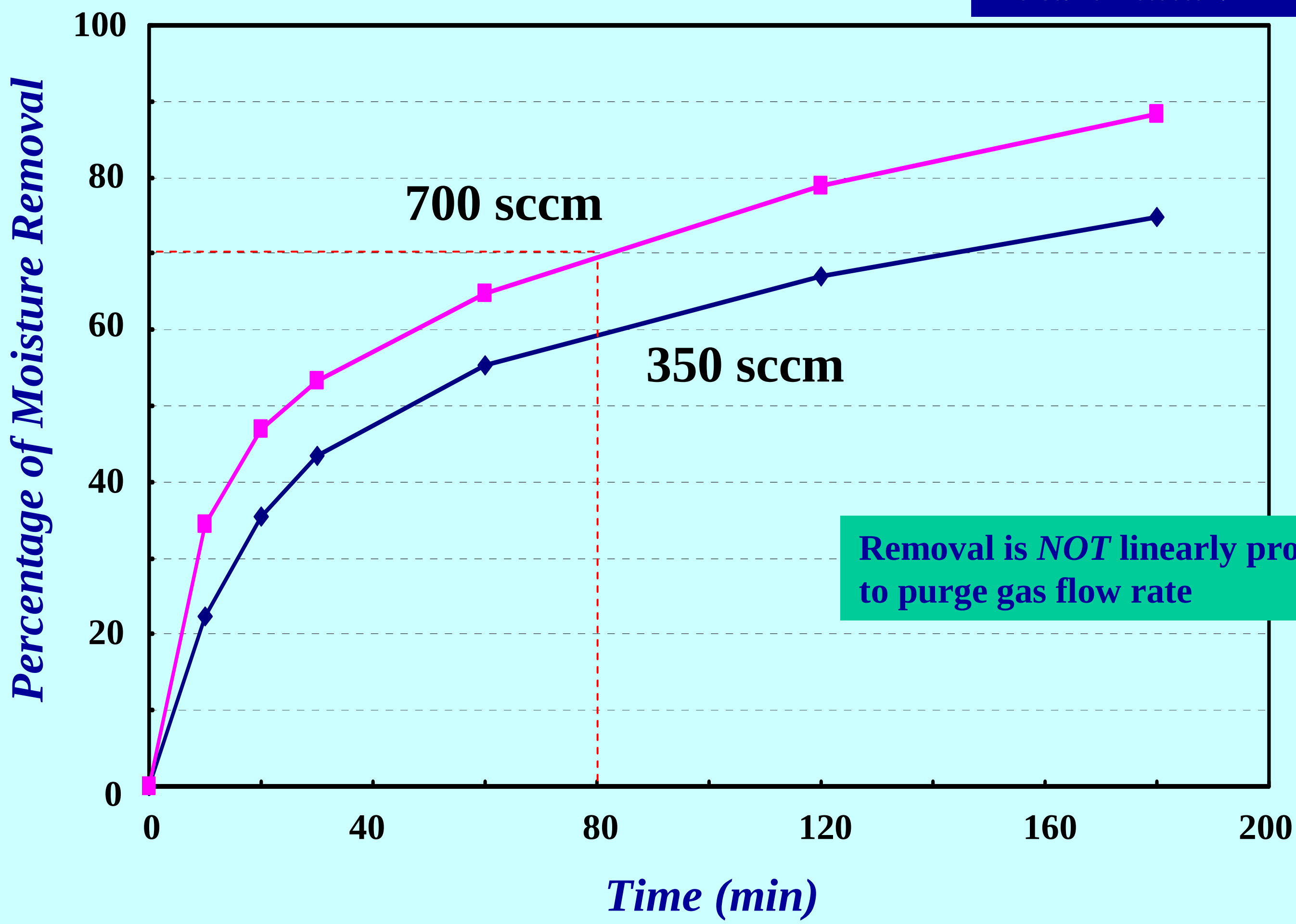




Parametric Study – Purge Flow Rate

Test Section: EPSS pipe with 1.5 inch OD and 36 inch length. Initially the whole system was equilibrated with 181 ppb of moisture at 25 ^{0}C. Isothermal purge with 0.2 ppb purge gas

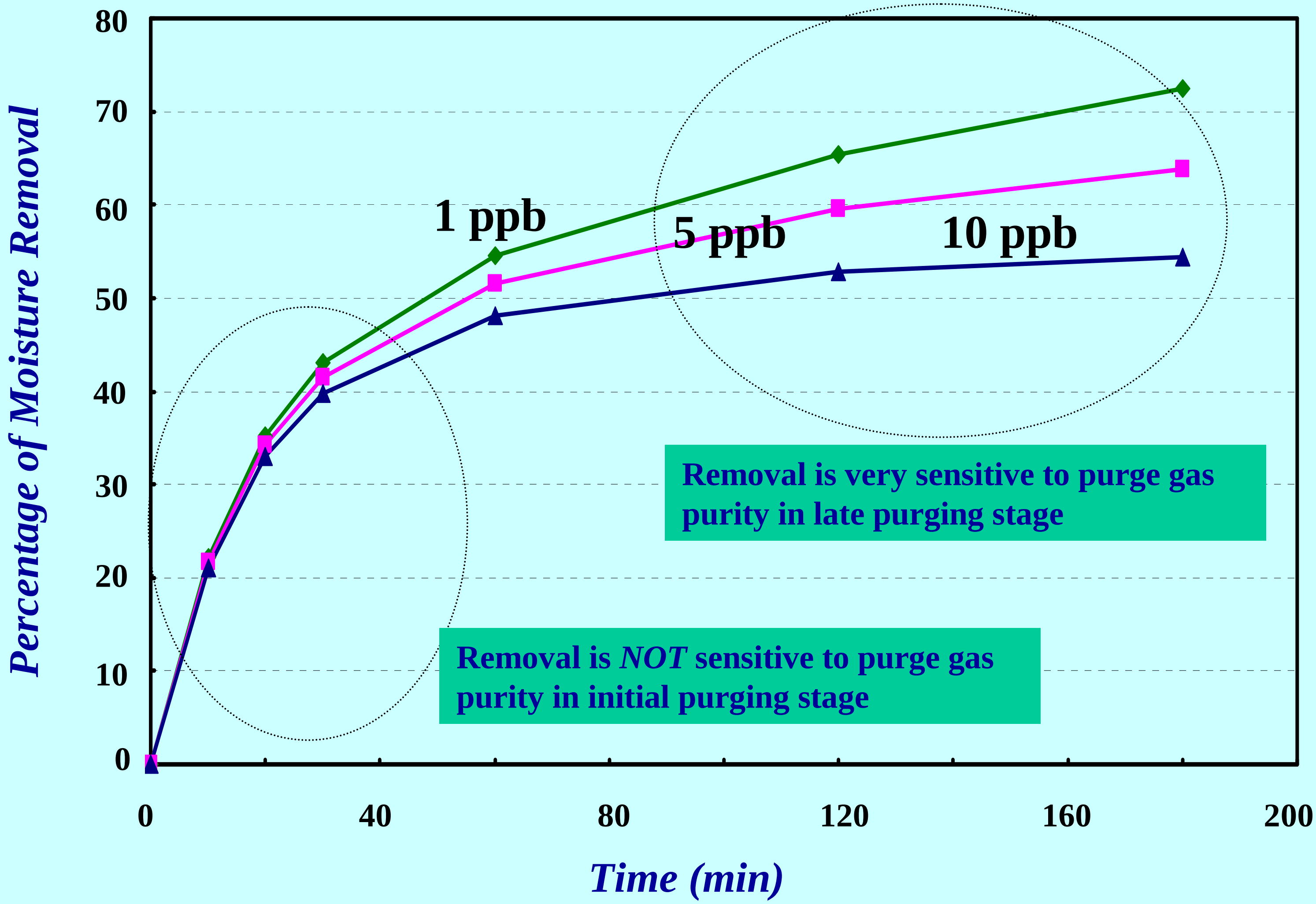
Moisture Detector: APIMS



Removal is *NOT* linearly proportional to purge gas flow rate

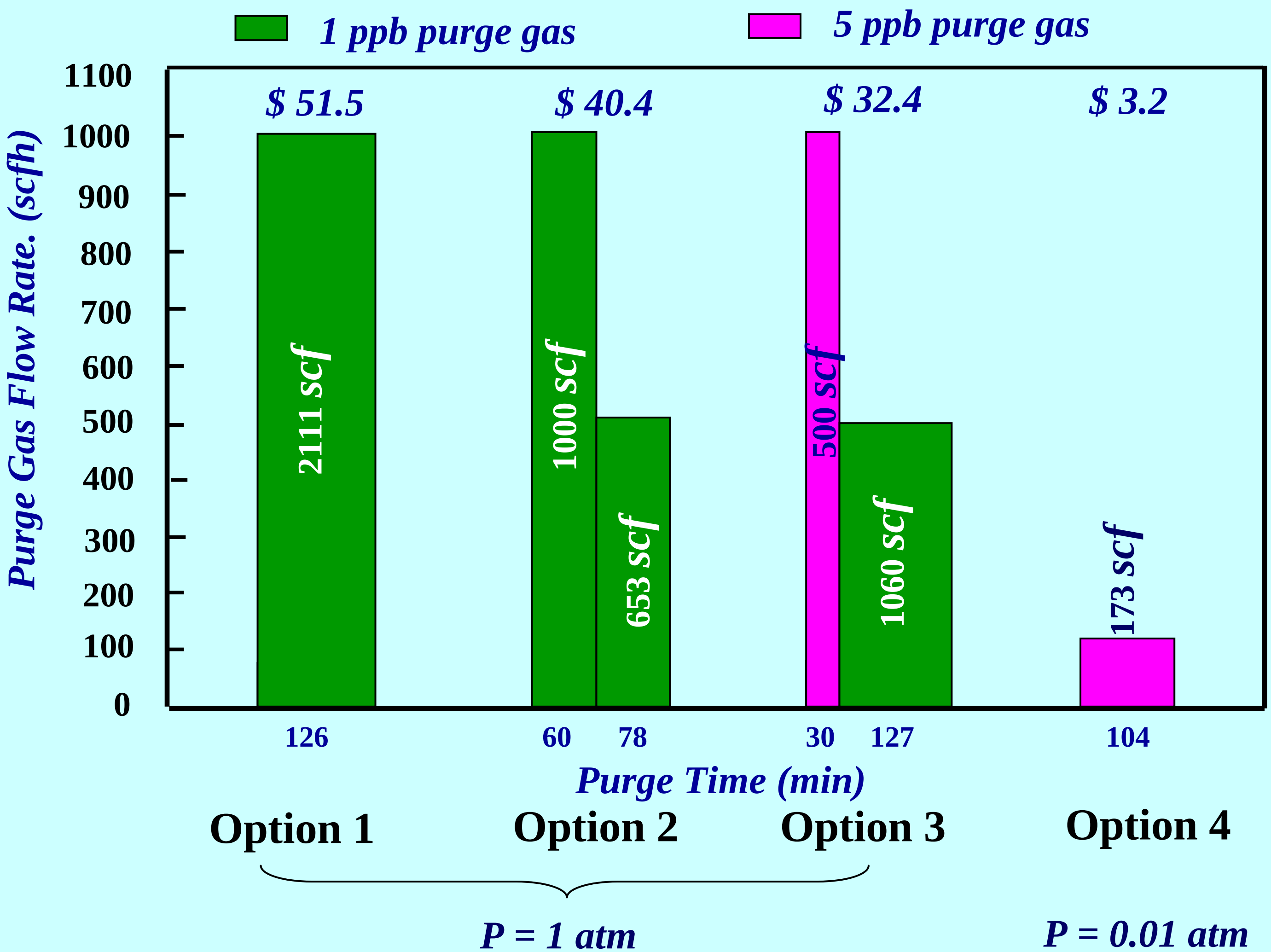
Parametric Study – Purge Gas Purity

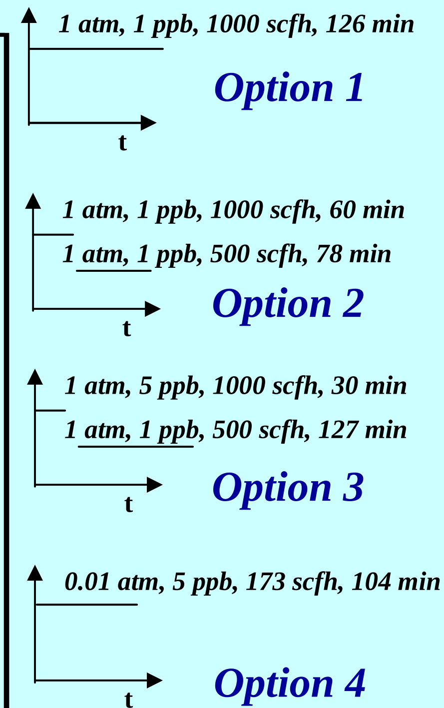
Test Section: EPSS pipe with 1.5 inch OD and 36 inch length. Initially the whole system was equilibrated with 181 ppb of moisture at 25 ^{0}C. Isothermal purge with 350 sccm purge gas



Low-ESH Impact Purge Strategies

Sample: 10 meter, 1.5 inch OD; Initially was equilibrated with 200 ppb of moisture at 25 ^{O}C. Isothermal purge with different purge options



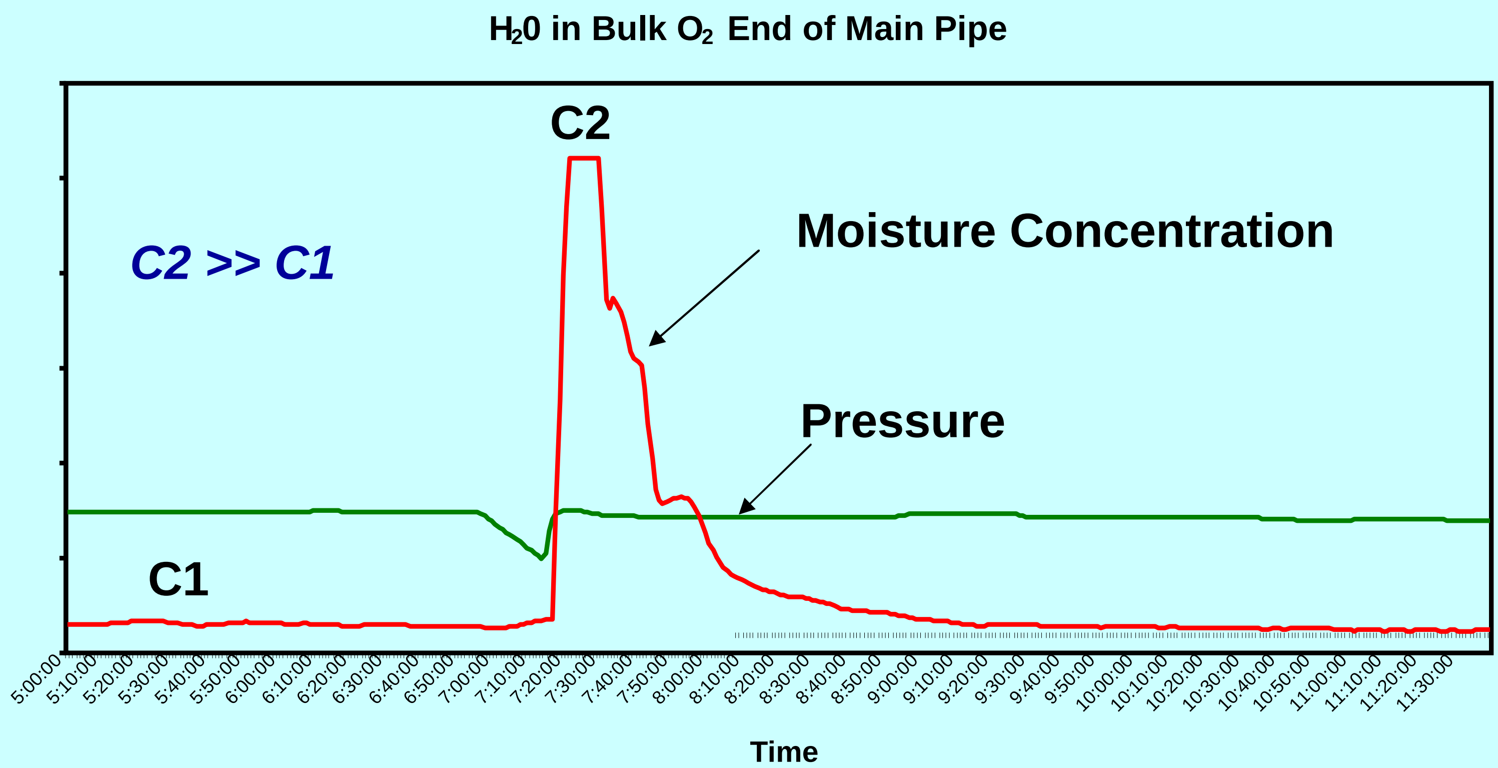


Cost includes:

1. **Power Consumption;**
2. **Purifier Replacement;**
3. **Vacuum Pump Depreciation;**
4. **Houseline N_2**

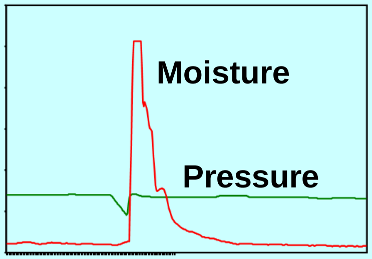
System Disturbance – Pressure Fluctuation

Figure was provided by Intel Fab. Actual values on both Y-axes were removed due to confidentiality



Any perturbation in a steady state system that changes gas phase concentration will destroy the current system equilibrium between pipe wall and gas phase, vice versa.

System Disturbance – Pressure Fluctuation

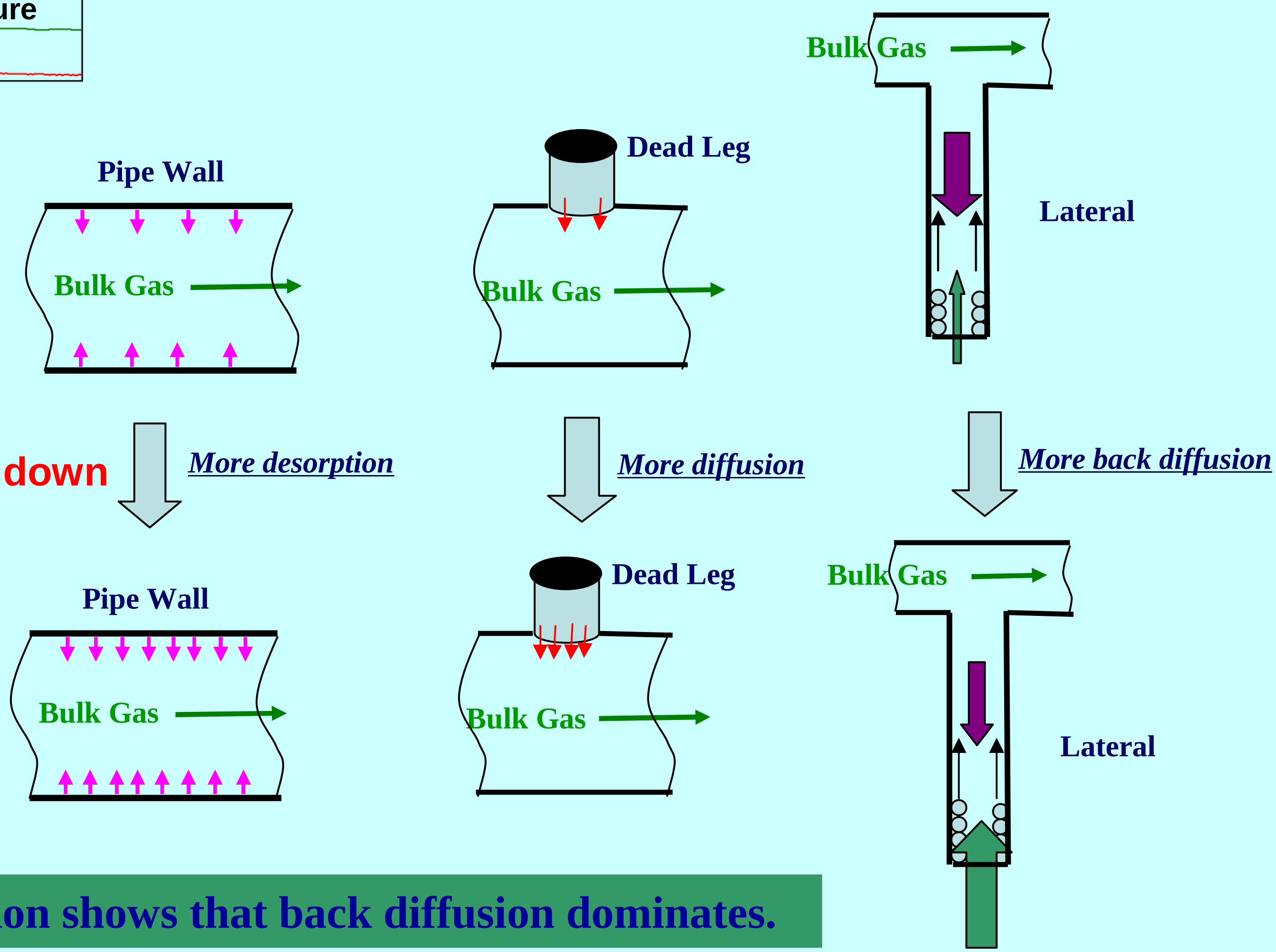


Where is moisture mainly from?

P=P1

When pressure drops down

P=P2



Model simulation shows that back diffusion dominates.

Conclusion

- **Cleaning of moisture contaminated UHP gas delivery system is a slow process. The purging process must be optimized.**
- **Different components (transfer pipes, filters, flow controllers, valves, regulators) have different moisture outgassing rates. Smaller interior surface area and surface finishes with less roughness are desired.**
- **Dead leg and back diffusion can cause contamination to the main stream. The number of dead legs should be minimized. Heating dead legs can partially decrease contamination from the dead leg. At laterals, only critical flow rates are required to block back diffusion.**
- **The comprehensive model in this research can help us to optimize purging processes with minimized time and cost. It also can allow us to predict moisture removal in main pipes and sub-pipes.**
- **System perturbation should be avoided.**

Future Plans

- Set up mathematical modeling for valves, regulators and MFCs (figuring out the equivalent length as a pipe); improve the comprehensive model.
- More study on system perturbation.
- Continue working with Intel; initiate similar applications and studies for other members; prepare a software package for purging/cleaning scenario study.

Acknowledgements

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- Paul Swift, Undergraduate student, University of Arizona