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### **BlowView-H2: cutting-edge simulation for hydrogen tank liner optimization**

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# BlowView-H2: Cutting-edge Simulations for Hydrogen Tank Liner Optimization

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Numerical Simulation and Process Modelling Team  
AMP-COMP

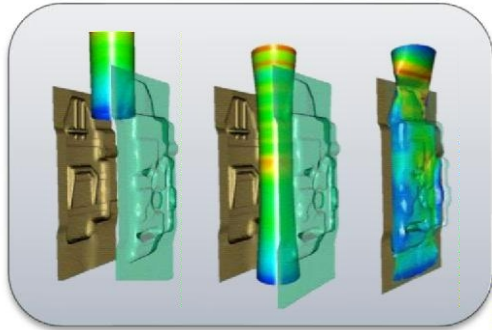
Annual Blow Molding Conference 2024  
Crown Plaza Atlanta SW, October 7-9 2024  
Peachtree City, GA , USA



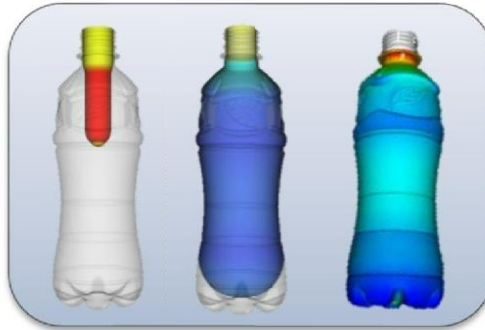
# Overview

- **Introduction to NRC's BlowView simulation software**
- **Objectives of the Blow Molded Plastic Liner (BMPL) simulation study**
- **BMPL simulation & optimization results**
- **BMPL H<sub>2</sub> permeation model and simulation case studies:**
  - Case 1 : Isothermal Case: Constant air temperature, and constant H<sub>2</sub> temperature & pressure
  - Case 2: Variable H<sub>2</sub> temperature & pressure
  - Case 3 : Pressure/Temp Variation during the Filling and Emptying Cycle
- **Conclusion & what's next ?**

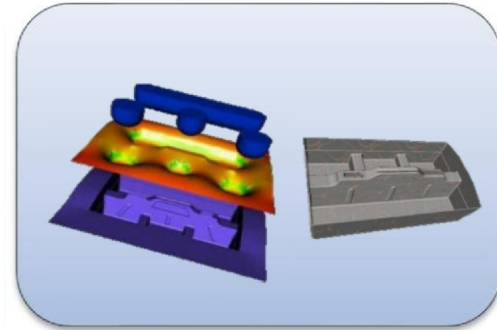
# NRC's BlowView Simulation Software



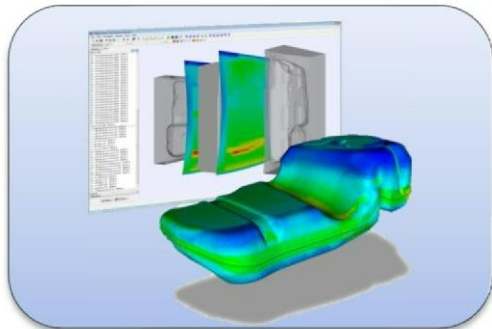
**Extrusion Blow Molding**



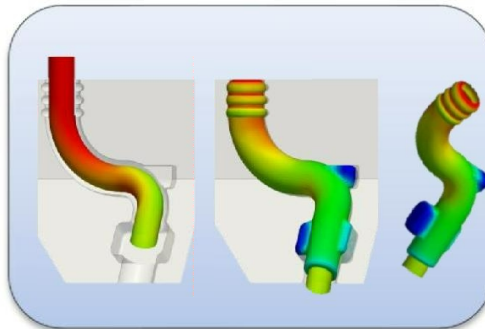
**Stretch Blow Molding**



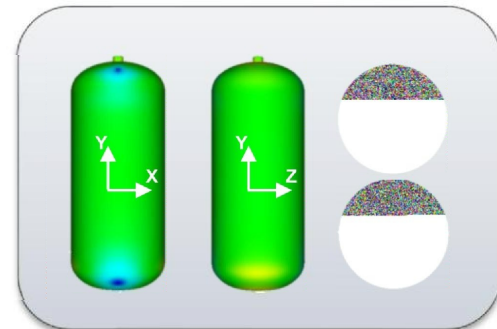
**Thermoforming**



**Twin-Sheet EBM**



**Suction Blow Molding**

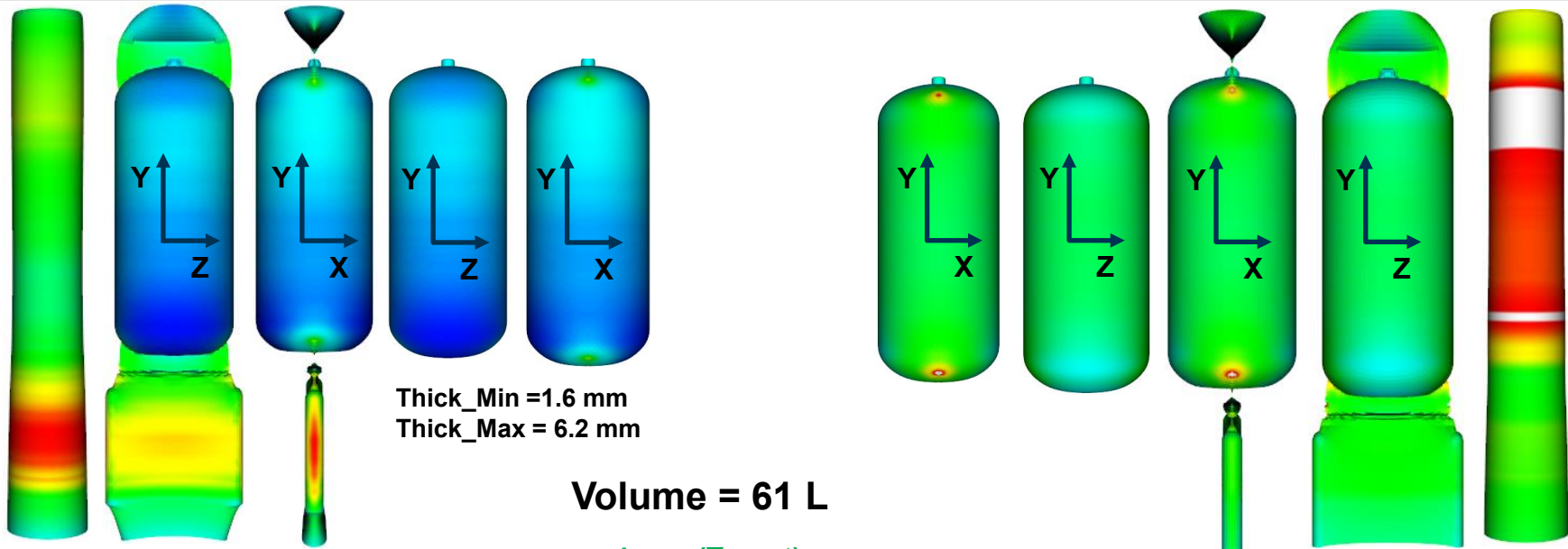


**H2 Liners**

# Objectives

- **Simulate a BMPL provided by industrial Partner using a PA6 resin (i.e., Durethan BC550Z);**
- **Optimize the process parameters to enhance uniformity in liner thickness for lightweighting;**
- **Evaluate the permeability performance of the BMPL under variable surrounding air temperatures, and internal H<sub>2</sub> temperatures and pressures;**
- **Simulate the filling and emptying cycle to predict pressure and temperature variations within the tank, as well as across the liner and composite layer.**

# H2 Liner Simulation & Optimization Results



## Initial Profile

Parison Length : 1432 mm  
Parison Weight : 4281 g  
Part Weight : 1759 g  
Average Part Thickness: 2.2 mm

Thick\_Min = 1.6 mm  
Thick\_Max = 6.2 mm

Volume = 61 L

4 mm (Target)

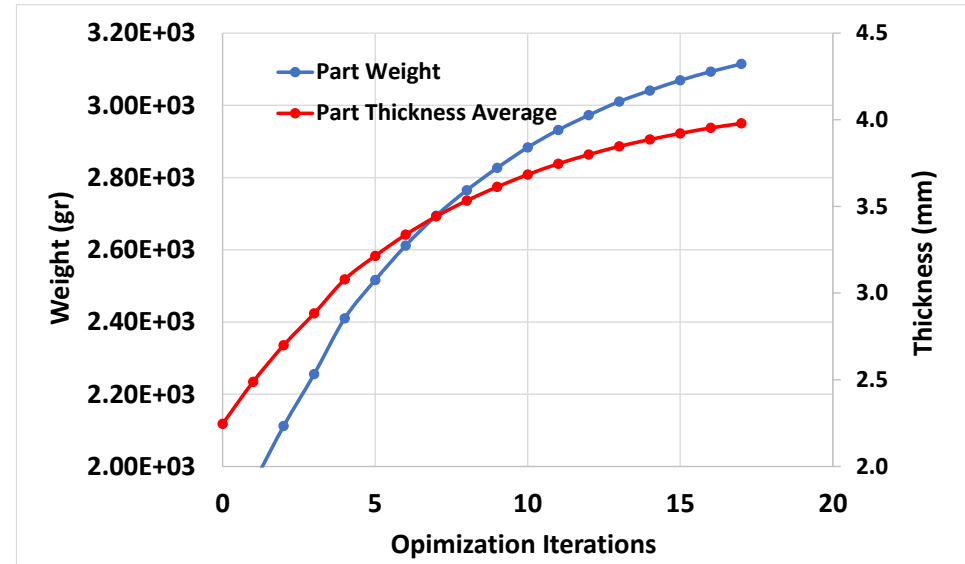
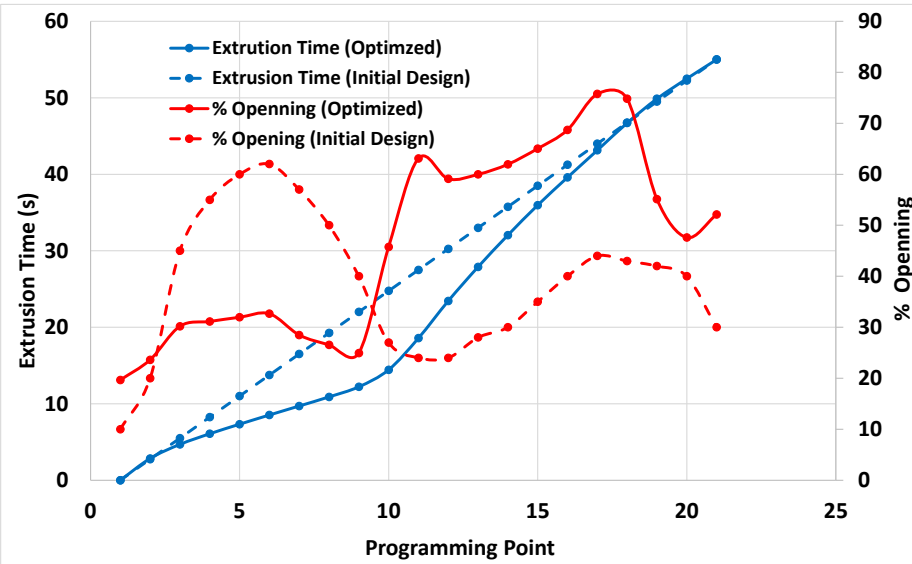
1.0 2.5 4.0 5.5 7.0 8.5

Thickness (mm)

## Optimized Profile

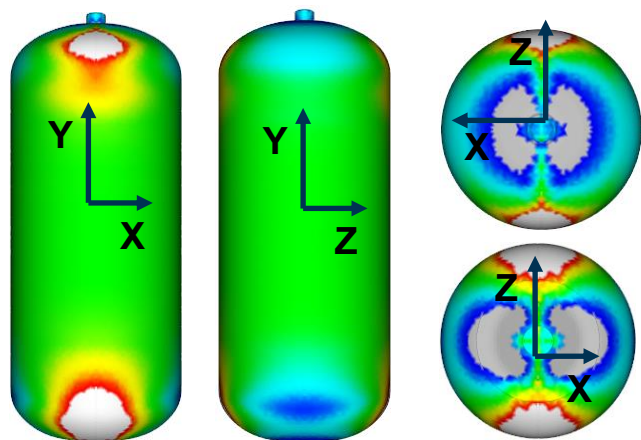
Parison Length : 1299 mm  
Parison Weight : 5089 g  
Part Weight : 3158 g  
Average Part Thickness: 4.0 mm

# H2 Liner Simulation & Optimization Results



# H<sub>2</sub> Permeability Analysis on Optimized Liner

Case 1 (Isothermal):  $T_{H_2} = 20^\circ\text{C}$ ,  $P_{H_2} = 70 \text{ MPa}$ ,  $T_{air} = 20^\circ\text{C}$

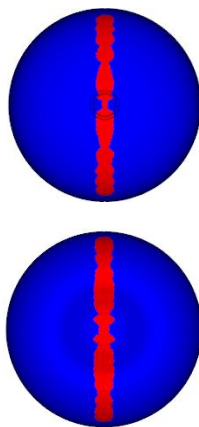


3.0 3.7 4.3 5.0

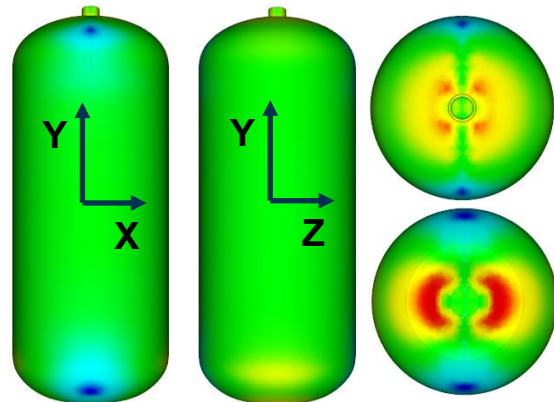
Thickness (mm)

Part Weight : 3158 g

Part Average Thickness: 4.0 mm



Pinch-off = 2.3 %



151.8 312.1 472.4 632.7

H<sub>2</sub> Flux Density (mg/day/m<sup>2</sup>)

Shell Surface = 0.839062 m<sup>2</sup>

Pinch-off Surface = 0.018724 m<sup>2</sup>

H<sub>2</sub>/Day through Shell Surface = 326.45 mg/Day

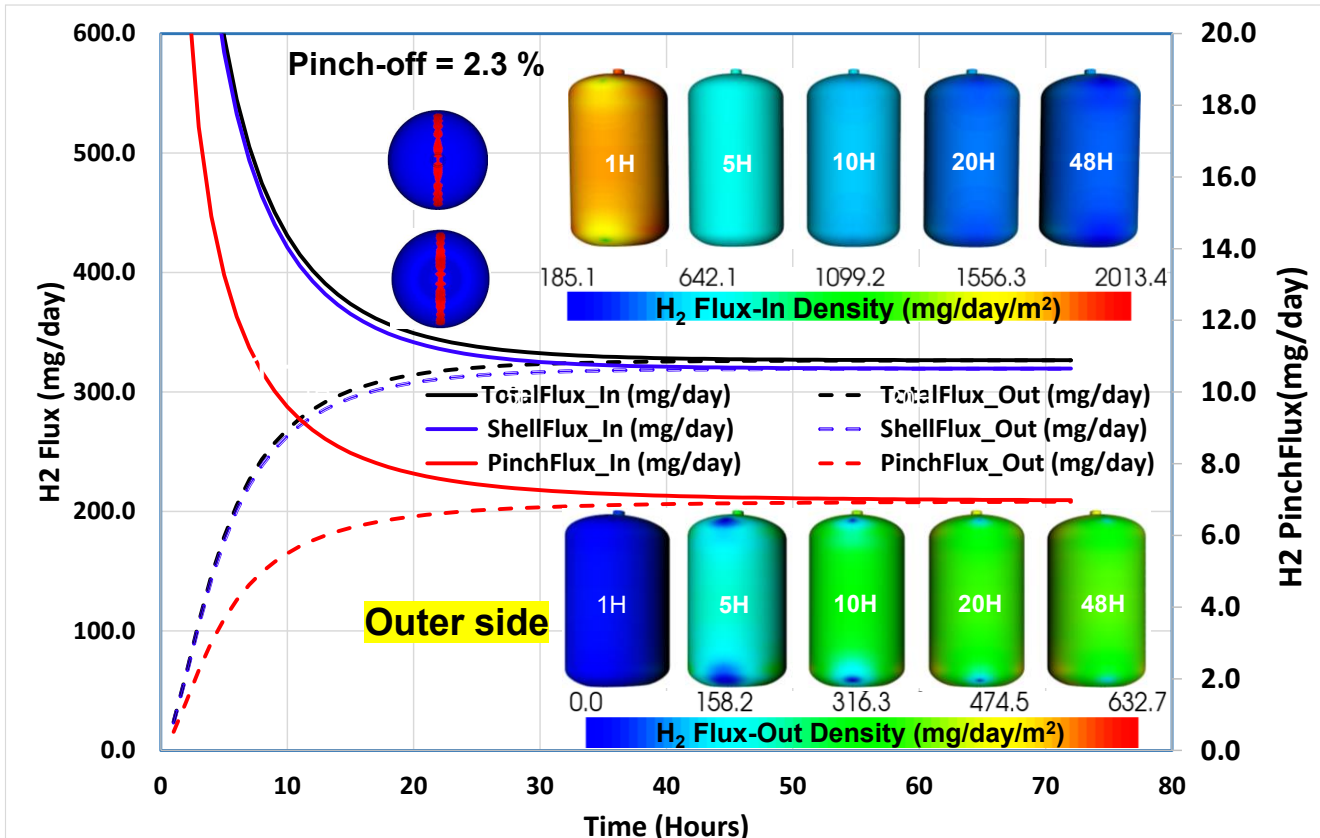
H<sub>2</sub>/Day through Pinch-off Surface = 6.60 mg/Day

Total H<sub>2</sub>/Day = 333.05 mg/Day = 5.17 NmL/hr/L

Note: Limit = 6 NmL/hr/L

# H<sub>2</sub> Permeability Analysis on Optimized Liner

Case 1 (Isothermal):  $T_{H_2} = 20^\circ\text{C}$ ,  $P_{H_2} = 70\text{ MPa}$ ,  $T_{air} = 20^\circ\text{C}$



# H2 Permeability Analysis on Optimized Liner

## Case 2 (Non-Isothermal): Time Depend P and T

### Case 2:

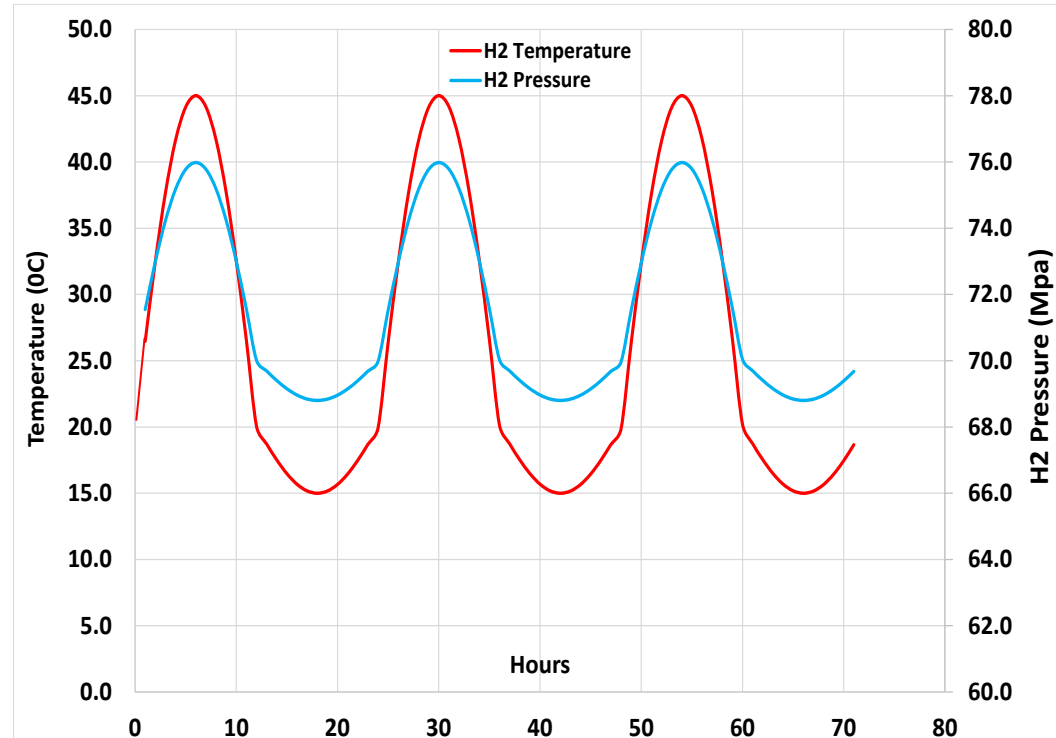
Initial liner  $T_{Init} = 20^{\circ}\text{C}$ ;  $P_{H2} = 0.0 \text{ MPa}$

Inner side  $T_{H2} = 20^{\circ}\text{C} + \text{Amp} \cdot \sin(2\text{PI}/24 \cdot \text{time})$ ;

Inner side (H2 Pressure obey to isochore transformation)

$P_{H2} / T_{H2} = (P_{H2} = 70 \times 10^6) / (T_{H2} = (273 + 20))$

Outer side  $T_{Air} = 20^{\circ}\text{C}$ ;  $P_{H2} = 0.0 \text{ MPa}$

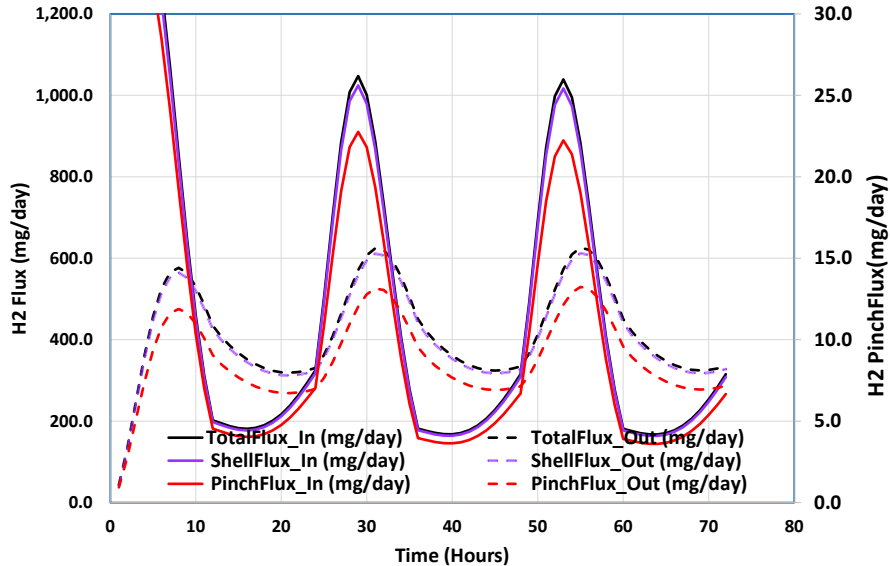


# H2 Permeability Analysis on Optimized Liner Case 2 (Non-Isothermal): Transient thermo-diffusion

$T_{H2} = 20^{\circ}\text{C} + \text{Amp. sin}(2\text{PI}/24*\text{time}); T_{Air} = 20^{\circ}\text{C}$

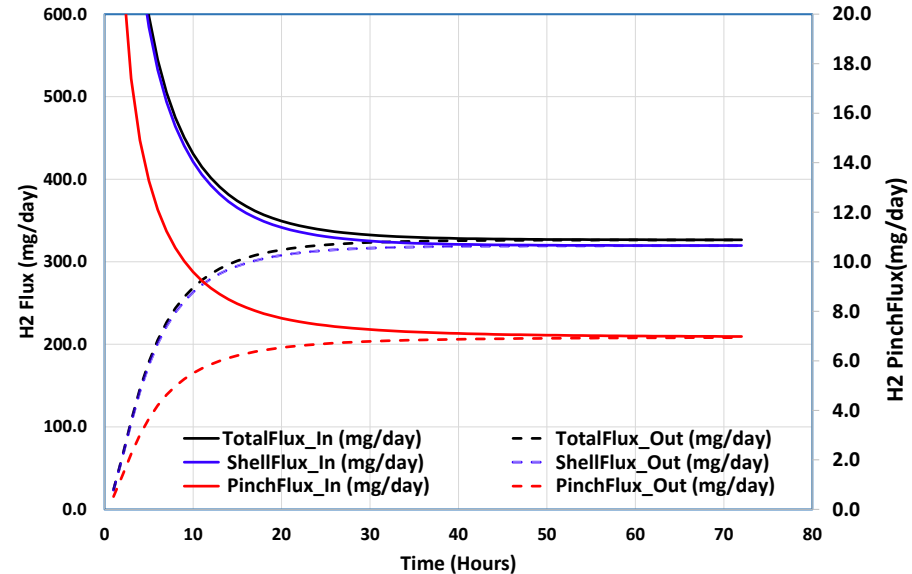
Isochore Transformation

$P_{H2}/T_{H2} = \text{constant}$



Isothermal:  $T_{H2} = 20^{\circ}\text{C}$  &  $T_{Air} = 20^{\circ}\text{C}$

$P_{H2} = 70 \text{ MPa}$



*Isothermal Transient case*

# H2 Permeability Analysis on Optimized Liner

## Case 3: Pressure/Temp Variation during the Filling and Emptying Cycle

### Filling Phase

Station Conditions

$$T_{H2\_Station} = 25^{\circ}C$$

$$P_{H2\_Station} = 90 \text{ MPa}$$

Reservoir Conditions

$$T_{H2\_R} = 25^{\circ}C$$

$$P_{H2\_R} = 1 \text{ MPa}$$

$$V_{H2\_R} = 61 \text{ L}$$

$$P_{H2\_R\_Max} = 70 \text{ MPa (cut-off pressure)}$$

### Emptying Phase

Reservoir Conditions

$$T_{H2\_R} = 25^{\circ}C$$

$$P_{H2\_R} = 70 \text{ MPa}$$

$$V_{H2\_R} = 61 \text{ L}$$

$$\text{EmptyingRate} = 1.1 \text{ kg/hr}$$

# H2 Permeability Analysis on Optimized Liner

## Case 3.1 : Pressure/Temp Variation during the Filling

Filling Phase Time = 5 min

Station Conditions

$$T_{H_2\_Station} = 25^\circ\text{C}$$

$$P_{H_2\_Station} = 90 \text{ MPa}$$

Reservoir Conditions

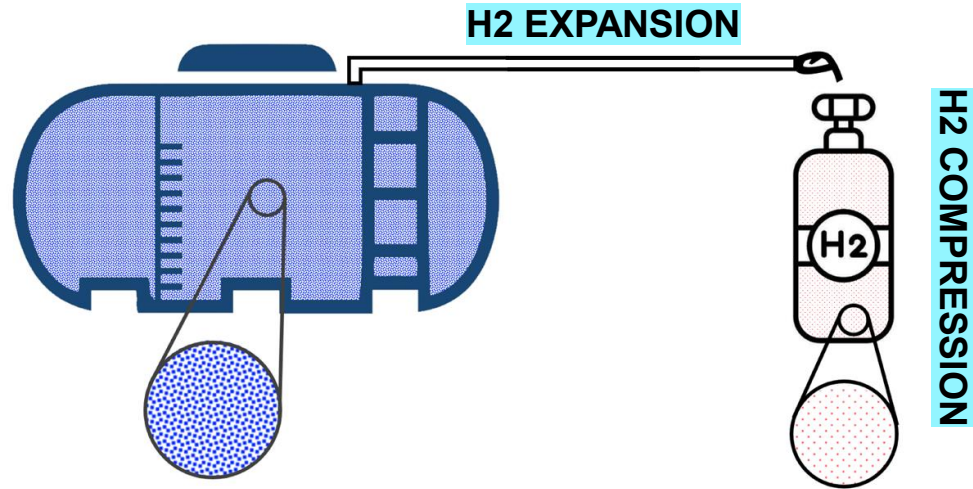
$$T_{H_2\_R} = 25^\circ\text{C}$$

$$P_{H_2\_R} = 1 \text{ MPa}$$

$$V_{H_2\_R} = 61 \text{ L}$$

$$P_{H_2\_R\_Max} = 70 \text{ MPa}$$

(cut-off pressure)



**Filling thermodynamic model assumptions**

Scenario 1 : Isothermal expansion in the station supply pipe

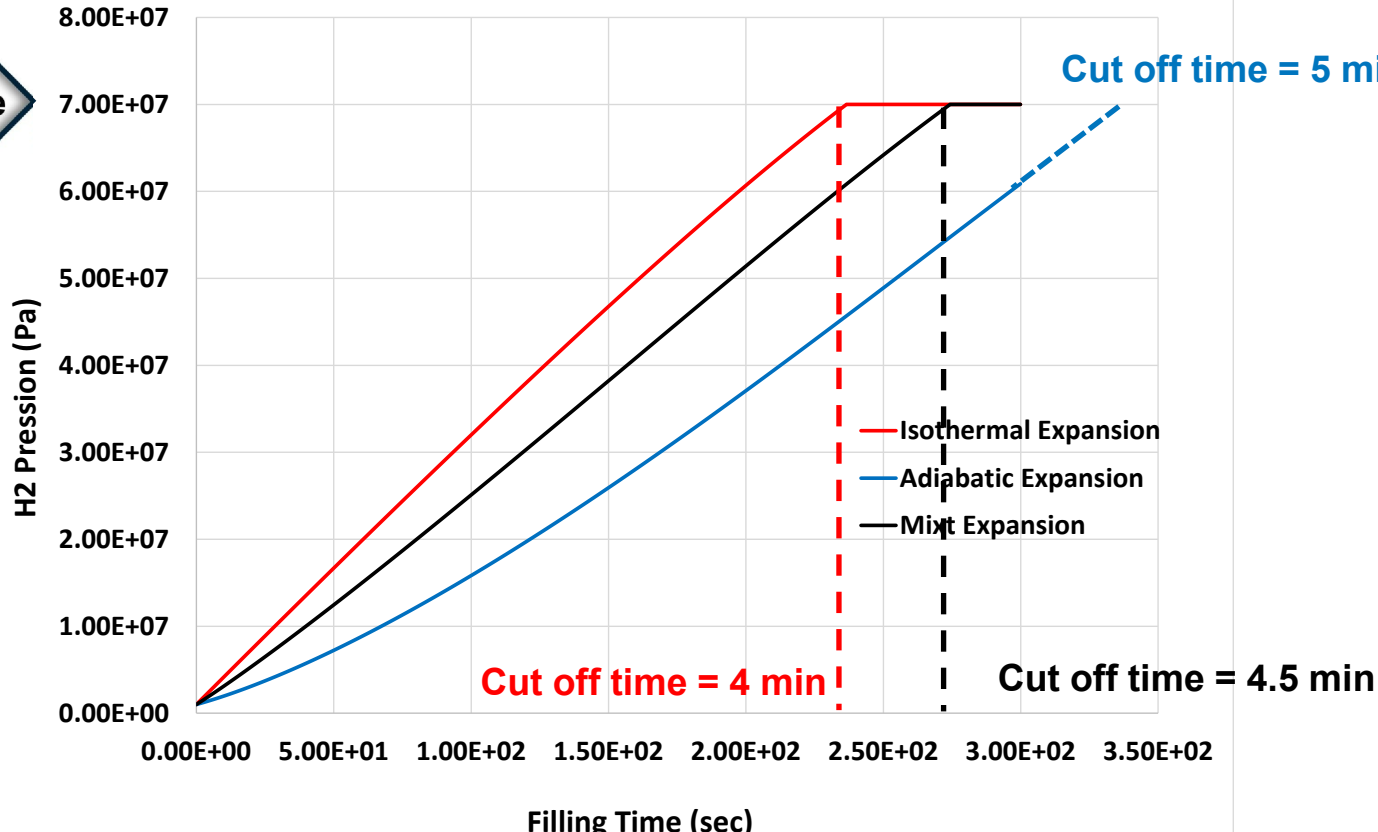
Scenario 2 : Adiabatic expansion in the station supply pipe

Scenario 3 : Mixed model

# H2 Permeability Analysis on Optimized Liner

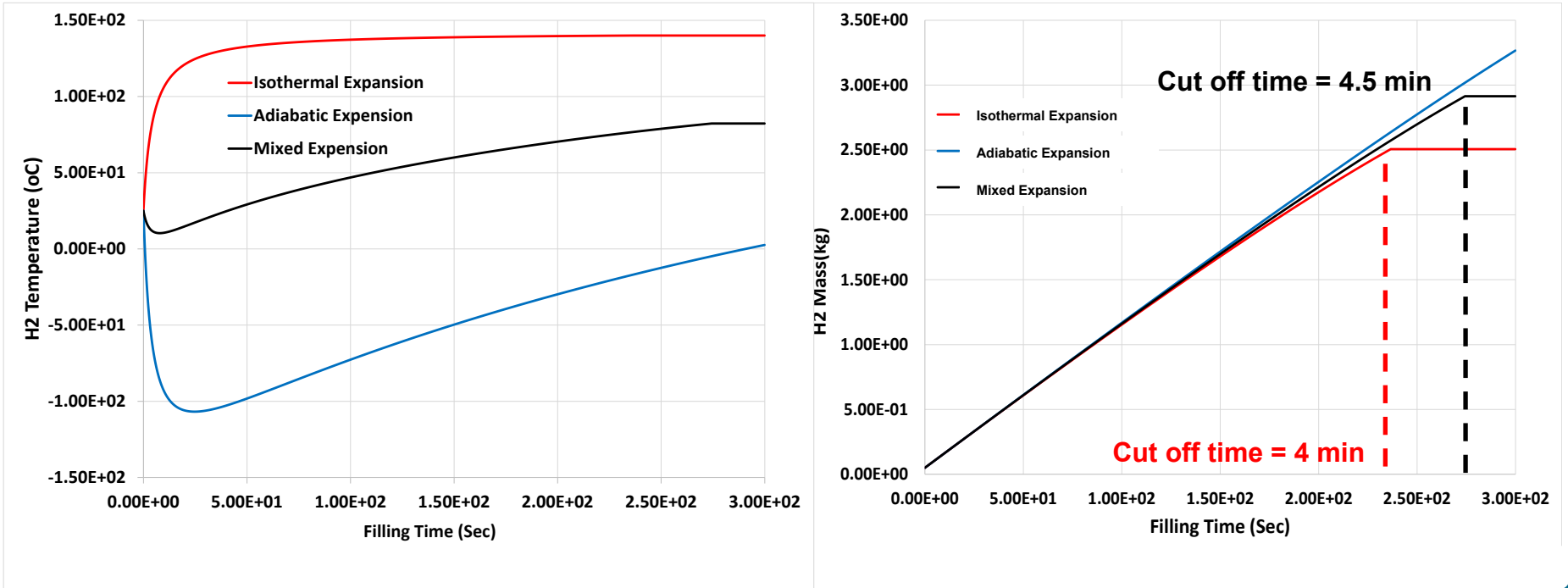
## Case 3.1: Pressure/Temp Variation during the Filling

Cut off Pressure



# H2 Permeability Analysis on Optimized Liner

## Case 3.1: Pressure/Temp Variation during the Filling



# H2 Permeability Analysis on Optimized Liner

## Case 3.2: Pressure/Temp Variation during the Emptying

### Emptying Phase

Reservoir Conditions

$$T_{H2\_R} = 25^{\circ}C$$

$$P_{H2\_R} = 70 \text{ MPa}$$

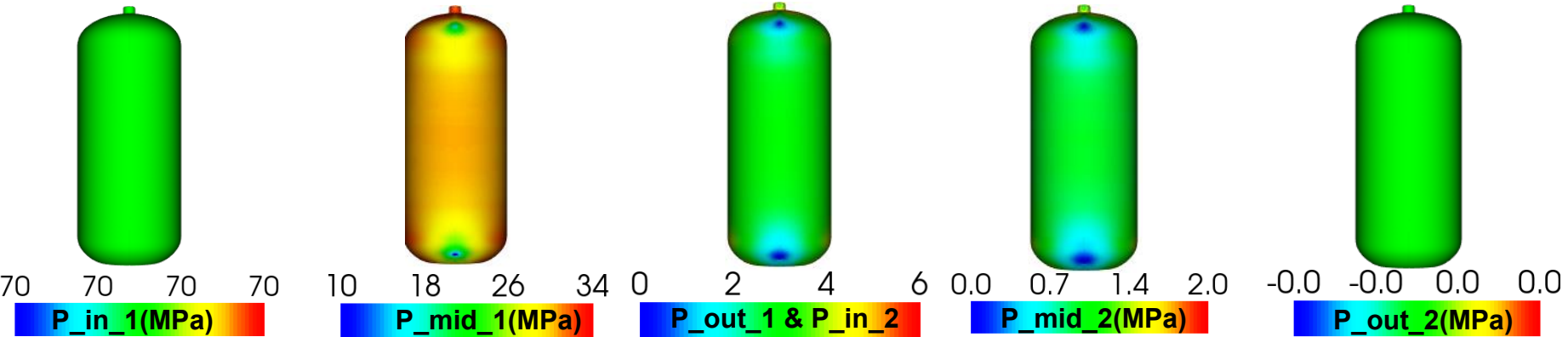
$$V_{H2\_R} = 61 \text{ L}$$

$$\text{EmptyingRate} = 1.1 \text{ kg/hr}$$



### H2 Pressure Evolution:

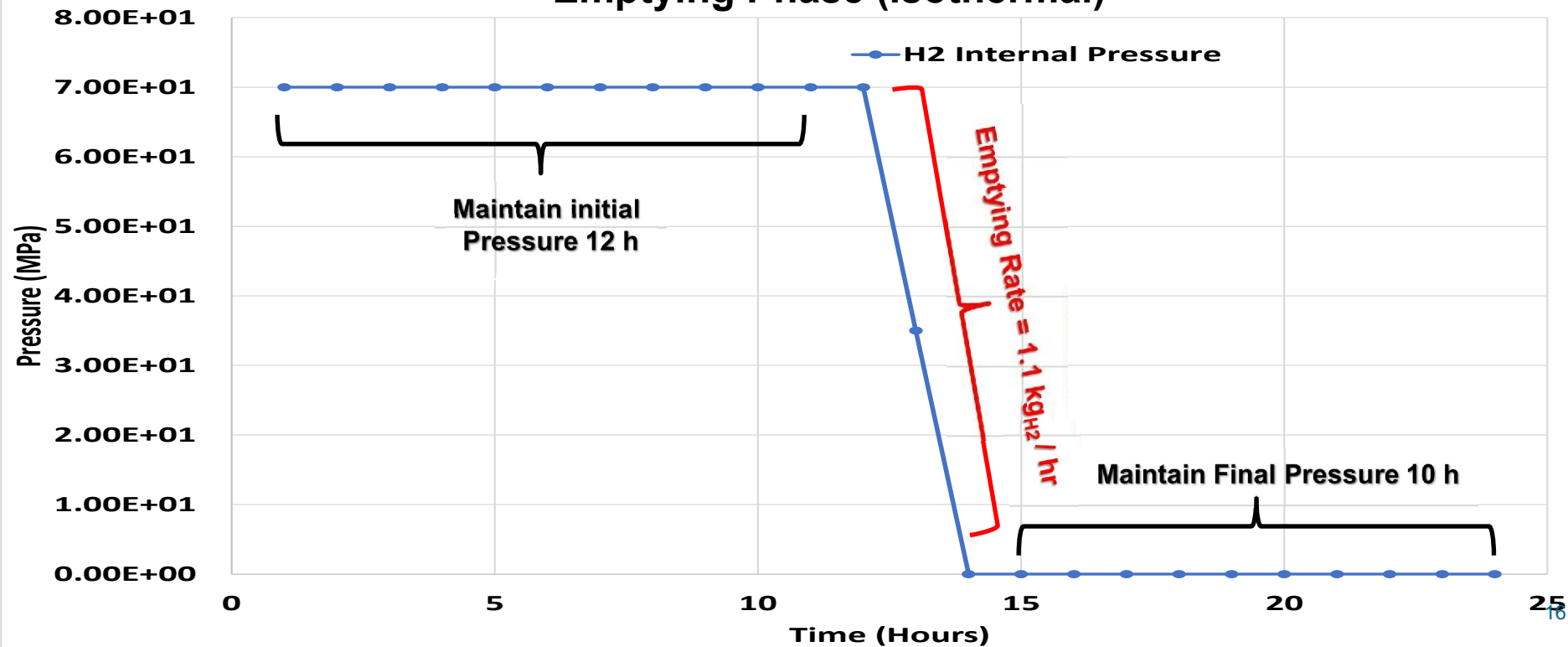
- Inside the H2 tank
- Through the Liner
- Interface Liner - Composite
- Through the Composite Layer



# H2 Permeability Analysis on Optimized Liner

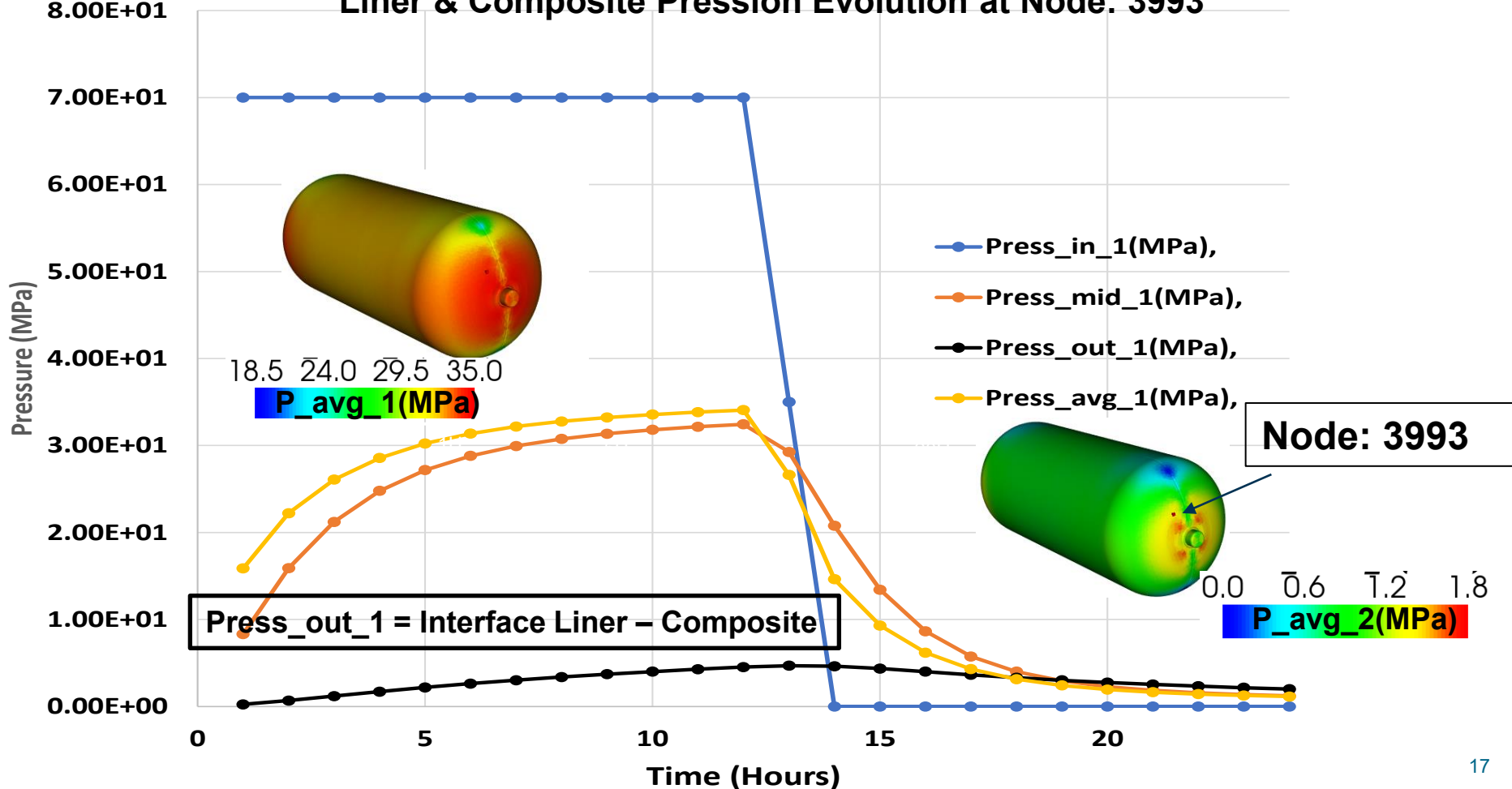
## Case 3.2: Pressure/Temp Variation during the Emptying Cycle

### Emptying Phase (Isothermal)



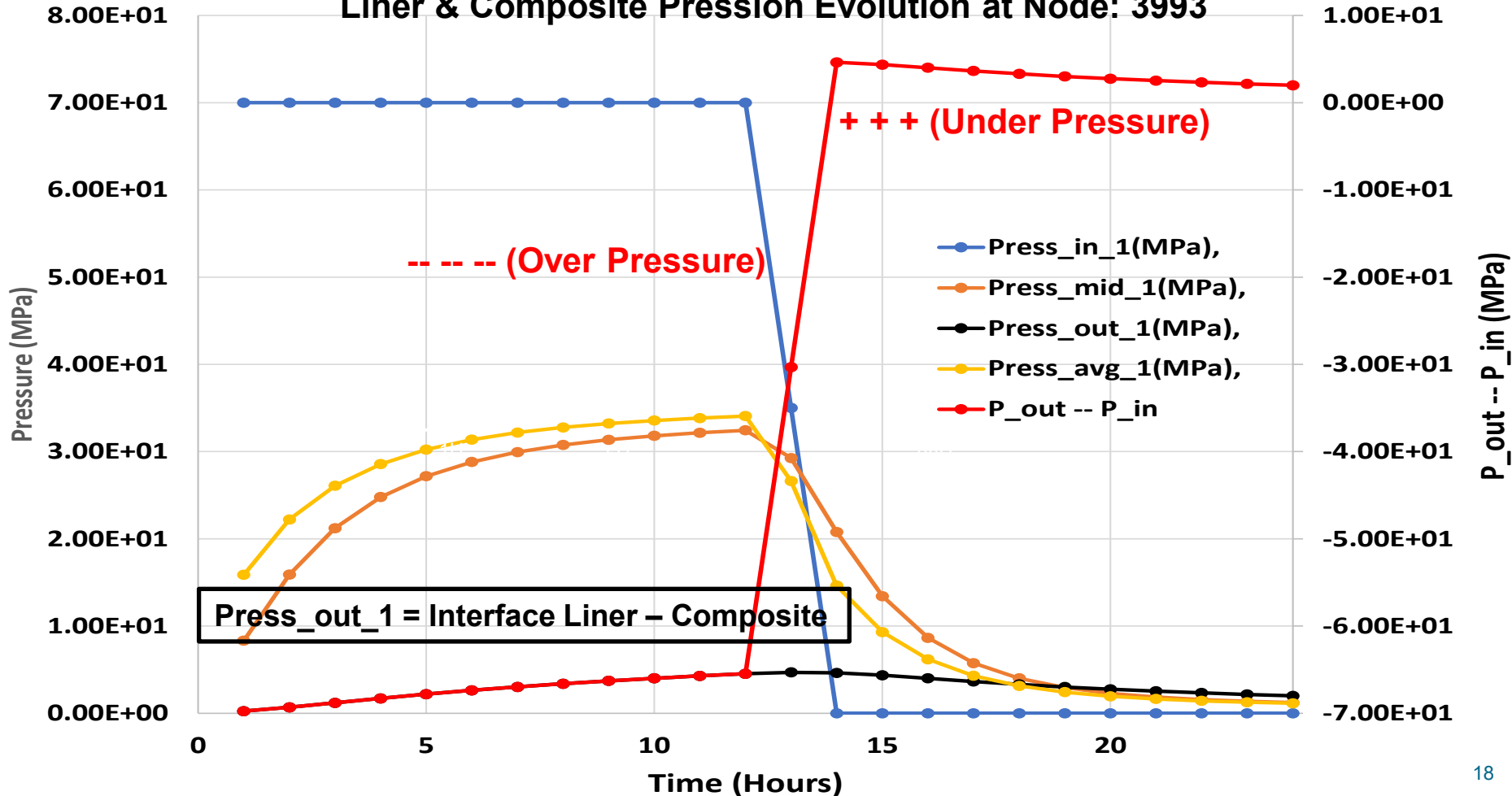
# Emptying Phase (Isothermal)

## Liner & Composite Pression Evolution at Node: 3993



# Emptying Phase (Isothermal)

## Liner & Composite Pressure Evolution at Node: 3993



# Conclusion & Future Developments

- **The permeability model has been improved by integrating the energy equation and the inclusion of the temperature effect on the transport coefficients**
- **Implementation of the thermodynamic model permitting :**
  - Predict H<sub>2</sub> temperature and pressure variations during filling and emptying cycles;
  - Predict the pressure and temperature distribution through the liner and the composite layer.

# Conclusion & Future Developments

- **Additional topics that are under investigation include:**
  - Predicting the exacerbation of liner-composite layer delamination during repeated tank filling and emptying cycles.
- **Coordinate, with industrial partners, validation studies based on experimental measurements.**

# Thank you !

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