Advancement in BlowView-H2 simulation software: design and optimization of thermoplastic liner for hyperbaric on-board hydrogen storage tanks

Benrabah, Zohir; Ilinca, Florin; Malo, Alain; Bournival, Sylvain; Bardetti, Anna

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Advancements in BlowView-H2 Simulation Software: Design and Optimization of Thermoplastic Liners for Hyperbaric On-board Hydrogen Storage Tanks

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Numerical simulation and Process Modelling Team
AMP-COMP

ITB's Advanced Mobility Fuels Summit 2024
The Sheraton Detroit Novi Hotel
21111 Haggerty Rd., Novi, MI 48375

Overview

- **Objectives of the simulation study**
- **Blow Molded Plastic Liner (BMPL) simulation & optimization analysis**
- **BMPL H_2 permeation simulation**
  - H2 Thermo-diffusion model in polymer
  - Variable external air temperature
  - Variable internal H2 temperature/pressure
- **Conclusion & what next ?**

Objectives

- Simulation analysis of a BMPL (provided by PO New Energies) using PA6 resin.
- Optimization of the processing parameters to improve uniformity of the liner thickness
- Modelling of H2 thermo-diffusion in polymer wall,
- Assess the BMPL permeability performance under different variable surrounding air temperature and internal H2 Temperature and pressure.

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  - Variable internal H2 temperature/pressure
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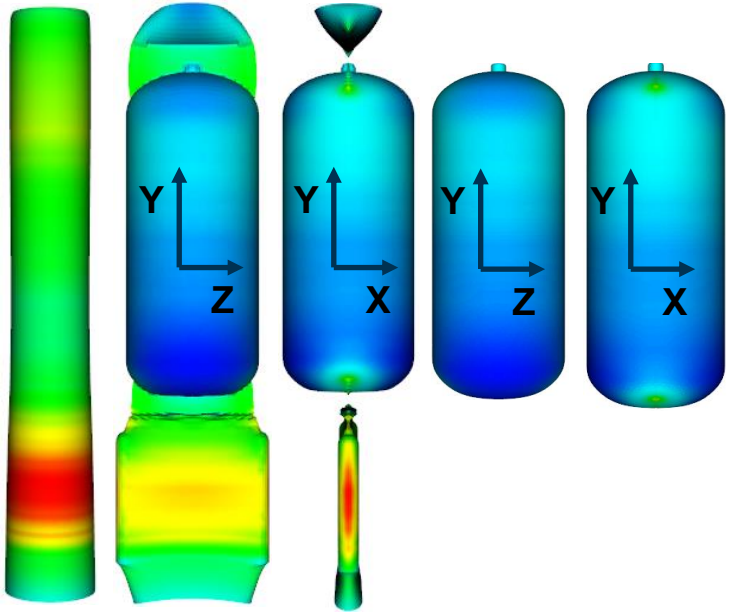
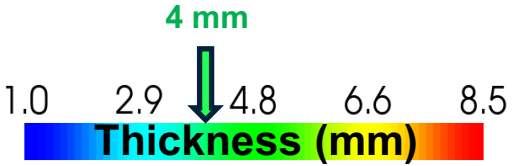
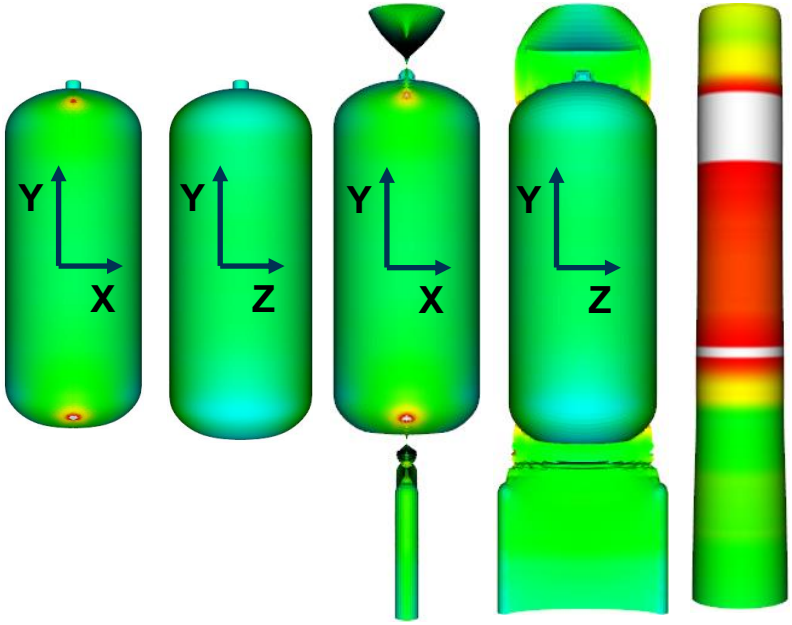
EBM H2 Liner simulation/optimization using PA6 (Durethan BC550Z)



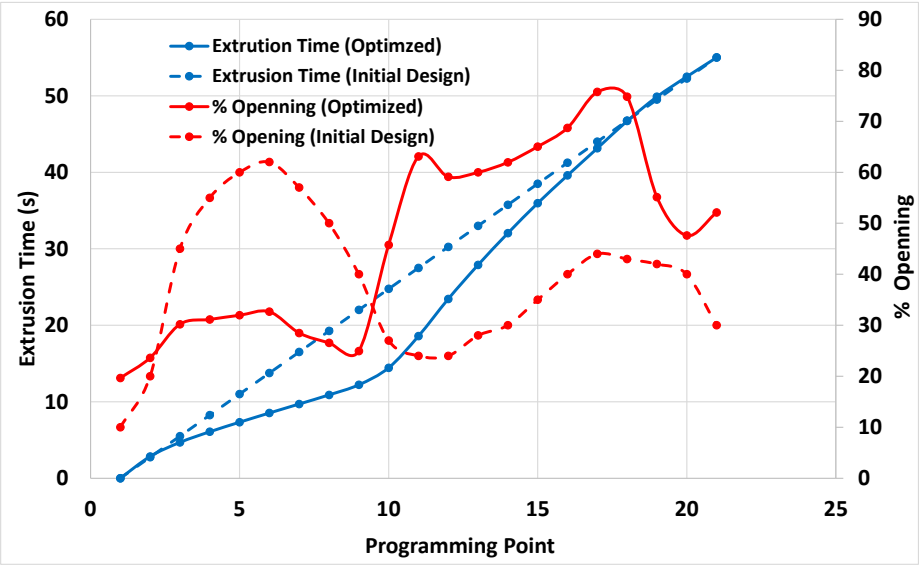
Initial Profile
Parison Length : 1432mm
Parison Weight : 4281 gr
Part Weight : 1759 gr
Part Average Thickness: 2.22 mm

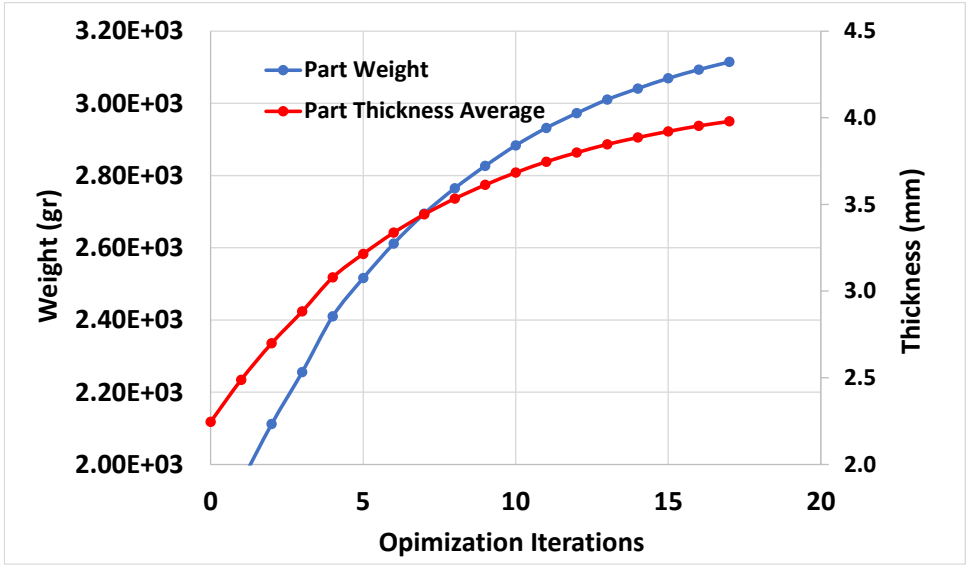




Optimized Profile
Parison Length : 1299mm
Parison Weight : 5089 gr
Part Weight : 3158 gr
Part Average Thickness: **3.99 mm**

EBM H2 Liner simulation/optimization using PA6 (Durethan BC550Z)





Overview

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Modelling H2 Thermo-diffusion in multilayer Polymer

Energy PDE

$$\frac{\partial}{\partial t}\left(\rho C_p T\right) - \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) = 0$$

$$T(x, t=0) = T_0\,(x)$$

$$k.\frac{\partial T(x=0,t)}{\partial x} = h_{in}\left(T_{H2}(t) - T(0,t)\right) \quad ; \; k.\frac{\partial T(x=L,t)}{\partial x} = h_{out}\left(T_{air}(t) - T(L,t)\right)$$

Diffusion PDE

$$\frac{\partial}{\partial t}\left(S_\infty \cdot \exp\left(\beta_s \cdot p_{H2} - \frac{\Delta H_s}{R \cdot T}\right) \cdot p_{H2}\right)$$

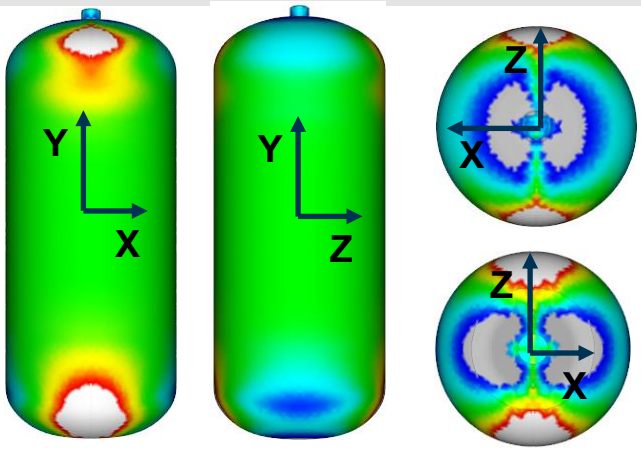
$$+\frac{\partial}{\partial x}\left(D_\infty \exp\left(\beta_D \cdot p_{H2} - \frac{E_D}{R \cdot T}\right)\frac{\partial}{\partial x}\left(S_\infty \cdot \exp\left(\beta_s \cdot p_{H2} - \frac{\Delta H_s}{R \cdot T}\right) \cdot p_{H2}\right)\right) = 0$$

$$p_{H2}(x, t=0) = p_{H2_0}\,(x)$$

$$p_{H2}(x=0,t) = p_{H2_{in}}\,(t) \; ; \; p_{H2}\,(x=L,t) = p_{H2_{out}}\,(t)$$

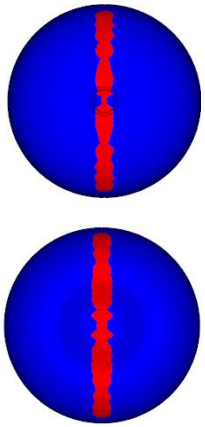
Benrabah Z., Ilinca F., Giraldeau F., Bournival S., Bardetti A. **Contribution to Modeling Hydrogen Permeation and Barrier Layer Optimization in Blow Molded Plastic Liners for an On-Board Compressed Hydrogen Tanks; International Journal of Hydrogen Energy, Nov., 2023**

H2 Permeability Analysis on Optimized PA6 (Durethan BC550Z) @ T =20^{0}C & 70MPa, Isothermal Steady State(monolayer)

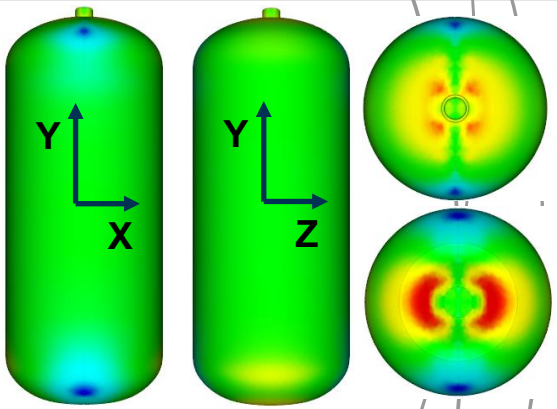


3.0 3.7 4.3 5.0

Thickness (mm)



(Pinch = 2.3 %)



151.8 312.1 472.4 632.7

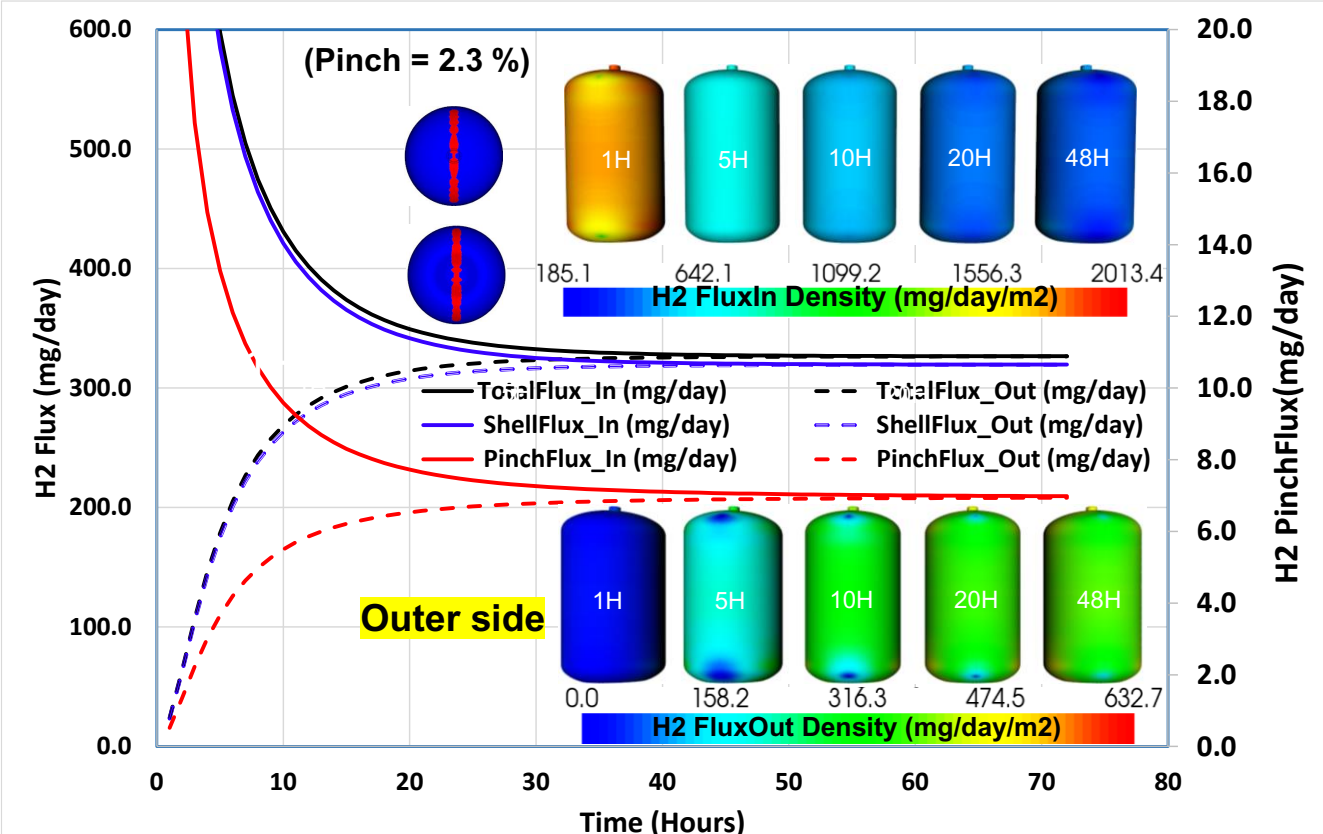
H2 Flux Density (mg/day/m2)

Part Weight : 3158 gr
Part Average Thickness: 3.99 mm

Shell Part Surface = 0.839062 m^2
Pinch-Off Part Surface = 0.018724 m^2
H2/Day through Shell Surface = 326.45 mg/Day
H2/Day through Pinch-Off Surface = 6.60 mg/Day
Total H2/Day = 333.05 mg/Day = 5.17 Nml/hr/L

Limit = 6 NmL/hr/L

H2 Permeability Analysis on Optimized PA6 (Durethan BC550Z) @ T =20^{0}C & 70MPa, Isothermal Transient



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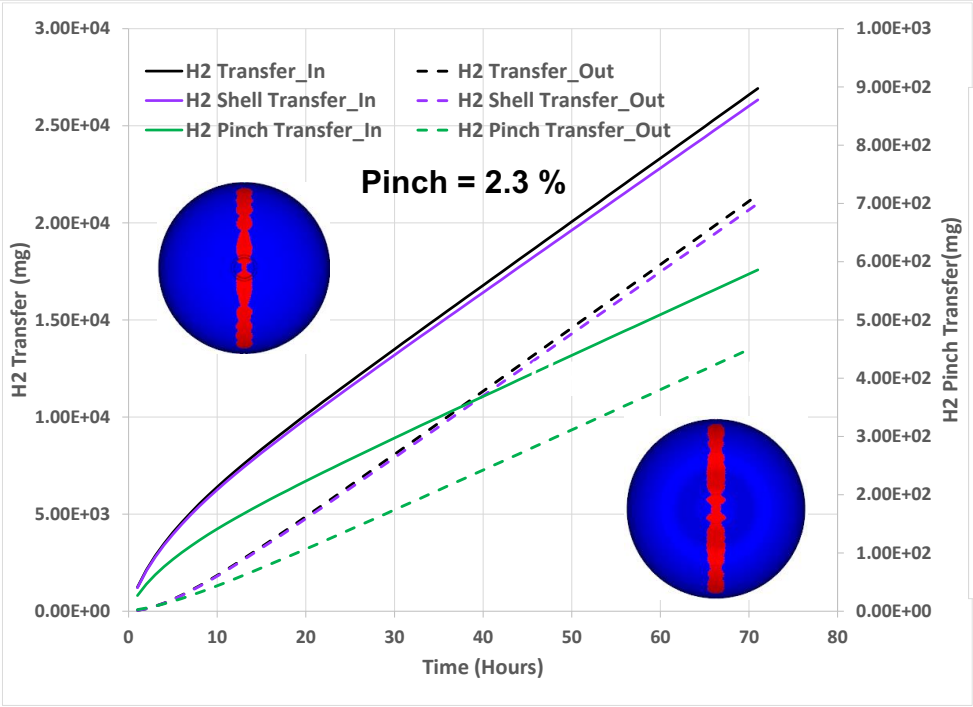
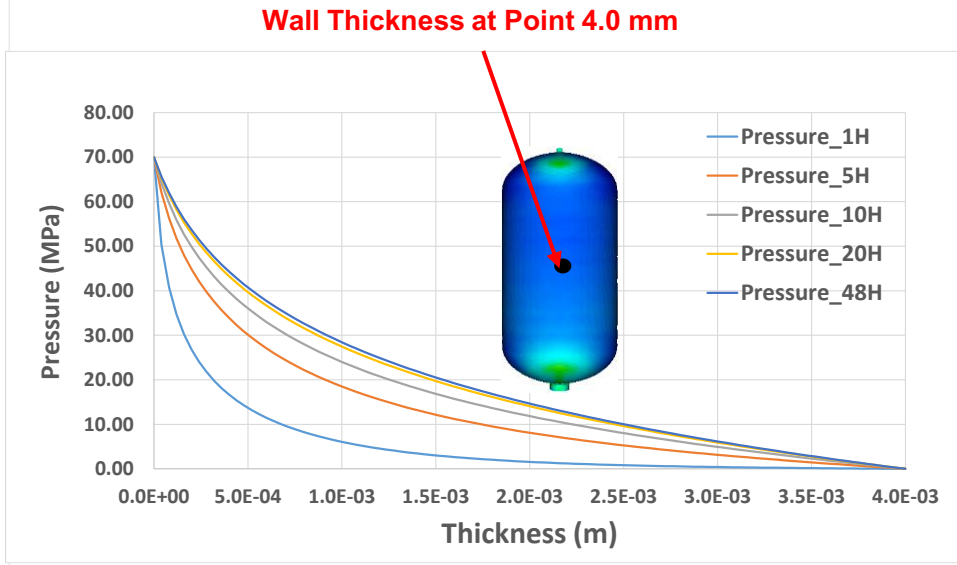




H2 Permeability Analysis on Optimized PA6 (Durethan BC550Z) with Time Depend Temperature Gradient

Simulation case 1:

Initial liner T_Init = 20^{0}C; P_H2 = 0.0 MPa

Inner side T_H2 = 20^{0}C; P_H2 = 70.0 MPa

Outer side T_Air = 20 ^{0}C + Amp . sin(2PI/24*time); P_H2 = 0.0 Mpa

Amp = 25 when sin(2PI/24*time) > 0 ; Amp = 5 when sin(2PI/24*time) < 0

Simulation case 2:

Initial liner T_Init = 20^{0}C; P_H2 = 0.0 MPa

Inner side T_H2 = 20 ^{0}C +Amp . sin(2PI/24*time); P_H2 = 70.0 MPa

Outer side T_Air = 20 ^{0}C; P_H2 = 0.0 MPa

Simulation case 3:

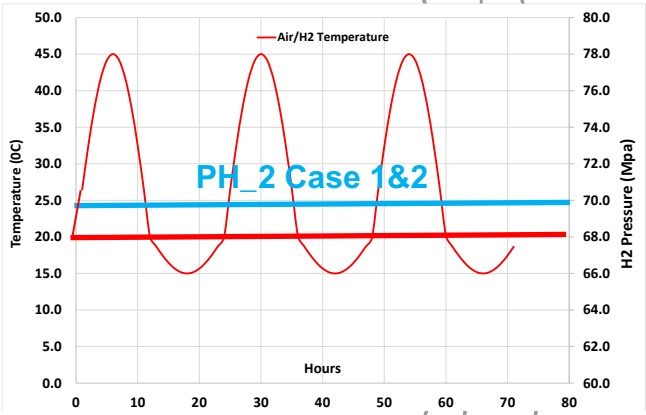
Initial liner T_Init = 20^{0}C; P_H2 = 0.0 MPa

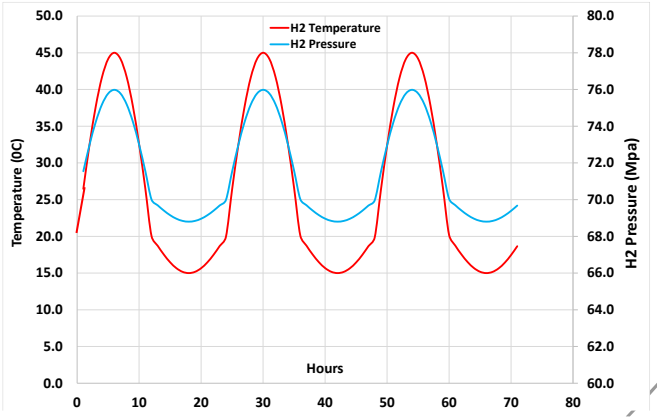
Inner side T_H2 = 20 ^{0}C +Amp . sin(2PI/24*time);

Inner side (H2 Pressure obey to isochore transformation)

P_H2 /T_H2 = (P_H2 = 70 x 10^6) / (T_H2 = (273+ 20))

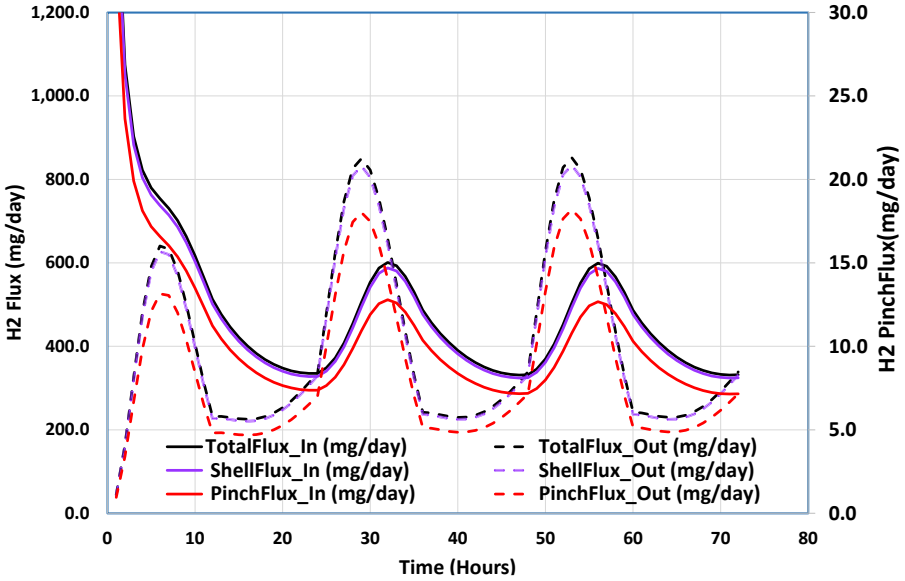
Outer side T_Air = 20 ^{0}C; P_H2 = 0.0 MPa



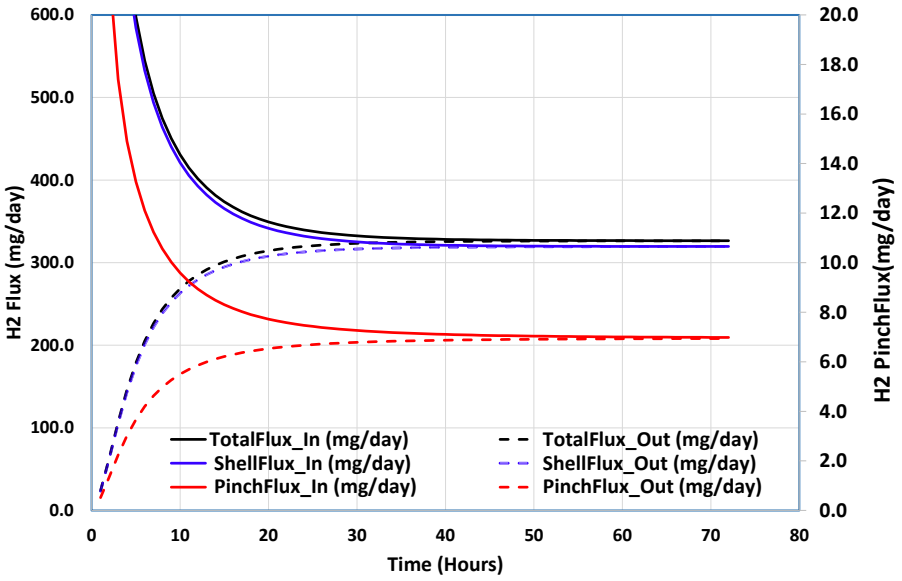


H2 Permeability Analysis on Optimized PA6 @ Transient thermo-diffusions simulation

T_H2 = 20^{0}C; T_Air = 20 ^{0}C + Amp . sin(2PI/24*time)
p_H2= 70MPa



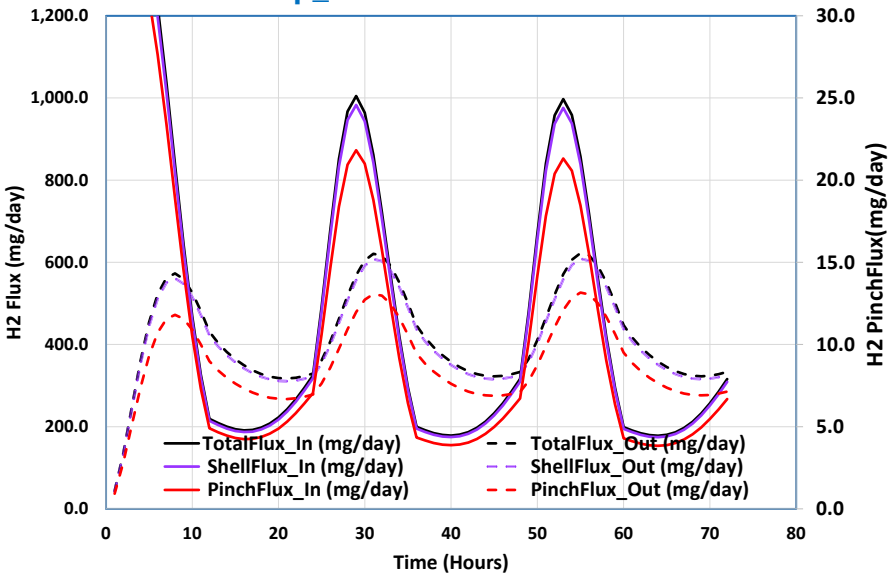
Isothermal: T_H2 =20^{0}C & T_Air =20 ^{0}C
p_H2= 70MPa



H2 Permeability Analysis on Optimized PA6 @ Transient thermo-diffusion simulation

T_H2 = 20 + Amp . sin(2PI/24*time); T_Air = 20^{0}C

p_H2= 70MPa



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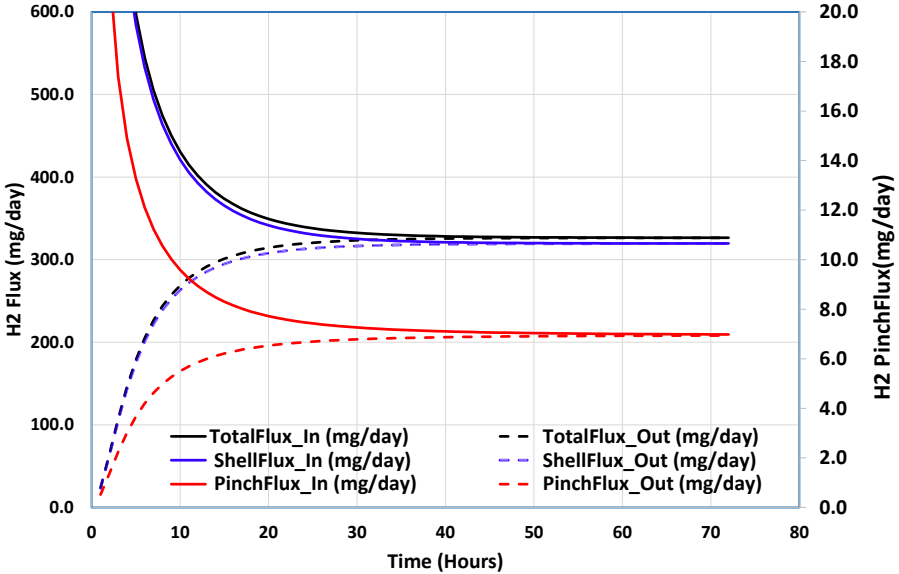
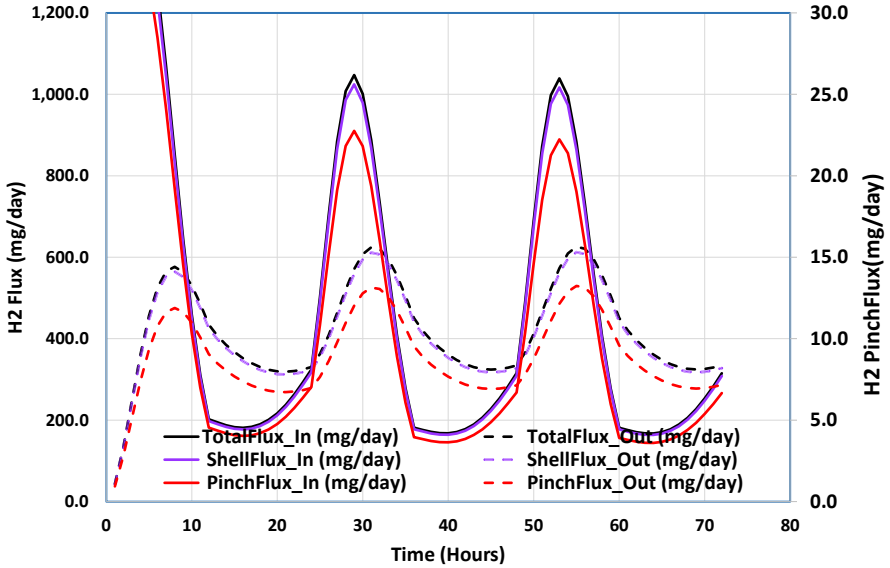


H2 Permeability Analysis on Optimized PA6 @ Transient thermo-diffusion simulation

T_H2 = 20 + Amp . sin(2PI/24*time); T_Air = 20^{0}C

Isochore Transformation
p_H2/T_H2 = constant



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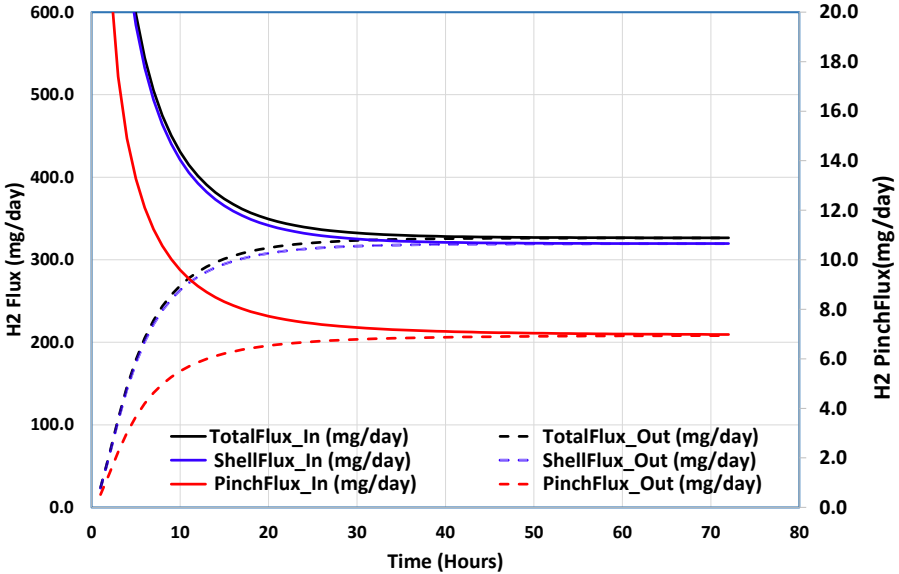

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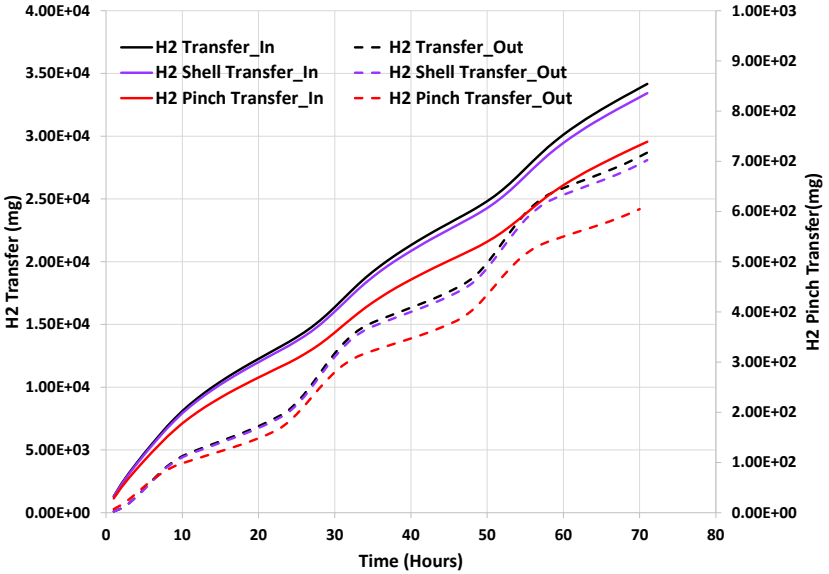

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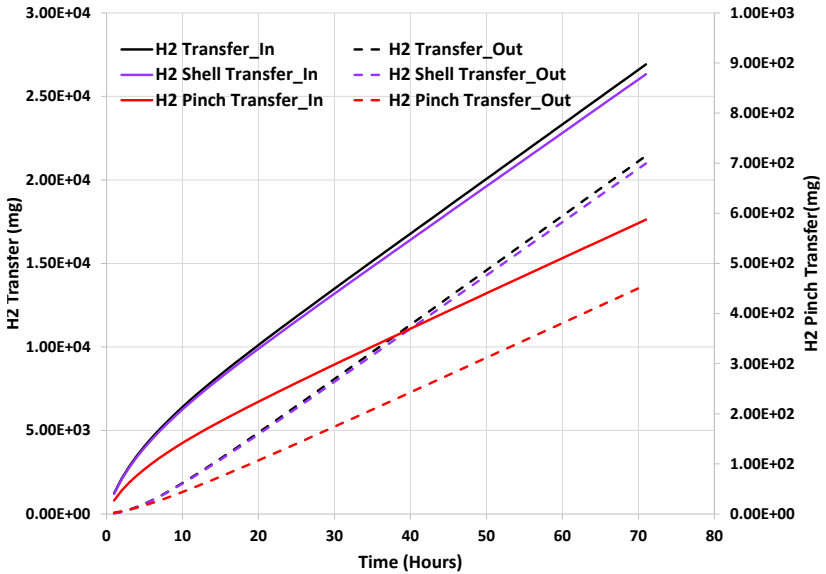

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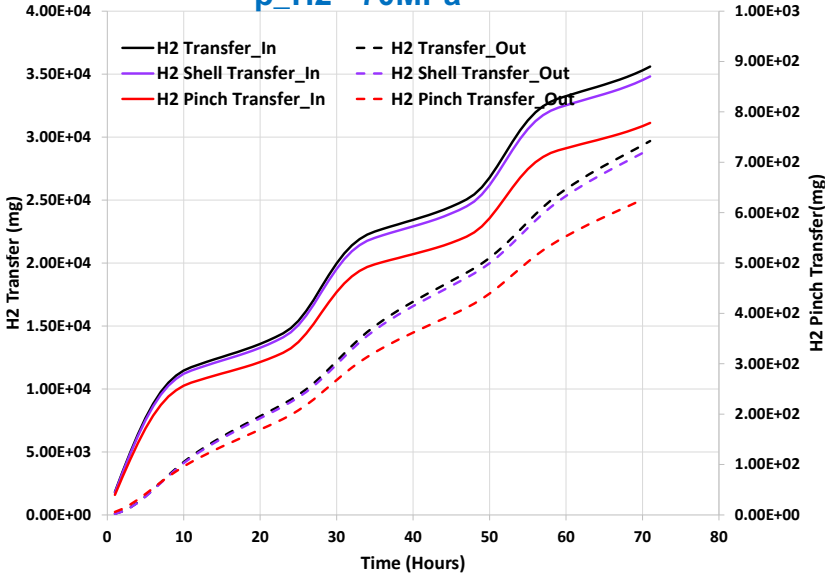

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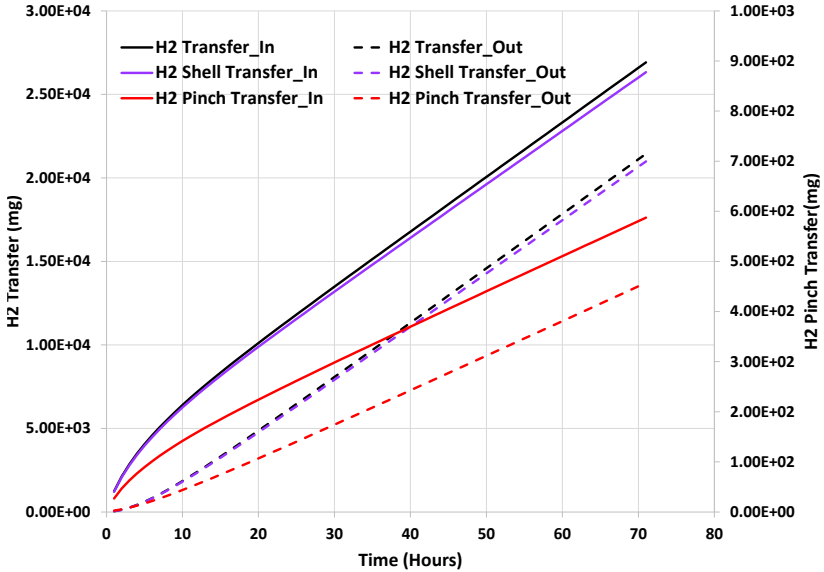

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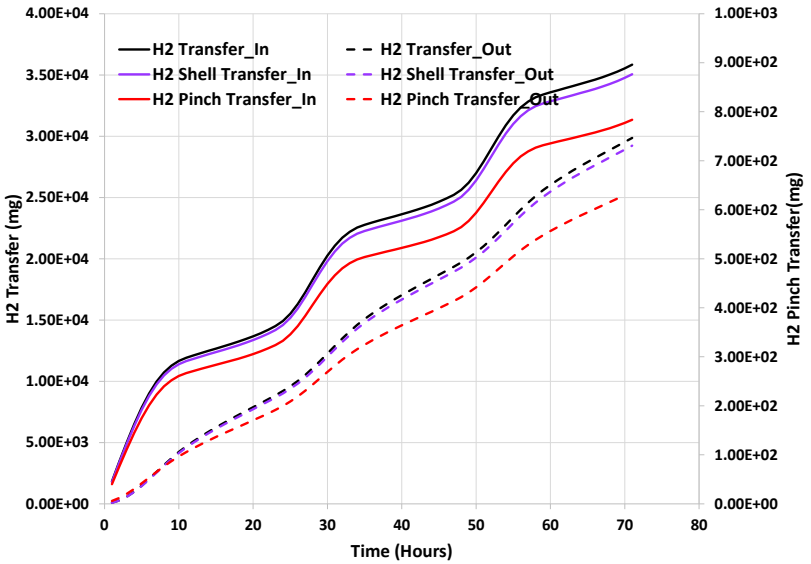

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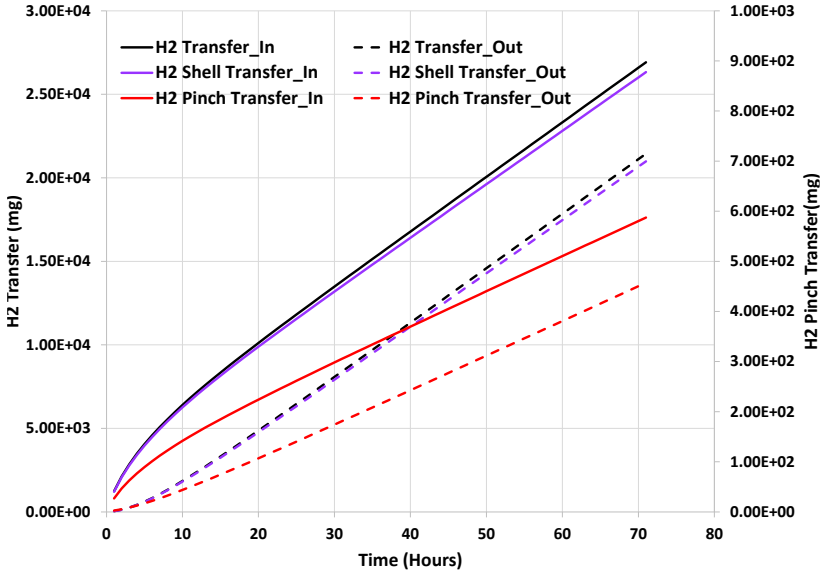

Conclusion & further developments

- **The permeability model has been improved by integrating the energy equation and the inclusion of the temperature effect on the transport coefficients;**

- **Continuing the enhancement of the permeability model by incorporating:**
  - **The thermodynamical model to account for pressure adjustment resulting from H2 losses during the permeation process and predict temperature variations due to the compression heating during the refiling & emptying phases;**
  - **The impact of the crystallinity in permeation model to expand its capabilities to semi –crystalline resins.**

Conclusion & further developments

- **Additional topics that will be investigated in the future include :**
  - **Modeling the cure process in the composite layer and analyzing liner delamination during curing.**
  - **Predicting the exacerbation of liner-composite layer delamination during repeated tank filling and emptying cycles.**

- **Coordinate with industrial partners simulation – validation study based on experimental measurements;**

- **The Office of Energy Research and Development (OERD) and AMP-COMP Program for supporting this project**
- **Our collaborators:**
  - P.O New Energies (Case Study)
  - LANXESS (PA6: Durethan BC550Z DUSXBL)

Thank you !

Contact : Zohir Benrabah

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