MODELLING OF MASS TRANSFER THROUGH THE BARRIER ENVELOPES OF VIPS

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Lionel FLANDIN, Bernard YRIEIX

IVIS 2015 – Nanjing – September 19th and 20th, 2015

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INTRODUCTION

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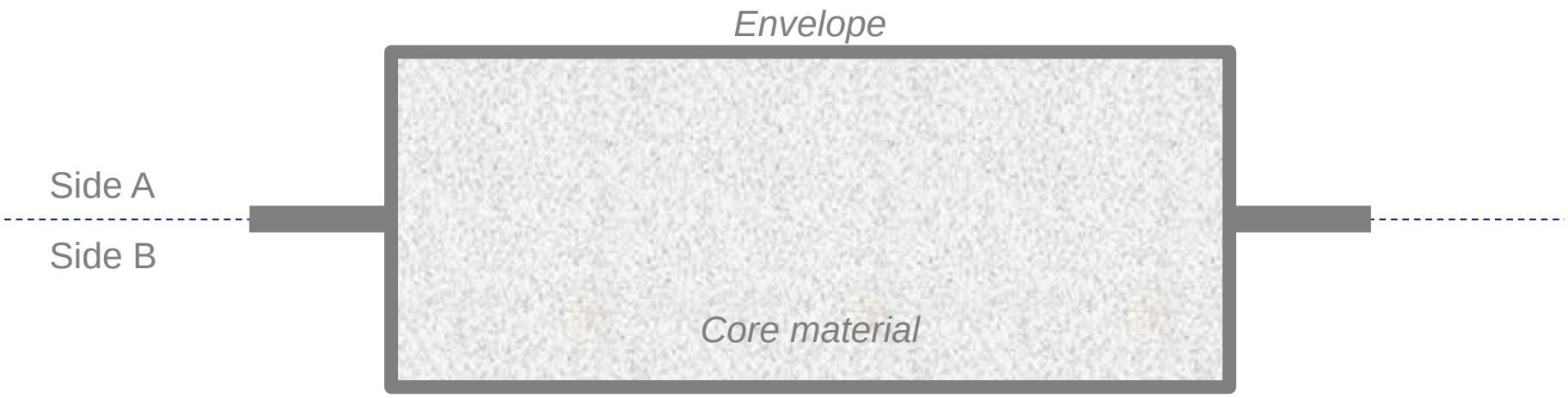
- **Hygrothermal behaviour of VIPs**



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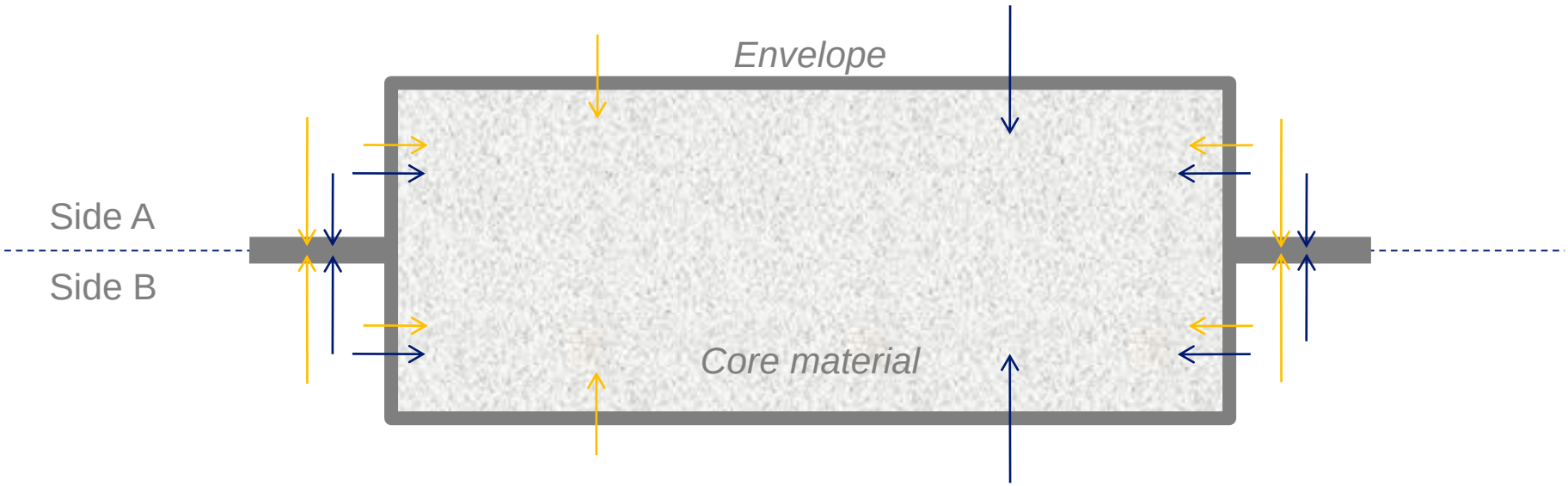

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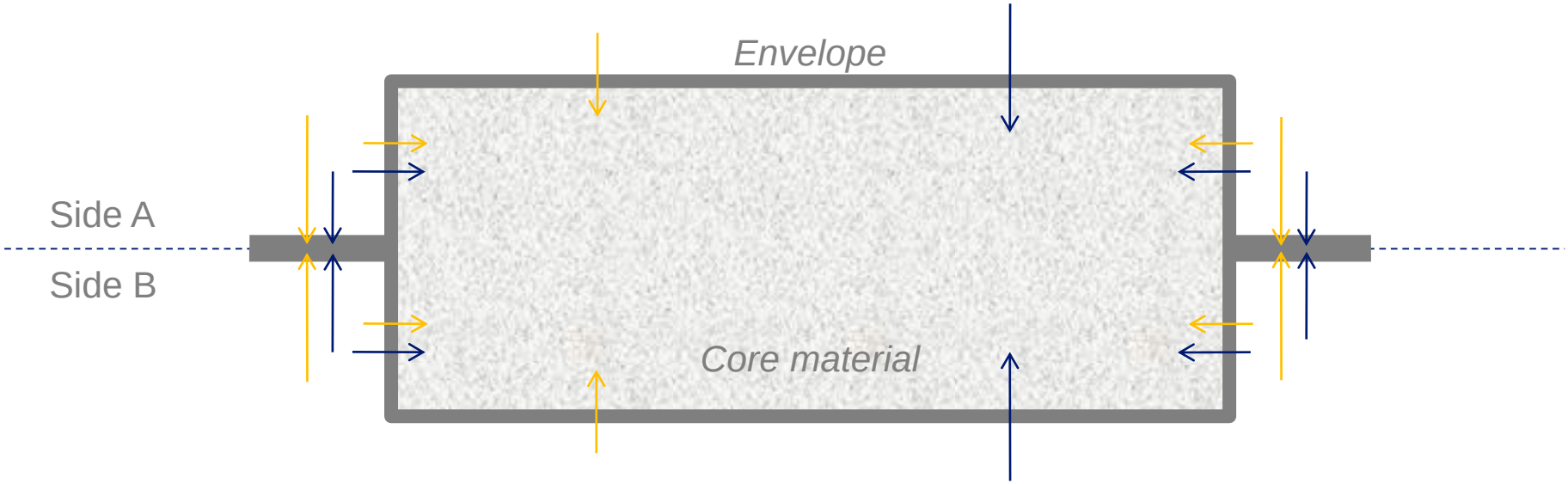

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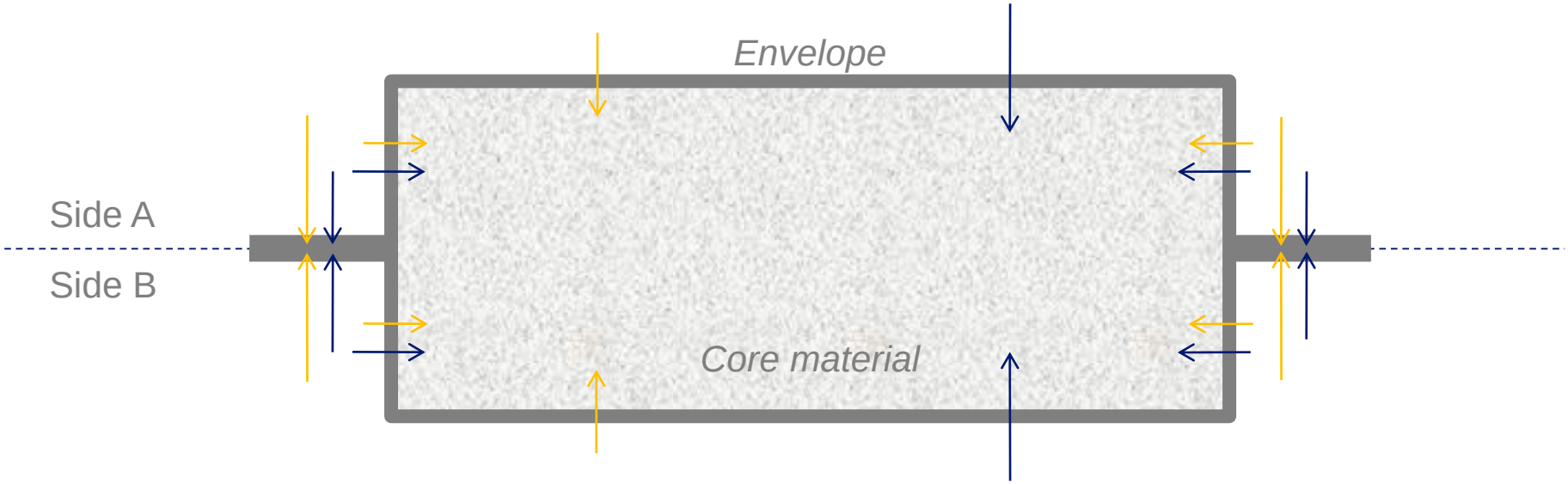

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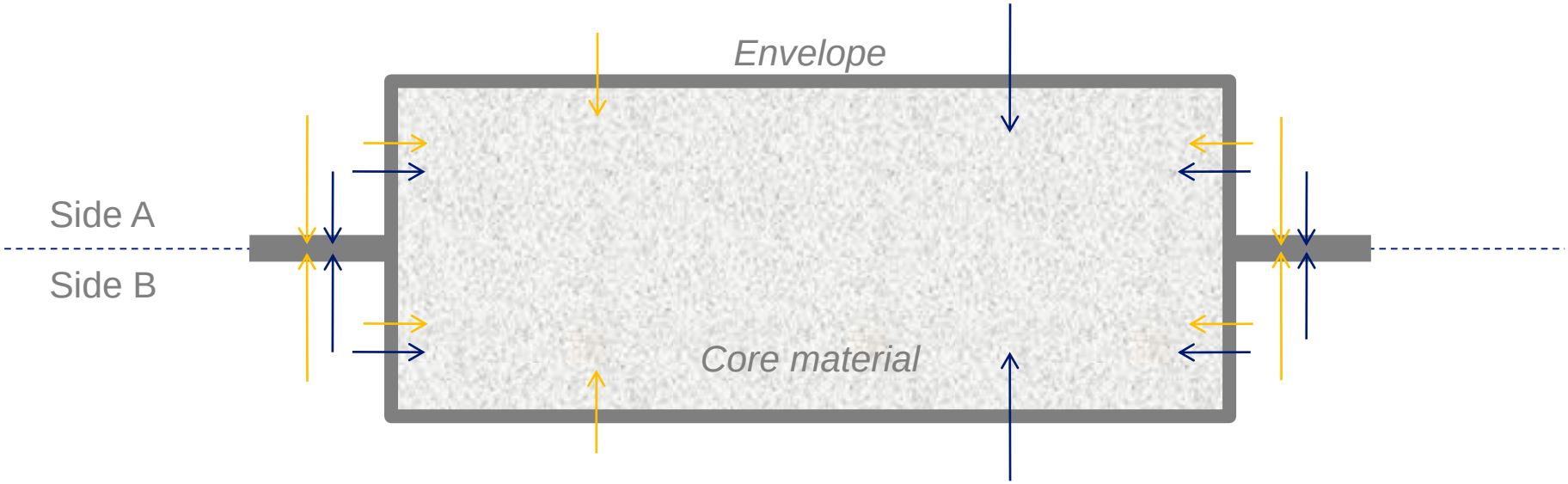

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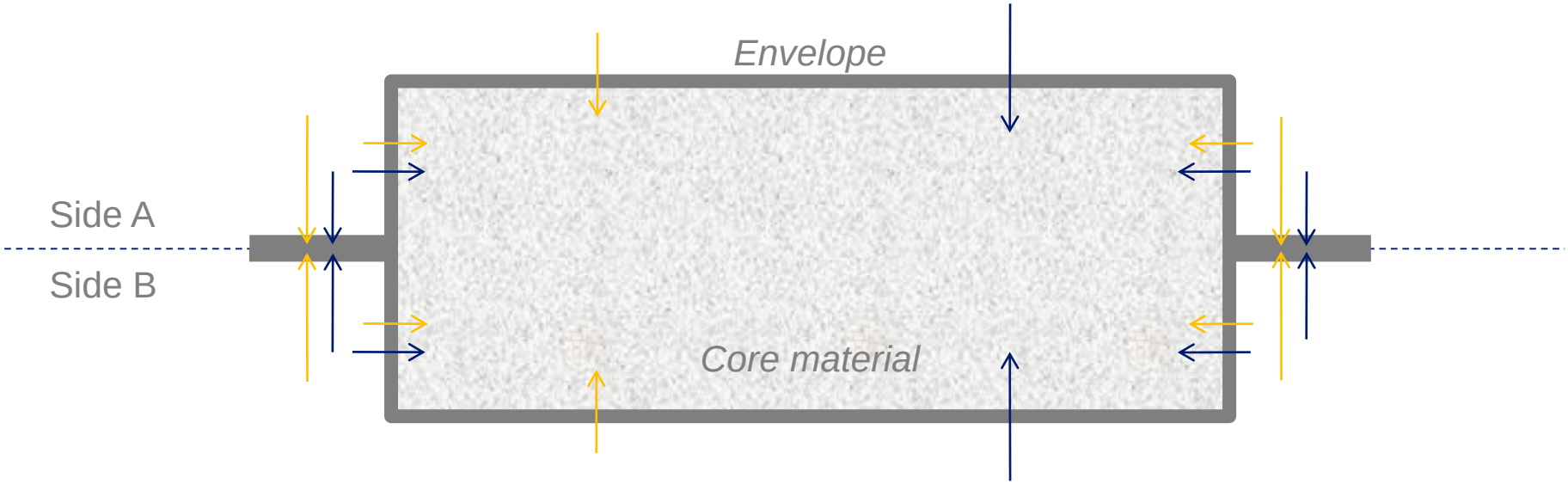

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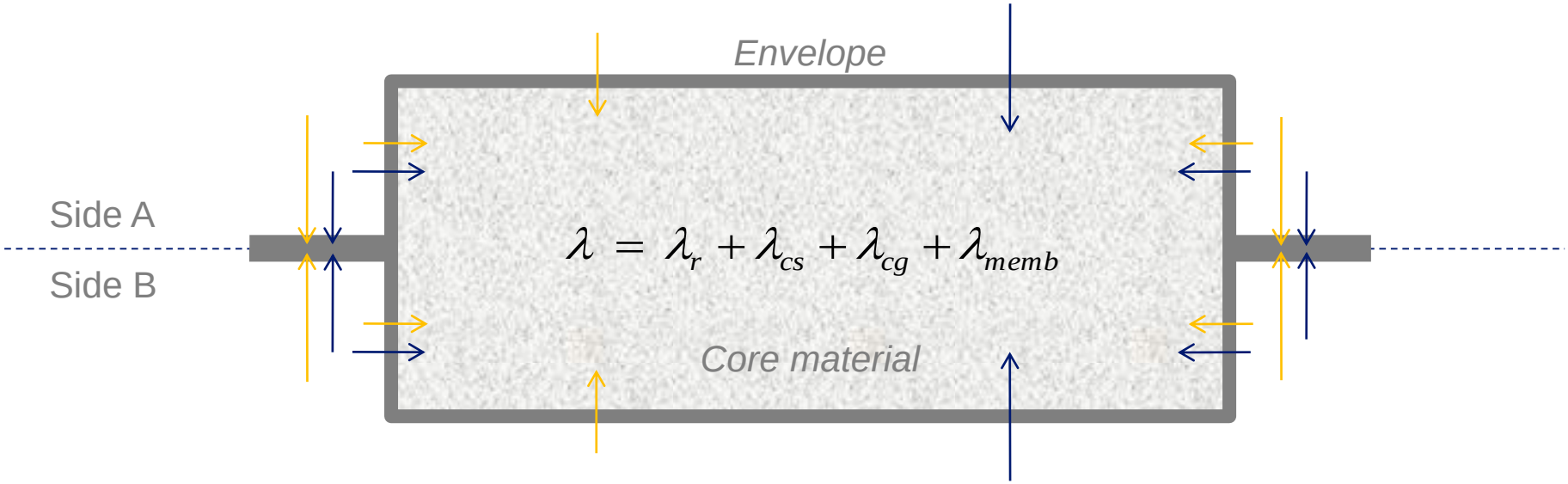

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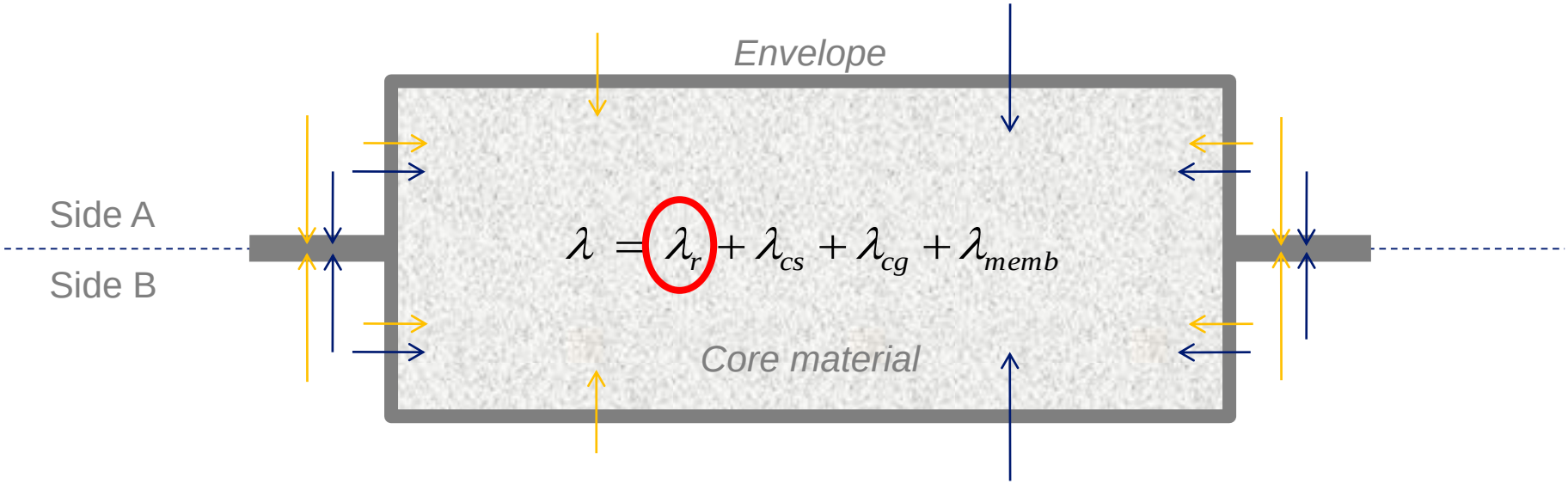

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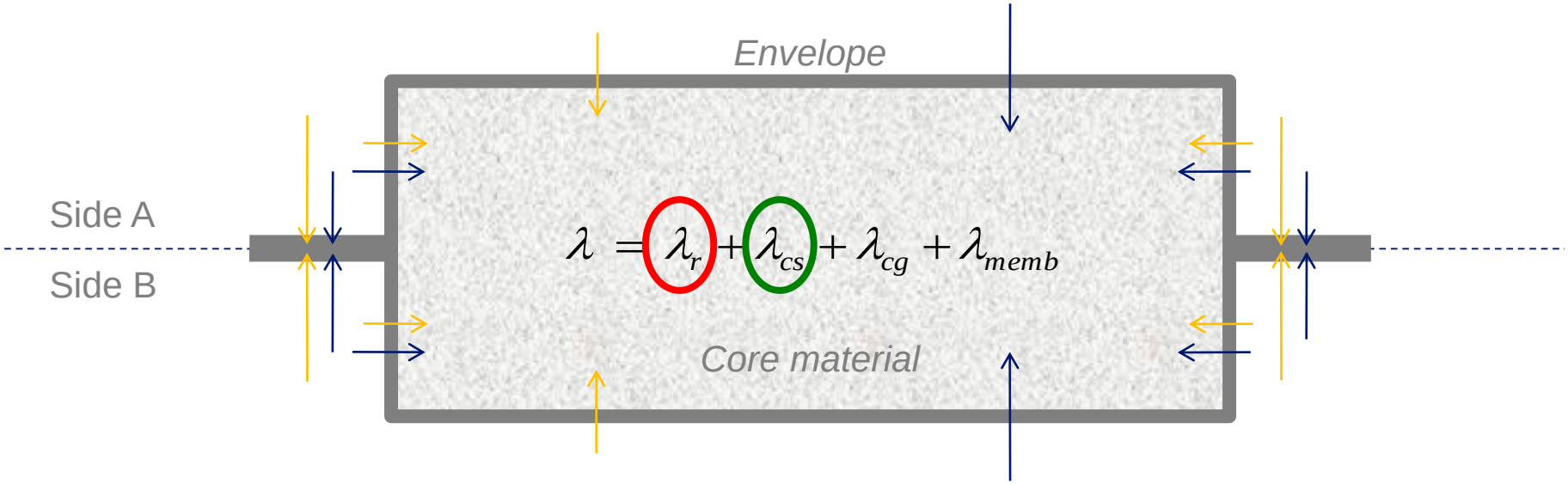

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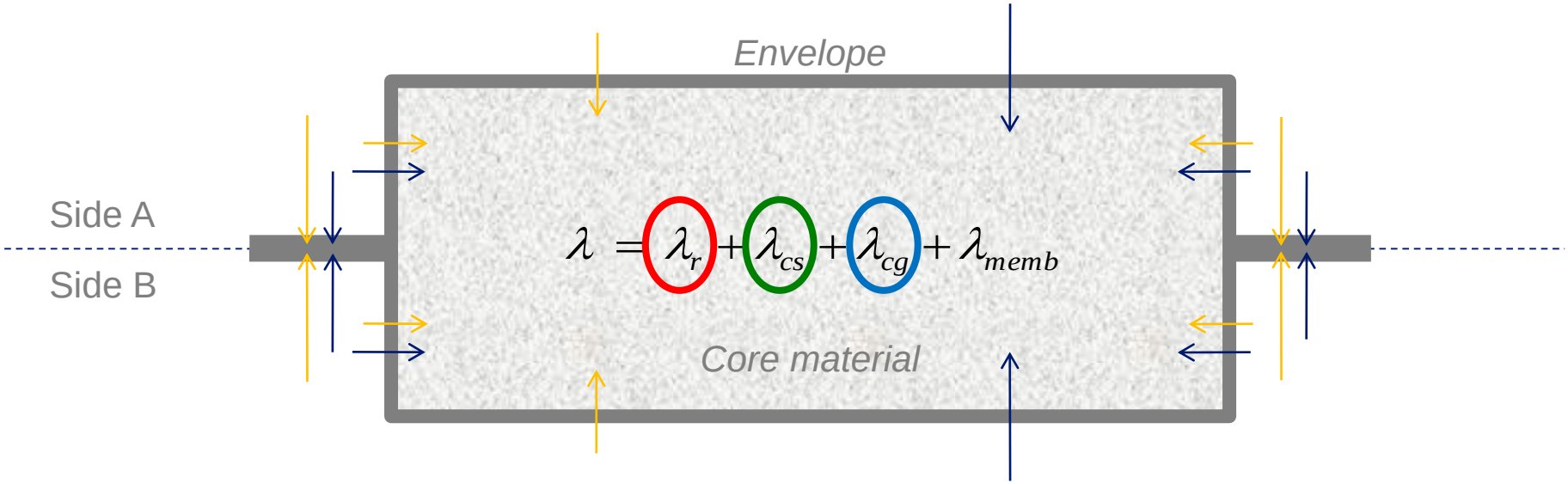

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+ pore size distribution

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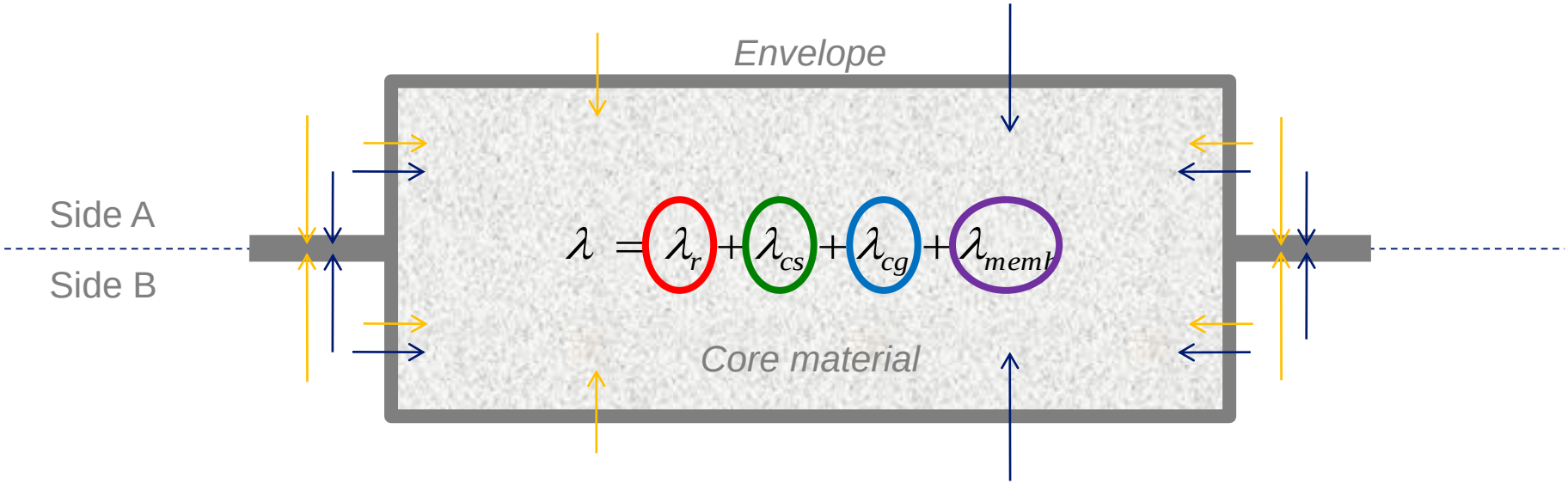

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Envelope Geometry

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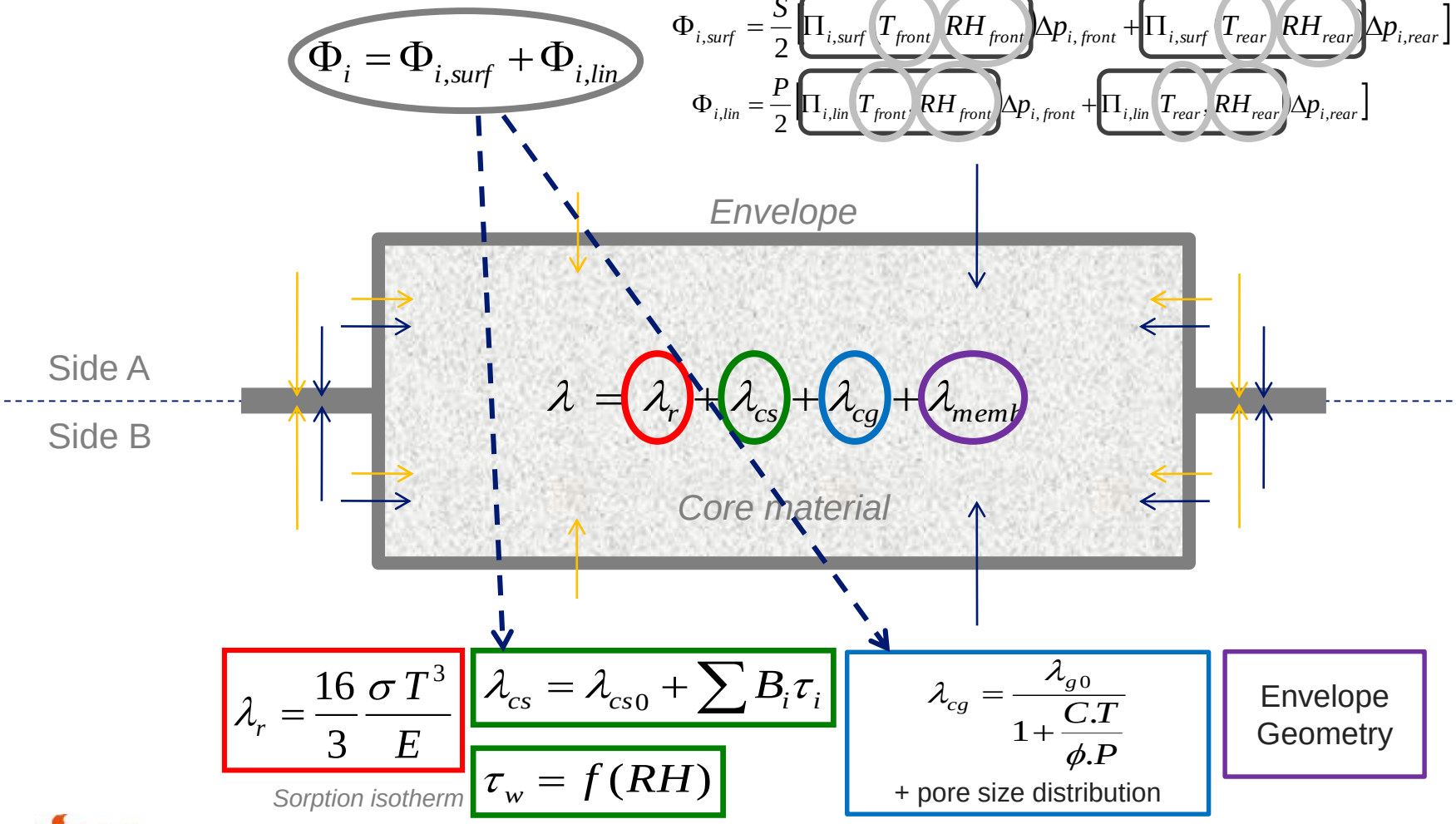

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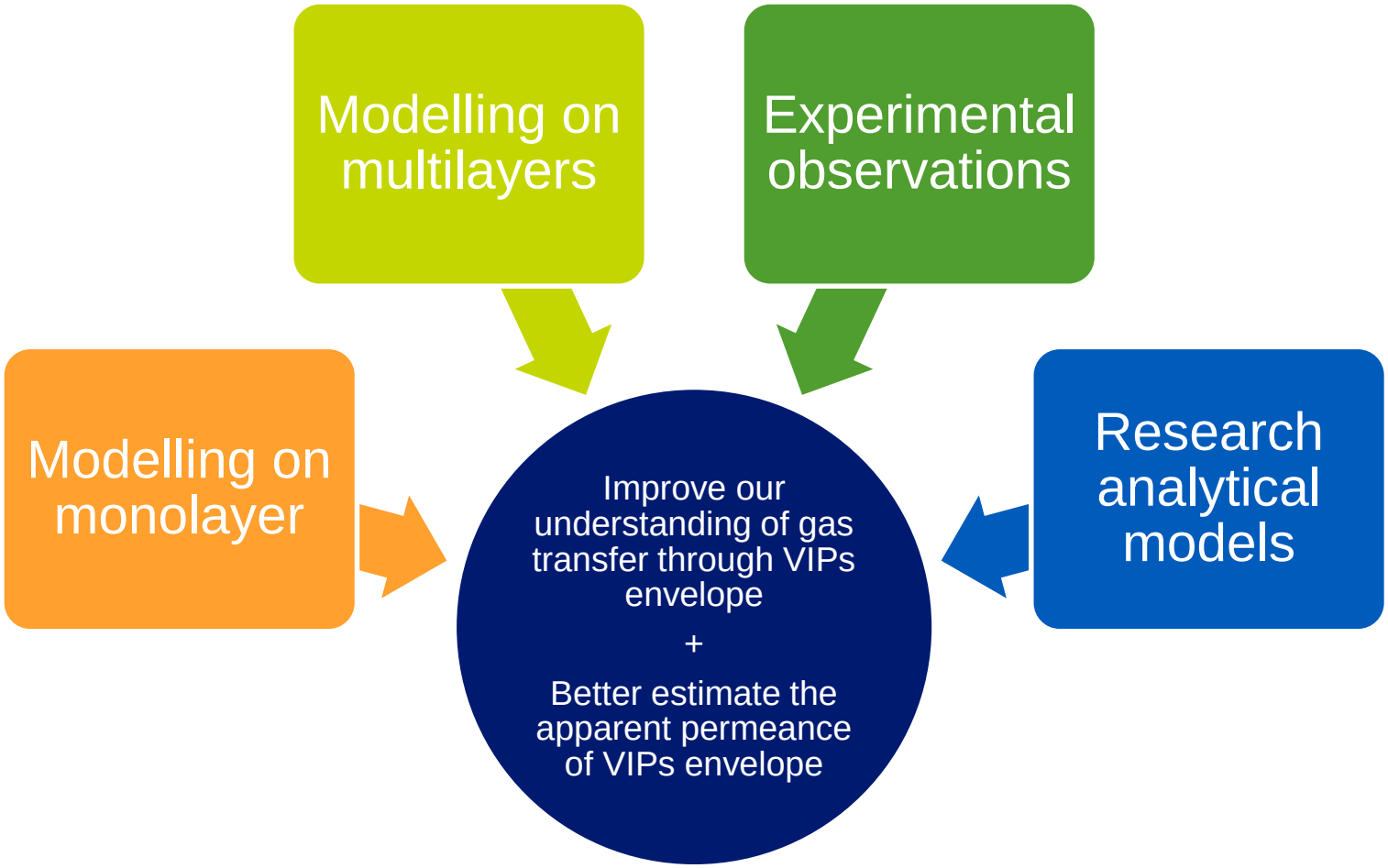

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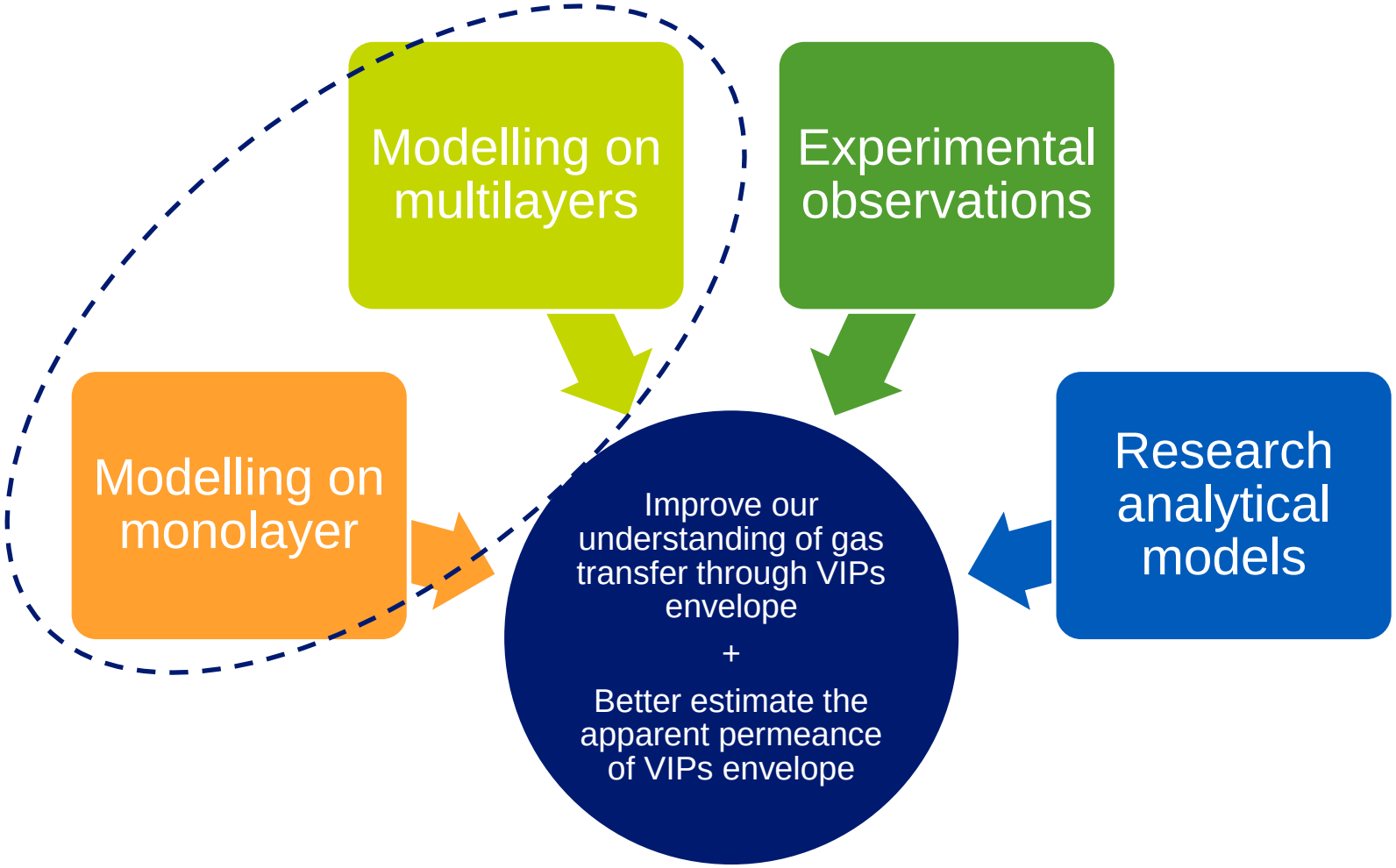

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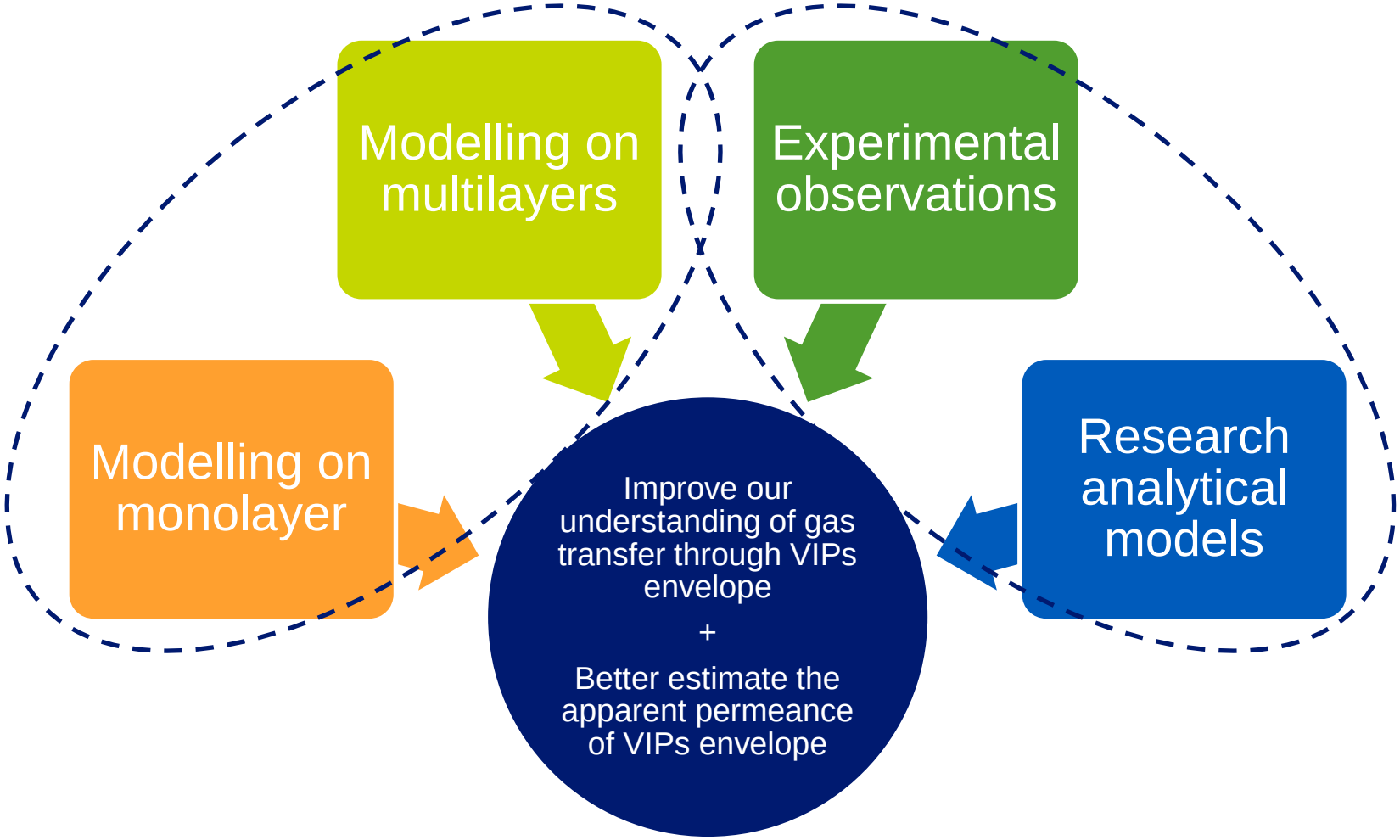
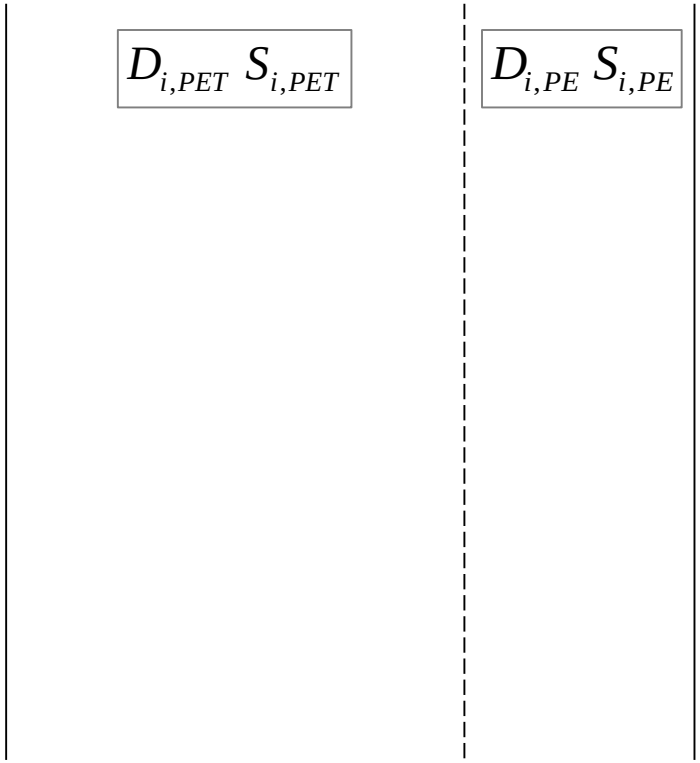


MODELLING APPROACH

BASICS PHENOMENA

- **Dissolution and molecular diffusion**



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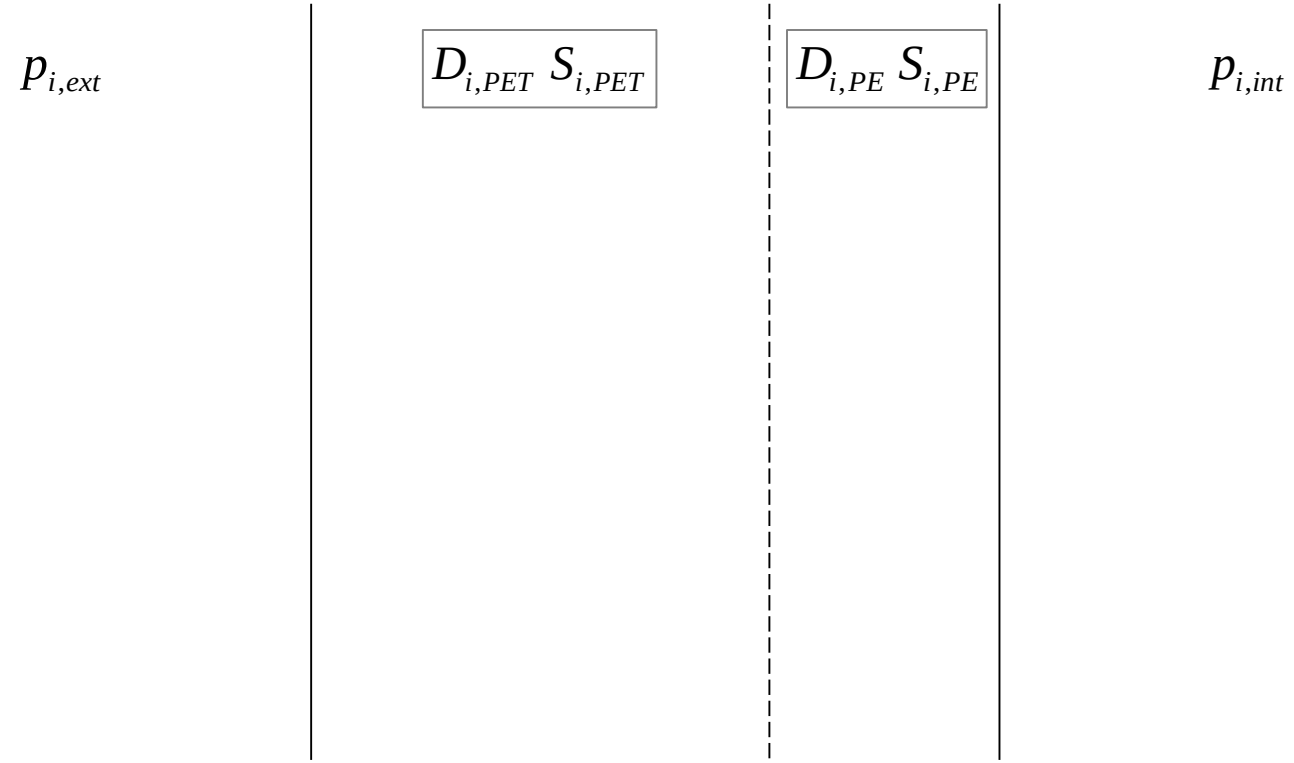

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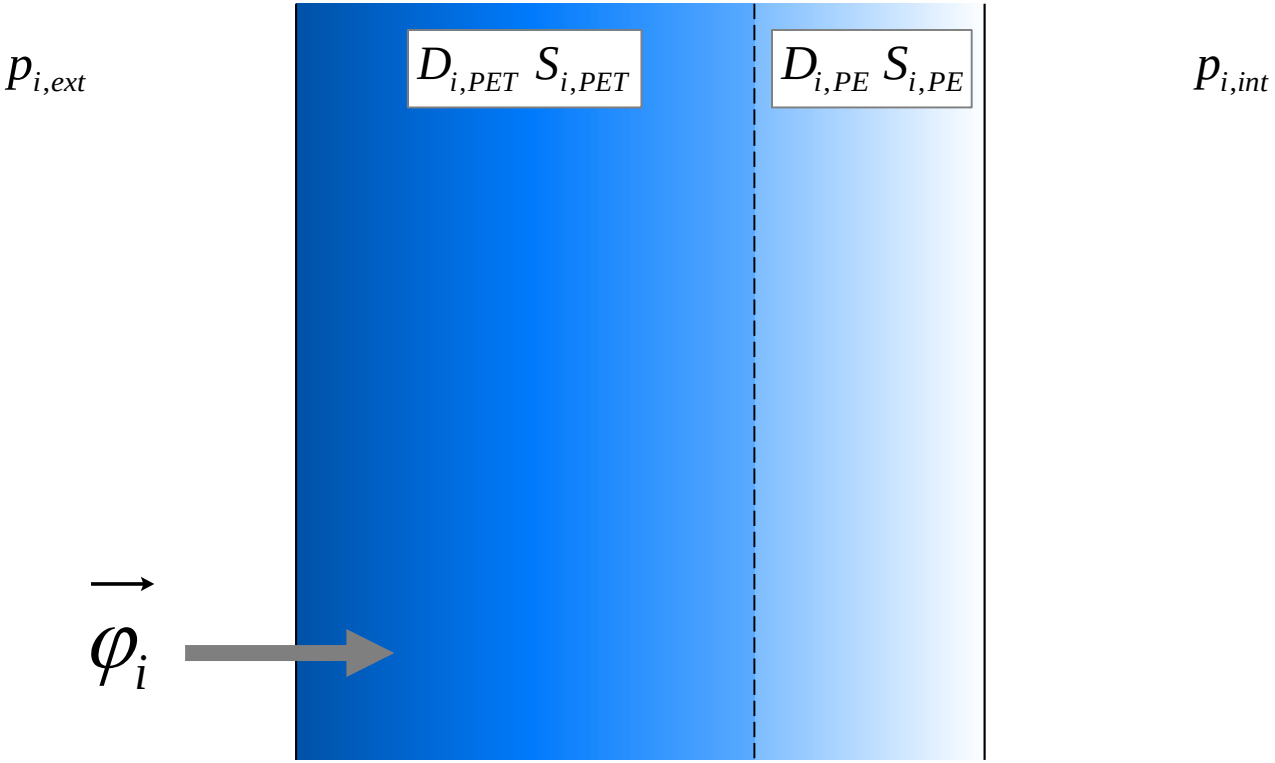

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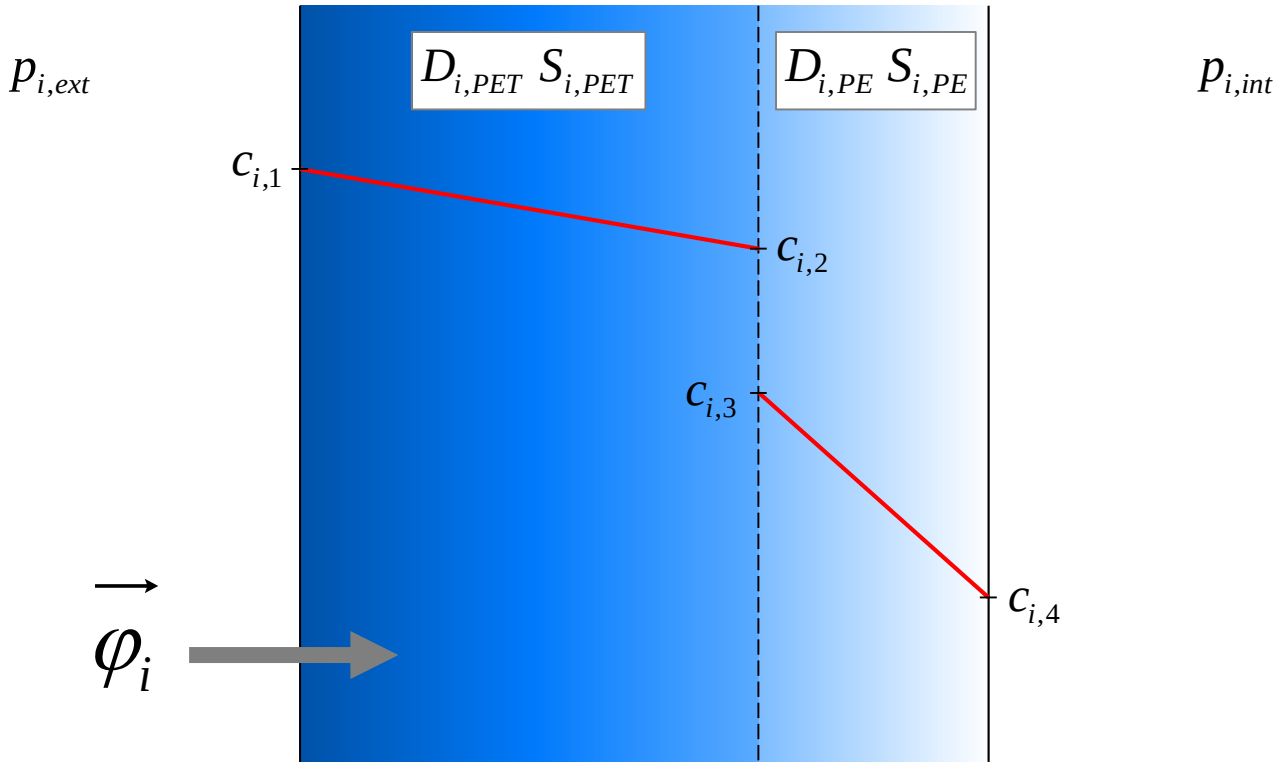

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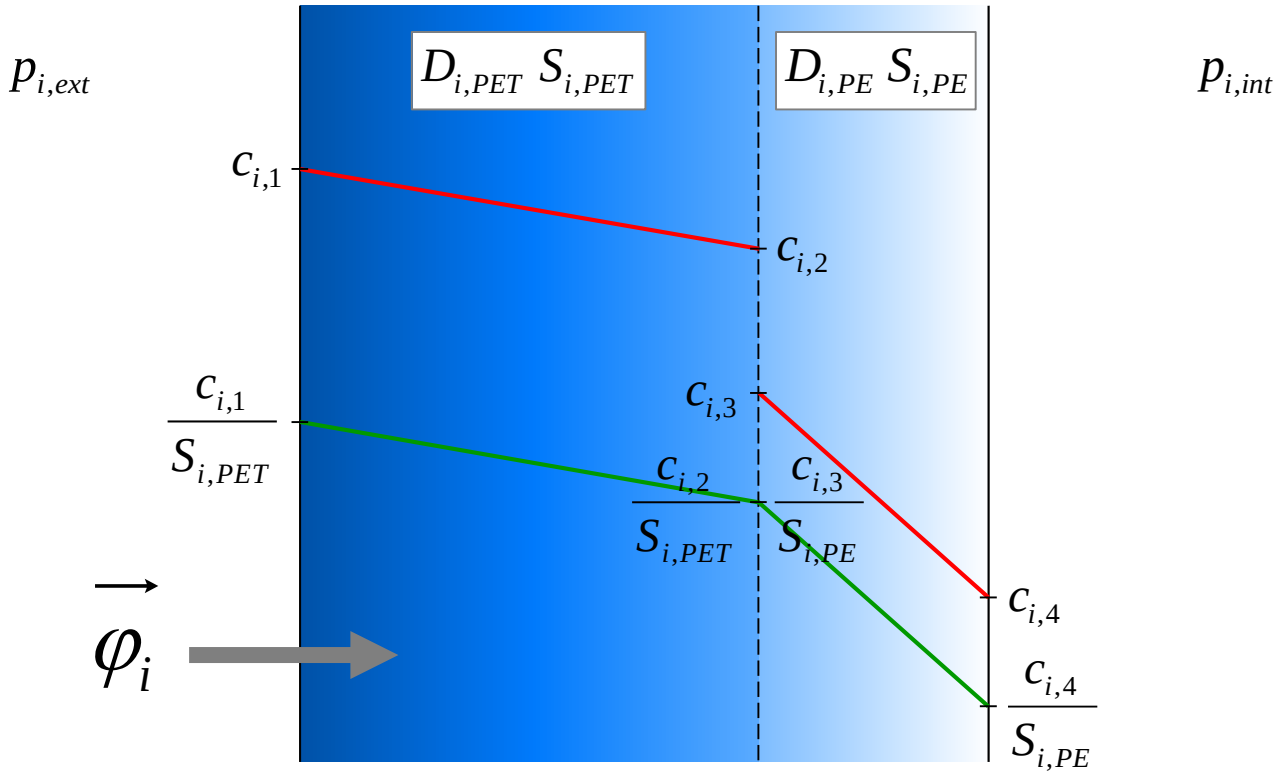

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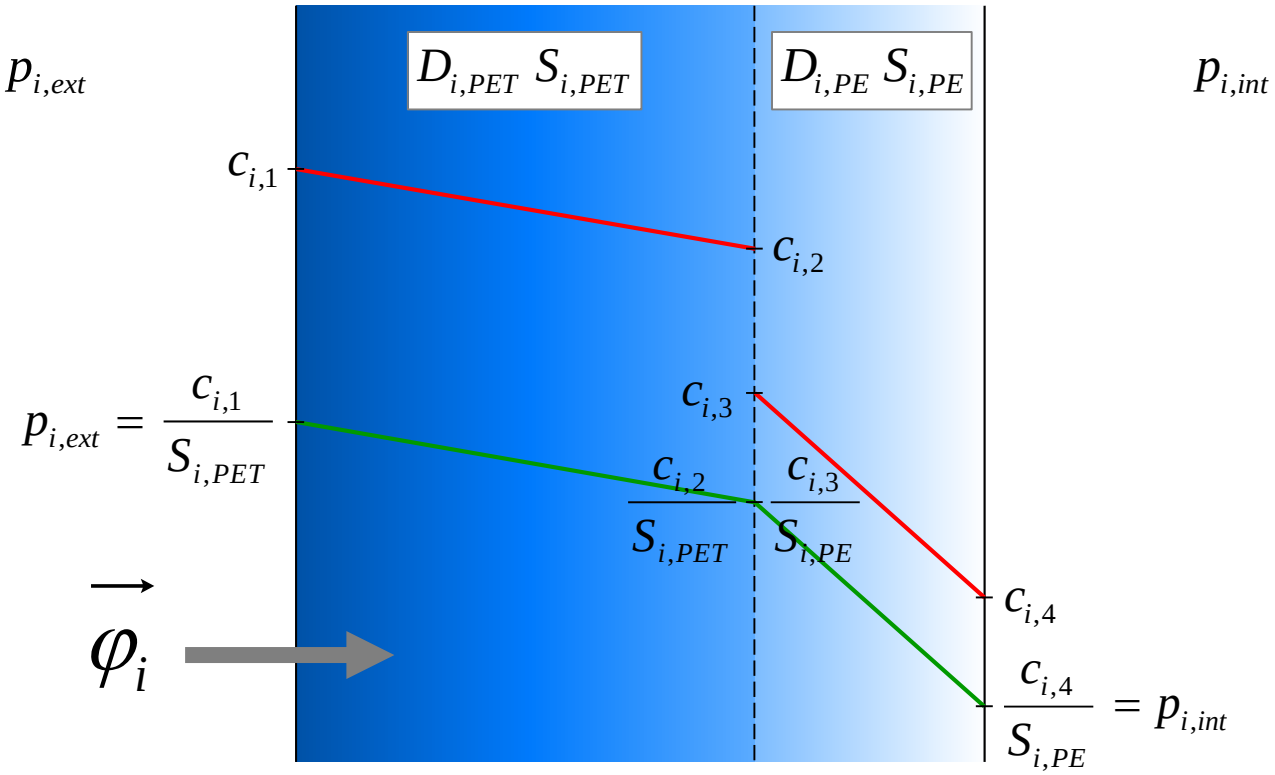

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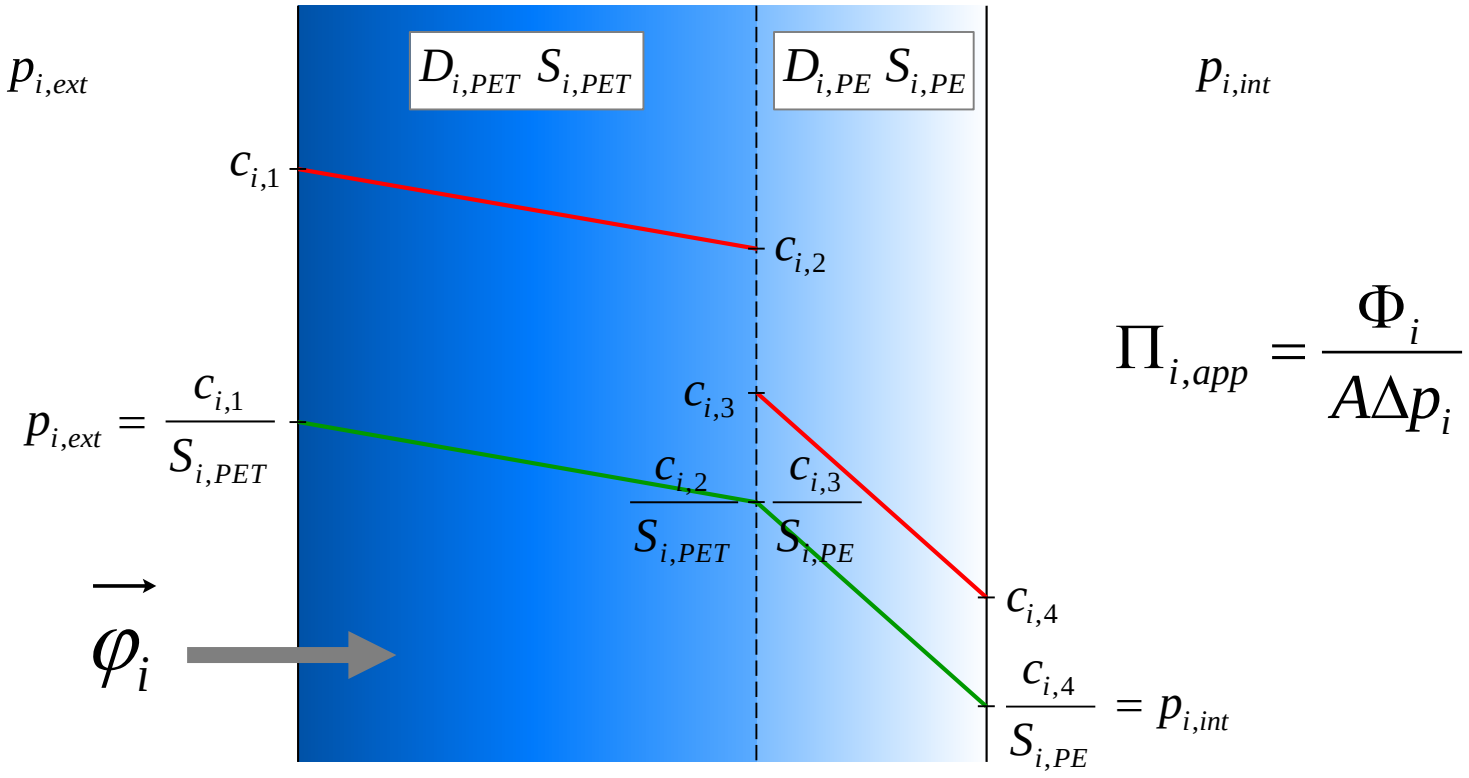

MODELLING APPROACH

- **Analogy between mass and heat transfer**

Analogy	Heat conduction	Molecular diffusion
Potential	Temperature T	Concentration/Solubility $\frac{c_i}{S_{i,j}}$
Flux	$\vec{\varphi} = -\lambda \nabla T$ Fourier's law	$\vec{\varphi_i} = -D_{i,j} S_{i,j} \nabla \frac{c_i}{S_{i,j}}$ Fick's law
Transitional regime	$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho c_p} \nabla^2 T$ Energy conservation	$\frac{\partial}{\partial t}\left(\frac{c_i}{S_{i,j}}\right) = D_{i,j} \nabla^2 \frac{c_i}{S_{i,j}}$ Mass conservation
	$\lambda \leftrightarrow D_{i,j} S_{i,j}$	$\rho c_p \leftrightarrow S_{i,j}$

MAIN STEPS OF MODELLING

- **MESHING**
  - Simail®
  - SMESH module from SALOME® Platform

- **THERMAL CALCULATION**
  - SYRTHES® software developed by EDF

- **PARAMETRIC STUDIES**
  - YACS module from SALOME® Platform

- **POST-PROCESSING**
  - Ensight® post-processing software

SOME RESULTS WITH PET M1F

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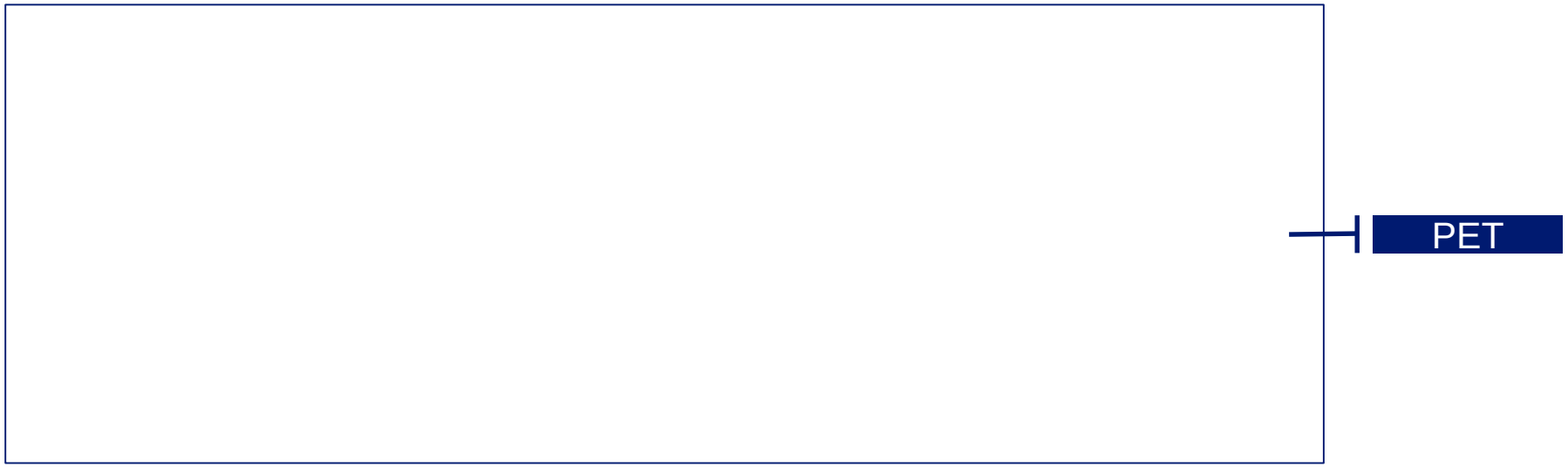
- **PET M1F 80nm**

$p_{i,ext}$



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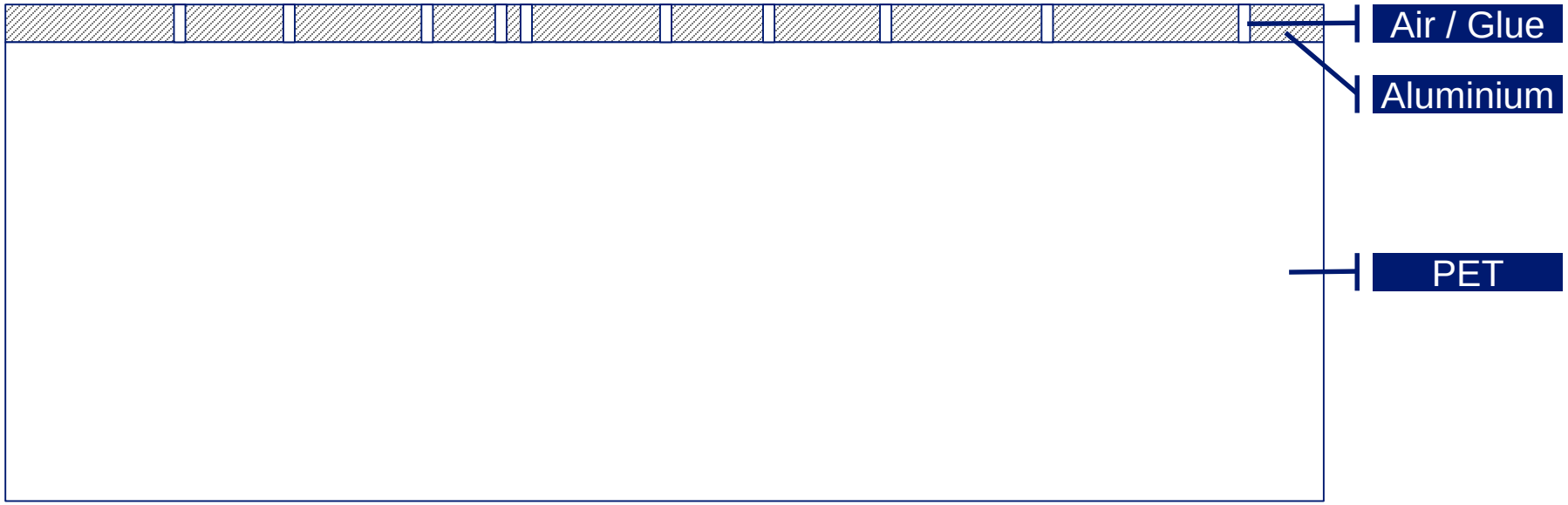

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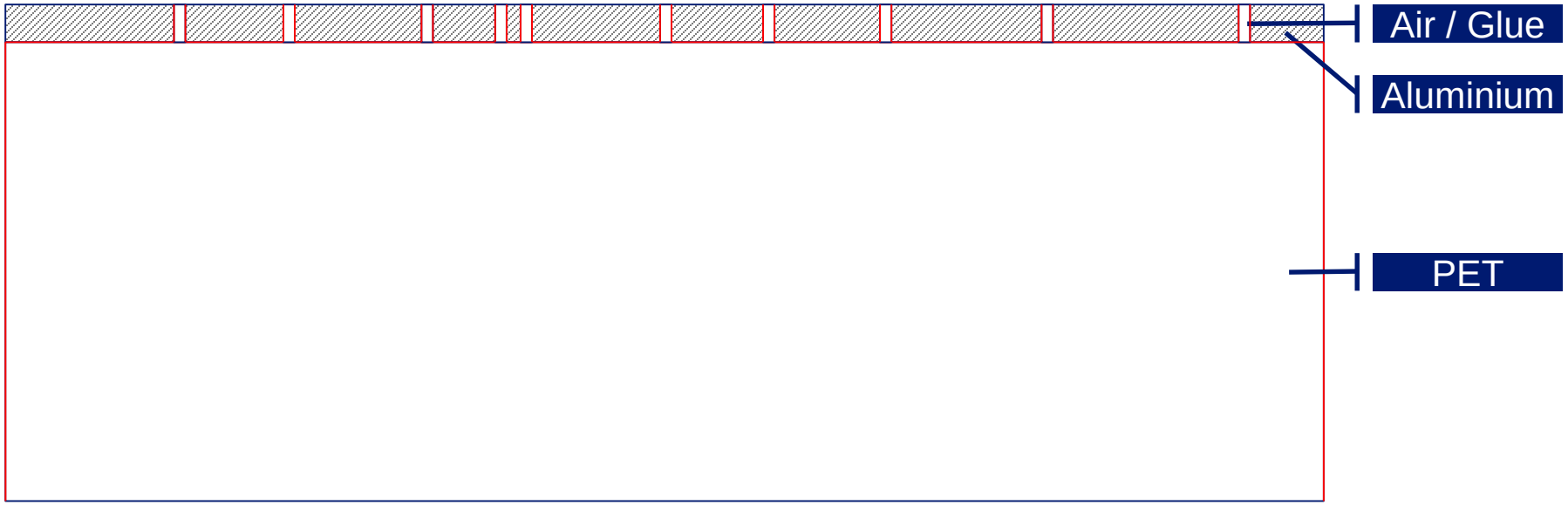

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Impermeable surface

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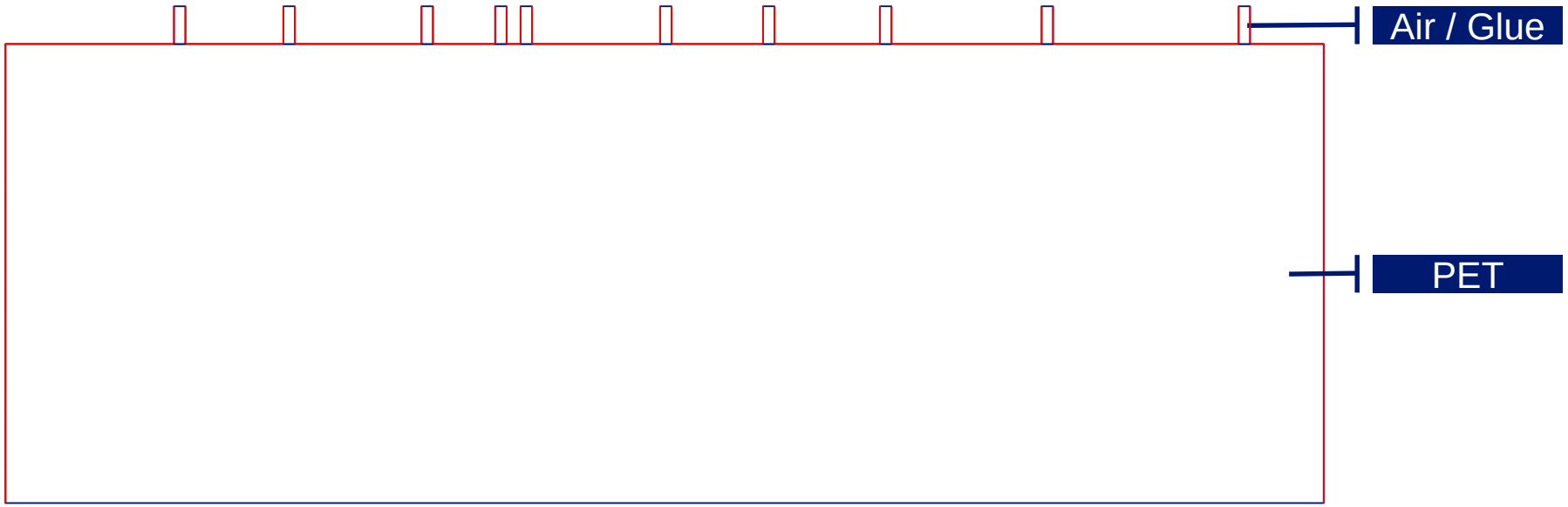

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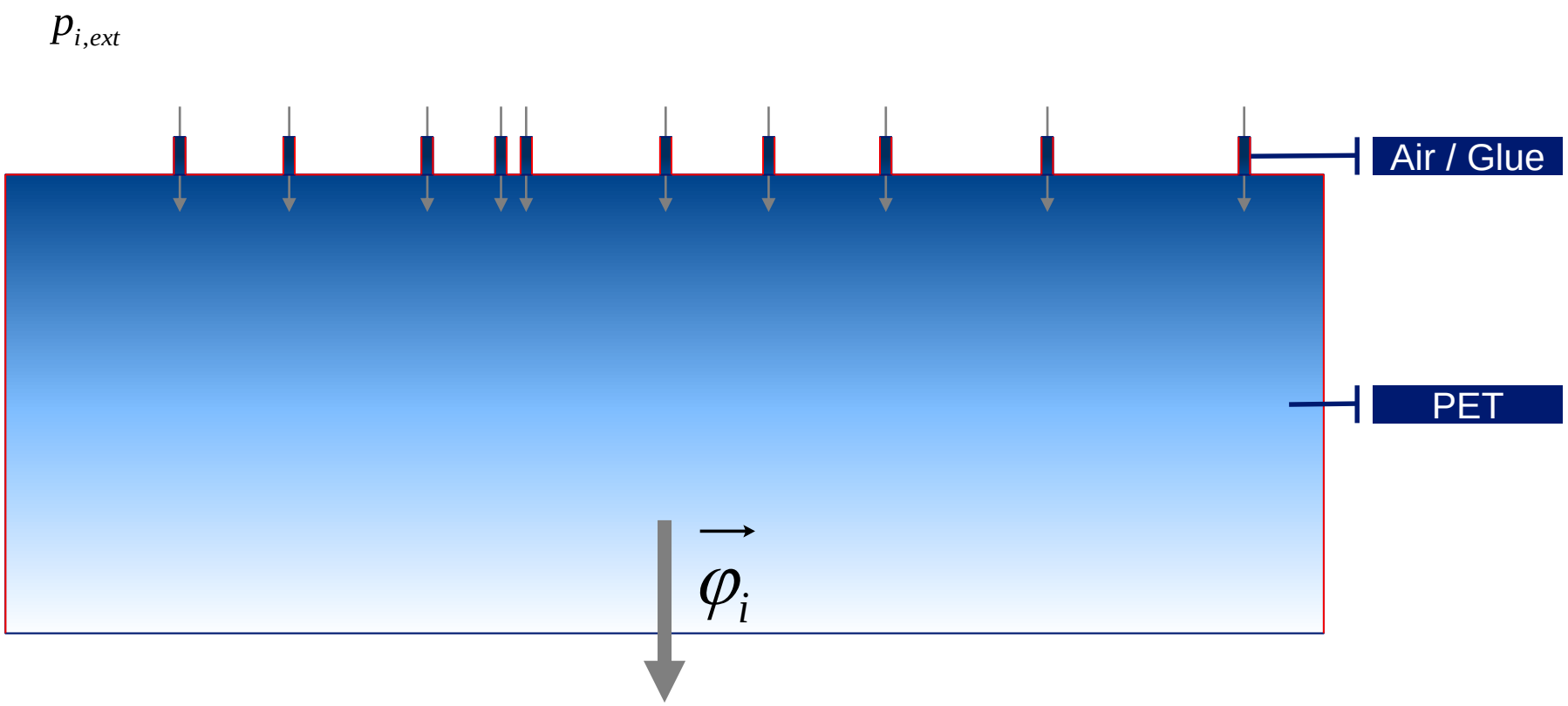

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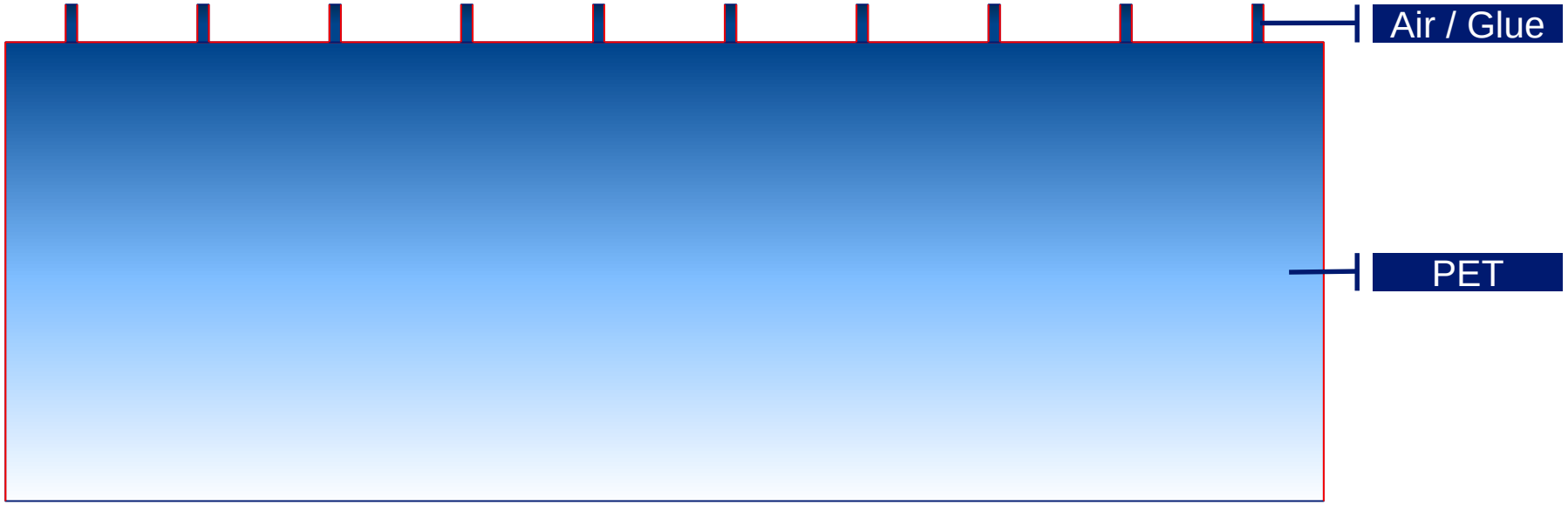

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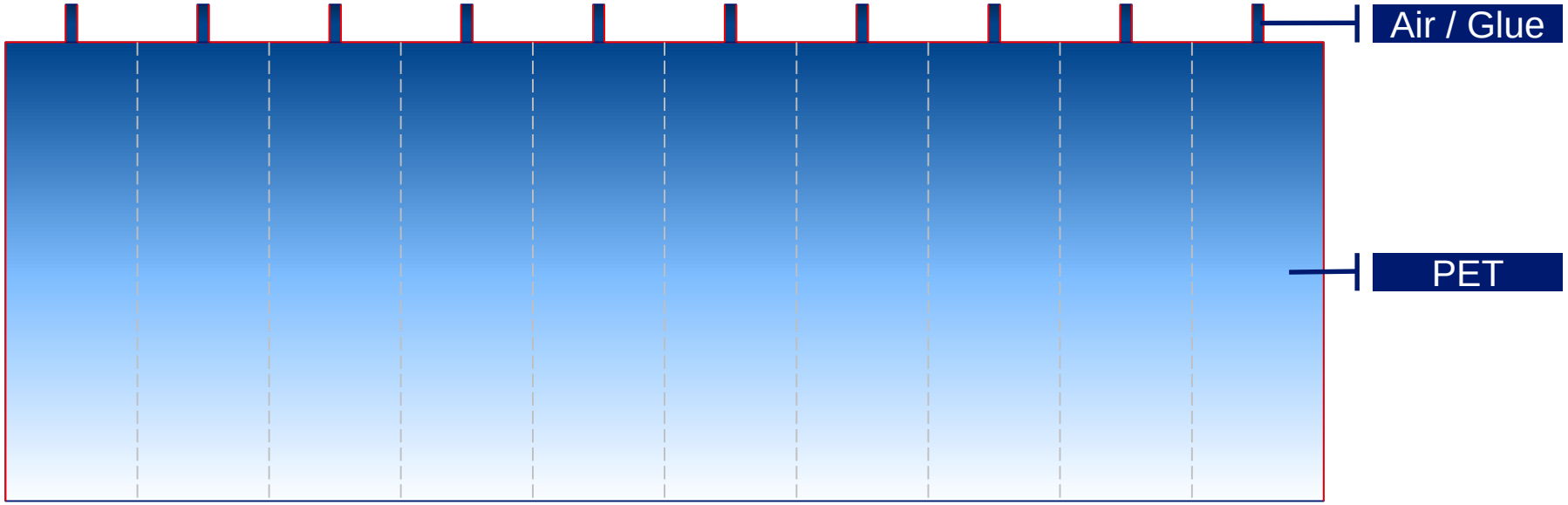

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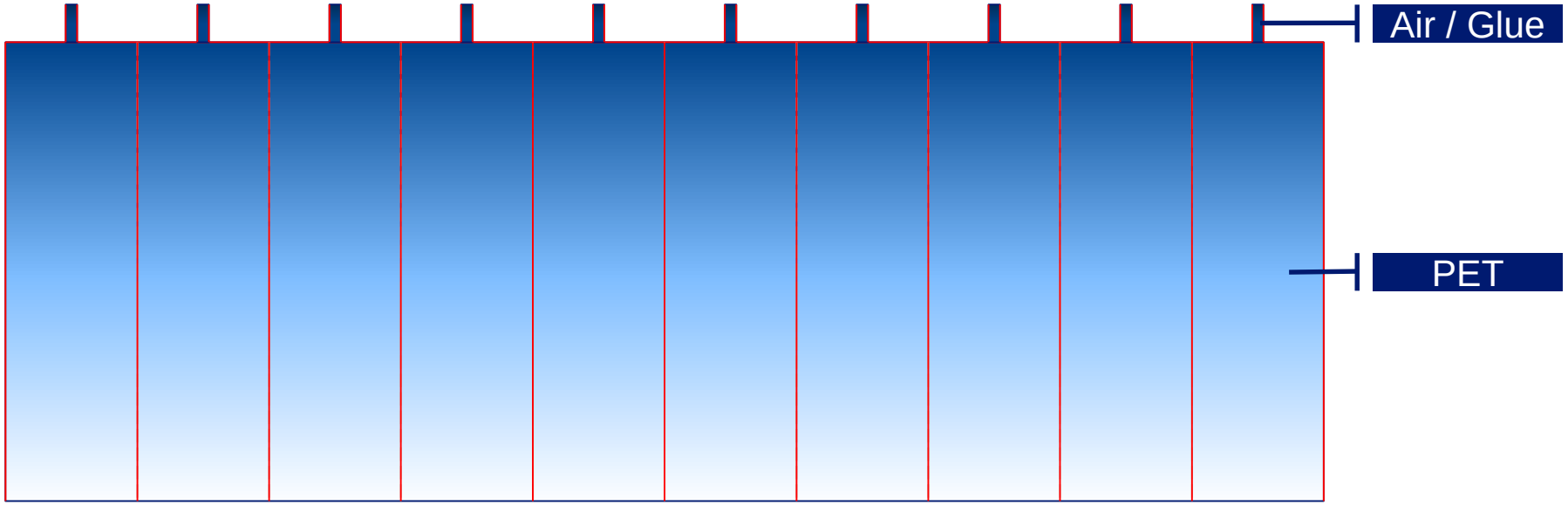

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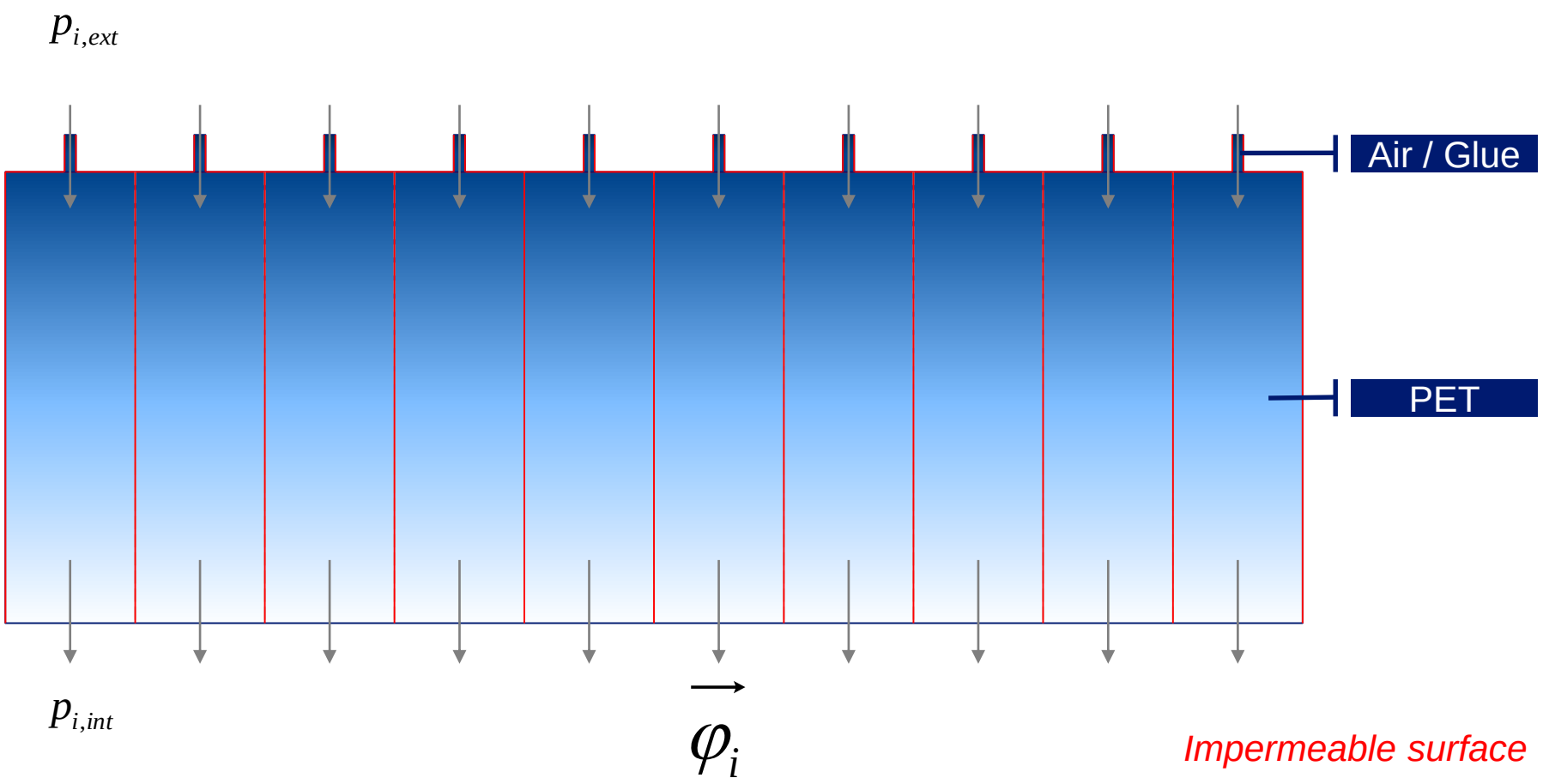

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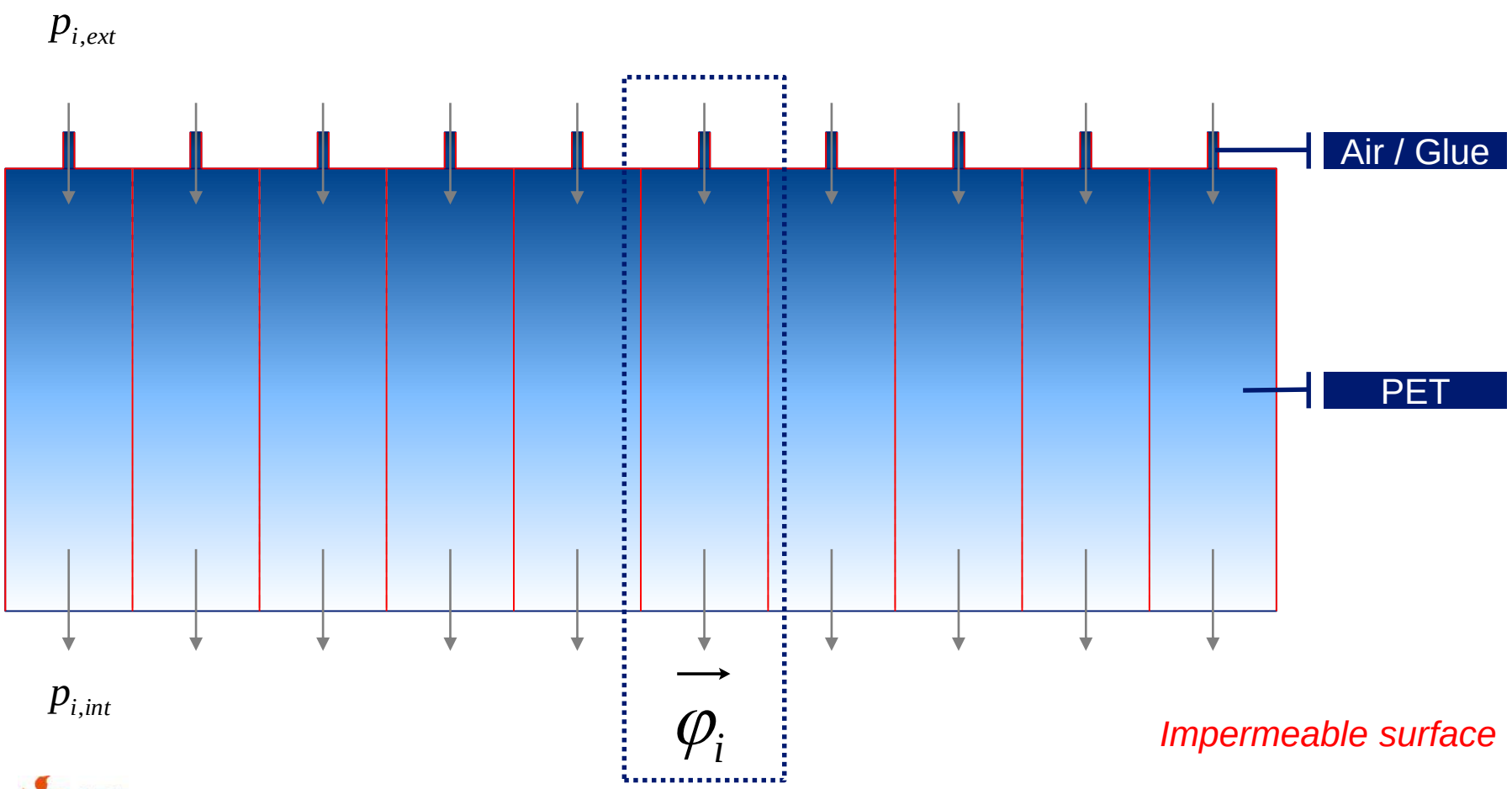

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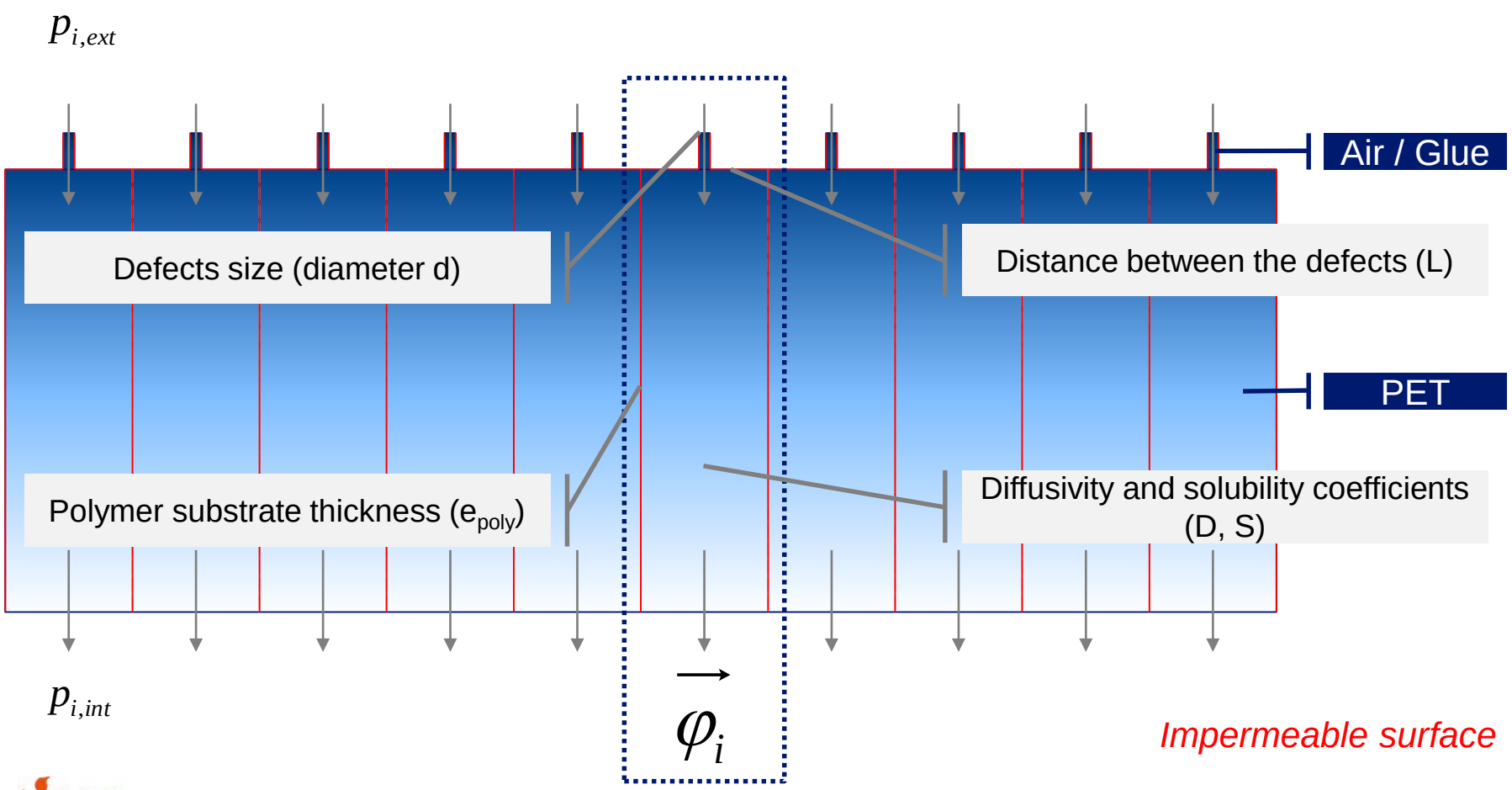

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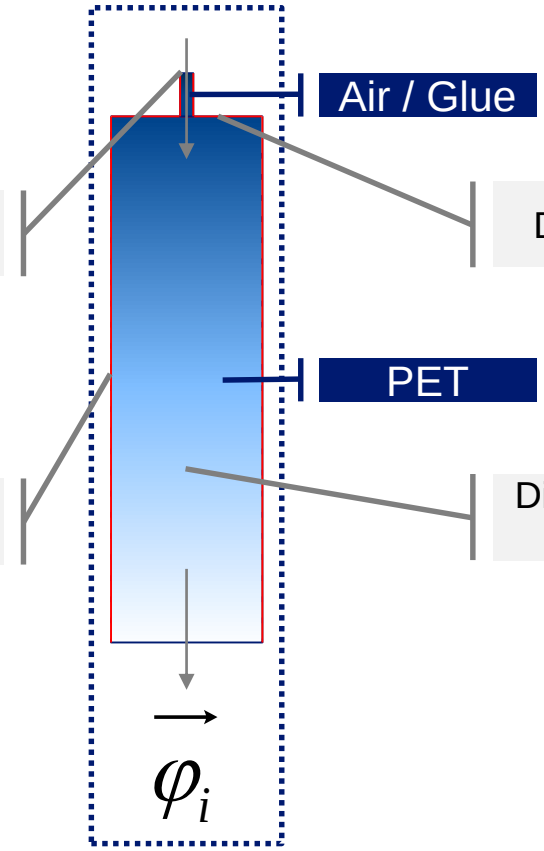

Defects size (diameter d)

Distance between the defects (L)

Polymer substrate thickness (e_{poly})

Diffusivity and solubility coefficients (D, S)

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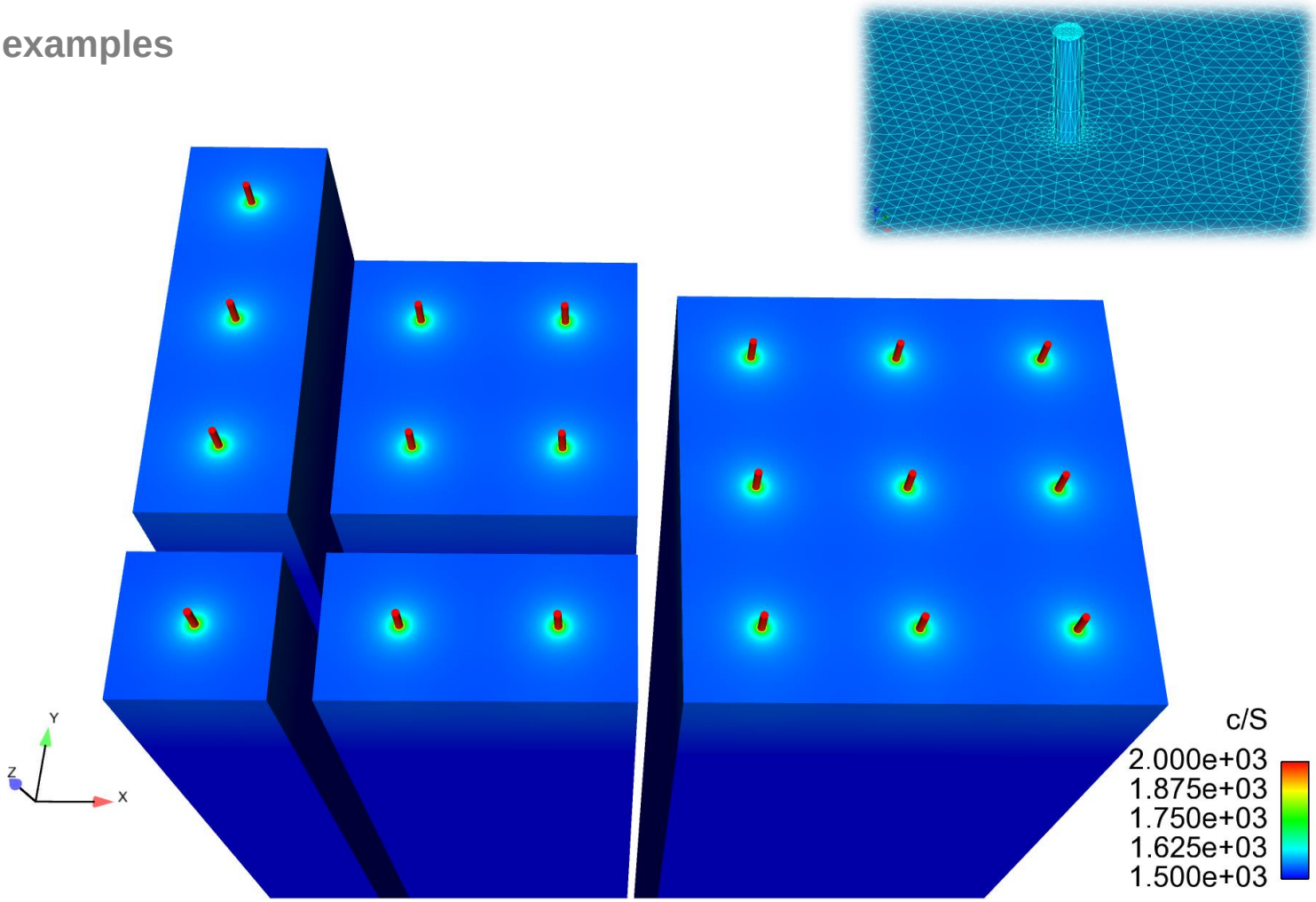

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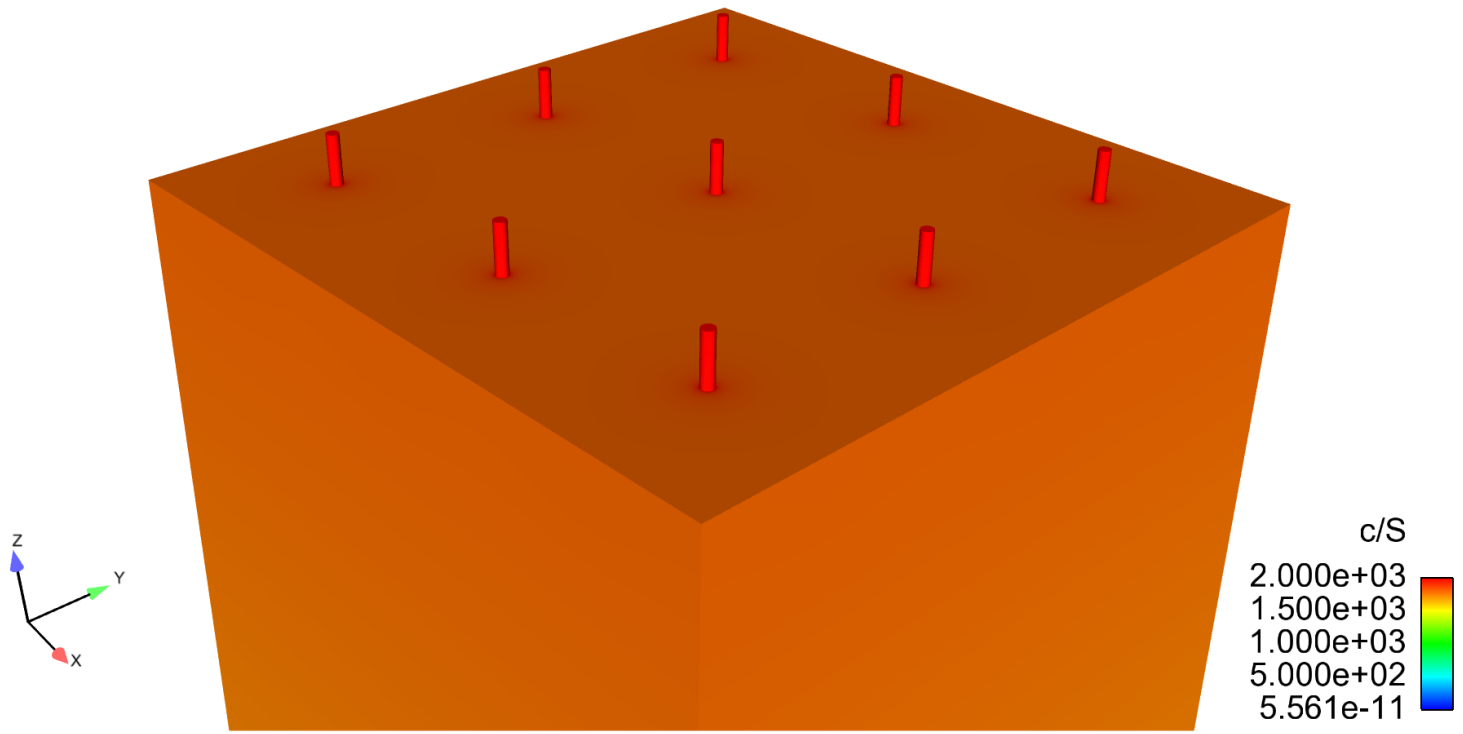

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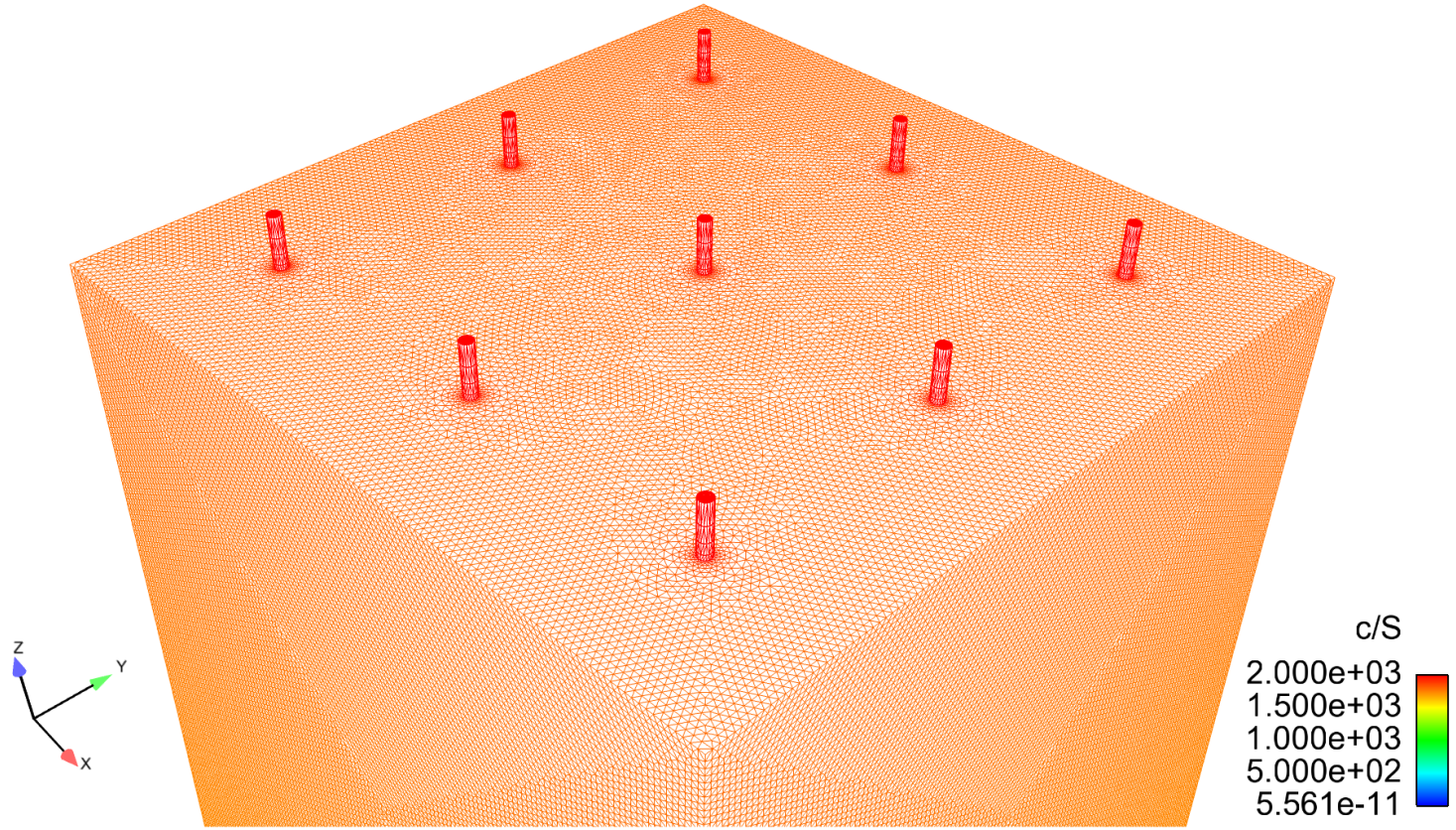
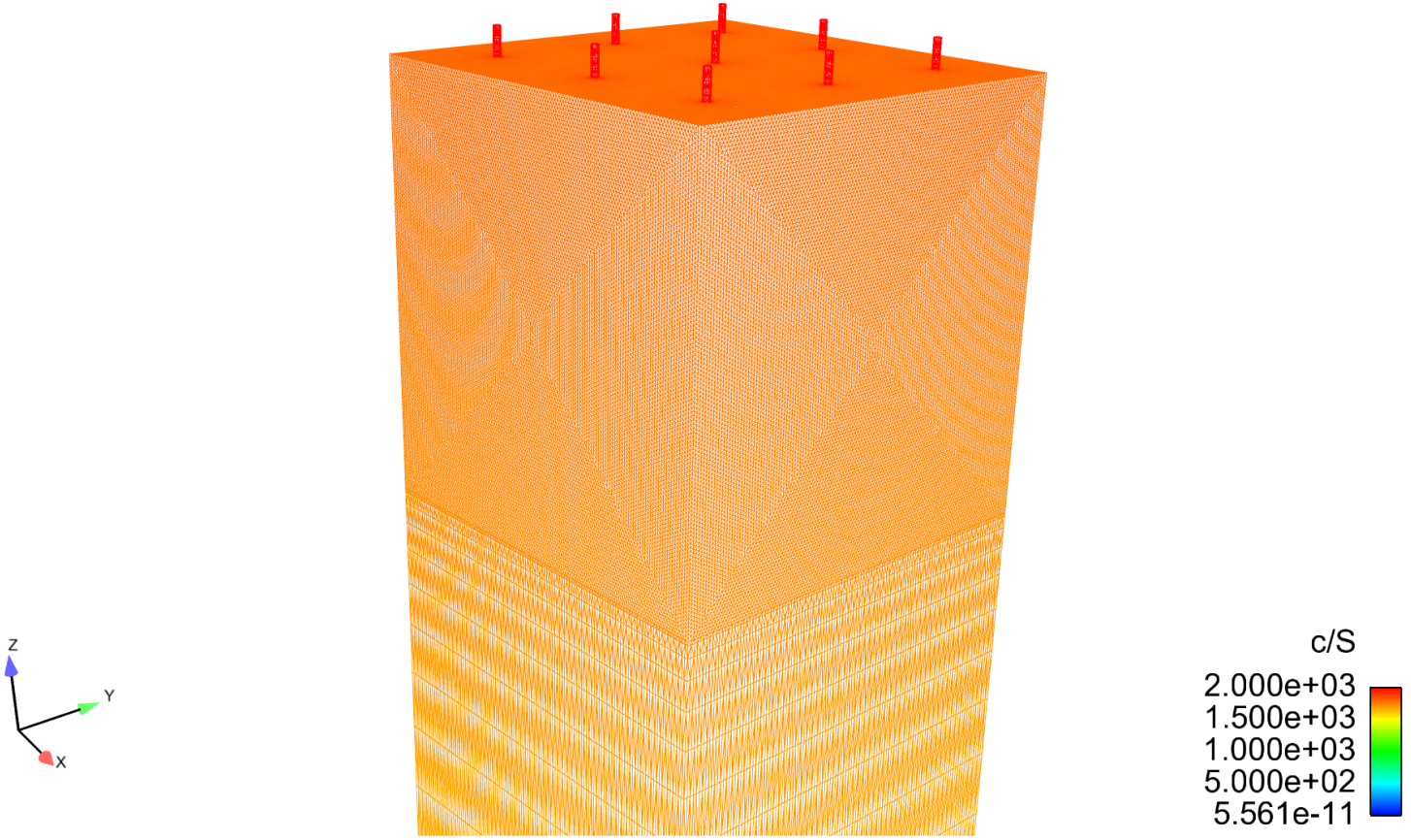


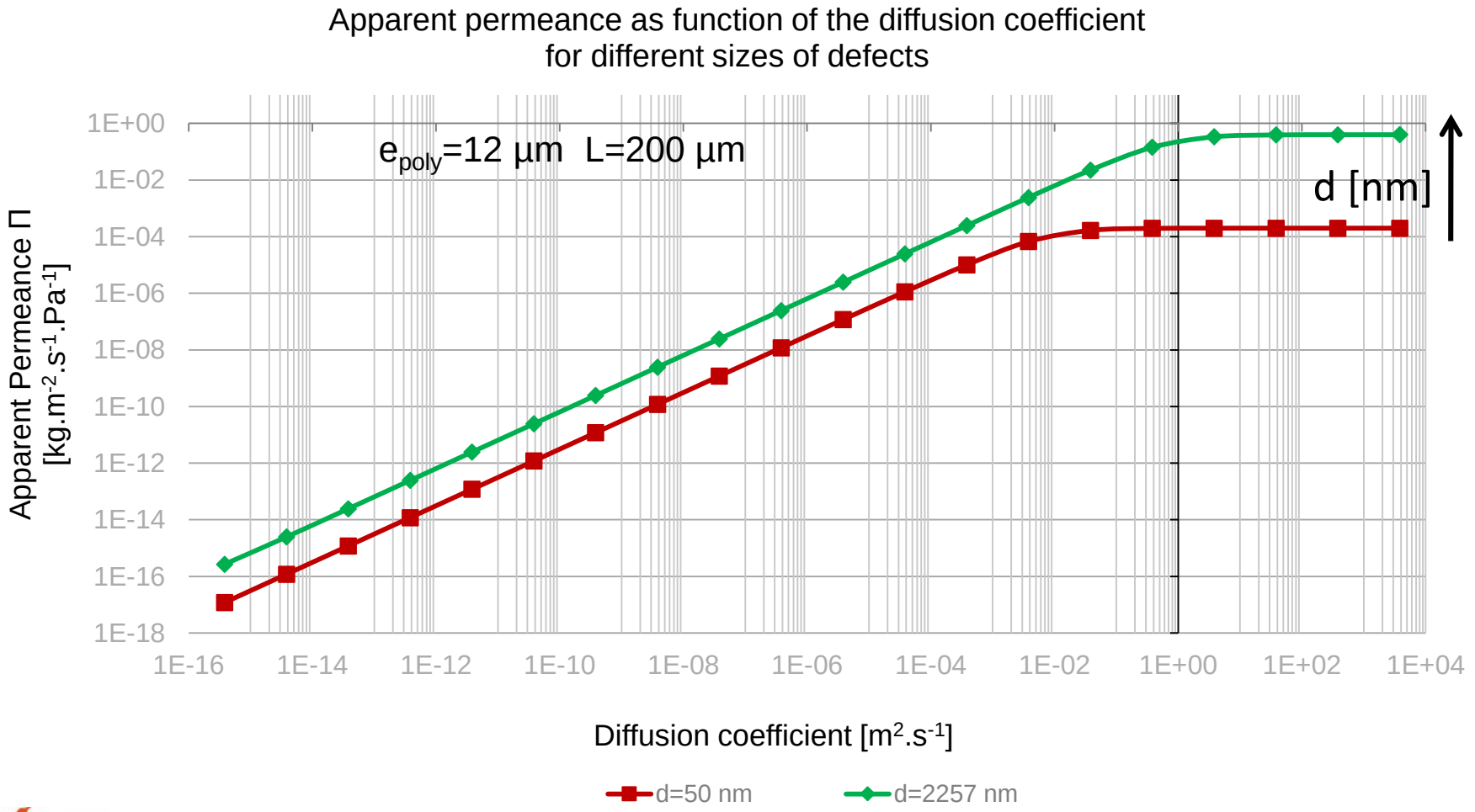
SOME RESULTS WITH PET M1F

- **Mesh examples**



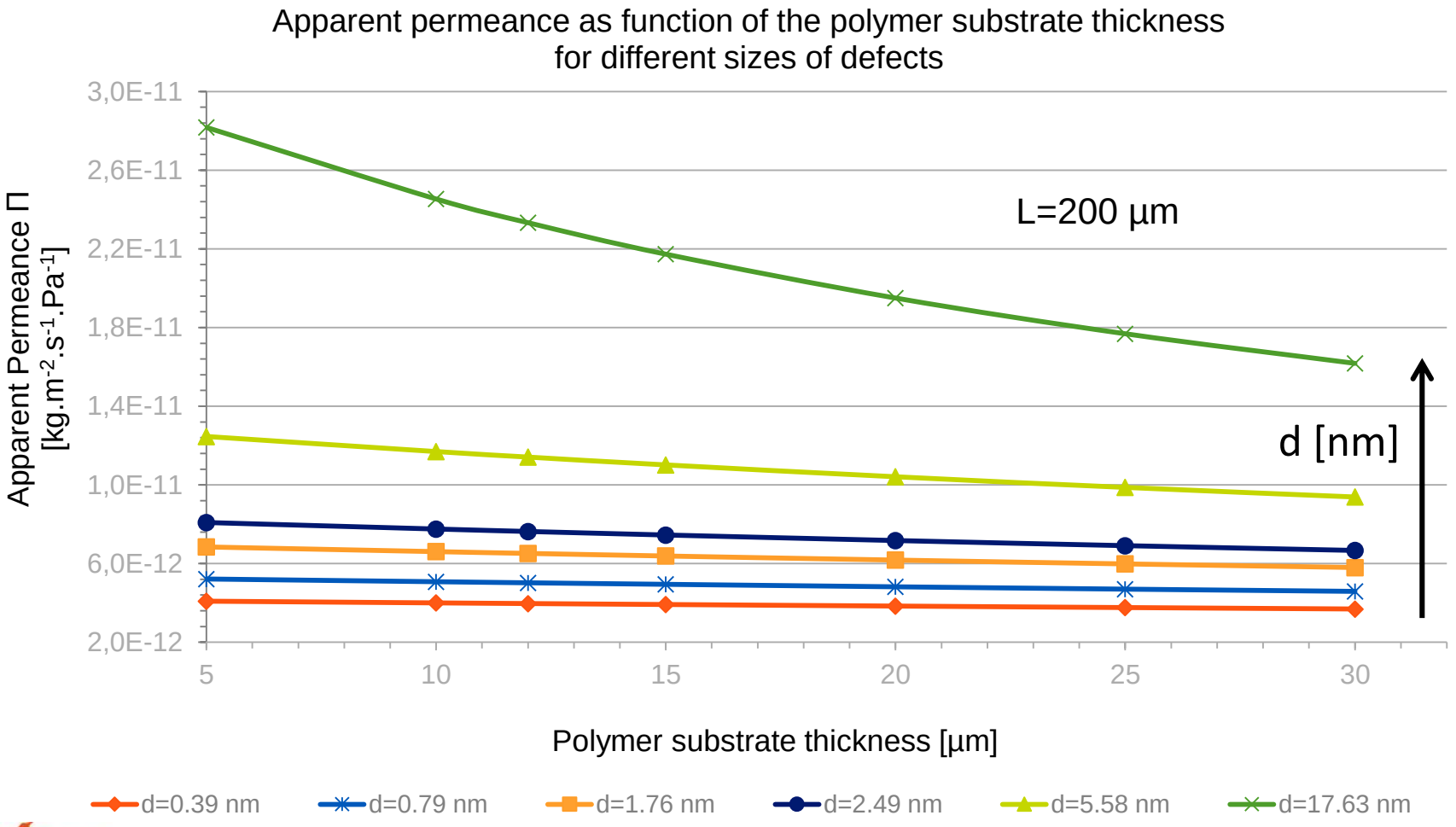
SOME RESULTS WITH PET M1F

- **Diffusivity and solubility coefficients (D, S)**



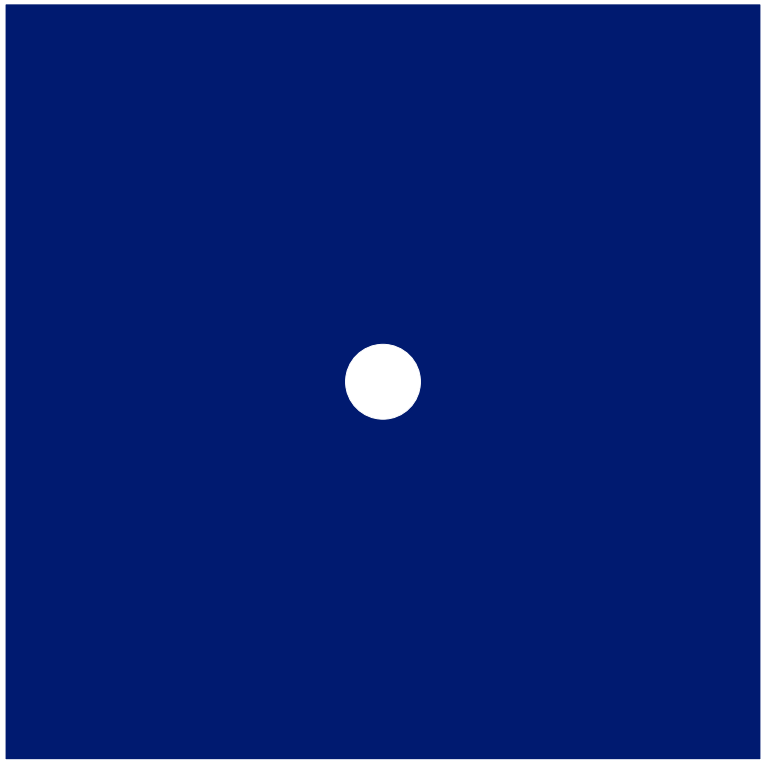
SOME RESULTS WITH PET M1F

- **Polymer substrate thickness (e_{poly})**



SOME RESULTS WITH PET M1F

- **Defects size (diameter d) and distance between the defects (L)**



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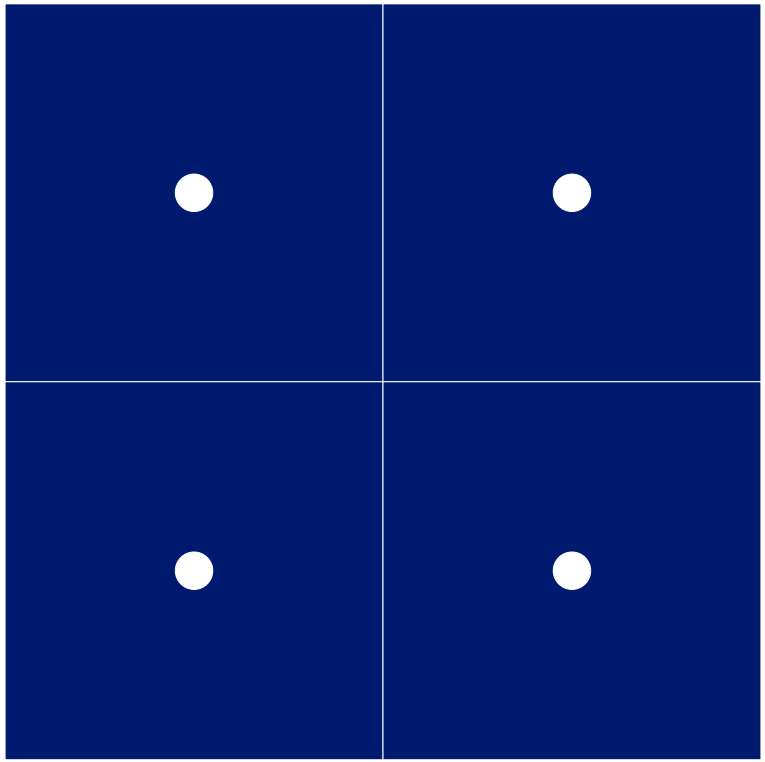

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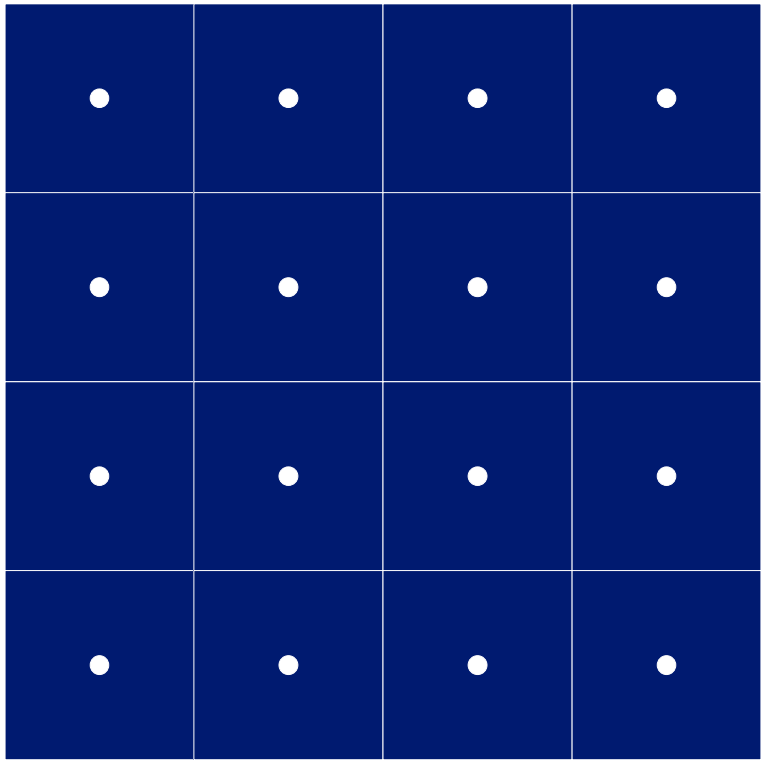

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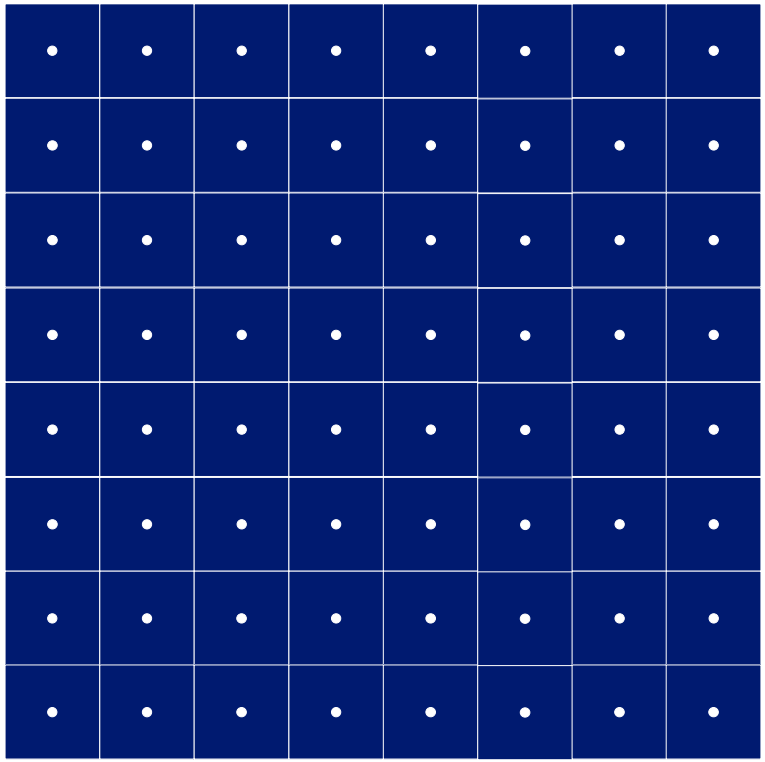

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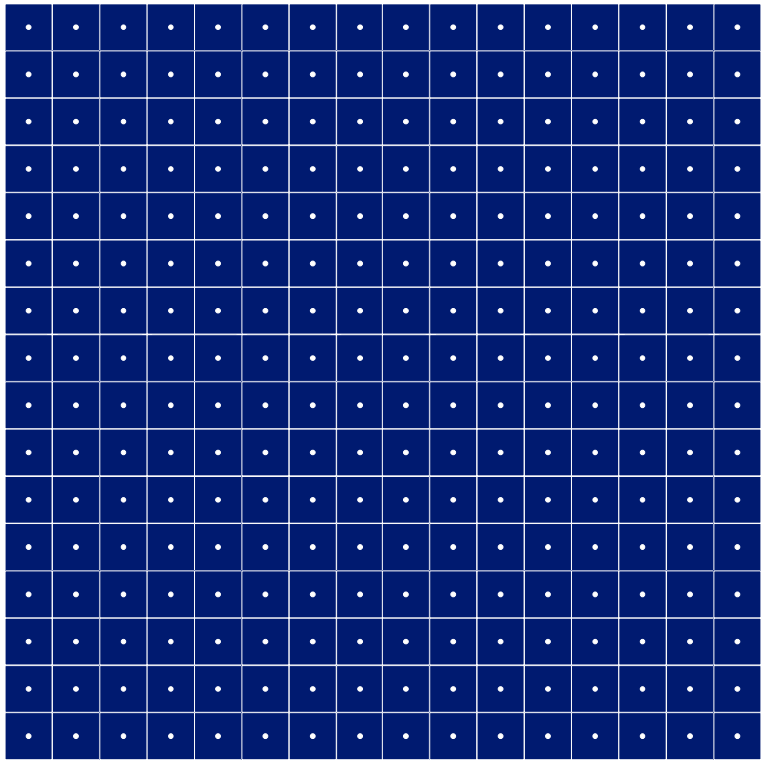

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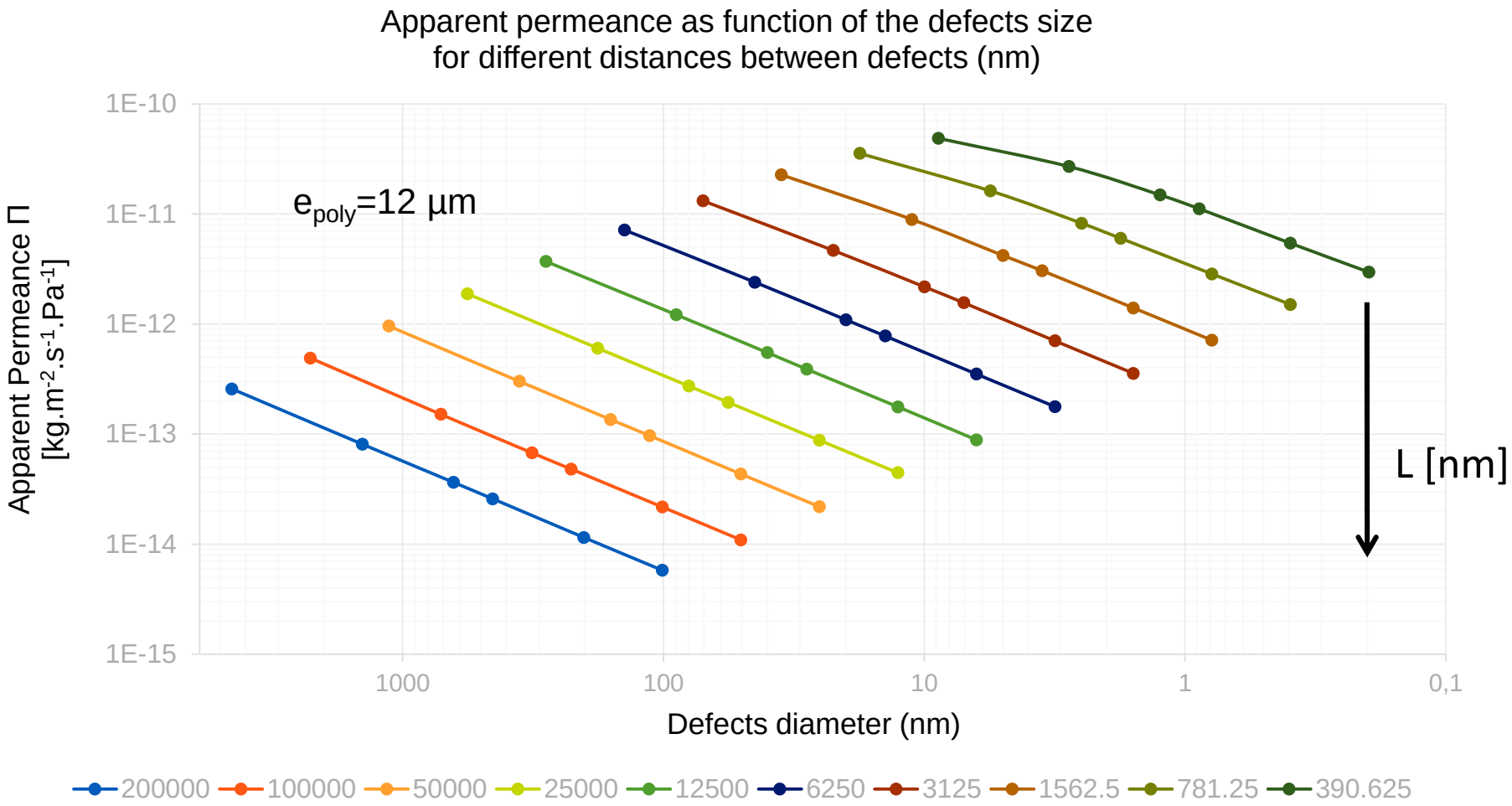

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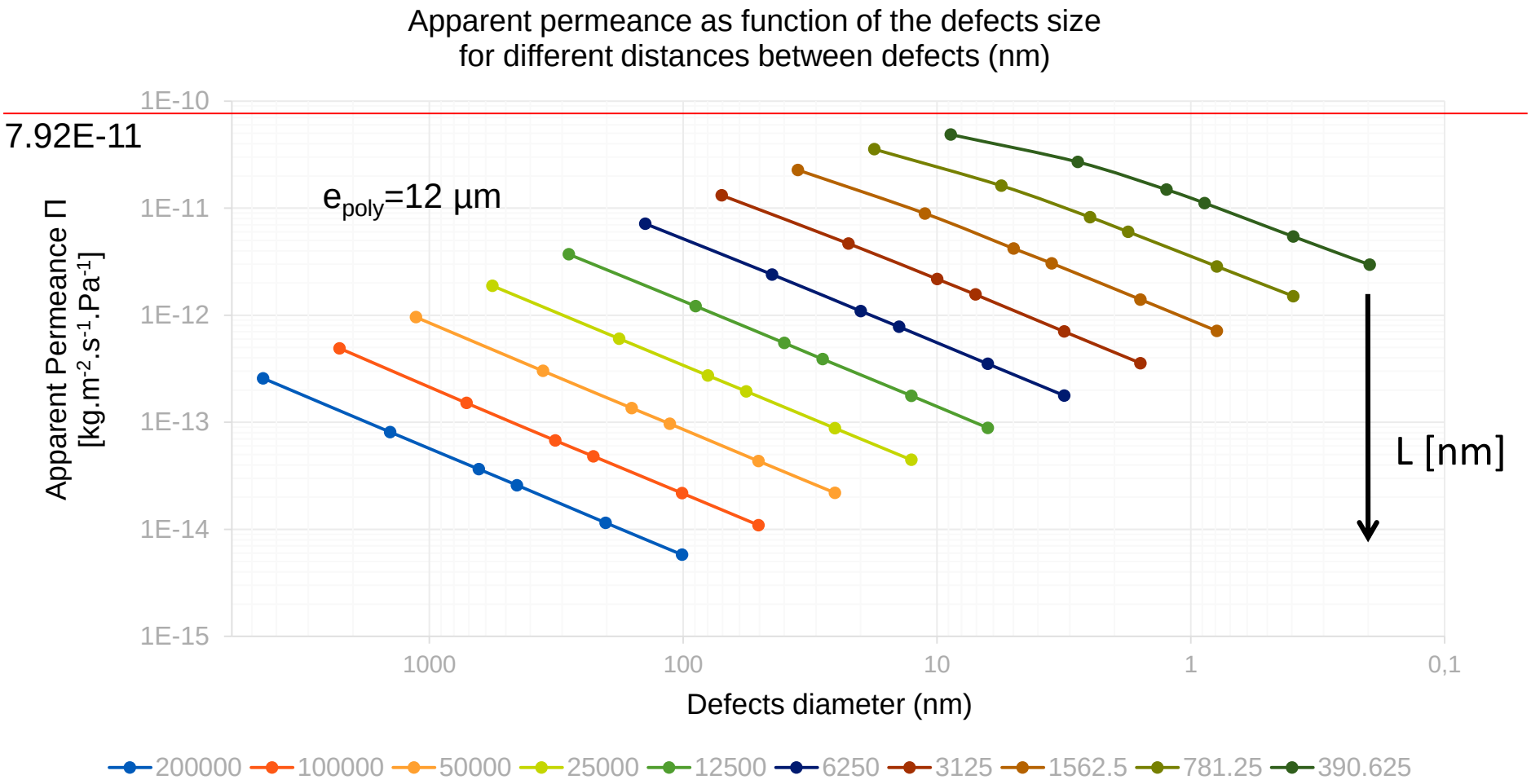

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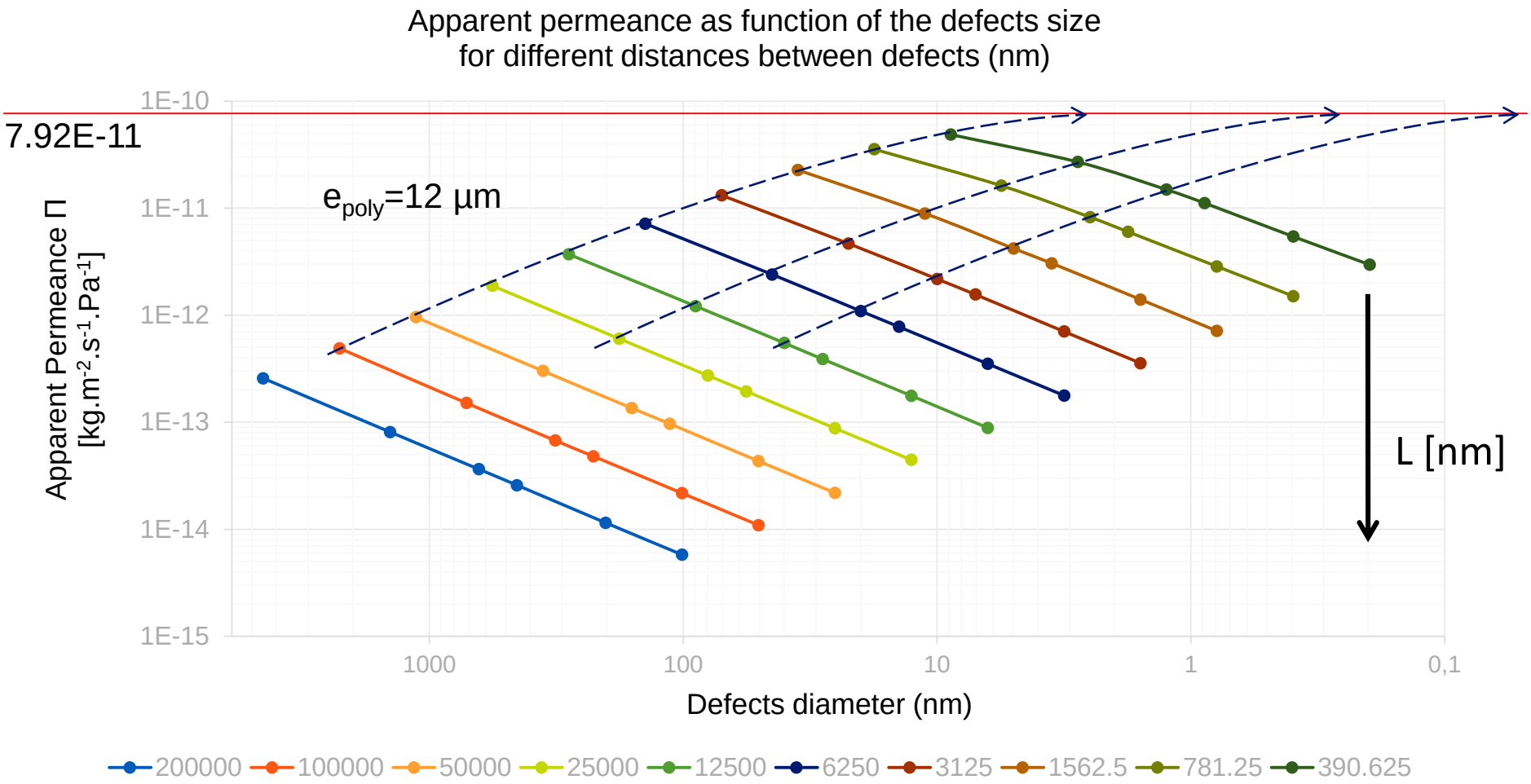
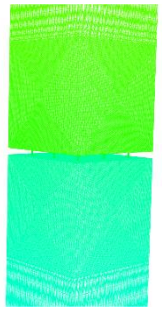
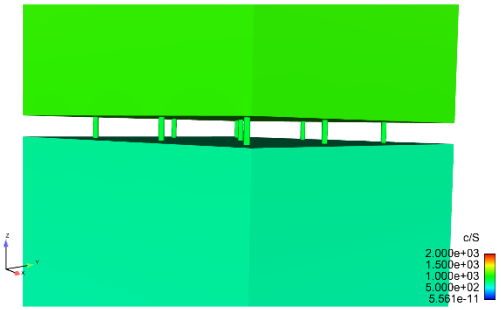


CONCLUSION AND OUTLOOK

CONCLUSION AND OUTLOOK

- **The gas transfer is not only regulated by the defects of the coating layer.**
- **The permeance gradually decreases with the thickness of the polymer substrate… and this effect tends to diminish when there are less defects.**
- **The permeance is more influenced by the distance between defects than the defects size.**
- **When the mean distance between defects is very small, the permeance of the PET M1F approaches that of the uncoated.**





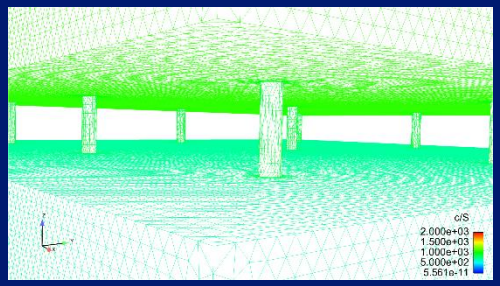
* OUTLOOK *

MULTILAYERS MODELLING

EXPERIMENTAL OBSERVATIONS

COMPARISON BETWEEN EXPERIMENTAL PERMEANCES AND CALCULATED PERMEANCES

RESEARCH ANALYTICAL MODEL



Thanks for listening