Sequence of Non-linear Real-Power Mass Transfer Resistances in Composite Thin Films: Optimal Layer Distribution and Permeance Ratio

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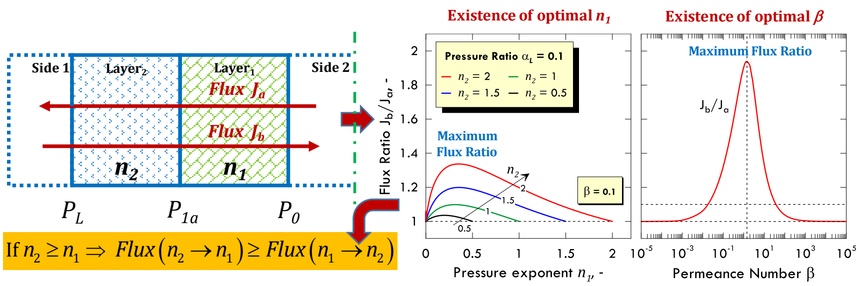
Introduction. This work focuses on determining the optimal permeance ratio and the optimal layer distribution in multilayer membranes and thin films, where each layer follows a flux law characterized by a real-valued exponent [1].: $Flux = \pi_i\left(P_1^{n_i} - P_2^{n_i}\right)$, which represents a significant generalisation of what found in literature [2].

Methodology. The following Figure illustrates the scheme of the considered problem. The permeating flux of a gas species through a multilayer membrane is a reference phenomenon of investigation, although also other mathematically-equivalent physical systems can be generally treated in the same manner. Specifically, the system is made of two layers, namely *Layer₁* and *Layer₂*, in each of which the mass transport of a certain species of interest is described by the general real-power flux law reported in Eq. 1. The variables $P_{1,i}$ and $P_{2,i}$ denote the represent the partial pressures at the opposite surfaces of the i^{th} layer. The permeances π_i are defined consistently. Without loss of generality, we suppose that $n_2 > n_1$.

$$Flux \equiv J = \pi_i\left(P_{1,i}^{n_i} - P_{2,i}^{n_i}\right),\ \ \{n_i, \pi_i\} \in \mathbb{R}^+,\ \ i \equiv \text{Layer} \tag{1}$$



Results and discussion. The novelties in this work are: i) Demonstration of the existence of an optimal permeance ratio between two layers, which is demonstrated to be equal to the inverse of the ratio of the respective maximum theoretical driving forces attainable in each layer; ii) Proof of the fact that such an optimal permeance ratio is a global optimum, and theoretical generalization of the optimality to any types of driving forces; iii) Discovery of the existence of an optimal value of the lower exponent n_1, which is a counter-intuitive result not reported previously; iv) Evidence that a finite virial-type linear combination of polynomial driving forces can be effectively approximated by the non-linear power law under investigation.. The significance of this study is further emphasized by the fact that the findings obtained are not only relevant to any type of composite membranes, such as metallic, ceramic, polymeric and/or hybrid ones, but to systems in which there is a flux of any physical quantity through thin films according to the above flux law.

Keywords: Distribution of Layers, Non-linear Resistances, Multilayer Membranes, Thin films

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References

[1] Caravella, A. et al. *Journal of Membrane Science* **2024**, *705,* 122877.
[2] Caravella, A. et al. *Journal of Membrane Science* **2023**, *683*, 121842.