Paneļdiskusijas "Inovācijas jūrai Latvijā"

Prezentācija

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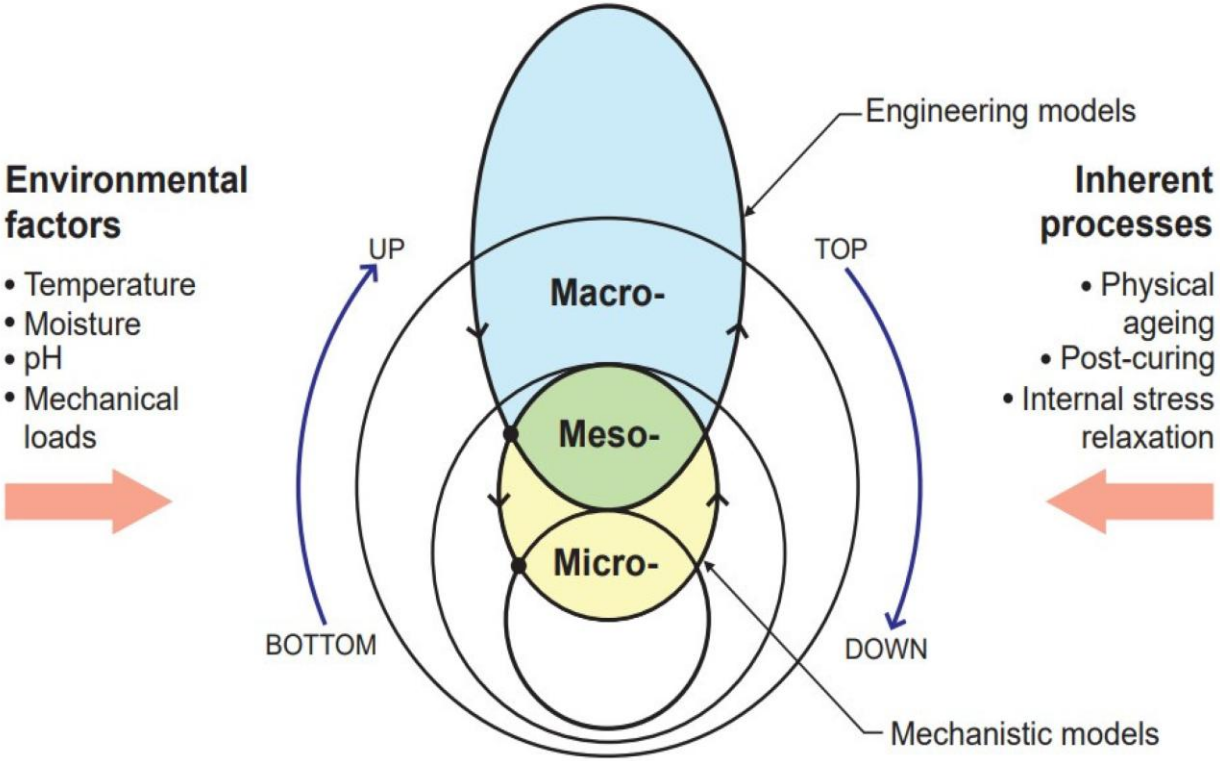
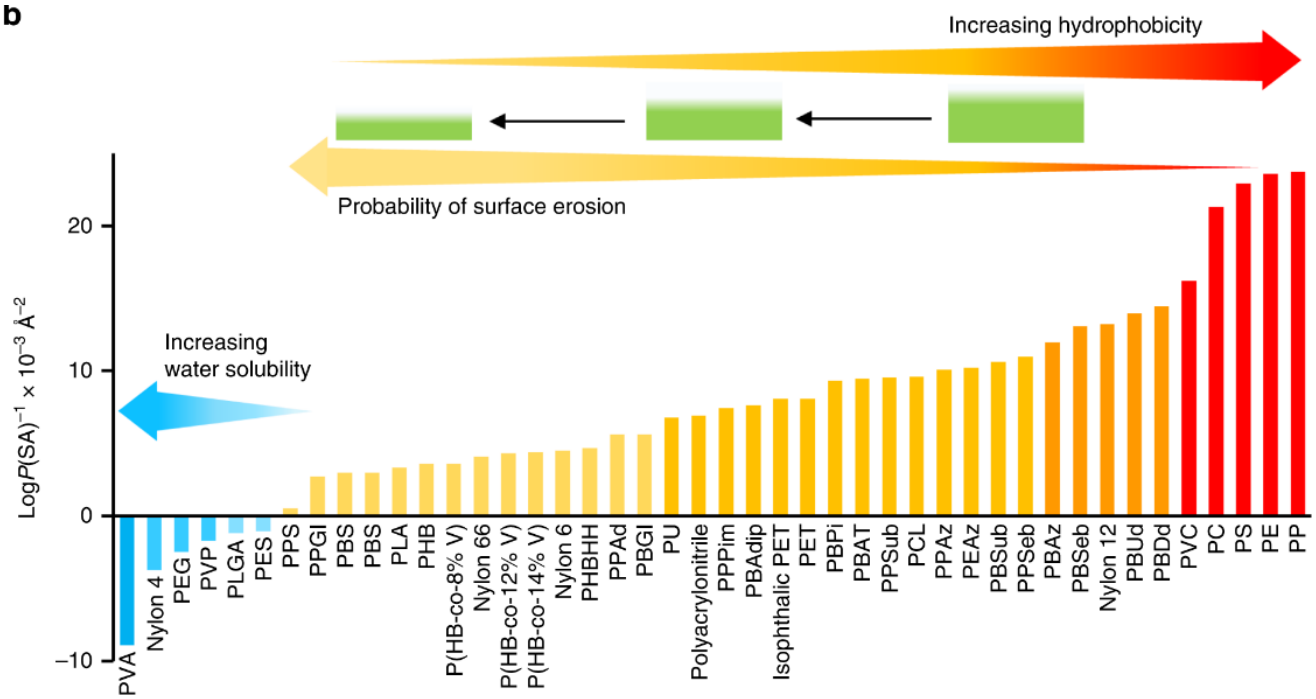
MARTE
Funded by the European Union

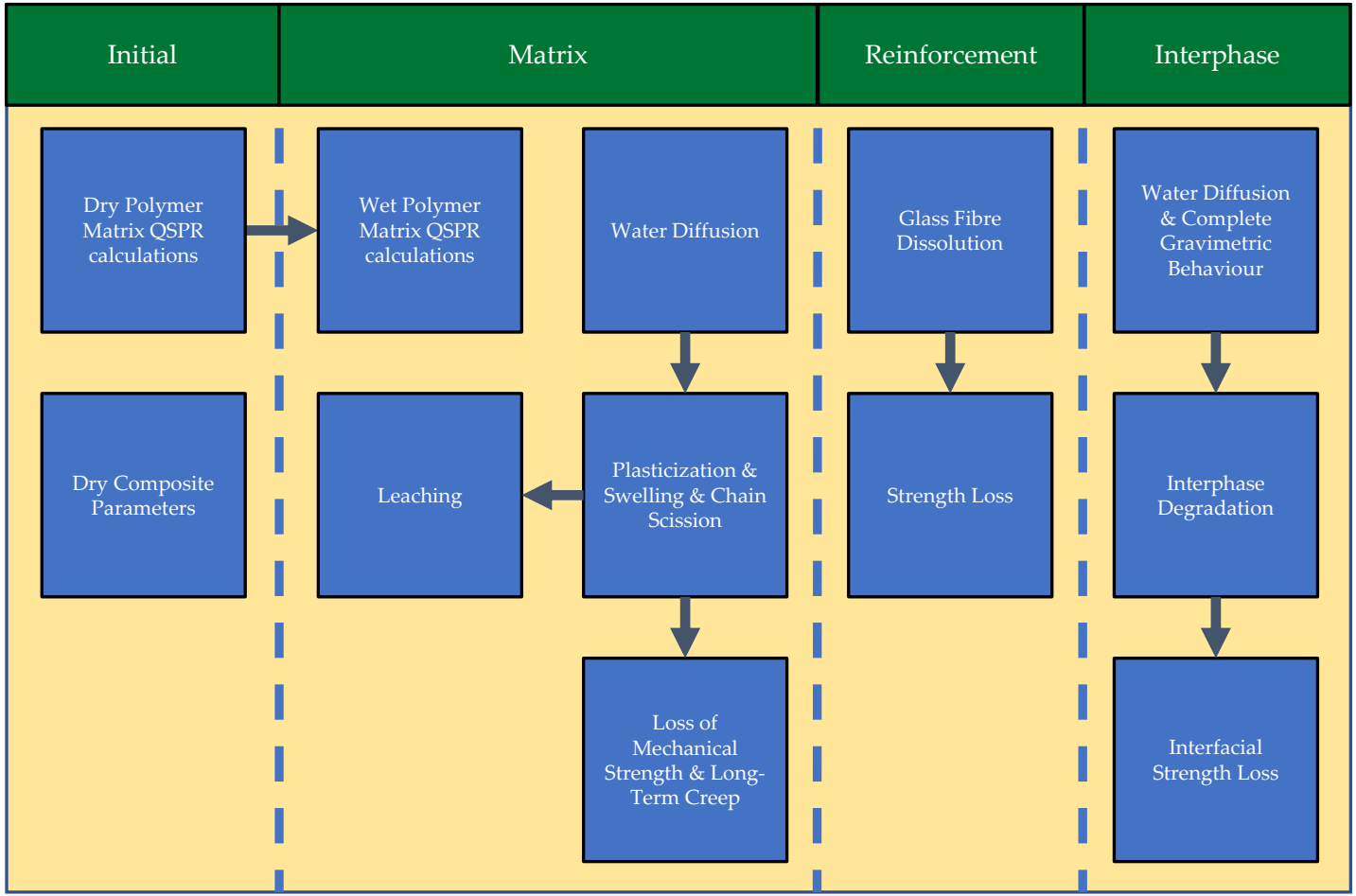


Modelling of Environmental Ageing of Polymers and Polymer Composites—Durability Prediction Methods. *Polymers* **2022**, *14*, 907.

The wide range of hydrophobicity of plastics



1. Min, K., Cuiffi, J.D. & Mathers, R.T. Ranking environmental degradation trends of plastic marine debris based on physical properties and molecular structure. Nat Commun 11, 727 (2020). https://doi.org/10.1038/s41467-020-14538-z


Initial
Matrix
Reinforcement
Interphase
Dry Polymer Matrix QSPR calculations
Wet Polymer Matrix QSPR calculations
Water Diffusion
Glass Fibre Dissolution
Water Diffusion & Complete Gravimetric Behaviour
Dry Composite Parameters
Leaching
Plasticization & Swelling & Chain Scission
Strength Loss
Interphase Degradation
Loss of Mechanical Strength & Long-Term Creep
Interfacial Strength Loss

Hydrolysis

- Hydrolysis of PA was studied by Mazan et al in [1]
- Hydrolysis of biodegradable polymers was studied by Vieira et al. in [2]. time-dependent decrease of tensile strength s of biodegradable PLA-PCL directly related to the decrease of molecular weight M_{n}

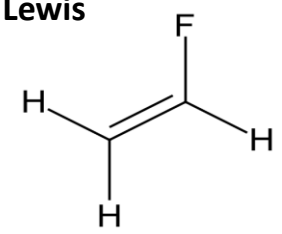
$$d_h = 1 - \frac{\sigma_t}{\sigma_0} = 1 - \frac{M_{nt}}{M_{n0}} = 1 - e^{-ut}$$

[1] Mazan, Tobiasz & Jørgensen, Jens & Echtermeyer, Andreas. (2015). Aging of polyamide 11. Part 3: Multiscale model predicting the mechanical properties after hydrolytic degradation. Journal of Applied Polymer Science. 132. 10.1002/app.42792

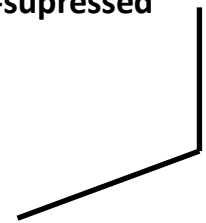
[2] Vieira, A.C.; Guedes, R.M.; Tita, V. Constitutive modeling of biodegradable polymers: Hydrolytic degradation and time-dependent behavior. Int. J. Solids Struct. **2014**, 51, 1164–1174

Summary of the Approach

Lewis



H-supressed



Connectivity Indices (Structure parameters):

- Zeroth-order Simple $^{0}\chi$
- Zeroth-order Valence $^{0}\chi^{v}$
- First-order Simple $^{1}\chi$
- First-order Valence $^{1}\chi^{v}$

Atomic indices:

- simple δ
- valence δ^{v}

Bond Indices:

- simple β
- valence β^{v}

QSPR (Quantitative Structure-Property) regression equations:

Properties as functions of connectivity indices. Available in J. Bicerano's Approach.

Predicted Properties

Krauklis, A. E. Technical report on QSPR, NTNU.