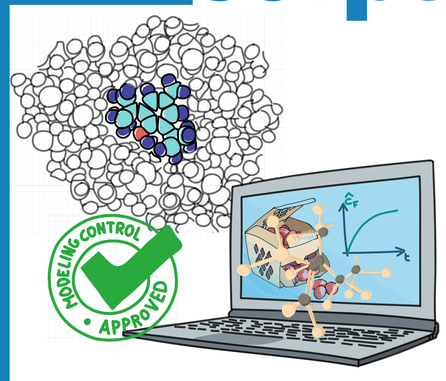
Prediction of diffusion and sorption properties for the circular economy

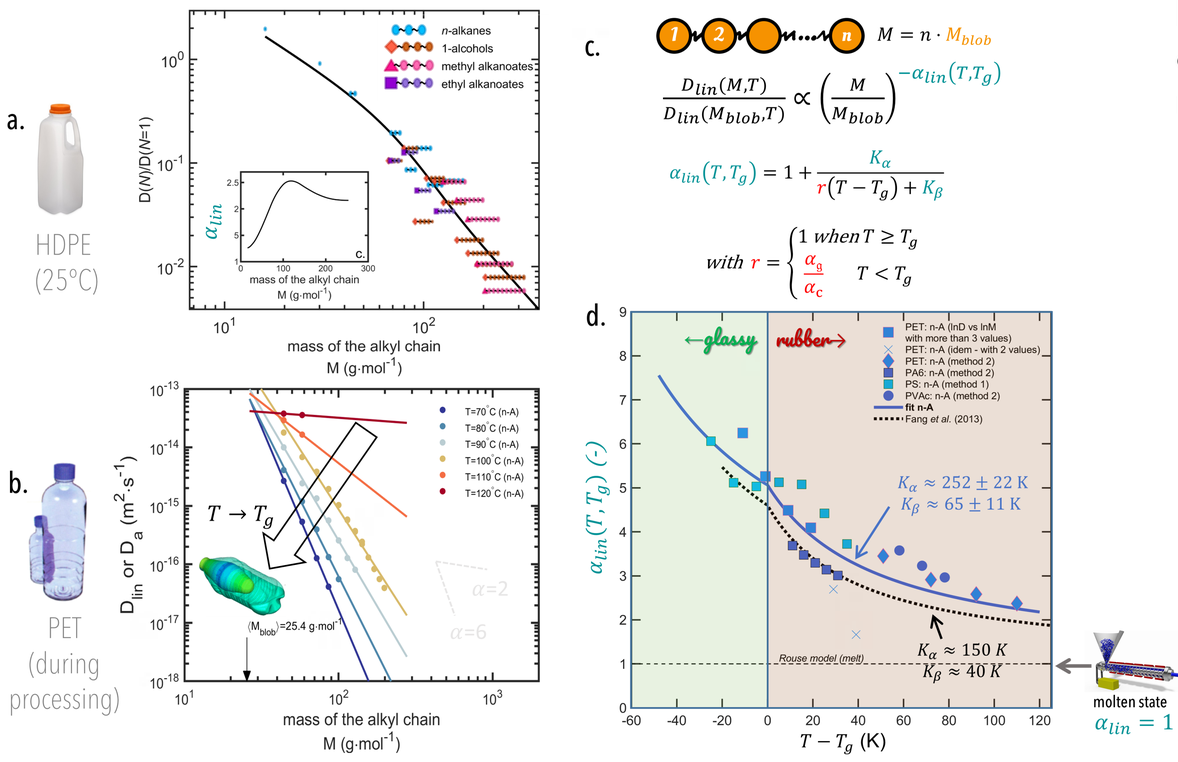


Summary

Mathematical prediction is at the core of the authorization of recycled materials for food contact. Risk assessment is carried out on worst-case chemical structures (with the highest migration rate and the highest hazard). Modeling across the scales offer to work with arbitrary chemical structures and to predict transport and thermodynamic properties for all conditions met by the materials (from thermoplastics to cellulosic materials) and food. These approaches feed the safe-by-design strategy developed by UMT.

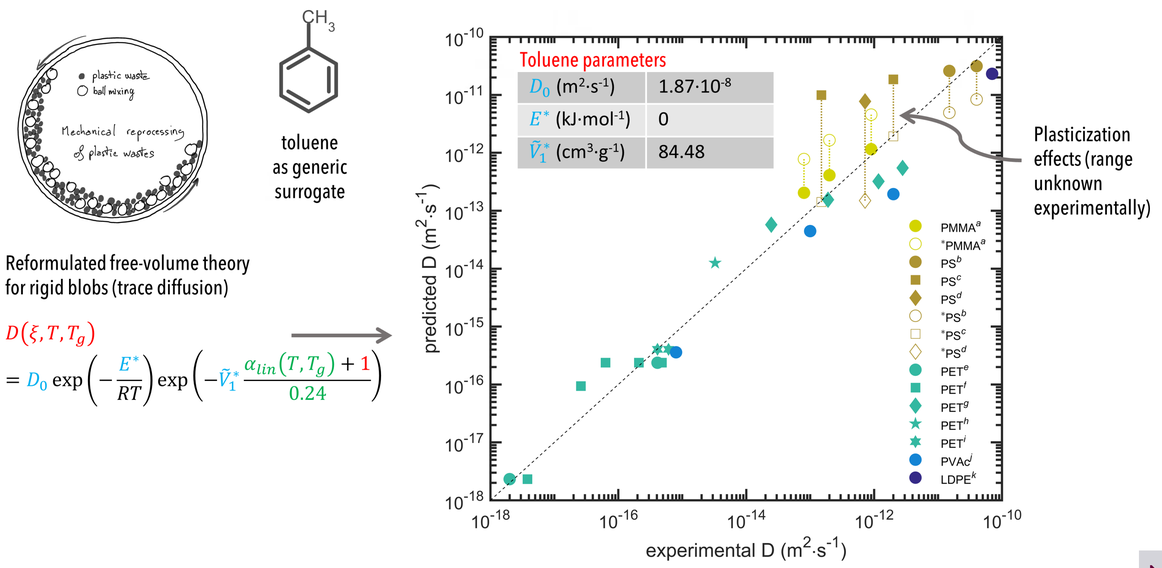
Prediction of diffusivities D_P in thermoplastics (from glassy to molten state)

With support from Fraunhofer Institute (IVV, Germany), a vast experimental campaign to complete a large database of D_P for homologous linear solutes in 12 polymers (rubbery or glassy). The new data validated our extended hole-free volume theory, which is actually the most comprehensive theory to predict D_P from molten down to glassy state.



Scaling laws and diffusion activation by temperature in (a) high density polyethylene (HDPE, T_g ~-110°C) in typical use conditions and (b) polyethylene terephtalate (PET, T_g ~80°C) in mechanical recycling process conditions; (c) scaling law relative to blob theory (e.g blob = ethyl group) and dependance of the exponence α_{lin} on the difference of $T - T_g$. The continuous curves represent the theoretical predictions and the symbols, the experimental values.

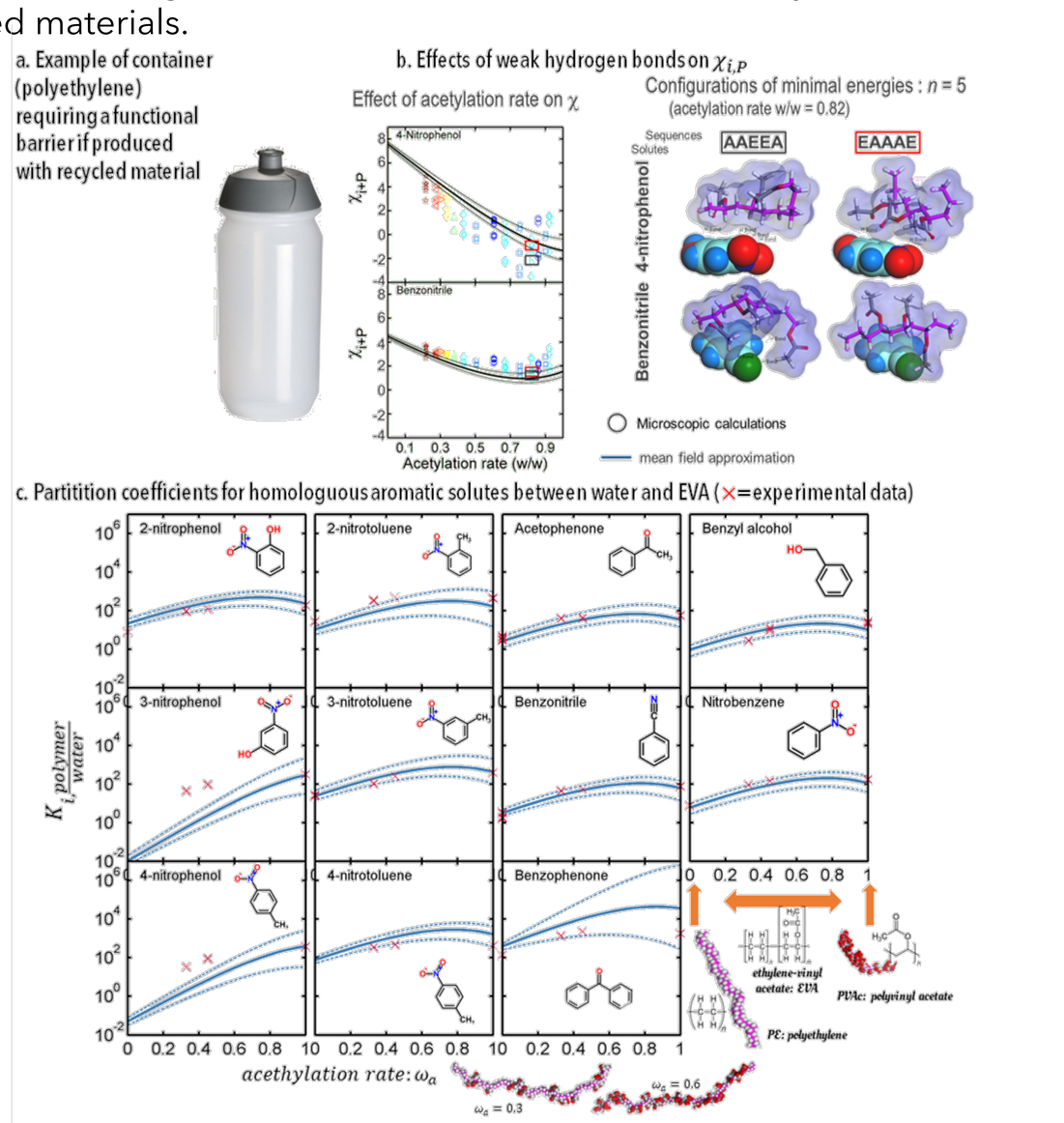
The drastic drop in the temperature dependence (represented by α_{lin}) is an essential property. This effect justifies the temperatures used for the decontamination of glassy polymers such as PET (10 to 20° C above their T_g). Conversely, it shows the very high risk of contamination of rubbery polymers (LDPE, HDPE and to a certain extent PP) in post-consumer recycled material.



Hole-free volume diffusivity model of toluene and its prediction in various polymers and temperatures (no fitting).

Prediction of activity and partition coefficients at atomic scale

Partition coefficients require measurements at thermodynamical equilibrium and are therefore particularly time-consuming to determine experimentally. With the support of the industry (Arkema, Solvay, the European association of producers of plastics), the existing 0.3 Kvalues published so far were extended to more than 6 Kvalues by using tailored molecular modeling for homo- and heteropolymers, hydroalcoholic solutions. The new computational methodology opened the design of new functional materials for not yet authorized recycled materials.

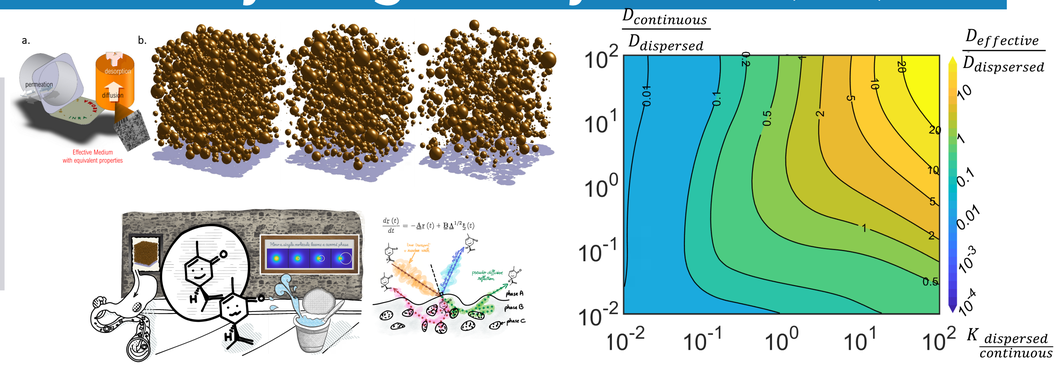


Prediction of partition coefficients at 40 ° C of homologous aromatic solutes between EVA (ethylene vinyl acetate) and water as a function of the acetylation rate of EVA. Because EVA is a random copolymer, two calculation methods were used: (b) by direct sampling of the segments of copolymers to account for the possibilities of hydrogen bonds and (c) in mean field (continuous curves, the 80% confidence interval is shown in dotted lines).

Future crises, choice of food simulants and test conditions, performances of functional barriers can be anticipated with an accuracy comparable of experiments without delay..

Mass transfer in foods calculated by Langevin Dynamics (LD)

New universal simulator based on LD-simulations



Effective diffusivity in emulsions based on ratio of diffusivities and relative chemical affinities

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