

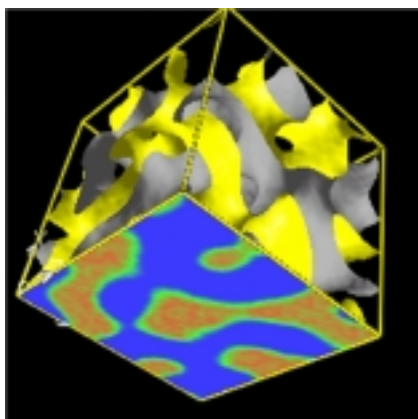
Technical Abstract No. 5

Polymer Blends for Gas Separation and Barrier Applications

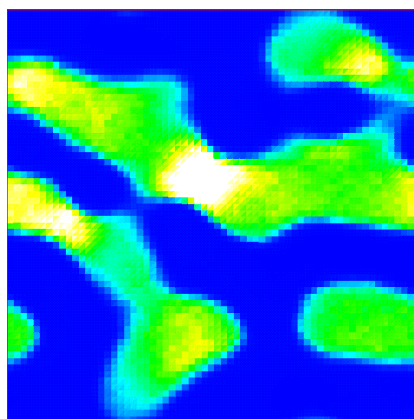
Polymer membranes for the separation of air and other gas mixtures are used in many medical and industrial applications. A successful polymer membrane should exhibit good selectivity between different gases, e. g., O₂ (oxygen) and N₂ (nitrogen) and simultaneously have a sufficiently high permeability. The laboratory design of such membranes requires big and costly experimental efforts. ***Palmyra* delivers accurate and reliable numerical predictions for the selectivity and permeability of various model samples in a short time, thus allowing one to concentrate the laboratory experiments on the most promising mixtures.**

Blends of polystyrene and polyisoprene (PS/PI) are often used for gas separation. The left figure below presents an arbitrary percolative morphology typical of PS/PI blends. This nanoscale morphology was calculated with the software package MesoDyn[®] of Accelrys[®] and fed into *Palmyra's* *GridMorph* for permeability predictions. From the *Palmyra* simulations,* the overall permeability and selectivity coefficients were obtained numerically.

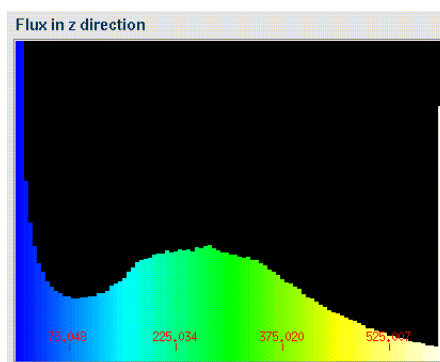
To better understand the local transport behaviour of composites, *Palmyra GridMorph* also allows one to visualize local properties such as gas fluxes in different directions (shown in the middle and right figures). This feature opens a novel route for computer-aided optimization of the membrane structure at a nanoscale level.



MesoDyn[®] structure of polystyrene/polyisoprene blend with compatibilizers: iso-surfaces and density slice showing polymer distributions.



Palmyra cut plane viewer: slice of the structure on the left, showing the magnitude of the oxygen flux in the z direction (from left to right).



Palmyra histogram with the magnitudes of the oxygen flux in the z direction (the same color scheme as for the middle figure).

*) Ref: G. Goldbeck-Wood, A. H. Widmann, U. W. Suter, A. A. Gusev, Europolymer Congress Eindhoven, July 2001.