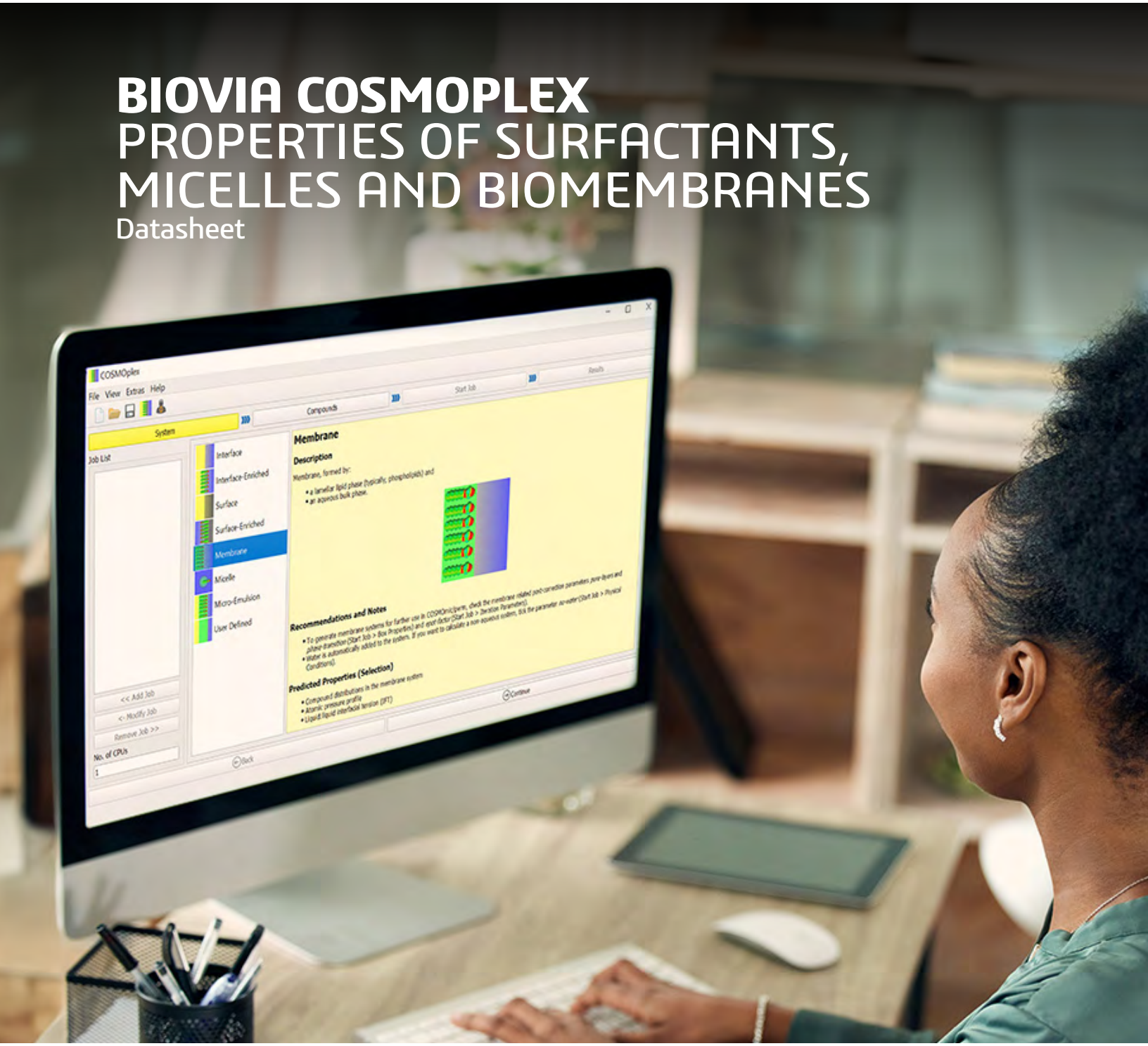
BIOVIA

3DEXPERIENCE®

BIOVIA COSMOPLEX
PROPERTIES OF SURFACTANTS, MICELLES AND BIOMEMBRANES
Datasheet



DASSAULT SYSTEMES

EFFICIENT TREATMENT OF SELF-ORGANIZING SYSTEMS

BIOVIA COSMOplex is a unique methodology extending COSMO-RS far into the regime of inhomogeneous systems, providing access to a series of physical-chemical properties. By this approach COSMOplex yields results usually generated by molecular dynamics (MD) at considerably lower cost.

Systems and physicochemical properties

- Distributions of neutral and ionic species
- Intrinsic passive permeation through biomembranes (pH dependent)
- Prediction of micelle formation including critical micelle concentrations (CMC)
- Partition coefficients and free energy profiles of micellar and biomembrane systems (e.g., SDS, DMPC, POPC, DPPC)
- Microemulsions, e.g. fish points, equivalent alkyl carbon numbers (EACN)
- Interfaces, e.g. interfacial tension

Your benefit

- COSMOplex is up to 10,000 times faster than MD
- Mechanistic prediction of micellar, microemulsion and membrane properties
- No additional fitting of parameters
- Easy to use graphical user interface

METHODOLOGY

BIOVIA COSMOplex is based on COSMO-RS theory which derives the thermophysical behavior of liquids from quantum mechanical DFT calculations.

By combining the chemical potential from COSMO-RS with atomic pressures in a given simulation geometry, the molecules distribute in space until equilibrium is reached.

Systematic calculation of a large number of positions, orientations and conformers results in a probability distribution and hence a free energy profile for the solutes or system components in the micelle, membrane or microemulsion.

PARTITIONING IN MICELLAR AND MEMBRANE SYSTEMS

Biomembranes: Example DMPC

A DMPC bilayer, taken from an MD simulation, is used to calculate the phospholipid-water partition coefficient log $K_{lip:w}$ of neutral an d ionic compounds of different kind.

With a RMSD = 0.62 (neutral compounds) and 0.70 (ions) to experimental data, the method gives very good results, without the need to fit parameters to a given training set.

BIOMEMBRANE PERMEATION

The mechanistic **BIOVIA COSMOplex** approach makes use of:

- Free energy profiles ΔG(z): throughout the biomembrane from chemical potentials μ(z),
- Diffusion coefficients D(z): membrane layer specific (e.g. water, polar head groups, alkyl tails).

BIOVIA COSMOplex results are compared to gold standard BLM experiments. A DMPC bilayer is used as reference to calculate intrinsic passive membrane permeation.

With R^2 = 0.92 and RMSD = 0.62 to experimental data, COSMOplex gives very good results.

This model is applicable to neutral compounds, pH dependent protonation states and permanent ions: pH dependence of permeation is taken into account.

SURFACTANTS

(Micro)emulsions

Surfactant containing systems such as (micro)emulsions can be handled with **BIOVIA COSMOplex**. The example to the right shows the distribution of oil, surfactant and water in a microemulsion system as simulated with COSMOplex. Even complex fish point diagrams can be calculated by COSMOplex.

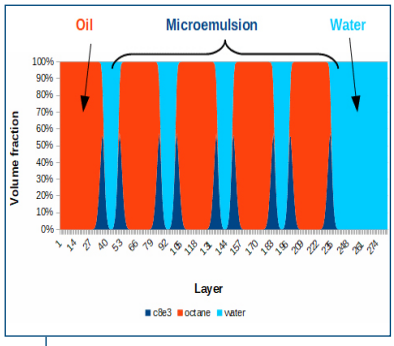


Figure 1: Distribution of oil, surfactant and water in a virtual Microemulsion testtube

Critical micelle concentrations

Critical micelle concentrations can be calculated for pure surfactant compounds, with a good agreement with the experiment, as shown to the right, and even mixtures of them.

Interfaces and interfacial tension

Due to its ability to simulate inhomogeneous systems, BIOVIA COSMOplex can also predict the concentration profile at a liquid-liquid interface and even the average orientation of the molecules. The left graph illustrates the internal pressure profile at the interface, which directly corresponds to the interfacial energy. By applying an additional correlation function, the interfacial tension between two liquid mixture can thus be predicted in a straight forward manner. The liquids can be complex and even contain surfactants.

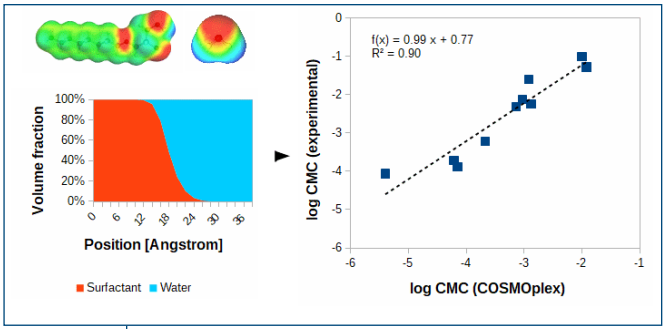


Figure 2: Distribution of surfactant and water in a layered system and predicted Critical Micelle Concentrations (CMC) for surfactants

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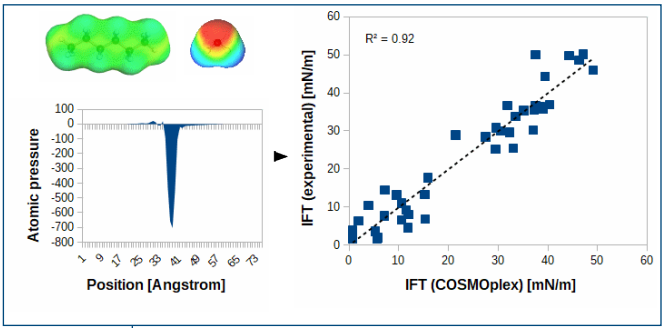

Figure 3: Pressure profile and derived interfacial tension (IFT) for a range of surfactants. The pressure profile at a liquid-liquid interface corresponds directly to the interfacial energy is used to predict the IFT.

MULTISCALE MODELS: BIOVIA COSMOPLEX

Skin penetration model

BIOVIA COSMOplex can simulate the self-assembly of biomembranes consisting of different membrane components, e.g. phospholipids, ceramides, cholesterol etc. It can even include small molecules such as penetration enhancers or potentially toxic molecules. The example below shows the predicted permeation of UV-filter molecules through skin, where COSMOplex was used to generate the bio-membranes and **BIOVIA COSMOplex** and BIOVIA COSMOtherm were used for diffusion constants, free energies and partitioning coefficients, which are all required for the used skin permeation model.

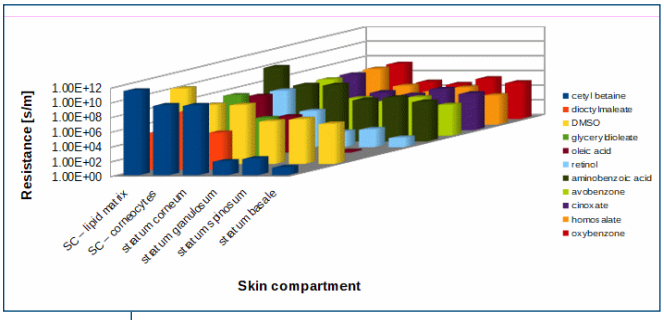

Figure 4: Prmeation of UV-filter molecules through skin as predicted by COSMOplex.

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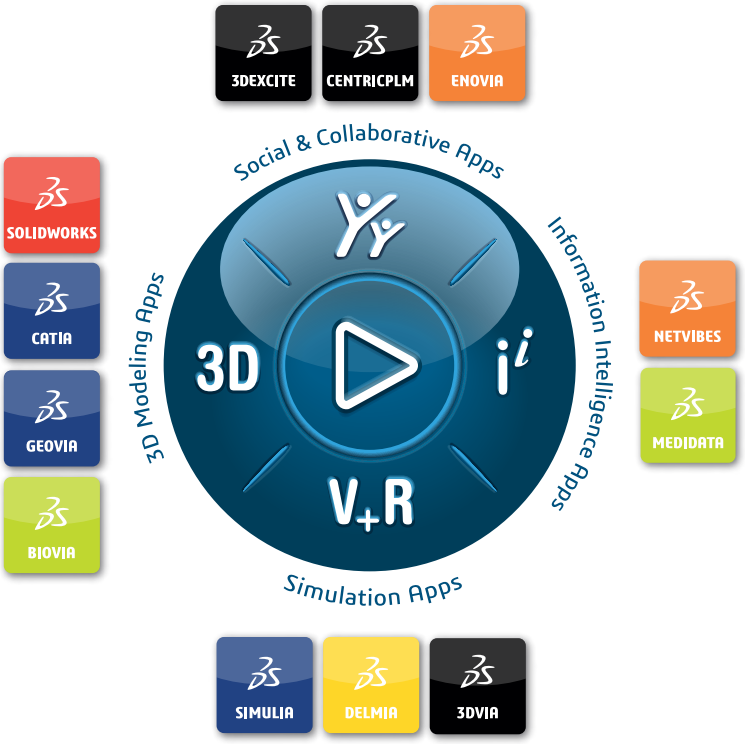

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