

COSMOthermX Version 18 (March 2018)

Key features of the release at a glance:

- Batch functionality and revised database handling and search features in COSMOthermX
- New features (compressible liquid and real gas) for many applications.
- Fundamentally revised and improved algorithms for many properties (IFT, solubility, IL, ..)
- Improved theory for the high quality prediction level BP-TZVPD-FINE.

COSMOperm:

- COSMOperm, an extension of COSMOmic to calculate membrane permeabilities has been included in the COSMOtherm release.

Features of the release in detail:

1. New, extended and revised graphical user interface COSMOthermX functionality

Batch processing: The new graphical user interface supports the submission of batches of molecules, which allows for the calculation of a property over a series of molecules.

Remote submission of jobs: The COSMOtherm calculation can now be submitted on a remote linux server. This enables the user to easily handle many or very time-consuming jobs.

Project tree. The jobs can now be handled in projects and can thus be easier administrated.

New database structure: The preinstalled databases and COSMObases are now delivered and handled by an SQL database. The access is much faster and additional feature could be implemented into the database search. Databases in the format of older COSMOtherm releases can be converted to new format.

Optimized database interface: Search new molecules has become easier, faster and more powerful. It is now possible to paste molecules names, CAS-numbers or even SMILES into the window and retrieve all molecules within just a few seconds.

Other changes: The FlatSurf and Interfacial Tension panels have been contracted to the Interfacial Properties panel. Other changes include the Similarity, Multiple Solvents and COSMOmic panels.

2. New, extended and revised COSMOtherm functionality

Improved compound loading: Due to changes in the COSMOtherm code, molecules are loaded faster, which speeds up jobs with many molecules or series of many small jobs.

New feature: The concept of the so-called "**mixture compound**" (`name.mix` files) has been introduced into COSMOtherm. The MIX-file concept allows the simple application of **composites** (such as *ionic liquids*, *salts*, or salts with *crystal water*) or **mixtures** with fixed mixture ratio (such as *brine*, which is a rock salt solution in water with a fixed composition). The pseudo-compounds thus defined can be treated like a single regular compound in the workflow of COSMOtherm. This allows a significant simplification of the treatment of composites and mixtures with fixed mixture ratio. Moreover, the treatment of such specialty compounds now is generally available throughout all COSMOtherm functionality and property prediction panels. The source files of the mixture compounds or composites (i.e. the COSMO-, ENERGY- and VAP-files of the mixture compound's components) is stored internally in the MIX-file, thus avoiding any compatibility and ambiguity issues. Note, that this feature is not yet available in the graphical user interface COSMOthermX.

New feature: Extension of COSMOtherm **gas phase related** property predictions (currently vapor pressure, boiling point, enthalpy of vaporization, Henry law constant, free energy of solvation, density) towards critical conditions. This was achieved by a combination of regular COSMO-RS theory (which is based on the assumption of incompressible liquid and ideal gas phase) with **Equation-of-State** (EoS) methodologies and their according mixing rules (MRs). Note, that this feature is not yet available in the graphical user interface COSMOthermX.

New feature: Extension of COSMOtherm **VLE and LLE phase diagram** predictions. It is now possible to compute the **temperature** or **pressure glide** function for *isobaric* or *isothermal* phase diagrams. The glide function assumes the mole fraction concentration in the gas phase **y** to be fixed and the concentration in the liquid phase **x** to be the dependent function of **y**. Thus the glide option computes the VLE and LLE phase diagram based on a different fulcrum compared to the regular default VLE and LLE computation. Note, that this feature is not yet available in the graphical user interface COSMOthermX.

Enhanced feature: Extension of the native COSMOtherm **density** and molar volume prediction with temperature and mixture dependence. In previous versions of COSMOtherm this feature was available for pure compounds at room temperature only. The density model now has been extended to predict the density of mixtures at any temperature $\rho(T,x)$ without loss of prediction quality compared to the old model. Note, that this feature is not yet available in the graphical user interface COSMOthermX.

Enhanced feature: Extension of the native COSMOtherm **viscosity** prediction model with temperature dependence. The viscosity model now has been extended to predict the viscosity of pure compounds at any temperature $\eta(T)$ without loss of prediction quality compared to the old

room temperature-only model. Note, that this feature is not yet available in the graphical user interface COSMOthermX.

New feature: A model for the prediction of **diffusion coefficient** (DC) has been developed and implemented. The $D(T,x)$ model is applicable to self-diffusion of pure compounds, to compounds at infinite dilution in a solvent, and to mixtures at any temperature. Note, that this feature is not yet available in the graphical user interface COSMOthermX.

New feature: A model for the prediction of **liquid thermal conductivity** (LTC) has been developed and implemented. The $\kappa(T,x)$ model is applicable pure compounds and to mixtures at any temperature. Note, that this feature is not yet available in the graphical user interface COSMOthermX.

New and extended feature: The computation of **temperature series** (for *isothermal* fixed-pressure properties) or **pressure series** (for *isobaric* fixed-temperature properties) has been generally implemented and is now available for all property calculations that are available in COSMOtherm. In addition to the input of the number of temperature or pressure steps of the series it is now also possible to give a temperature or pressure increment. Note, that this feature is not yet available in all panels of the graphical user interface COSMOthermX.

New feature: Input of **experimental** temperature dependent pure compound **density** for the use in **polymer** predictions. The input of $\rho_{\text{exp}}(T)$ is possible via parameters for DIPPR105 equation, DIPPR116 equation, or a polynomial expansion. In addition, it is possible to input pairs of density and temperature, which will be fitted by COSMOtherm to a polynomial. The experimental density values can be utilized in the free volume calculations necessary for polymer predictions. Note, that this feature is not yet available in the graphical user interface COSMOthermX.

Revised and improved feature: The Interfacial Tension (**IFT**) prediction and the **Flatsurf** functionality for the computation of surface free energy properties have been combined for easier use, and re-implemented into the command line version of COSMOtherm. Thus it is now possible to compute IFT also in the commandline version of COSMOtherm.

Revised and improved feature: The **solubility** multiple solute and multiple solvent screening have been unified for easier use, and re-implemented into the command line version of COSMOtherm. Thus it is now possible to compute multiple solvent solubility screening also in the commandline version of COSMOtherm. In addition, the **reference solubility** functionality has been revised fundamentally and is now also available for both multiple solute and multiple solvent screening.

Revised and improved feature: The Ionic Liquid capacity and selectivity screening (**IL screening**) option has been unified for easier use, and re-implemented into the command line version of COSMOtherm. Thus it is now possible to compute IL screenings also in the commandline version of COSMOtherm.

Revised and improved feature: The **COSMOmeso** functionality, i.e. the fitting of COSMOtherm computed activity coefficients to Flory-Huggins and DPD simulation parameters has been unified for easier use, and re-implemented into the command line version of COSMOtherm. Thus it is

now possible to compute COSMOmeso parameters also in the commandline version of COSMOtherm.

3. Improved accuracy and applicability of COSMO*therm* predictions

Our “best quality” computation level **BP-TZVPD-FINE** theory has been enhanced further.

Current BP-TZVPD-FINE level includes the following features:

- Modified hydrogen bonding to reduce the noise for extreme σ values (Mar 2018)
- New enthalpy contribution for strongly networking solvents, i.e. water (Dec 2017)
- Hydrogen-Bonding Corrected Misfit (HBCMF) (Dec. 2016)
- Residual Dielectric Correction (RDC) (Dec. 2014)
- Dispersion energies based on Grimme D3 method (Dec. 2013)
- Dispersion correction to the HB interaction energy (Dec. 2013)
- Entropic contribution of HB acceptor sites (Dec. 2012)
- New hydrogen bonding physics (Dec. 2011)
- Steric hindrance for hydrogen bonding (Dec. 2011)
- Inclusion of some hydrogen bonding cooperativity effects (Dec. 2011)
- New quantum chemical level (BP-TZVPD) (Dec. 2011)
- Improved cavity construction (FINE-cavity) (Dec. 2011)

Parameter set improvements: Enhanced sets of COSMO*therm* parameters for high level (BP-TZVPD-FINE), production level (BP-TZVP-COSMO, and DMOL3-PBE), and screening level (BP-SVP-AM1) sigma-profiles were obtained from a careful reconsideration of fit data and conformer choice for all compounds involved in the fitting and validation procedure.

The reference states of the chemical potentials computed by COSMO*therm* have been revised. Now the chemical potentials of the liquid state and the gas phase are collated with somewhat more physically meaningful numbers. Note that this change does not affect the differences of chemical potentials. I.e. all of the observable properties computed by COSMO*therm*, as well as all properties that are not directly measurable, but are based on differences of chemical potentials (such as activity coefficients, or free energy of solvation) will remain untouched by the change of the reference state.