Combination of COSMO-RS and cubic EoS

In order to be as predictive as possible, the newly implemented combination of COSMO-RS theory with Equation-of-State methodologies (COSMO-RS-EoS) is able to give accurate predictions of mixture activity coefficients and many other properties for non-compressible systems and in most cases also reasonable predictions of pure component properties, all necessary information like EoS parameters, component-selective temperature and pressure, activity factors, activity coefficients of the components in the mixture and their derivatives can be directly calculated within COSMOTherm.

Calculation of binary interaction parameters

Due to its tremendous influence on the calculated phase diagram and the fact that the temperature-dependent binary interaction parameters \(k_{ij}\) will not be available for most of the mixture systems and temperatures of interest, a simple and efficient calculation/estimation method for these parameters is of great importance.

Since there are no adjustable parameters in the mHV1 mixing rule – which gives reasonable results for a broad range of systems – we developed a calculation method which allows reasonable predictions of bubble-point and dew-point temperatures in a reasonable time.

Workflow improvements

Although the developed algorithms and calculation methods for isothermal and isobaric calculations are very similar, the isobaric procedure proves to be more time-consuming due to the temperature dependence of the COSMO-RS activity coefficients and the necessity to use empirical parameters \(C_i\). In the case of the isothermal procedure, the activity coefficients calculated at the critical point and mixture EoS parameters have to be recalculated in each mixture cycle, what would make the resulting algorithm way too time-consuming to be efficiently usable. We therefore developed a new procedure which allows reasonable predictions of bubble-point and dew-point temperatures in a reasonable time.

Calculation of compressible/supercritical systems

As already mentioned in the introductory part, a major disadvantage of COSMO-RS theory is its limitation in incompressible systems. In the second case, an error might be introduced, because the temperature dependent activity coefficients are calculated at a different temperature. Unfortunately, the developed COSMO-RS-EoS combination allows reasonable predictions of compressible systems which are only partially accessible with existing procedures.

Combination of Equation-of-State methods with COSMO-RS

In order to be as predictive as possible, the newly implemented combination of COSMO-RS theory with Equation-of-State methodologies (COSMO-RS-EoS) is able to give accurate predictions of mixture activity coefficients and many other properties for non-compressible systems and in most cases also reasonable predictions of pure component properties, all necessary information like EoS parameters, component-selective temperature and pressure, activity factors, activity coefficients of the components in the mixture and their derivatives can be directly calculated within COSMOTherm.

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