

Differences between COSMO-RS, COSMO-RS(OI) and COSMO-SAC

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After the great success of COSMO-RS (A. Klamt, COSMOLogic), similar models were developed by different groups in the world. While the details of the commercial COSMO-RS model are not completely published, the other models are fully described in the open literature.

For an excellent introduction to COSMO calculations and the COSMO-RS-model see "A. Klamt, "From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design", Elsevier 2005". The book discusses many aspects in great detail but does not always give sufficient information, to which extend the results of the model are influenced by the different extensions like orthogonal sigma profiles etc.

COSMO-SAC was developed by Lin and Sandler (S.-T. Lin and S. I. Sandler, "A Priori Phase Equilibrium Prediction from a Segment Contribution Solvation Model", *Ind. Eng. Chem. Res.* **2002**, *41*, 899-913) and was implemented in the Aspen simulator.

The Aspen Property Plus Product Information states:

The implementation in Aspen Plus for COSMO-SAC adapts the effective sigma profile approach so that it requires only two parameters, component volume and sigma profile. The component surface area will be calculated as follows:

$$A = \sum_i p_i(\sigma_i), i = 1, 2, \dots, 51$$

A quantum mechanical calculation should give you all three parameters for each component. Then if necessary, you can convert the original sigma profile form to the effective sigma profile form as defined above for Aspen Plus.

If your COSMO output is from a program like Gaussian, the program should provide you the details on how to calculate these three parameters for each component from the COSMO output. The procedure may vary depending on how the quantum mechanical calculation is carried out. Aspen Plus cannot provide such a procedure for conversion.

A detailed description of COSMO-SAC together with results can be found at http://www.aspentech.com/publication_files/TP50.pdf

The COSMO-RS(OI) model was developed by Grensemann and Gmehling ("Performance of a Conductor-Like Screening Model for Real Solvents Model in Comparison to Classical Group Contribution Methods", *Ind. Eng. Chem. Res.*, **44** (5), 1610 -1624, 2005). During the development, a large amount of data from the DDB were used to verify the validity of the different model modifications.

COSMO-RS-models primarily calculate the chemical potential of a component via the shielding charge density in an ideal conductor. Other important interactions like dispersive forces and hydrogen-bonding are modeled in much less detail.