Using the VT-2005 database

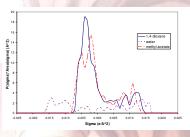
A step-by-step tutorial on predicting liquid-phase activity coefficients using the VT-2005 sigma profiles and the COSMO-SAC-VT-2005 program

Richard Oldland, Eric Mullins, Michael Zwolak, Kevin Seavey, and Y. A. Liu

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This presentation shows how to use VT-2005 sigma profiles with the COSMO-SAC-VT-2005 program to predict activity coefficients



1. Overview of sigma profiles



2. Outline of the COSMO-SAC model



3. Using the COSMO-SAC-VT-2005 program

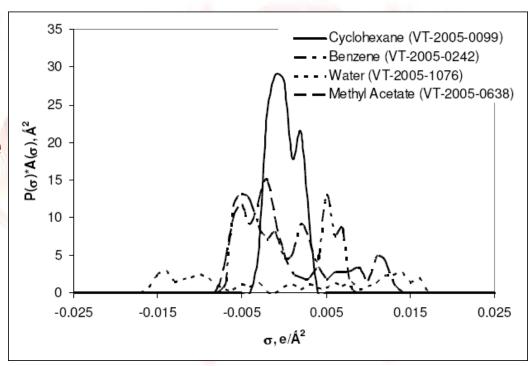
The sigma profile depicts the surface charge distribution over the entire molecule.

Graphically: Area vs. charge/Area

Unique to each molecule

Profiles are stored in a database

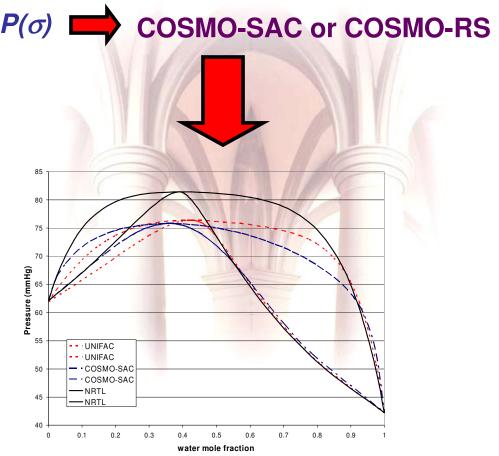
Sigma profiles are not specific to a COSMO extension



Sigma profile $[P(\sigma)]$ = the probability a specific surface segment will have a specific charge density.

COSMO models use sigma profiles to predict physical properties.

- Solubility (SLE)
- Vapor-Liquid (VLE)
- Partition coefficients (K_{OW})
- pKa



We develop the VT-2005 sigma-profile database containing over 1200 molecules.

Chemical components including alcohols, alkanes, fluorocarbons, ketones, aldehydes, solvents, etc.

The molecules contain the following elements: C, O, H, N, I, CI, F, Br, P, F

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Building the VT-2004 database

A step-by-step tutorial on generating VT-2004-consistent sigma profiles using the Accelrys Materials Studio Dmol3 software package.

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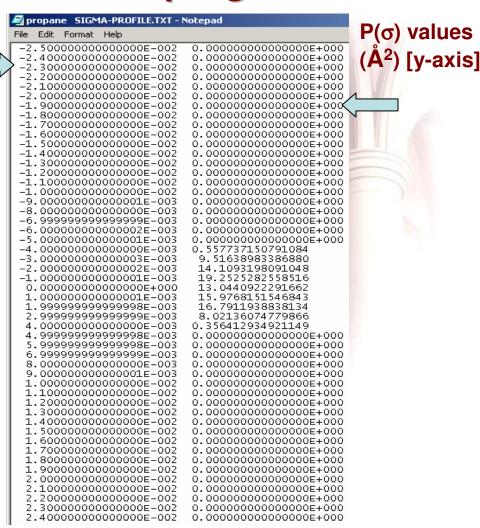


We create sigma profiles in a format that is usable with COSMO-SAC-VT-2005 program.

Sigma values (e/Ų) [x-axis]

The output file 'Chemical' Sigma-profile.txt is located in the 'C:\Profiles\' directory by default.Å

We can either use this file directly in the COSMO-SAC program or we can plot it in MS Excel.



Lin and Sandler (2002) develop the continuumsolvation model COSMO-SAC

Model traits

- Extension to COSMO
- Liquid phase interactions
- Thermodynamically consistent

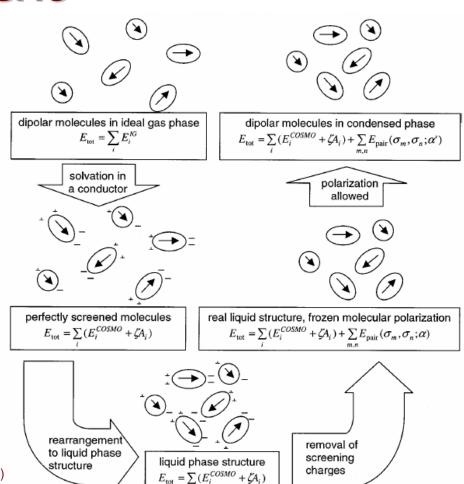
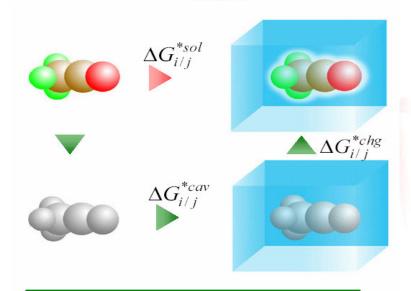


Figure from: Lin and Sandler (2002a)



We begin with the definition of the solvation free energy (ΔG_{sol})



 $\Delta G_{i/j}^{*sol}$: solvation free energy

 $\Delta G_{i/j}^{*cav}$: cavity formation free energy

 $\Delta G_{i/j}^{*chg}$: charging free energy

i/j: solute i in solvent j

c: total molar concentration

We break the real solvation process into two "ideal" steps:

- 1. Cavity formation
- 2. Charge restoration

Previous models for the activity coefficient use the free energy of solvation.

$$\ln \gamma_{i/S} = \frac{\Delta G_{i/S}^{*sol} - \Delta G_{i/i}^{*sol}}{RT} + \ln \frac{c_S}{c_i}$$

In terms of the solvation free energy (Ben-Naim (1987))

$$\ln \gamma_{i/S} = \frac{\Delta G_{i/S}^{*res} - \Delta G_{i/i}^{*res}}{RT} + \ln \gamma_{i/S}^{SG}$$

In terms of the charge restoring free energy. (Lin and Sandler (2002a))

The authors approximate the solvation process with the charge restoration free energy. We calculate this quantity with sigma profiles and activity coefficients for each surface segment.

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The COSMO-SAC model predicts the activity coefficient using the sigma profile.

$$\ln \gamma_{i/S} = \frac{\Delta G_{i/S}^{*res} - \Delta G_{i/i}^{*res}}{RT} + \ln \gamma_{i/S}^{SG}$$

Starting with the charge restoring free energy

$$\frac{\Delta G_{i/S}^{*res}}{RT} = \sum_{\sigma_m} \left[n_i \left(\sigma_m \right) \frac{\Delta G_{\sigma_m/S}^{*res}}{RT} \right] = n_i \sum_{\sigma_m} p_i \left(\sigma_m \right) \ln \Gamma_S \left(\sigma_m \right)$$

$$\frac{\Delta G_{i/i}^{*res}}{RT} = \sum_{\sigma_m} \left[n_i \left(\sigma_m \right) \frac{\Delta G_{\sigma_m/i}^{*res}}{RT} \right] = n_i \sum_{\sigma_m} p_i \left(\sigma_m \right) \ln \Gamma_i \left(\sigma_m \right)$$
 profile and the segment activity coefficient

In terms of the sigma

$$\ln \gamma_{i/S} = n_i \sum_{\sigma_m} p_i(\sigma_m) \left[\ln \Gamma_S(\sigma_m) - \ln \Gamma_i(\sigma_m) \right] + \ln \gamma_{i/S}^{SG}$$

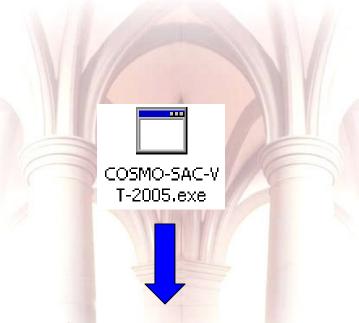


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We provide the COSMO-SAC-VT-2005 program to predict activity coefficients

The COSMO-SAC-VT-2005 program is:

- FORTRAN90 based
- Open literature
- Quick to run
- Binary mixtures only
- •Easily upgradeable for ternary and quaternary mixtures



Calculates liquid-phase activity coefficients for mole fractions ranging from 0.005-0.995 in steps of 0.01

Locate the pure component sigma profiles





This program is compatible with sigma profiles in a format similar to the VT-2005 sigma profiles.

COSMO-SAC-VT-2005.exe requires the <u>profile name</u> AND <u>location</u>.

We store our sigma profiles in a central directory "C:\Profiles" to make them easy to locate. Create the directories "C:\Profiles" and "C:\Profiles\Gammas" at this time.

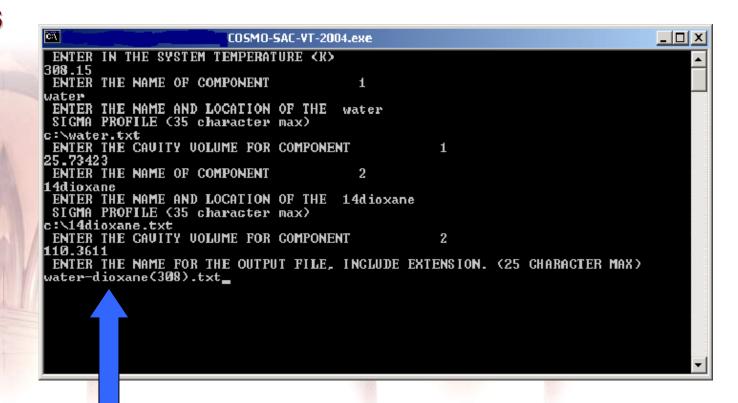
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Run "COSMO-SAC-VT-2005.exe" and follow the MS-

DOS prompts

Required inputs:

- System temperature
- Species names
- VT-2005 sigma profiles
- Cavity volumes
- Output file name



Creates the output file in the directory "C:\Profiles\Gammas" by default.

COSMO-SAC-VT-2005.exe creates an output text file

The output file is in the format: Mole fraction component $1, \gamma_1, \gamma_2, Ln(\gamma_1), Ln(\gamma_2)$

We can use the output to compare activity coefficient predictions or to predict physical properties

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Congratulations!



You have successfully used the COSMO-SAC model, COSMO-SAC-VT-2005.exe, to predict liquid-phase activity coefficients for a binary mixture.



Acknowledgements



We used the following articles in developing this procedure.

- Klamt, Andreas, G. Shüürmann, "COSMO-A New Approach to Dielectric Screening in Solvents with Explicit Expressions for the Screening Energy and Its Gradient", *J. Chem. Soc. Perkin Trans.*, **2**, 799, (1993).
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