M winmostar tutorial Gromacs Calculation of Solubility/Chi/DPD Parameters

V11.6.5

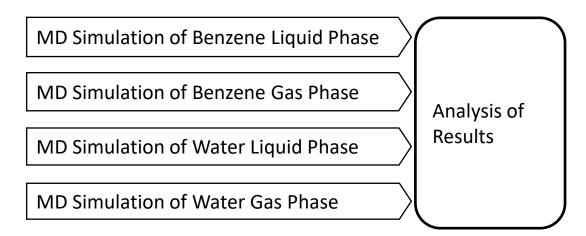
30 March 2024 X-Ability Co., Ltd.

About This Manual

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult <u>Beginner's Guide</u>.
- For those who wish to explore the details of each feature, please refer to <u>Winmostar User Manual</u>.
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
 - <u>Winmostar Introductory Training Session</u>: This guide only introduces the operation methods of the Basic Tutorial.
 - <u>Winmostar Basic Training Session</u>: We will cover the theoretical background, explanations on interpreting results, operational methods of the Basic Tutorial, and procedures for some tutorials beyond the basic level.
 - <u>Individual Training Session</u>: You can freely customize the training content according to your preferences.
- If you are unable to proceed with the operations as outlined in this manual, please first consult <u>Frequently asked questions</u>.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using <u>Contact page</u>. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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Overview

 In this tutorial, we calculate the cohesive energy of benzene (component A) and water (component B), the Hildebrand solubility parameters for both components, the Flory-Huggins parameter (χ) between water and benzene, and the DPD A_{ij} parameter.



Note :

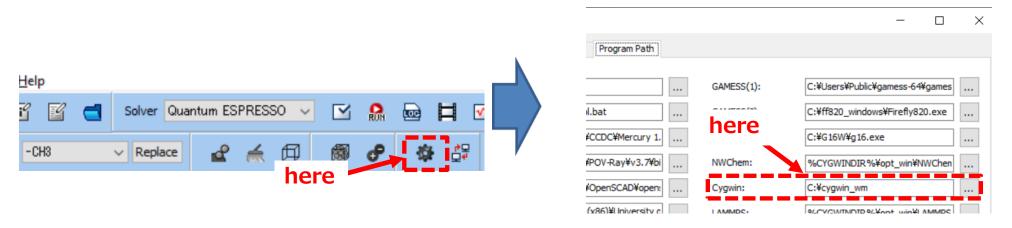
- The number of steps required for equilibration varies with the type of molecule and initial density.
- Larger step counts in the 'main calculation' lead to better reproducibility and more reliable results.
- The type of force field and interaction calculation conditions significantly affect the calculation results.
- Although the calculation of water vapor phase is not necessary when using a rigid water model, it
 is currently required by Winmostar[™] for the energy file, so the calculation will be performed.

Operating Environment Settings

- To use this feature, it is necessary to set up Cygwin.
- <u>https://winmostar.com/en/installation/</u> Set up Cygwin by following the configuration steps outlined in the installation instructions.

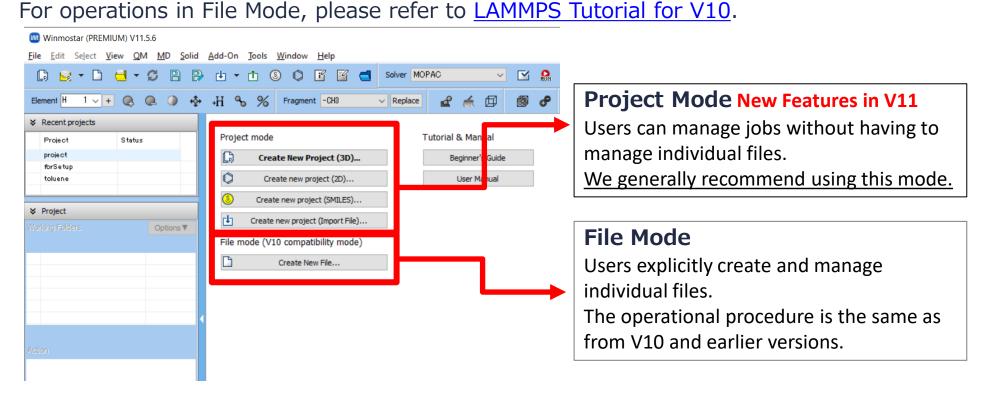


• By default, it is installed directly under C:, but you can install it in a location of your choice by changing the 'Program Path' > 'Cygwin' in Winmostar Preference.



Operating Modes of Winmostar V11

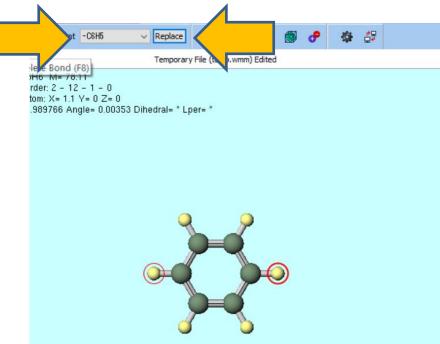
V11 offers two operating modes: **Project Mode** and **File Mode**. This manual focuses on operations in Project Mode.



A. Modeling of the System (Component A Liquid Phase)

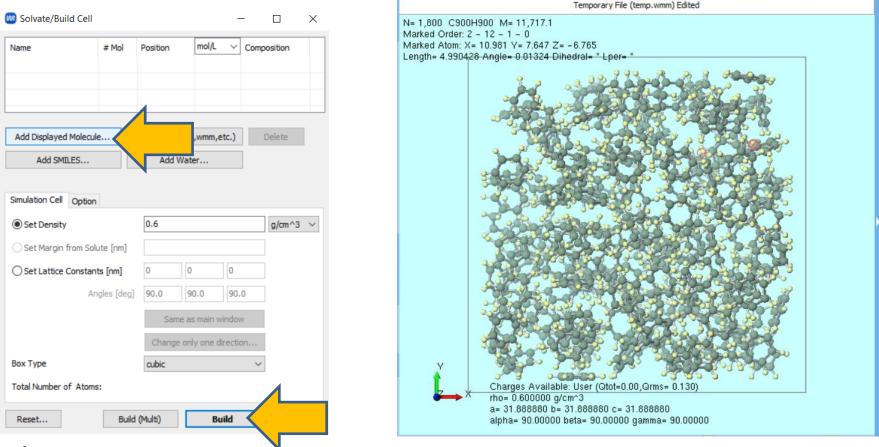
For basic operations, please refer to Gromacs Basics tutorial.

- A. Click File | New Project, enter 'solub_param' in Project name, and click Save.
- B. Select '-C6H5' from **Fragment** and click **Replace** to create benzene.
- C. Click *P* Assign Charges Automatically and then click OK.
- D. Click **Export File and save as '**benzene_am1bcc.mol2'.



A. Modeling of the System (Component A Liquid Phase)

- A. Click Solvate/Build Cell.
- B. Click Add Displayed Molecule, enter '150', and click OK.
- C. Click **Build**.



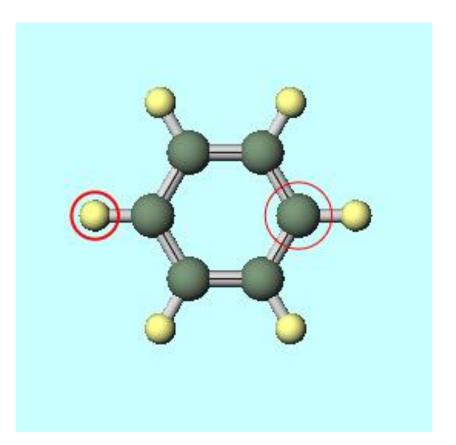
B. Execution of Calculation (Component A Liquid Phase)

- A. Select **Gromacs** from **Solver**, and open **Markflow Setup**.
- B. Click **OK**, and if 'Assigned force field parameters' is displayed, click **OK** again.
- C. Change Simulation time of 2nd job to '50'.
- D. Adjust **Simulation time**, **Temperature**, **Pressure** as needed (no changes needed for this tutorial).
- E. If you want to finish the calculation quickly by reducing computational accuracy, change **Precision** of **all jobs** from **1st** to **3rd** to 'Low'.
- F. Click + next to # of jobs once.
- G. Click **OK**, adjust settings in **Job Setting** window as needed, and then click **Run**.

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				+ -	
Minimize ~	Temperature [K]	300.	Pressure [atm]	1.	
10.	# of snapshots	50	Initial velocity	From parent 🔍	
ndition	Precision	Medium	√ De	tals	
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C. Modeling of the System (Component A Vapor Phase)

- A. Click 🛃 Import File and select benzene_am1bcc.mol2 saved in P. 6.
- B. In Import File dialog, click Discard and import.



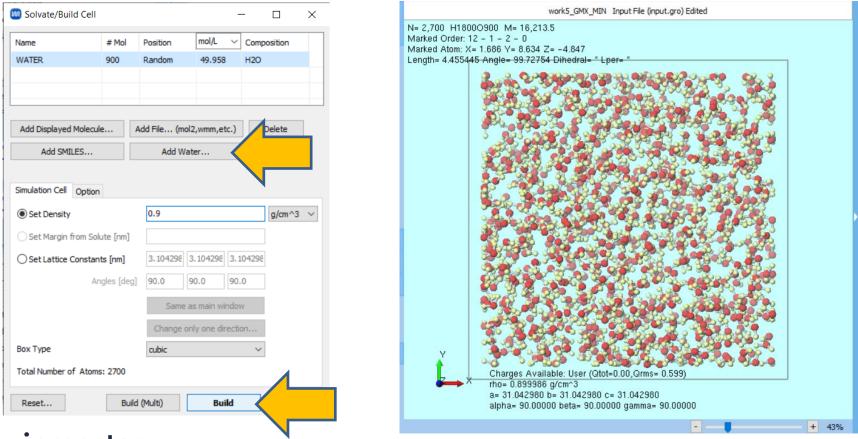
D. Execution of Calculation (Component A Vapor Phase)

- A. Open **(Workflow Setup)**.
- B. Click No when prompted 'Do you want to continue from previous run?'.
- C. Click **OK** when 'Create Cell' is displayed.
- D. Click **OK** in **Assign force field parameters** window, and then click **OK** again when 'Assigned force field parameters' is displayed.
- E. Change **Preset** to 'Isolated system NVT Equilibration'.
- F. Change **Simulation time**, **Temperature**, **Pressure** as needed (no changes are needed for this tutorial).
- G. If you want to speed up the calculation by lowering the calculation accuracy, change **Precision** of **1st** and **2nd jobs** to 'Low'.
- H. Click + next to # of jobs once.
- I. Change **Initial velocity** of **3rd job** to 'From Parent'.
- J. Click **OK**, then adjust settings as needed in **Job Setting** window and click **Run**.

Proceed to 'IX. Result Analysis' if only the solubility parameter of component A is needed.

E. Modeling of the System (Component B Liquid Phase)

- A. Click **Solvate/Build Cell**.
- B. Click Add Water, enter '900', and click OK.
- C. Enter '0.9' in Set Density, and click Build.

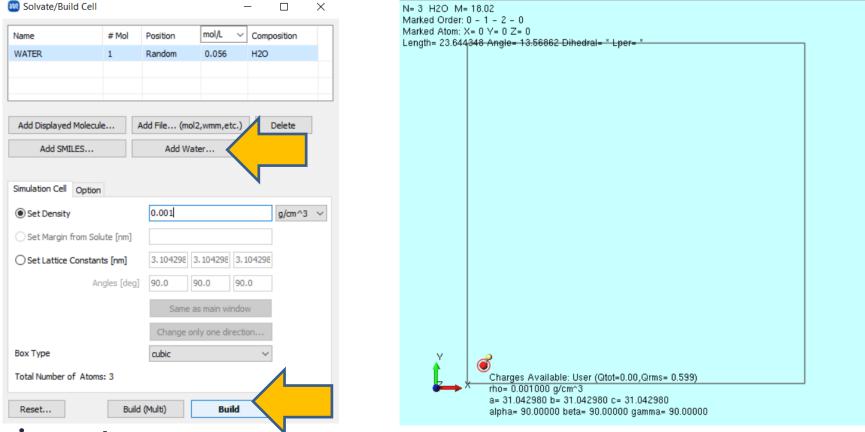


F. Execution of Calculation (Component B Liquid Phase)

- A. Open 🗹 (Workflow Setup).
- B. If prompted 'Do you want to continue from previous run?', click No.
- C. Click **OK**, and when 'Assigned force field parameters' is displayed, click **OK**.
- D. Change **Preset** to 'Fluid/Amorphous NPT Equilibration'.
- E. Change Simulation time of 2nd job to '50'.
- F. Adjust **Simulation time**, **Temperature**, **Pressure** as needed (no changes are needed for this tutorial).
- G. If you want to shorten the calculation time, change **Precision** of **all jobs** from **1st** to **3rd** to 'Low'.
- H. Click + next to # of jobs once.
- I. Click **OK**, adjust the settings in **Job Setting** window as needed, and then click **Run**.

G. Execution of Calculation (Component B Vapor Phase)

- A. Click 🚳 Solvate/Build Cell.
- B. Click Add Water, enter '1', and click OK.
- C. Enter '0.001' in Set Density, and click Build.



G. Execution of Calculation (Component B Vapor Phase)

- A. Open **(Workflow Setup)**.
- B. If prompted 'Do you want to continue from previous run?', click No.
- C. Click **OK**, and when 'Assigned force field parameters' is displayed, click **OK**.
- D. Change **Preset** to 'Isolated system NVT Equilibration'.
- E. Adjust **Simulation time**, **Temperature**, **Pressure** as needed (no changes are needed for this tutorial).
- F. If you want to shorten the calculation time, change **Precision** of **1st** and **2nd jobs** to 'Low'.
- G. Click + next to # of jobs once.
- H. Change **Initial velocity** of **3rd job** to 'From Parent'.
- I. Click **OK**, adjust the settings in **Job Setting** window as needed, and then click **Run**.

- A. After all calculations are completed, click Analyses | Chi/DPD Parameter, and then click Molecule A tab.
- B. Click Select for Liquid Phase's edr File, and select gmx_mdrun.edr under work4_GMX_NPT.
- C. Click Select for Liquid Phase's gro File, and select gmx_mdrun.gro under work4_GMX_NPT.
- D. Click Select for Vapor Phase's edr File, and select gmx_mdrun.edr under work7_GMX_NVT.

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Import Last Coordinate (gro)		
Radial Distribution Function	Chi/Solubility Parameters	- 🗆 ×
Diffusion Constant/Mean Square Displacement	Molecule A Molecule B Chi / Aij	
Scattering Function	Molecule & Molecule B Chi / Alj	
Velocity Autocorr./Vibration Spectrum	Liquid Phase edr File (not selected)	Select
Static Dielectric Constant		
Shear Viscosity	gro File (not selected)	Select
Density Profile		
Free Volume	Vapor Phase edr File (not selected)	Select
Hildebrand Solubility Parameter		
Chi/DPD Parameter		
Bond/Angle/Dihedral Distribution		
Normal Mode Analysis		

A. The **Hildebrand solubility parameter** δ of **Molecule A** (in this case, benzene) and **DPD Parameter** A_{ii} between **Molecule As** are output at the following location. (Be careful of the units when comparing with literature values, etc.)

Chi/Solubility Parameters		_		×				
Molecule A Molecule B Chi / Aij								
Liquid Phase edr File C:¥winmos	11¥UserData¥solub_parar	n.wmpjdata¥work4_G	Select					
gro File C:¥winmos	11¥UserData¥solub_parar	n.wmpjdata¥work4_G	Select					
Vapor Phase edr File C:¥winmos	11¥UserData¥solub_parar	n.wmpjdata¥work7_G	Select					
Properties								
Molar Volume	Vma	[m^3/mol]	7.82025e-05					
Temperature	Temperature T [K]		299.916	299.916				
Isothermal Compressibility	Kt	[J/m^3]	7.66133e-10					
Dimensionless Compressibility	K=Vma/(R*T*Kt)	[-]	40.93386		Intra-species			
DPD Parameter	Aii=(K-1)/(0.2*rho)	[-]	39.53847	$\langle _$	DPD Parameters			
Liquid Potential Energy	El	[kJ/mol]	21.2239					
Vapor Potential Energy	Ev	[kJ/mol]	53.5775					
Cohesive Energy dE=Ev-El		[kJ/mol]	32.35360		Cohesive Energy			
Solubility Parameter	da=sqrt(dE/Vma)	[(J/cm^3)^1/2]	20.34000		Solubility Paramet			
Reset		Excel	Close					

To determine the χ parameter and the DPD parameter A_{ij} :

- A. Click Molecule B tab.
- B. Click Select next to Liquid Phase's edr File, and select gmx_mdrun.edr under work11_GMX_NPT.
- C. Click Select next to Liquid Phase's gro File, and select gmx_mdrun.gro under work11_GMX_NPT.
- D. Click Select next to Vapor Phase's edr File, and select gmx_mdrun.edr under work14_GMX_NVT.

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Vapor Phase edr File C:¥w	inmos11¥UserData¥solub_para	m.wmpjdata¥work14_	(Select]	
Molar Volume	Vmb	[m^3/mol]	1.81817e-05		
Temperature	т	[K]	300.001		
Isothermal Compressibility	Kt	[J/m^3]	5.24488e-10		
Dimensionless Compressibility	K=Vmb/(R*T*Kt)	[-]	13.89767		Intra-species
DPD Parameter	Aii=(K-1)/(0.2*rho)	[-]	12.76997		-
Liquid Potential Energy	El	[kJ/mol]	-46.4469		DPD Parameters
Vapor Potential Energy	Ev	[kJ/mol]	0		L
Cohesive Energy	dE=Ev-El	[kJ/mol]	46.44690		
Solubility Parameter	db=sqrt(dE/Vmb)	[(J/cm^3)^1/2]	50.54301		Solubility Parame
Reset		Excel	Close		

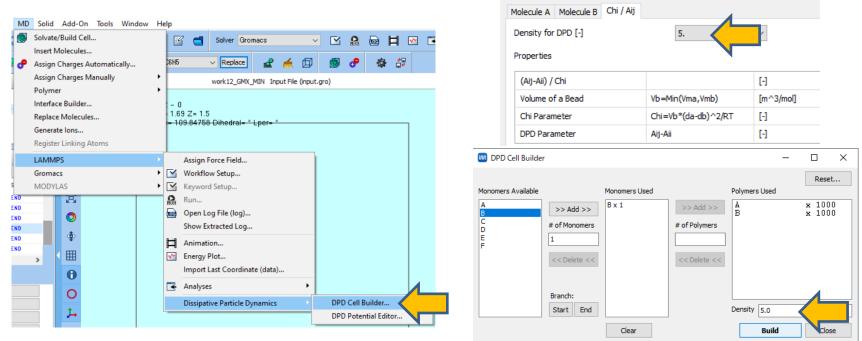
A. In **Chi/Aij tab**, **x** parameter and **DPD parameter** ($A_{ij} - A_{ii}$) are displayed.

Chi/Solubility Parameters	4	-	- 🗆	×	
Molecule A Molecule B Chi /	Aij				
Density for DPD [-]	5.	\sim			
Properties					
(Aij-Aii) / Chi		[-]	1.45000		
Volume of a Bead	Vb=Min(Vma,Vmb)	[m^3/mol]	1.8182E-005	;	
Chi Parameter	Chi=Vb*(da-db)^2/RT	[-]	6.65027		X Parameter
DPD Parameter	Aij-Aii	[-]	9.64290		Inter-species
					DPD Parameters
Citation					
R. D. Groot and P. B. Warren	n, J. Chem. Phys., 107 (11), 199	7.			
Reset		Exc	el Clos	e	
				-	

Supplementary: Setting up DPD Calculations

- A. If you are not performing DPD calculations, skip this section.
- B. For detailed settings for DPD calculations, refer to 'Winmostar™ LAMMPS Tutorial on Dissipative Particle Dynamics'.
- C. When creating a system in **MD | LAMMPS | Dissipative Particle Dynamics | DPD Cell Builder**, enter the value displayed in **Density for DPD** field in **Chi/Aij tab** of **Chi/Solubility Parameters** window into **Density** field.

M Chi/Solubility Parameters



Supplementary: Setting up DPD Calculations

- A. Next, in **MD | LAMMPS | Dissipative Particle Dynamics | DPD Potential Editer**, under **Nonbond tab**, for A-A and B-B interactions, specify the intraspecies DPD parameter A_{ij} obtained for MonomerA and MonomerB, respectively, in **MonomerA**, **MonomerB tabs**. However, unify the value for either component 1 or 2. For A-B interactions, input the sum of the adopted intraspecies DPD parameter and the obtained interspecies DPD parameter ($A_{ij} A_{ij}$).
- B. The calculation of the DPD parameters for water-benzene was referenced from the literature [A. Maiti and S. McGrother, J. Chem. Phys., 120 (3), 2004, 1594.].

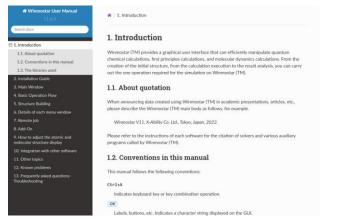
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new	Mass	Bond	Nonbond			
	i	j	Aij	Rcut		
	A	A	15.00	1.000	1	
	A	В	15.00	1.000		
	В	В	15.00	1.000		
			20	1	Set	
				-	000	
New Delete			0	К	Cance	el

In this example, the value for the intraspecies parameter of H2O is adopted, and values are rounded to the nearest decimal point.

Finally

• For detailed information on each feature, please refer to Winmostar User Manual.





Winmostar User Manual

Scenes from Winmostar Training Session

- If you wish to practice the contents of this guide, please consider attending <u>Winmostar Introductory Training Session</u>, <u>Winmostar Basic Training Session</u>, or <u>Individual Training Session</u>. (See page 2 for details.)
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