

### Winmostar tutorial Gromacs Vapor Pressure - Surface Tension V7.025

# X-Ability Co., Ltd. <u>question@winmostar.com</u> 2017/8/8



## Configure

#### You must set up Cygwin to use Gromacs on Winmostar.

 Obtain the installer for Cygwin, which contains the all programs needed by Winmostar, at <u>https://winmostar.com/en/manual\_en.html</u>.

2. Installation Guides for Solvers
For Windows
cygwin_wm_v7_20160926.exe(418MB)
(For Experts)NWChem/Gromacs/Amber Build with Cygwin
GAMESS Installation Guide
LAMMPS Installation Guide

• When you change the installation path for Cygwin from the default one, specify it on the preference panel.





#### Note

- The simulation steps required are dependent on molecular species and initial density.
- To obtain accurate and reproducible results, you have to set long simulation time.
- The method for interaction calculations and/or the force field also affect the simulation results.
- Insert vacuum layer as needed before executing calculations for equilibrium.



#### I. Build a simulation cell

In this tutorial, we'll calculate the saturated vapor pressure and surface tension with a vapor-liquid equilibration.

- 1. Click **MD** | Solvate/Build Cell.
- 2. Uncheck Put the molecule on main window as solute.
- 3. Click Add water. Set Enter # of molecules to 500.
- 4. Click OK.

	ile on main windov	v as solute:			
Name	# Mol	Position	mol/L 🗸	Composition	
					Add water
Add V	Water	A	dd .mol2 File	Delete	Enter # of molecules 500
Simulation Cell	Option				
Set Density [	[g/cm^3]	0.6			
Set Distance	from Solute [nm]				
🔿 Set Box Size	[nm]			Import	
	Angles	90.0	90.0 90.	0	
Box Type		cubic		~	



#### Build a simulation cell Ι.

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Y=6.2800)2=

- 1. Set Set Density to 0.9.
- 2. Click **Build**.





#### I. Build a simulation cell

- 1. Click Edit | Solvate/Build Cell.
- 2. On Expand, set Width to 50, then click Expand.
- 3. Click OK.





#### I. Build a simulation cell

Click the icon of red X camera, then zoom out the camera. Vapor – liquid equilibration system has been built.



2017/8/8



#### II. Equilibration

- 1. Click MD | Gromacs | Keywords Setup.
- 2. Click Reset.
- 3. Click **# of Threads** to parallel number, then click **OK**.
- 4. Click MD | Gromacs | Start Gromacs.
- 5. Save the coordinate file as **spce500k.gro**, the topology file as **spce500k.top**.

Ø		Groma	ics Setup		_	
Exten	ding Simulation		# of Threads		2	
Preset	Minimize (fast)	¥	MPI (for Remo	te Job)	1 Pr	
Basic A	dvance Output	Interaction Other	Automatic Option	s For	ce Field	
Run Con	trol		Temperature C	ouplin	g	
dt [ps]		0.002	tcoupl		berendsen	$\sim$
nsteps		5000	tc-grps		System	
Total time	e: N/A		ref-t [K]		300.0	
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🖌 Fix rai	ndom seed		pcoupltype		isotropic	$\sim$
gen-seed		12345	ref-p [bar]		1.0	
Explici	itly set gen-temp	[K] 300.	tau-p [ps]		1.0	
			compressibility [/b	ar]	4.5e-5	
			refcoord-scaling		no	$\sim$
	OK	Cancel	Load		Save	Reset
Соруі	right (C)	2017 X-A	bility Co.	, Lto	d. All rig	ghts
		resei	ved.			



### II. Equilibration

- 1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
- 2. Check Extending Simulation.
- 3. Set Preset to NVT (fast), ref-t [K] to 500, then click OK.
- 4. Click MD | Gromacs | Start Gromacs.

<b>3</b>	Groma	acs Setup	- 🗆 🗾			
Extending Simulation		# of Threads	2			
Preset NVT (fast)	$\boldsymbol{<}$	MPI (for Remote Job)	1 Processes			
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Run Control		Temperature Coupling	I			
dt [ps]	0.002	tcoupl	berendsen 🗸			
nsteps	5000	tc-grps	System			
Total time: 10 ps		ref-t [K]	500			
integrator	md 🗸	tau-t [ps]	1.0			
Velocity Generation		Pressure Coupling				
gen-vel	yes 🗸 🗸	pcoupl	no 🗸			
Fix random seed		pcoupltype	isotropic 🗸 🗸 🗸			
gen-seed	12345	ref-p [bar]	1.0			
Explicitly set gen-temp	[K] 300.	tau-p [ps]	1.0			
		compressibility [/bar]	4.5e-5			
		refcoord-scaling	no v			
ок		Load	Save Reset			
Copyright (	2017 X-AI	bility Co.,Ltd. A	All rights			
	reser	ved.				



#### III. Product run

- 1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
- 2. Set nsteps to 250000, gen-vel to no, then click OK.
- 3. Click MD | Gromacs | Start Gromacs.

¢			(	Groma	ics Setup	)		-		>
🖌 Exte	nding Simu	lation			# of Thre	ads	2			
Preset	NVT (f	ast)		¥	🗌 MPI (fo	r Remote	Job) 1	Pr	ocesse	:5
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Run Co	ntrol				Tempera	ture Cou	pling			
dt [ps]			0.002		coupl		ber	rendsen	~	•
nsteps			250000				Sys	tem		
Total tim	ne: 500 p	s			ref-t [K]		300	).0		
integrat	or		md	~	tau-t [ps]		1.0			
¥elocit	y Genera	tion			Pressure	Coupling	)			
gen-vel			ho				no		~	•
🖌 Fix r	andom see	d			pcoupltype	9	isol	tropic	~	¢.
gen-see	:d		12345		ref-p [bar]		1.0			
Expli	citly set ge	en-temp [	[K] 300.		tau-p [ps]		1.0			
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	OK					Load	Sav	/e	Rese	ət
(	Copyr	ight	201	7 X-	Ability	Co.,L	td. A	ll righ	ts	
			•	rese	erved.					



#### IV. Analyze

- 1. Click MD | Gromacs | Energy Plot.
- 2. Open the edr file selected by default.
- 3. Click Calc Ave, then open the gro file selected by default.

[Pres-ZZ] indicates vapor pressure(vapor-liquid pressure, the unit is bar),

[#Surf\*SurfTen] indicates the product of number of interfaces (2 in this case) multiplied by surface tension (the unit is bar\*nm).

20	0	energy	_ave.log.dos	- D ×
Energy terms Temperature Pressure	Stat All	istics over 250001 steps [ 10.00 statistics are over 25001 points	00 through 510.0000 ps ], 29 data Err Est. BMSD Tot-Drift	sets
∀ir-XX         ∀ir-XY         ∀ir-XZ         ∀ir-YX         ∀ir-YY         ∀ir-YZ         ∀ir-ZX         ∀ir-ZZ         Pres-XX         Pres-XY	LLI (Court Court Court Poter Tota Temp Press Vir-1 Vir-1 Vir-1 Vir-1 Vir-1 Vir-1 Vir-1 Vir-1 Vir-1 Vir-1 Vir-1 Vir-1 Vir-1 Vir-1 Vir-1	R)         5.00378           R)         5.00378           sub (SR)         -37.0888           - recip.         0.860051           trial         -31.225           trial         -12.452           trial         -1.17412           trial         -1.17412           trial         -0.0534983           trial         -0.054955           trial         -19.47612           trial         -19.47612           trial         -19.47612	0.019 0.329461 -0.0674196 0.12 0.685914 0.436155 0.0097 0.0611801 0.0346324 0.11 0.542085 0.403368 0.0047 0.264021 0.0233712 0.12 0.485174 0.426739 0.19 10.5864 0.937904 1.1 111,463 1.4721 1.5 391.806 2.08302 1.5 239.042 -0.371305 1.4 238.313 -3.9262 1.5 392.389 4.88406 0.98 237.707 0.442537 1.4 238.309 -3.83966 0.98 237.719 0.406208 1.4 383.712 -6.15202 2.4 162.568 -1.54788 0.42 100 88 1.14344	(kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol) (kJ/mol)
Draw Close mol	Pres Pres Pres Pres Pres Pres Lamb	-0.512764           -YX         -0.00622886           YY         -18.6126           -YZ         0.0266161           -ZX         -0.510424           -ZY         0.030644           -ZY         16.2886           #Surffen         443.5           stem         49.834           -System         1	0,44 100,693 1,70306 0,42 100,88 1,133 0,95 162,054 2,12677 0,66 100,604 -3,91869 0,44 100,692 1,66785 0,65 100,609 -3,90393 0,71 159,4 3,8374 16 2173,7 44,534 0,19 10,5954 0,937904 0 0 0	(bar) (bar) (bar) (bar) (bar) (bar) (bar) (bar) (bar) (k) ()
YMIN     YMAX       Redraw     Excel	Reference: R. S	Sakamaki <i>et al.</i> , J.	Chem. Phys., 134,	124708 (20

reserved.

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2017/8/8



#### IV. Analyze

- 1. Click MD | Gromacs | Density Profile.
- 2. Open default files for 3 times.
- 3. Click **Draw** to draw Density distribution toward the z axis.

If you need the density of liquid or gas phase respectively, click **Excel** to obtain csv file. Try distribution fitting configurations on various graphing softwares.



2017/8/8