Calculation Details

Use the species Aspen as example. The calculation procedures for the other two species are quite similar.

1) Details of obtaining the volumes weights (Pages 1—10)

RH=0 only pores in lignin and empty pores

	pore diam.(nm)	vol(cc)	ad.water(g)	wall substance mass(g)
lignin	0.63	1.67E-020	0.1894	
	0.95	7.70E-030		

RH=5% M=1.79% water(g) 0.0179

Assume 0.63 nm pores are generated in cellulose and hemi-cellul. According to their mass ratio

	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
lignin	0.63	1.67E-02	0	0.1894
	0.95	7.70E-03	0	

	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
cellulose	0.63	3.440E-03	3.195E-03	0.0816

	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
hemi-cellul.	0.63	1.583E-02	0.0147	0	0.3754

RH=10% M=2.59% water(g) 0.0259

Assume 0.63 nm pores are continuely generated in cellulose and hemi-cellul.

	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
lignin	0.63	1.67E-02	0	0.1894
	0.95	7.70E-03	0	

	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
cellulose	0.63	4.549E-03	4.623E-03	0.0816

	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
hemi-cellul.	0.63	2.094E-02	0.02128	0.3754

RH=15% M=3.35% water(g) 0.0335

Assume 0.95 nm pores begin to be generated in hemi-cellul.

I need consider transit from 0.63nm pore to 0.95nm pore here for hemicell.

Old Pores total water(g) 2.767E-02

	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
lignin	0.63	1.67E-02	0	0.1894
	0.95	7.70E-03	0	

	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
cellulose	0.63	4.549E-03	4.939E-03	0.0816

	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
hemi-cellul.	0.63	2.094E-02	0.02273	0.3754

First for hemi-cellul. 5% 0.63nm pore transit to 0.95nm (Vol increase 2.27 times)

New Pores 1 addit.water1 (g) 5.831E-03 total water(g) 2.868E-02

	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
lignin	0.63	1.67E-02	0	0.1894
	0.95	7.70E-03	0	

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	4.549E-03	4.939E-03	0.0816

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.989E-02	0.02159	0.3754
	0.95	2.376E-03	2.146E-03	

Then for cellul. and hemi-cellul. left water mass is generated by newly formed 0.63 nm pore according to their mass ratio

New Pores 2	addit.water1 (g)	4.822E-03		total water (g)	3.350E-02
lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)	
	0.63	1.67E-02	0	0.1894	
	0.95	7.70E-03	0		

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	5.342E-03	5.800E-03	0.0816

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.354E-02	0.02555	0.3754
	0.95	2.376E-03	2.146E-03	

RH=25% M=4.59% water(g) 0.0459

Assume 0.95nm pores are initally generated in cellulose

Assume 0.95nm pores are continuely generated in hemi- cellulose

Old Pores	total water(g)	3.390E-02		
lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.67E-02	0	0.1894
	0.95	7.70E-030		

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	5.342E-03	5.852E-03	0.0816

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.354E-02	0.02578	0.3754
	0.95	2.376E-03	2.259E-03	

First for hemi-cellul. And cellul. 10% 0.63nm pore transit to 0.95nm (Vol increase 2.27 times)

New Pores 1	addit. water1(g)	1.200E-02		total water(g)	3.697E-02
lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)	
	0.63	1.67E-02	0	0.1894	
	0.95	7.70E-03	0		

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	4.808E-03	5.267E-03	0.0816
	0.95	1.213E-03	1.153E-03	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.118E-02	0.02321	0.3754
	0.95	7.719E-03	7.340E-03	

Then for cellul. and hemi-cellul. left water mass is generated by newly formed 0.63 nm pore according to their mass ratio

New Pores 2	addit. water1(g)	8.933E-03		total water(g)	4.590E-02

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.67E-020	0.1894	
	0.95	7.70E-030		

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	6.264E-03	6.862E-03	0.0816
	0.95	1.213E-03	1.153E-03	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.788E-02	0.03054	0.3754
	0.95	7.719E-03	7.340E-03	

RH=35% M=5.83% water(g) 0.0583

Assume 0.95nm pores are continuely generated in hemi- cellulose
New 0.63nm pores are formed

A. 60% 0.63nm lignin pore begin to be filled

Old Pores total water(g) 0.0554

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.67E-02	9.002E-03	0.1894
	0.95	7.70E-030		
cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	6.264E-03	6.924E-03	0.0816
	0.95	1.213E-03	1.174E-03	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.788E-02	0.03082	0.3754
	0.95	7.719E-03	7.473E-03	

B for hemi-cellul. And cellul. 5% 0.63nm pore transit to 0.95nm (Vol increase 2.27 times)

New Pores additional water(g) 0.0029 total water(g) 5.726E-02

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.67E-02	9.002E-03	0.1894
	0.95	7.70E-030		

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	5.950E-03	6.578E-03	0.0816
	0.95	1.924E-03	1.862E-03	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.649E-02	0.02928	0.3754
	0.95	1.088E-02	1.054E-02	

C for cellul. and hemi-cellul. left water mass is generated by newly formed 0.63 nm pore according to their mass ratio

New Pores 2 additional water(g) 0.0010 total water(g) 5.830E-02

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.67E-02	9.002E-03	0.1894
	0.95	7.70E-030		

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	6.119E-03	6.764E-03	0.0816
	0.95	1.924E-03	1.862E-03	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.726E-02	0.03014	0.3754

0.95 1.088E-02 1.054E-02

RH=45% M=7.02% water(g) 0.0702

1.6nm pore begins to generate in hemi-cellulose

the other 40% 0.63nm lignin pore are filled with water (all 0.63nm pores in lignin are filled with water)

Old Pores total water(g) 0.0658

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.67E-02	1.601E-02	0.1894
	0.95	7.70E-03	0	

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	6.119E-03	6.824E-03	0.0816
	0.95	1.924E-03	1.891E-03	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.726E-02	0.03041	0.3754
	0.95	1.088E-02	1.070E-02	

A. for hemi-cellul. 5% 0.95nm pore swell to 1.6nm, vol. increase to 2.84 times

New Pores1 additional water(g) 0.0044 total water(g) 6.676E-02

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.67E-02	1.601E-02	0.1894
	0.95	7.70E-03	0	

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	6.119E-03	6.824E-03	0.0816
	0.95	1.924E-03	1.891E-03	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.726E-02	0.03041	0.3754
	0.95	1.034E-02	1.016E-02	
	1.6	1.545E-03	1.465E-03	

B. for hemi-cellul. And cellul. 7% 0.63nm pore swell to 0.95nm, vol. increase to 2.27 times

New Pores2 additional water(g) 0.0034 total water(g) 6.937E-02

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.67E-02	1.601E-02	0.1894
	0.95	7.70E-03	0	

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	5.690E-03	6.346E-03	0.0816
	0.95	2.896E-03	2.846E-03	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.535E-02	0.02828	0.3754
	0.95	1.467E-02	1.442E-02	
	1.6	1.545E-03	1.465E-03	

C for cellul. and hemi-cellul. 80% left water mass is generated by newly formed 0.63 nm pore according to their mass ratio

for lignin 20% left water mass is generated by newly formed 0.63nm pore

New Pores3 additional water(g) 0.0008 total water(g) 7.020E-02

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.69E-02	1.618E-02	0.1894

0.95 7.90E-03 0

cellulosepore diam.(nm) vol(cc) ads. water(g) wall substance mass(g)
0.63 5.797E-03 6.466E-03 0.0816
0.95 2.896E-03 2.846E-03

hemi-cellul.pore diam.(nm) vol(cc) ads. water(g) wall substance mass(g)
0.63 2.585E-02 0.02883 0.3754
0.95 1.467E-02 1.442E-02
1.6 1.545E-03 1.465E-03

RH=55% M=8.34% water(g) 0.0834
0.95 pore in lignin begin to be filled by water
A .lignin 60% 0.95 nm pores are filled with water
Old Pores total water(g) 0.0758
lignin pore diam.(nm) vol(cc) ads. water(g) wall substance mass(g)
0.63 1.69E-02 1.681E-02 0.1894
0.95 7.90E-03 4.42E-03

cellulosepore diam.(nm) vol(cc) ads. water(g) wall substance mass(g)
0.63 5.797E-03 6.517E-03 0.0816
0.95 2.896E-03 2.883E-03

hemi-cellul.pore diam.(nm) vol(cc) ads. water(g) wall substance mass(g)
0.63 2.585E-02 0.02905 0.3754
0.95 1.467E-02 1.460E-02
1.6 1.545E-03 1.477E-03

B. for hemi-cellul. 10% 0.95nm pore swell to 1.6nm, vol. increase to 2.84 times

New Pores 1 additional water(g) 0.0076 total water(g) 7.828E-02
lignin pore diam.(nm) vol(cc) ads. water(g) wall substance mass(g)
0.63 1.69E-02 1.681E-02 0.1894
0.95 7.90E-03 4.417E-03

cellulosepore diam.(nm) vol(cc) ads. water(g) wall substance mass(g)
0.63 5.797E-03 6.517E-03 0.0816
0.95 2.896E-03 2.883E-03

hemi-cellul.pore diam.(nm) vol(cc) ads. water(g) wall substance mass(g)
0.63 2.585E-02 0.0291 0.3754
0.95 1.320E-02 0.0131
1.6 5.712E-03 5.460E-03

C. for hemi-cellul., cellul. 12% 0.63nm pore swell to 0.95nm, vol. increase to 2.27 times

New Pores 1 additional water(g) 0.0051 total water(g) 8.259E-02
lignin pore diam.(nm) vol(cc) ads. water(g) wall substance mass(g)
0.63 1.69E-02 1.681E-02 0.1894
0.95 7.90E-03 4.417E-03

cellulosepore diam.(nm) vol(cc) ads. water(g) wall substance mass(g)
0.63 5.102E-03 5.735E-03 0.0816
0.95 4.475E-03 4.454E-03

hemi-cellul.pore diam.(nm) vol(cc) ads. water(g) wall substance mass(g)
0.63 2.274E-02 0.0256 0.3754

0.95	2.024E-02	0.0202
1.6	5.712E-03	5.460E-03

D for cellul. and hemi-cellul. 80% left water mass is generated by newly formed 0.63 nm pore according to their mass ratio

for lignin 20% left water mass is generated by newly formed 0.63nm pore

New Pores 1 additional water(g) 0.0008 total water(g) 8.340E-02

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.69E-02	1.697E-02	0.1894
	0.95	7.90E-03	4.417E-03	

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	5.204E-03	5.850E-03	0.0816
	0.95	4.475E-03	4.454E-03	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.322E-02	0.0261	0.3754
	0.95	2.024E-02	0.0202	
	1.6	5.712E-03	5.460E-03	

RH=65% M=9.89% water(g) 0.0989

accessible OH reach max, no new 0.63nm pore can be generated

the other 40% lignin 0.95 nm pores are filled with water

Old Pores total water(g) 0.0870

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.69E-02	1.689E-02	0.1894
	0.95	7.90E-03	7.51E-03	

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	5.204E-03	5.883E-03	0.0816
	0.95	4.475E-03	4.511E-03	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.322E-02	0.02625	0.3754
	0.95	2.024E-02	2.041E-02	
	1.6	5.712E-03	5.530E-03	

A. for hemi-cellul. 14% 0.95nm pore swell to 1.6nm, vol. increase to 2.84 times

New Pores1 additional water(g) 0.0119 total water(g) 9.190E-02

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.69E-02	1.689E-02	0.1894
	0.95	7.90E-03	7.506E-03	

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	5.204E-03	0.0059	0.0816
	0.95	4.475E-03	0.0045	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.322E-02	0.0262	0.3754
	0.95	1.741E-02	0.0175	
	1.6	1.376E-02	0.0133	

B. for cellul. And lignin 10.5% 0.63nm pore swell to 0.95nm, vol. increase to 2.27 times

for hemi-cellul. 16% 0.63 nm pore swell to 0.95nm

New Pores2 additional water(g) 0.0070 total water(g) 9.888E-02

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.51E-02	1.511E-02	0.1894
	0.95	1.19E-02	1.133E-02	

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	4.658E-03	0.0053	0.0816
	0.95	5.715E-03	0.0058	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.950E-02	0.0220	0.3754
	0.95	2.584E-02	0.0260	
	1.6	1.376E-02	0.0133	

RH=75% M=12.03% water(g) 0.1203

accessible OH reach max, no new 0.63nm pore can be generated

Old Pores total water(g) 0.0999

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.51E-02	1.541E-02	0.1894
	0.95	1.19E-02	1.15E-02	

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	4.658E-03	5.295E-03	0.0816
	0.95	5.715E-03	5.803E-03	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.950E-02	0.0222	0.3754
	0.95	2.584E-02	0.0262	
	1.6	1.376E-02	0.0135	

A. for hemi-cellul. 22% 0.95nm pore swell to 1.6nm, vol. increase to 2.84 times

New Pores1 additional water(g) 0.0204 total water(g) 1.099E-01

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.51E-02	1.541E-02	0.1894
	0.95	1.19E-02	1.146E-02	

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	4.658E-03	0.0053	0.0704
	0.95	5.715E-03	0.0058	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.950E-02	0.0222	0.3754
	0.95	2.016E-02	0.0205	
	1.6	2.991E-02	0.0293	

B. for cellul. And lignin 19% 0.63nm pore swell to 0.95nm, vol. increase to 2.27 times for hemi-cellul. 26.5% 0.63 nm pore swell to 0.95nm

New Pores2 additional water(g) 0.0104 total water(g) 1.203E-01

lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.22E-02	1.248E-02	0.1894
	0.95	1.84E-02	1.773E-02	

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	3.773E-03	0.0043	0.0816
	0.95	7.724E-03	0.0078	

hemi-cellul.pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	1.433E-02	0.0163	0.3754
0.95	3.189E-02	0.0324	
1.6	2.991E-02	0.0293	

RH=85% M=15.39% water(g) 0.1539

Old Pores total water(g) 0.1215

lignin pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	1.22E-02	1.278E-02	0.1894
0.95	1.84E-02	1.79E-02	

cellulose pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	3.773E-03	4.313E-03	0.0816
0.95	7.724E-03	7.888E-03	

hemi-cellul.pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	1.433E-02	0.0164	0.3754
0.95	3.189E-02	0.0326	
1.6	2.991E-02	0.0297	

A. for hemi-cellul. 32% 0.95nm pore swell to 1.6nm, vol. increase to 2.84 times

New Pores1 additional water(g) 0.0324 total water(g) 1.398E-01

lignin pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	1.22E-02	1.278E-02	0.1894
0.95	1.84E-02	1.79E-02	

cellulose pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	3.773E-03	4.313E-03	0.0816
0.95	7.724E-03	7.888E-03	

hemi-cellul.pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	1.433E-02	0.0164	0.3754
0.95	2.168E-02	0.0221	
1.6	5.889E-02	0.0584	

B. for cellul. And lignin 37% 0.63nm pore swell to 0.95nm, vol. increase to 2.27 times
for hemi-cellul.43% 0.63 nm pore swell to 0.95nm

New Pores2 additional water(g) 0.0141 total water(g) 1.539E-01

lignin pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	7.71E-03	8.054E-03	0.1894
0.95	2.87E-02	2.79E-02	

cellulose pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	2.377E-03	2.717E-03	0.0816
0.95	1.089E-02	1.112E-02	

hemi-cellul.pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	8.170E-03	0.0093	0.3754
0.95	3.567E-02	0.0364	
1.6	5.889E-02	0.0584	

RH=90% M=18.29% water(g) 0.1829

Old Pores total water(g) 0.1546

lignin pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	7.71E-03	8.148E-03	0.1894
0.95	2.87E-02	2.81E-02	

cellulose pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)

0.63	2.377E-03	2.724E-03	0.0816
0.95	1.089E-02	1.116E-02	

hemi-cellul.pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	8.170E-03	0.0094	0.3754
0.95	3.567E-02	0.0365	
1.6	5.889E-02	0.0586	

A. for hemi-cellul. 30% 0.95nm pore swell to 1.6nm, vol. increase to 2.84 times

New Pores1 additional water(g) 0.0283 total water(g) 1.738E-01

lignin pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	7.71E-03	8.148E-03	0.1894
0.95	2.87E-02	2.81E-02	

cellulose pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	2.377E-03	2.724E-03	0.0816
0.95	1.089E-02	1.116E-02	

hemi-cellul.pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	8.170E-03	0.0094	0.3754
0.95	2.497E-02	0.0256	
1.6	8.928E-02	0.0888	

B. for cellul. And lignin 39% 0.63nm pore swell to 0.95nm, vol. increase to 2.27 times
for hemi-cellul. 46% 0.63 nm pore swell to 0.95nm

New Pores2 additional water(g) 0.0091 total water(g) 1.829E-01

lignin pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	4.70E-03	4.970E-03	0.1894
0.95	3.55E-02	3.47E-02	

cellulose pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	1.450E-03	1.662E-03	0.0816
0.95	1.300E-02	1.331E-02	

hemi-cellul.pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	4.412E-03	0.0051	0.3754
0.95	3.350E-02	0.0343	
1.6	8.928E-02	0.0888	

RH=95% M=20.5% water(g) 0.205

2.2 nm pore begin to generate in hemicellulose

Old Pores total water(g) 0.1835

lignin pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	4.70E-03	5.028E-03	0.1894
0.95	3.55E-02	3.50E-02	

cellulose pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	1.450E-03	1.666E-03	0.0816
0.95	1.300E-02	1.335E-02	

hemi-cellul.pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
0.63	4.412E-03	0.0051	0.3754
0.95	3.350E-02	0.0344	
1.6	8.928E-02	0.0889	

A. for hemi-cellul. 5% 1.6nm pore swell to 2.2nm, vol. increase to 1.89 times

New Pores 1	additional water(g)		0.0215	total water(g)	1.873E-01
lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)	
	0.63	4.70E-03	5.028E-03	0.1894	
	0.95	3.55E-02	3.50E-02		

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.450E-03	1.666E-03	0.0816
	0.95	1.300E-02	1.335E-02	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	4.412E-03	0.0051	0.3754
	0.95	3.350E-02	0.0344	
	1.60	8.482E-02	0.0845	
	2.20	8.437E-03	8.273E-03	

B for hemi-cellul. 22% 0.95nm pore swell to 1.6nm, vol. increase to 2.84 times

New Pores 2	additional water(g)		0.0177	total water(g)	2.006E-01
lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)	
	0.63	4.70E-03	5.028E-03	0.1894	
	0.95	3.55E-02	3.50E-02		

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	1.450E-03	1.666E-03	0.0816
	0.95	1.300E-02	1.335E-02	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	4.412E-03	0.0051	0.3754
	0.95	2.613E-02	0.0268	
	1.60	1.058E-01	0.1053	
	2.20	8.437E-03	8.273E-03	

C. for cellul. And lignin 33% 0.63nm pore swell to 0.95nm, vol. increase to 2.27 times
for hemi-cellul. 39% 0.63 nm pore swell to 0.95nm

New Pores 3	additional water(g)		0.0044	total water(g)	2.050E-01
lignin	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)	
	0.63	3.15E-03	3.369E-03	0.1894	
	0.95	3.91E-02	3.85E-02		

cellulose	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	9.714E-04	1.117E-03	0.0816
	0.95	1.408E-02	1.446E-02	

hemi-cellul.	pore diam.(nm)	vol(cc)	ads. water(g)	wall substance mass(g)
	0.63	2.691E-03	0.0031	0.3754
	0.95	3.004E-02	0.0308	
	1.60	1.058E-01	0.1053	
	2.20	8.437E-03	8.273E-03	

2) R codes for smoothing of PSD

```
# species: aspen
lnr1 <- seq(log(0.1), log(3.6), by = 0.02)      # generate pore size evenly in the range  [0.1-3.6] nm
lnr1.pdf <- dnorm(lnr1, log(0.63), 0.15)
r1 <- exp(lnr1)

lnr2 <- seq(log(0.1), log(3.6), by = 0.02)
lnr2.pdf <- dnorm(lnr2, log(0.95), 0.15)

lnr3 <- seq(log(0.1), log(3.6), by = 0.02)
lnr3.pdf <- dnorm(lnr3, log(1.6), 0.15)

lnr4 <- seq(log(0.1), log(3.6), by = 0.02)
lnr4.pdf <- dnorm(lnr4, log(2.2), 0.15)

lnr <- seq(log(0.1), log(3.6), by=0.02)
lnr.pdf <- lnr1.pdf + lnr2.pdf + lnr3.pdf + lnr4.pdf
r <- exp(lnr)

# RH =0%, using total pore vol. at each pore size as weights
# cellulose --No pore
 cellul.wt1_00 <-0
 cellul.wt2_00 <-0
 cellul.wt3_00 <-0
 cellul.wt4_00 <-0
 cellul_p_00 <- cellul.wt1_00* lnr1.pdf + cellul.wt2_00*lnr2.pdf + cellul.wt3_00*lnr3.pdf +
  cellul.wt4_00*lnr4.pdf                              # this is the pore distribution of lnW

 # hemicellulose -NO PORE
 hemi.cellul.wt1_00 <-0
 hemi.cellul.wt2_00 <-0
 hemi.cellul.wt3_00 <-0
 hemi.cellul.wt4_00 <-0
 hemi.cellul_p_00 <- hemi.cellul.wt1_00* lnr1.pdf + hemi.cellul.wt2_00*lnr2.pdf  +
  hemi.cellul.wt3_00*lnr3.pdf + hemi.cellul.wt4_00*lnr4.pdf

 # lignin ---pore
 lig.wt1_00<- 1.67e-2
 lig.wt2_00 <- 0.77e-2
 lig.wt3_00 <- 0
 lig.wt4_00 <- 0
 lig_p_00 <- lig.wt1_00* lnr1.pdf + lig.wt2_00*lnr2.pdf + lig.wt3_00*lnr3.pdf + lig.wt4_00*lnr4.pdf

# cell wall pore
wall_p_00 <- cellul_p_00 + hemi.cellul_p_00 + lig_p_00

plot(c(0.35, 3.6), range(c(cellul_p_00, hemi.cellul_p_00, lig_p_00, wall_p_00)),  type = "n",  log="x", xlab= "cell
  wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore size distribution at
  RH =0%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_00, lwd=1.5, col="red")
lines(r, hemi.cellul_p_00, lwd=1.5)
lines(r, lig_p_00, col="blue", lwd=1.5)
lines(r, wall_p_00, col="green", lwd=1.5)
```

```
 legend(1.5, 0.02, c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5, 1.5,1.5),
  col=c("red", "black", "blue", "green"), cex = 1.2)


# save the data, record the data as a dataframe
H_0 <- rep("H = 0", length(r))
PSD_00 <- data.frame(r, cellul_p_00, hemi.cellul_p_00, lig_p_00, wall_p_00, H_0)
names(PSD_00) <- c("d", "PAC", "PAH", "PAL", "Total pores", "H")

# write the dataframe to a file
write.csv(PSD_00, file= "PSD_00.csv",  row.names= FALSE, quote = FALSE)

 # RH =5%, using total pore vol at each pore size as weights
 # cellulose
 cellul.wt1_05 <- 3.440e-3
 cellul.wt2_05 <-0
 cellul.wt3_05 <-0
 cellul.wt4_05 <-0
 cellul_p_05 <- cellul.wt1_05* lnr1.pdf + cellul.wt2_05*lnr2.pdf + cellul.wt3_05*lnr3.pdf +
  cellul.wt4_05*lnr4.pdf

 # hemicellulose
 hemi.cellul.wt1_05 <-1.583e-2
 hemi.cellul.wt2_05 <-0
 hemi.cellul.wt3_05 <-0
 hemi.cellul.wt4_05 <-0
 hemi.cellul_p_05 <- hemi.cellul.wt1_05* lnr1.pdf + hemi.cellul.wt2_05*lnr2.pdf  +
  hemi.cellul.wt3_05*lnr3.pdf + hemi.cellul.wt4_05*lnr4.pdf

 # lignin ---pore
 lig.wt1_05<- 1.67e-2      # pore empty
 lig.wt2_05 <- 0.77e-2     # pore empty
 lig.wt3_05 <- 0
 lig.wt4_05 <- 0
 lig_p_05 <- lig.wt1_05* lnr1.pdf + lig.wt2_05*lnr2.pdf + lig.wt3_05*lnr3.pdf + lig.wt4_05*lnr4.pdf

# cell wall pore
wall_p_05 <- cellul_p_05 + hemi.cellul_p_05 + lig_p_05

plot(c(0.35, 3.6), range(c(cellul_p_05, hemi.cellul_p_05, lig_p_05, wall_p_05)),  type = "n",  log ="x", xlab= "cell
  wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore size distribution at
  RH =5%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_05, lwd=1.5, col="red")
lines(r, hemi.cellul_p_05, lwd=1.5)
lines(r, lig_p_05, col="blue", lwd=1.5)
lines(r, wall_p_05, col="green", lwd=1.5)

 legend(1.5, 0.08, c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5, 1.5,1.5),
  col=c("red", "black", "blue", "green"), cex = 1.2)

# record the data as a dataframe
H_05 <- rep("H = 5%", length(r))
PSD_05 <- data.frame(r, cellul_p_05, hemi.cellul_p_05, lig_p_05, wall_p_05, H_05)
names(PSD_05) <- c("d", "PAC", "PAH", "PAL", "PAT", "H")

# write the dataframe to a file
```

```
write.csv(PSD_05, file= "PSD_05.csv", row.names= FALSE, quote = FALSE)

 # RH =10%, using total pore vol at each pore size as weights
 # cellulose
 cellul.wt1_10 <- 4.549e-3
 cellul.wt2_10 <-0
 cellul.wt3_10 <-0
 cellul.wt4_10 <-0
 cellul_p_10 <- cellul.wt1_10* lnr1.pdf + cellul.wt2_10*lnr2.pdf + cellul.wt3_10*lnr3.pdf +
  cellul.wt4_10*lnr4.pdf

 # hemicellulose -
 hemi.cellul.wt1_10 <-2.094e-2
 hemi.cellul.wt2_10 <-0
 hemi.cellul.wt3_10 <-0
 hemi.cellul.wt4_10 <-0
 hemi.cellul_p_10 <- hemi.cellul.wt1_10* lnr1.pdf + hemi.cellul.wt2_10*lnr2.pdf + hemi.cellul.wt3_10*lnr3.pdf
  + hemi.cellul.wt4_10*lnr4.pdf

 # lignin ---pore
 lig.wt1_10<- 1.67e-2      # pore empty
 lig.wt2_10 <- 0.77e-2     # pore empty
 lig.wt3_10 <- 0
 lig.wt4_10 <- 0
 lig_p_10 <- lig.wt1_10* lnr1.pdf + lig.wt2_10*lnr2.pdf + lig.wt3_10*lnr3.pdf + lig.wt4_10*lnr4.pdf

# cell wall pore
wall_p_10 <- cellul_p_10 + hemi.cellul_p_10 + lig_p_10

plot(c(0.35, 3.6), range(c(cellul_p_10, hemi.cellul_p_10, lig_p_10, wall_p_10)),  type = "n", log="x", xlab= "cell
  wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore size distribution at
  RH =10%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_10, lwd=1.5, col="red")
lines(r, hemi.cellul_p_10, lwd=1.5)
lines(r, lig_p_10, col="blue", lwd=1.5)
lines(r, wall_p_10, col="green", lwd=1.5)

 legend(1.5, 0.10, c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5, 1.5,1.5),
  col=c("red", "black", "blue", "green"), cex = 1.2)

 # RH =15%, using total pore vol at each pore size as weights
 # cellulose
 cellul.wt1_15 <- 5.342e-3
 cellul.wt2_15 <-0
 cellul.wt3_15 <-0
 cellul.wt4_15 <-0
 cellul_p_15 <- cellul.wt1_15* lnr1.pdf + cellul.wt2_15*lnr2.pdf + cellul.wt3_15*lnr3.pdf +
  cellul.wt4_15*lnr4.pdf

 # hemicellulose -
 hemi.cellul.wt1_15 <-2.354e-2
 hemi.cellul.wt2_15 <-2.376e-3
 hemi.cellul.wt3_15 <-0
 hemi.cellul.wt4_15 <-0
 hemi.cellul_p_15 <- hemi.cellul.wt1_15* lnr1.pdf + hemi.cellul.wt2_15*lnr2.pdf  +
  hemi.cellul.wt3_15*lnr3.pdf + hemi.cellul.wt4_15*lnr4.pdf
```

```
 # lignin ---pore
 lig.wt1_15<-  1.67e-2      # pore empty
 lig.wt2_15 <- 0.77e-2     # pore empty
 lig.wt3_15 <- 0
 lig.wt4_15 <- 0
 lig_p_15 <- lig.wt1_15* lnr1.pdf + lig.wt2_15*lnr2.pdf + lig.wt3_15*lnr3.pdf + lig.wt4_15*lnr4.pdf

# cell wall pore
wall_p_15 <- cellul_p_15 + hemi.cellul_p_15 + lig_p_15

plot(c(0.35, 3.6), range(c(cellul_p_15, hemi.cellul_p_15, lig_p_15, wall_p_15)),  type = "n",  log="x", xlab= "cell
  wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore distribution at RH
  =15%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_15, lwd=1.5, col="red")
lines(r, hemi.cellul_p_15, lwd=1.5)
lines(r, lig_p_15, col="blue", lwd=1.5)
lines(r, wall_p_15, col="green", lwd=1.5)

 legend(1.5, 0.10, c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5, 1.5,1.5),
  col=c("red", "black", "blue", "green"), cex = 1.2)

# record the data as a dataframe
H_15 <- rep("H = 15%", length(r))
PSD_15 <- data.frame(r, cellul_p_15, hemi.cellul_p_15, lig_p_15, wall_p_15, H_15)
names(PSD_15) <- c("d", "PAC", "PAH", "PAL", "PAT", "H")

# write the dataframe to a file
write.csv(PSD_15, file= "PSD_15.csv", row.names= FALSE, quote = FALSE)


 # RH =25%, using total pore vol at each pore size as weights
 # cellulose
 cellul.wt1_25 <- 6.264e-3
 cellul.wt2_25 <- 1.213e-3
 cellul.wt3_25 <-0
 cellul.wt4_25 <-0
 cellul_p_25 <- cellul.wt1_25* lnr1.pdf + cellul.wt2_25*lnr2.pdf + cellul.wt3_25*lnr3.pdf +
  cellul.wt4_25*lnr4.pdf

 # hemicellulose -
 hemi.cellul.wt1_25 <-2.788e-2
 hemi.cellul.wt2_25 <-7.719e-3
 hemi.cellul.wt3_25 <-0
 hemi.cellul.wt4_25 <-0
 hemi.cellul_p_25 <- hemi.cellul.wt1_25* lnr1.pdf + hemi.cellul.wt2_25*lnr2.pdf  +
  hemi.cellul.wt3_25*lnr3.pdf + hemi.cellul.wt4_25*lnr4.pdf

 # lignin ---pore
 lig.wt1_25<-  1.67e-2      # pore empty
 lig.wt2_25 <- 0.77e-2     # pore empty
 lig.wt3_25 <- 0
 lig.wt4_25 <- 0
 lig_p_25 <- lig.wt1_25* lnr1.pdf + lig.wt2_25*lnr2.pdf  + lig.wt3_25*lnr3.pdf + lig.wt4_25*lnr4.pdf
# cell wall pore
wall_p_25 <- cellul_p_25 + hemi.cellul_p_25 + lig_p_25
```

```
plot(c(0.35, 3.6), range(c(cellul_p_25, hemi.cellul_p_25, lig_p_25, wall_p_25)),  type = "n", log="x", xlab= "cell
  wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore distribution at RH
  =25%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_25, lwd=1.5, col="red")
lines(r, hemi.cellul_p_25, lwd=1.5)
lines(r, lig_p_25, col="blue", lwd=1.5)
lines(r, wall_p_25, col="green", lwd=1.5)

 legend(1.5, 0.12, c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5, 1.5,1.5),
  col=c("red", "black", "blue", "green"), cex = 1.2)

 H_25 <- rep("H = 25%", length(r))
PSD_25 <- data.frame(r, cellul_p_25, hemi.cellul_p_25, lig_p_25, wall_p_25, H_25)
names(PSD_25) <- c("d", "PAC", "PAH", "PAL", "PAT", "H")

# write the dataframe to a file
write.csv(PSD_25, file= "PSD_25.csv", row.names= FALSE, quote = FALSE)

# ================================================================
# RH =35% , using total pore vol at each pore size as weights
 # cellulose
 cellul.wt1_35 <- 6.119e-3
 cellul.wt2_35 <- 1.924e-3
 cellul.wt3_35 <-0
 cellul.wt4_35 <-0
 cellul_p_35 <- cellul.wt1_35* lnr1.pdf + cellul.wt2_35*lnr2.pdf + cellul.wt3_35*lnr3.pdf +
  cellul.wt4_35*lnr4.pdf

 # hemicellulose -
 hemi.cellul.wt1_35 <-2.726e-2
 hemi.cellul.wt2_35 <-1.088e-2
 hemi.cellul.wt3_35 <-0
 hemi.cellul.wt4_35 <-0
 hemi.cellul_p_35 <- hemi.cellul.wt1_35* lnr1.pdf + hemi.cellul.wt2_35*lnr2.pdf  +
  hemi.cellul.wt3_35*lnr3.pdf + hemi.cellul.wt4_35*lnr4.pdf

 # lignin ---pore
 lig.wt1_35<-  1.67e-2      # 60% OF pore filled
 lig.wt2_35 <- 0.77e-2     # pore empty
 lig.wt3_35 <- 0
 lig.wt4_35 <- 0
 lig_p_35 <- lig.wt1_35* lnr1.pdf + lig.wt2_35*lnr2.pdf  + lig.wt3_35*lnr3.pdf + lig.wt4_35*lnr4.pdf

# cell wall pore
wall_p_35 <- cellul_p_35 + hemi.cellul_p_35 + lig_p_35

plot(c(0.35, 3.6), range(c(cellul_p_35, hemi.cellul_p_35, lig_p_35, wall_p_35)),  type = "n", log="x", xlab= "cell
  wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore distribution at RH
  =35%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_35, lwd=1.5, col="red")
lines(r, hemi.cellul_p_35, lwd=1.5)
lines(r, lig_p_35, col="blue", lwd=1.5)
lines(r, wall_p_35, col="green", lwd=1.5)
```

```
 legend(1.5, 0.12, c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5, 1.5,1.5),
  col=c("red", "black", "blue", "green"), cex = 1.2)

 # record the data as a dataframe
H_35 <- rep("H = 35%", length(r))
PSD_35 <- data.frame(r, cellul_p_35, hemi.cellul_p_35, lig_p_35, wall_p_35, H_35)
names(PSD_35) <- c("d", "PAC", "PAH", "PAL", "PAT", "H")

# write the dataframe to a file
write.csv(PSD_35, file= "PSD_35.csv", row.names= FALSE, quote = FALSE)


# RH =45% , using total pore vol at each pore size as weights
 # cellulose
 cellul.wt1_45 <- 5.797e-3
 cellul.wt2_45 <- 2.896e-3
 cellul.wt3_45 <-0
 cellul.wt4_45 <-0
 cellul_p_45 <- cellul.wt1_45* lnr1.pdf + cellul.wt2_45*lnr2.pdf  + cellul.wt3_45*lnr3.pdf +
  cellul.wt4_45*lnr4.pdf

 # hemicellulose -
 hemi.cellul.wt1_45 <-2.585e-2
 hemi.cellul.wt2_45 <- 1.467e-2
 hemi.cellul.wt3_45 <-1.545e-3
 hemi.cellul.wt4_45 <-0
 hemi.cellul_p_45 <- hemi.cellul.wt1_45* lnr1.pdf + hemi.cellul.wt2_45*lnr2.pdf  +
  hemi.cellul.wt3_45*lnr3.pdf + hemi.cellul.wt4_45*lnr4.pdf

 # lignin ---pore
 lig.wt1_45<-  1.69e-2      # pore filled
 lig.wt2_45 <- 7.90e-3      # pore empty
 lig.wt3_45 <- 0
 lig.wt4_45 <- 0
 lig_p_45 <- lig.wt1_45* lnr1.pdf + lig.wt2_45*lnr2.pdf  + lig.wt3_45*lnr3.pdf + lig.wt4_45*lnr4.pdf

# cell wall pore
wall_p_45 <- cellul_p_45 + hemi.cellul_p_45 + lig_p_45

plot(c(0.35, 3.6), range(c(cellul_p_45, hemi.cellul_p_45, lig_p_45, wall_p_45)),  type = "n", log="x",  xlab= "cell
  wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore distribution at RH
  =45%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_45, lwd=1.5, col="red")
lines(r, hemi.cellul_p_45, lwd=1.5)
lines(r, lig_p_45, col="blue", lwd=1.5)
lines(r, wall_p_45, col="green", lwd=1.5)

 legend(1.5, 0.12, c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5, 1.5,1.5),
  col=c("red", "black", "blue", "green"), cex = 1.2)

 # record the data as a dataframe
H_45 <- rep("H = 45%", length(r))
PSD_45 <- data.frame(r, cellul_p_45, hemi.cellul_p_45, lig_p_45, wall_p_45, H_45)
names(PSD_45) <- c("d", "PAC", "PAH", "PAL", "PAT", "H")

# write the dataframe to a file
```

```
write.csv(PSD_45, file= "PSD_45.csv", row.names= FALSE, quote = FALSE)

# RH =55% , using total pore vol at each pore size as weights
 # cellulose
 cellul.wt1_55 <- 5.204e-3
 cellul.wt2_55 <- 4.475e-3
 cellul.wt3_55 <-0
 cellul.wt4_55 <-0
 cellul_p_55 <- cellul.wt1_55* lnr1.pdf + cellul.wt2_55*lnr2.pdf  + cellul.wt3_55*lnr3.pdf +
  cellul.wt4_55*lnr4.pdf

 # hemicellulose -
 hemi.cellul.wt1_55 <-2.322e-2
 hemi.cellul.wt2_55 <-2.024e-2
 hemi.cellul.wt3_55 <-5.712e-3
 hemi.cellul.wt4_55 <-0
 hemi.cellul_p_55 <- hemi.cellul.wt1_55* lnr1.pdf + hemi.cellul.wt2_55*lnr2.pdf  +
  hemi.cellul.wt3_55*lnr3.pdf + hemi.cellul.wt4_55*lnr4.pdf

 # lignin ---pore
 lig.wt1_55<-  1.69e-2      # pore filled
 lig.wt2_55 <- 7.90e-3     # 60%  pore filled
 lig.wt3_55 <- 0
 lig.wt4_55 <- 0
 lig_p_55 <- lig.wt1_55* lnr1.pdf + lig.wt2_55*lnr2.pdf  + lig.wt3_55*lnr3.pdf + lig.wt4_55*lnr4.pdf

# cell wall pore
wall_p_55 <- cellul_p_55 + hemi.cellul_p_55 + lig_p_55

plot(c(0.35, 3.6), range(c(cellul_p_55, hemi.cellul_p_55, lig_p_55, wall_p_55)),  type = "n",  log="x", xlab= "cell
  wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore distribution at RH
  =55%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_55, lwd=1.5, col="red")
lines(r, hemi.cellul_p_55, lwd=1.5)
lines(r, lig_p_55, col="blue", lwd=1.5)
lines(r, wall_p_55, col="green", lwd=1.5)

 legend(1.5, 0.11, c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5, 1.5,1.5),
  col=c("red", "black", "blue", "green"), cex = 1.2)

 # record the data as a dataframe
H_55 <- rep("H = 55%", length(r))
PSD_55 <- data.frame(r, cellul_p_55, hemi.cellul_p_55, lig_p_55, wall_p_55, H_55)
names(PSD_55) <- c("d", "PAC", "PAH", "PAL", "PAT", "H")

# write the dataframe to a file
write.csv(PSD_55, file= "PSD_55.csv", row.names= FALSE, quote = FALSE)



 # RH =65% , using total pore vol at each pore size as weights
 # cellulose
 cellul.wt1_65 <- 4.658e-3
 cellul.wt2_65 <- 5.715e-3
 cellul.wt3_65 <-0
 cellul.wt4_65 <-0
```

```
cellul_p_65 <- cellul.wt1_65* lnr1.pdf + cellul.wt2_65*lnr2.pdf  + cellul.wt3_65*lnr3.pdf +
 cellul.wt4_65*lnr4.pdf

# hemicellulose -
hemi.cellul.wt1_65 <-1.950e-2
hemi.cellul.wt2_65 <-2.584e-2
hemi.cellul.wt3_65 <-1.376e-2
hemi.cellul.wt4_65 <-0
hemi.cellul_p_65 <- hemi.cellul.wt1_65* lnr1.pdf + hemi.cellul.wt2_65*lnr2.pdf  +
 hemi.cellul.wt3_65*lnr3.pdf + hemi.cellul.wt4_65*lnr4.pdf

# lignin ---pore
lig.wt1_65<-  1.51e-2     # pore filled
lig.wt2_65 <- 1.19e-2     # pore filled
lig.wt3_65 <- 0
lig.wt4_65 <- 0
lig_p_65 <- lig.wt1_65* lnr1.pdf + lig.wt2_65*lnr2.pdf  + lig.wt3_65*lnr3.pdf + lig.wt4_65*lnr4.pdf

# cell wall pore
wall_p_65 <- cellul_p_65 + hemi.cellul_p_65 + lig_p_65

plot(c(0.35, 3.6), range(c(cellul_p_65, hemi.cellul_p_65, lig_p_65, wall_p_65)),  type = "n", log="x", xlab= "cell
 wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore distribution at RH
 =65%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_65, lwd=1.5, col="red")
lines(r, hemi.cellul_p_65, lwd=1.5)
lines(r, lig_p_65, col="blue", lwd=1.5)
lines(r, wall_p_65, col="green", lwd=1.5)

 legend(1.5, 0.12, c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5, 1.5,1.5),
 col=c("red", "black", "blue", "green"), cex = 1.2)

 # record the data as a dataframe
H_65 <- rep("H = 65%", length(r))
PSD_65 <- data.frame(r, cellul_p_65, hemi.cellul_p_65, lig_p_65, wall_p_65, H_65)
names(PSD_65) <- c("d", "PAC", "PAH", "PAL", "PAT", "H")

# write the dataframe to a file
write.csv(PSD_65, file= "PSD_65.csv", row.names= FALSE, quote = FALSE)

 # RH =75% , using total pore vol at each pore size as weights
 # cellulose
 cellul.wt1_75 <- 3.773e-3
 cellul.wt2_75 <- 7.724e-3
 cellul.wt3_75 <-0
 cellul.wt4_75 <-0
 cellul_p_75 <- cellul.wt1_75* lnr1.pdf + cellul.wt2_75*lnr2.pdf  + cellul.wt3_75*lnr3.pdf +
 cellul.wt4_75*lnr4.pdf

 # hemicellulose -
 hemi.cellul.wt1_75 <-1.433e-2
 hemi.cellul.wt2_75 <-3.189e-2
 hemi.cellul.wt3_75 <-2.991e-2
 hemi.cellul.wt4_75 <-0
 hemi.cellul_p_75 <- hemi.cellul.wt1_75* lnr1.pdf + hemi.cellul.wt2_75*lnr2.pdf  +
 hemi.cellul.wt3_75*lnr3.pdf + hemi.cellul.wt4_75*lnr4.pdf
```

```
 # lignin ---pore
 lig.wt1_75<-  1.22e-2     # pore filled
 lig.wt2_75 <- 1.84e-2     # pore filled
 lig.wt3_75 <- 0
 lig.wt4_75 <- 0
 lig_p_75 <- lig.wt1_75* lnr1.pdf + lig.wt2_75*lnr2.pdf  + lig.wt3_75*lnr3.pdf + lig.wt4_75*lnr4.pdf

# cell wall pore
wall_p_75 <- cellul_p_75 + hemi.cellul_p_75 + lig_p_75

plot(c(0.35, 3.6), range(c(cellul_p_75, hemi.cellul_p_75, lig_p_75, wall_p_75)),  type = "n",  log="x", xlab= "cell
  wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore distribution at RH
  =75%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_75, lwd=1.5, col="red")
lines(r, hemi.cellul_p_75, lwd=1.5)
lines(r, lig_p_75, col="blue", lwd=1.5)
lines(r, wall_p_75, col="green", lwd=1.5)

 legend(1.5, 0.15, c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5, 1.5,1.5),
  col=c("red", "black", "blue", "green"), cex = 1.2)

 # record the data as a dataframe
H_75 <- rep("H = 75%", length(r))
PSD_75 <- data.frame(r, cellul_p_75, hemi.cellul_p_75, lig_p_75, wall_p_75, H_75)
names(PSD_75) <- c("d", "PAC", "PAH", "PAL", "PAT", "H")

# write the dataframe to a file
write.csv(PSD_75, file= "PSD_75.csv", row.names= FALSE, quote = FALSE)

 # RH =85% , using total pore vol at each pore size as weights
 # cellulose
 cellul.wt1_85 <- 2.377e-3
 cellul.wt2_85 <- 1.089e-2
 cellul.wt3_85 <-0
 cellul.wt4_85 <-0
 cellul_p_85 <- cellul.wt1_85* lnr1.pdf + cellul.wt2_85*lnr2.pdf  + cellul.wt3_85*lnr3.pdf +
  cellul.wt4_85*lnr4.pdf

 # hemicellulose -
 hemi.cellul.wt1_85 <-8.170e-3
 hemi.cellul.wt2_85 <-3.567e-2
 hemi.cellul.wt3_85 <-5.889e-2
 hemi.cellul.wt4_85 <-0
 hemi.cellul_p_85 <- hemi.cellul.wt1_85* lnr1.pdf + hemi.cellul.wt2_85*lnr2.pdf  +
  hemi.cellul.wt3_85*lnr3.pdf + hemi.cellul.wt4_85*lnr4.pdf

 # lignin ---pore
 lig.wt1_85<-  7.71e-3     # pore filled
 lig.wt2_85 <- 2.87e-2     # pore filled
 lig.wt3_85 <- 0
 lig.wt4_85 <- 0
 lig_p_85 <- lig.wt1_85* lnr1.pdf + lig.wt2_85*lnr2.pdf + lig.wt3_85*lnr3.pdf + lig.wt4_85*lnr4.pdf

# cell wall pore
wall_p_85 <- cellul_p_85 + hemi.cellul_p_85 + lig_p_85
```

```
plot(c(0.35, 3.6), range(c(cellul_p_85, hemi.cellul_p_85, lig_p_85, wall_p_85)),  type = "n",  log="x", xlab= "cell
 wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore distribution at RH
 =85%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_85, lwd=1.5, col="red")
lines(r, hemi.cellul_p_85, lwd=1.5)
lines(r, lig_p_85, col="blue", lwd=1.5)
lines(r, wall_p_85, col="green", lwd=1.5)

 legend(0.33, 0.20, c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5,
 1.5,1.5), col=c("red", "black", "blue", "green"), cex = 1.2)

 H_85 <- rep("H = 85%", length(r))
PSD_85 <- data.frame(r, cellul_p_85, hemi.cellul_p_85, lig_p_85, wall_p_85, H_85)
names(PSD_85) <- c("d", "PAC", "PAH", "PAL", "PAT", "H")

# write the dataframe to a file
write.csv(PSD_85, file= "PSD_85.csv", row.names= FALSE, quote = FALSE)

 # RH =90% , using total pore vol at each pore size as weights
 # cellulose
 cellul.wt1_90 <- 1.450e-3
 cellul.wt2_90 <- 1.300e-2
 cellul.wt3_90 <-0
 cellul.wt4_90 <-0
 cellul_p_90 <- cellul.wt1_90 * lnr1.pdf + cellul.wt2_90*lnr2.pdf  + cellul.wt3_90*lnr3.pdf +
  cellul.wt4_90*lnr4.pdf

 # hemicellulose -
 hemi.cellul.wt1_90 <-4.412e-3
 hemi.cellul.wt2_90 <-3.350e-2
 hemi.cellul.wt3_90 <-8.928e-2
 hemi.cellul.wt4_90 <-0
 hemi.cellul_p_90 <- hemi.cellul.wt1_90* lnr1.pdf + hemi.cellul.wt2_90*lnr2.pdf  +
  hemi.cellul.wt3_90*lnr3.pdf + hemi.cellul.wt4_90*lnr4.pdf

 # lignin ---pore
 lig.wt1_90 <- 4.70e-3     # pore filled
 lig.wt2_90 <- 3.55e-2     # pore filled
 lig.wt3_90 <- 0
 lig.wt4_90 <- 0
 lig_p_90 <- lig.wt1_90* lnr1.pdf + lig.wt2_90*lnr2.pdf  + lig.wt3_90*lnr3.pdf + lig.wt4_90*lnr4.pdf

# cell wall pore
wall_p_90 <- cellul_p_90 + hemi.cellul_p_90 + lig_p_90

plot(c(0.35, 3.6), range(c(cellul_p_90, hemi.cellul_p_90, lig_p_90, wall_p_90)),  type = "n", log="x", xlab= "cell
 wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore distribution at RH
 =90%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_90, lwd=1.5, col="red")
lines(r, hemi.cellul_p_90, lwd=1.5)
lines(r, lig_p_90, col="blue", lwd=1.5)
lines(r, wall_p_90, col="green", lwd=1.5)
```

```
 legend(0.33, 0.24 , c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5,
 1.5,1.5), col=c("red", "black", "blue", "green"), cex = 1.2)

# RH =95% , using total pore vol at each pore size as weights
 # cellulose
 cellul.wt1_95 <- 9.714e-4
 cellul.wt2_95 <- 1.408e-2
 cellul.wt3_95 <-0
 cellul.wt4_95 <-0
 cellul_p_95 <- cellul.wt1_95 * lnr1.pdf + cellul.wt2_95*lnr2.pdf  + cellul.wt3_95*lnr3.pdf +
  cellul.wt4_95*lnr4.pdf

 # hemicellulose -
 hemi.cellul.wt1_95 <-2.691e-3
 hemi.cellul.wt2_95 <-3.004e-2
 hemi.cellul.wt3_95 <-1.058e-1
 hemi.cellul.wt4_95 <-8.437e-3

 hemi.cellul_p_95 <- hemi.cellul.wt1_95* lnr1.pdf + hemi.cellul.wt2_95*lnr2.pdf  +
  hemi.cellul.wt3_95*lnr3.pdf + hemi.cellul.wt4_95*lnr4.pdf

 # lignin ---pore
 lig.wt1_95 <- 3.15e-3     # pore filled
 lig.wt2_95 <- 3.91e-2     # pore filled
 lig.wt3_95 <- 0
 lig.wt4_95 <- 0
 lig_p_95 <- lig.wt1_95* lnr1.pdf + lig.wt2_95*lnr2.pdf + lig.wt3_95*lnr3.pdf + lig.wt4_95*lnr4.pdf

# cell wall pore
wall_p_95 <- cellul_p_95 + hemi.cellul_p_95 + lig_p_95

plot(c(0.35, 3.6), range(c(cellul_p_95, hemi.cellul_p_95, lig_p_95, wall_p_95)),  type = "n", log="x", xlab= "cell
  wall pore size (nm)", ylab = "d(culum.pore.vol)/d(pore_diam)  (cc/(g*nm))",  main = " pore distribution at RH
  =95%", cex.lab = 1.2, cex.axis = 1.2)

lines(r, cellul_p_95, lwd=1.5, col="red")
lines(r, hemi.cellul_p_95, lwd=1.5)
lines(r, lig_p_95, col="blue", lwd=1.5)
lines(r, wall_p_95, col="green", lwd=1.5)

 legend(0.33, 0.28, c("cellullose", "hemi-cellulose", "lignin", "cell wall" ), lty =c(1, 1, 1,1), lwd=c(1.5, 1.5,
  1.5,1.5), col=c("red", "black", "blue", "green"), cex = 1.2)

 # record the data as a dataframe
H_95 <- rep("H = 95%", length(r))
PSD_95 <- data.frame(r, cellul_p_95, hemi.cellul_p_95, lig_p_95, wall_p_95, H_95)
names(PSD_95) <- c("d", "PAC", "PAH", "PAL", "PAT", "H")

# write the dataframe to a file
write.csv(PSD_95, file= "PSD_95.csv", row.names= FALSE, quote = FALSE)
```