1. After extraction from the hansen.zip file, the directory will have the files listed below.

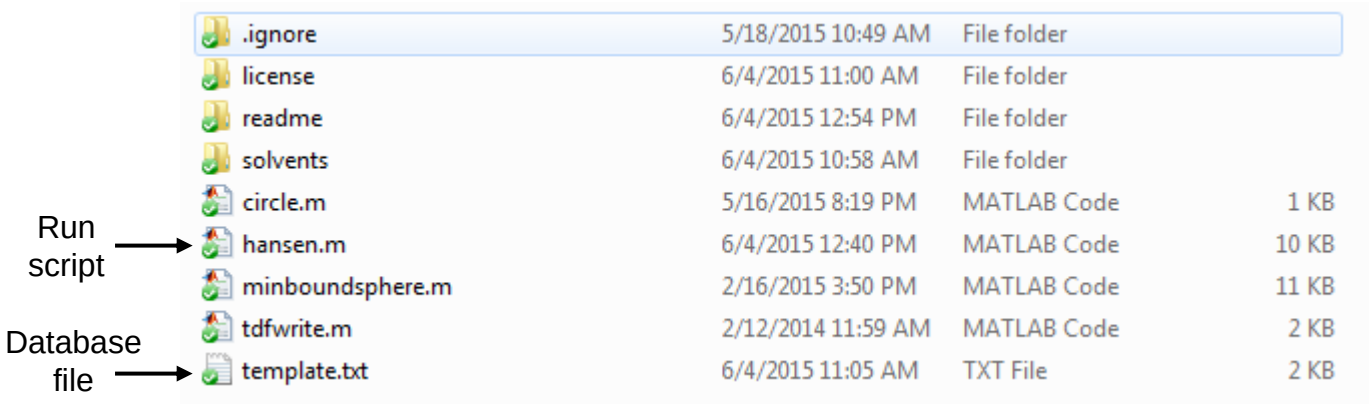
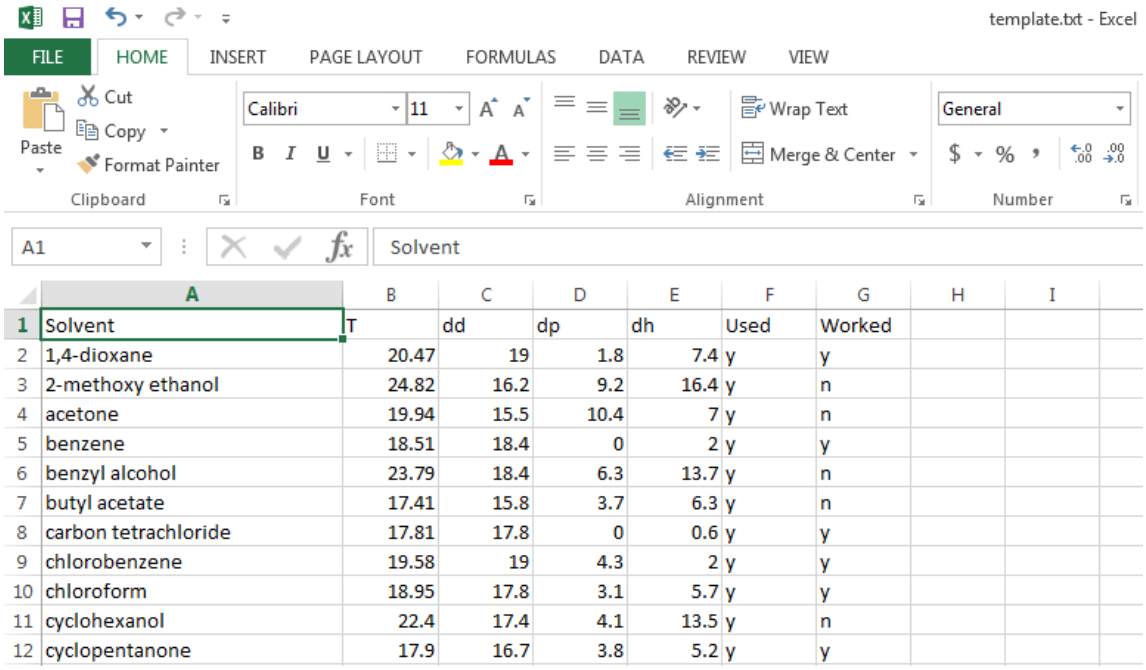


Figure 1: File list and their functions.

2. First task for using the program is to create a database file for the solvents. You can use the template file provided in the folder: template.txt. The .txt file can be edited in excel as shown in Figure 2.



	A	B	C	D	E	F	G	H	I
1	Solvent	T	dd	dp	dh	Used	Worked		
2	1,4-dioxane	20.47	19	1.8	7.4	y	y		
3	2-methoxy ethanol	24.82	16.2	9.2	16.4	y	n		
4	acetone	19.94	15.5	10.4	7	y	n		
5	benzene	18.51	18.4	0	2	y	y		
6	benzyl alcohol	23.79	18.4	6.3	13.7	y	n		
7	butyl acetate	17.41	15.8	3.7	6.3	y	n		
8	carbon tetrachloride	17.81	17.8	0	0.6	y	y		
9	chlorobenzene	19.58	19	4.3	2	y	y		
10	chloroform	18.95	17.8	3.1	5.7	y	y		
11	cyclohexanol	22.4	17.4	4.1	13.5	y	n		
12	cyclopentanone	17.9	16.7	3.8	5.2	y	y		

Figure 2: Database file with solvent names and corresponding T, δ_D, δ_P, δ_H values. Entries with "y" in the Used column is used for calculation. If the solvent is a good solvent, "y" is used in the Worked column and if the solvent is a bad solvent "n" is used in the Worked column.

3. To start the program, run the hansen.m file.

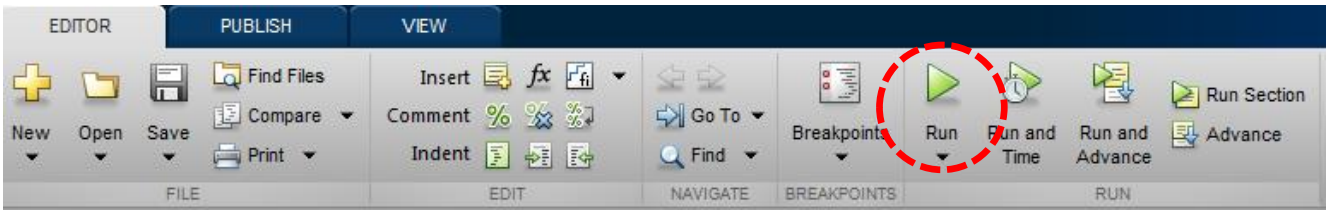


Figure 3: Running the program.

4. The program will ask for the database file. Select the database file and click open.

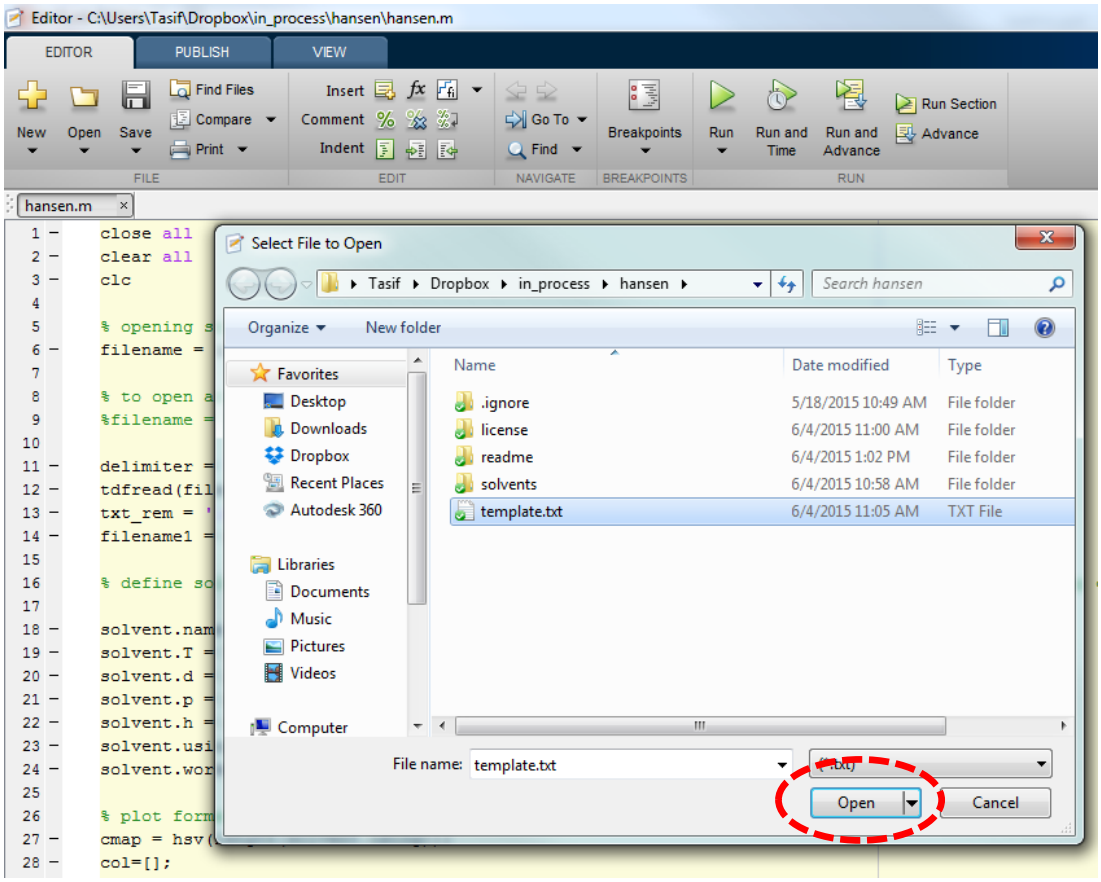


Figure 4: Opening the database file.

5. After running the script, a dialog window will appear denoting that the script ran successfully, as shown in Figure 5.

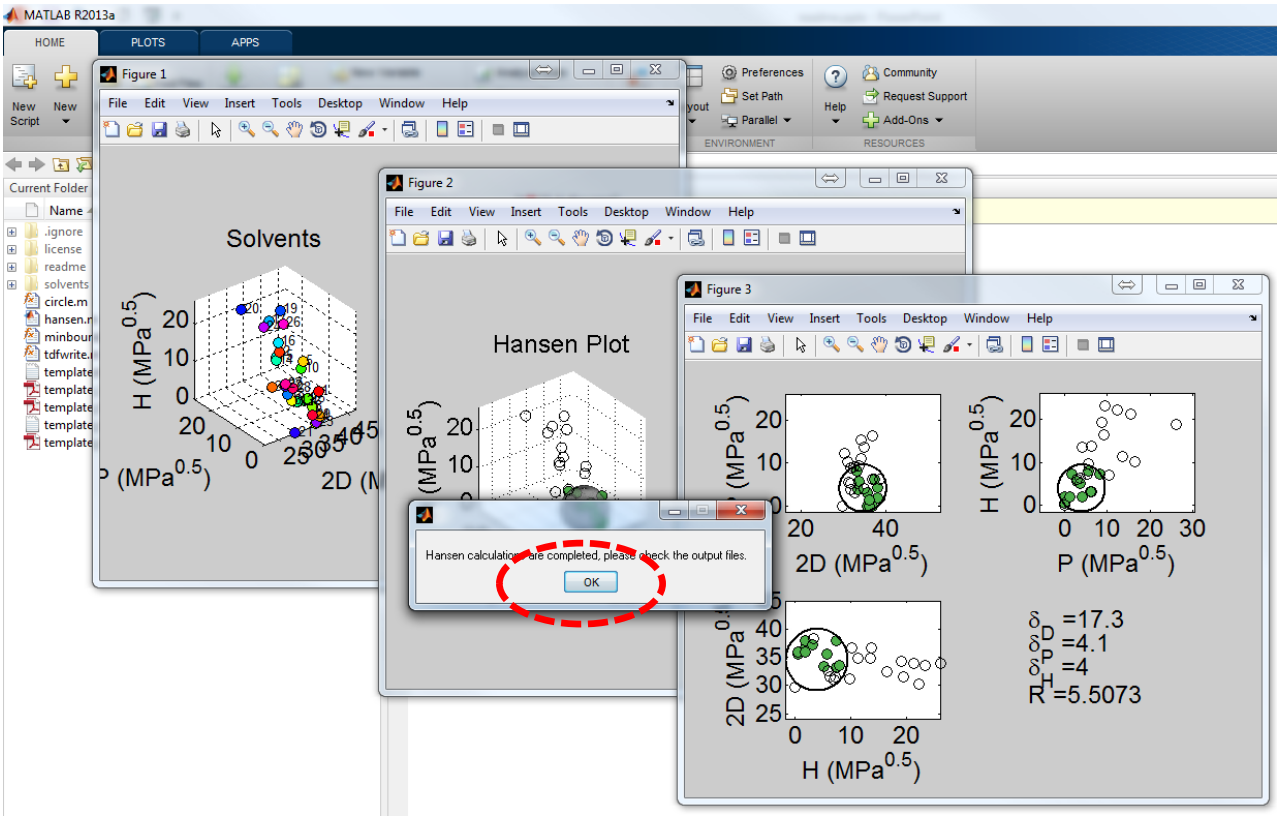


Figure 5: Dialog box denotes successful completion after running the script.

6. Three pdf files and a text file will be generated:

a. <filename>_solvents.pdf – shows all the solvents in hansen space.
b. <filename>_hansen.pdf – hansen plot where the good solvents are encapsulated within a sphere.
c. <filename>_2d.pdf – solvents are shown in 2d space for better visualization.
d. <filename>_report.txt –listing all the solvents and corresponding RED values.

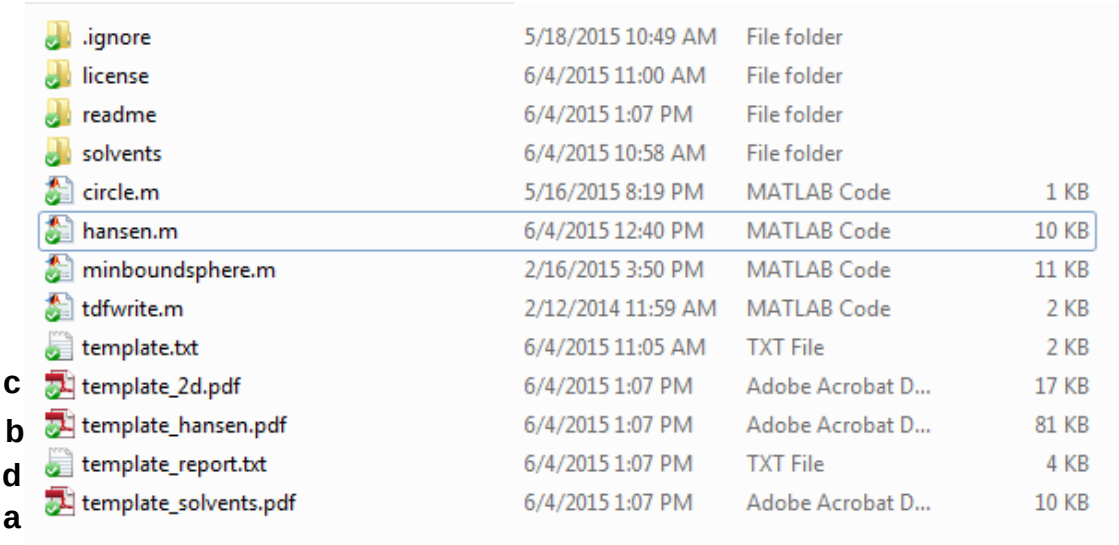


Figure 6: Generated figures after successfully running the script.

7. <filename>_solvents.pdf – The solvents are shown in hansen space. Name of the solvents are shown right to the plot, also a numerical value is assigned to each solvent.

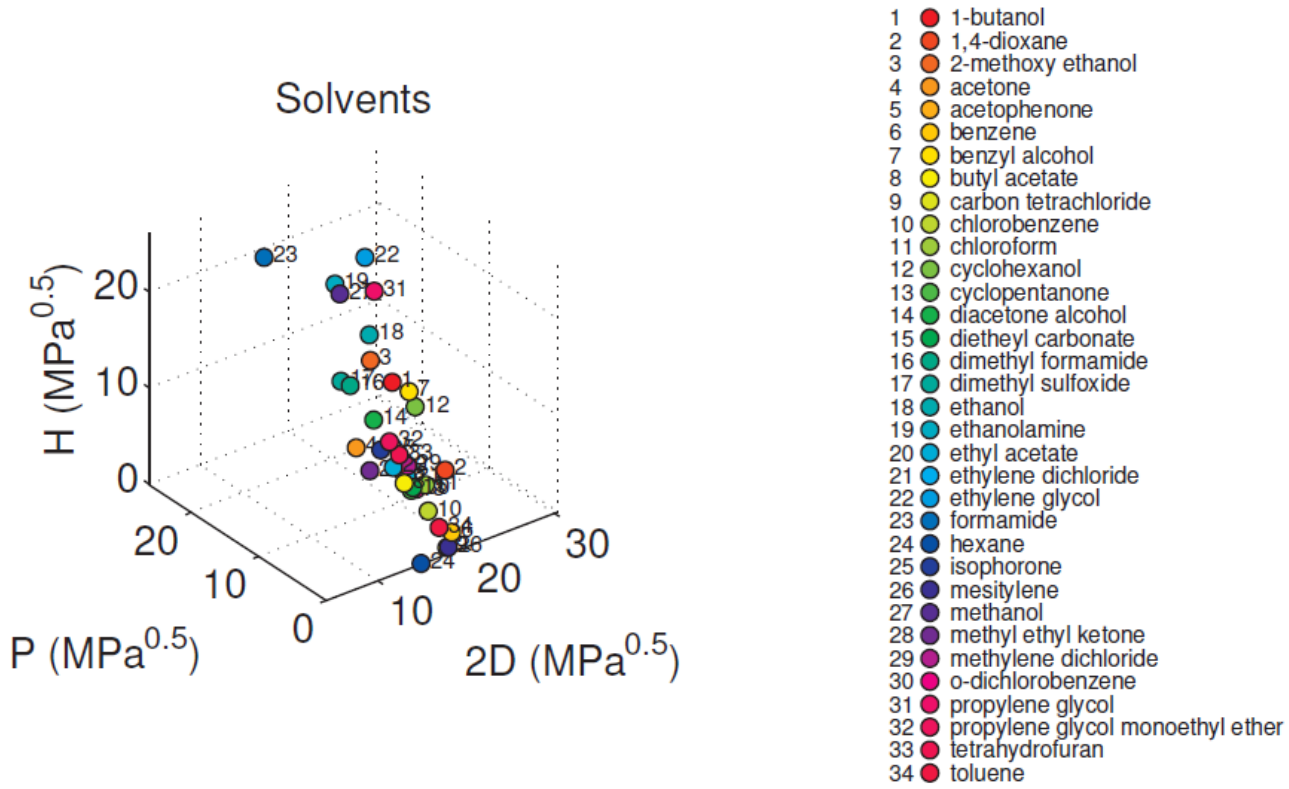


Figure 7: Solvents plot in hansen space.

8. <filename>_hansen.pdf – Good solvents (green circles) are encapsulated by a grey sphere. The bad solvents (empty circles) are outside the gray sphere.

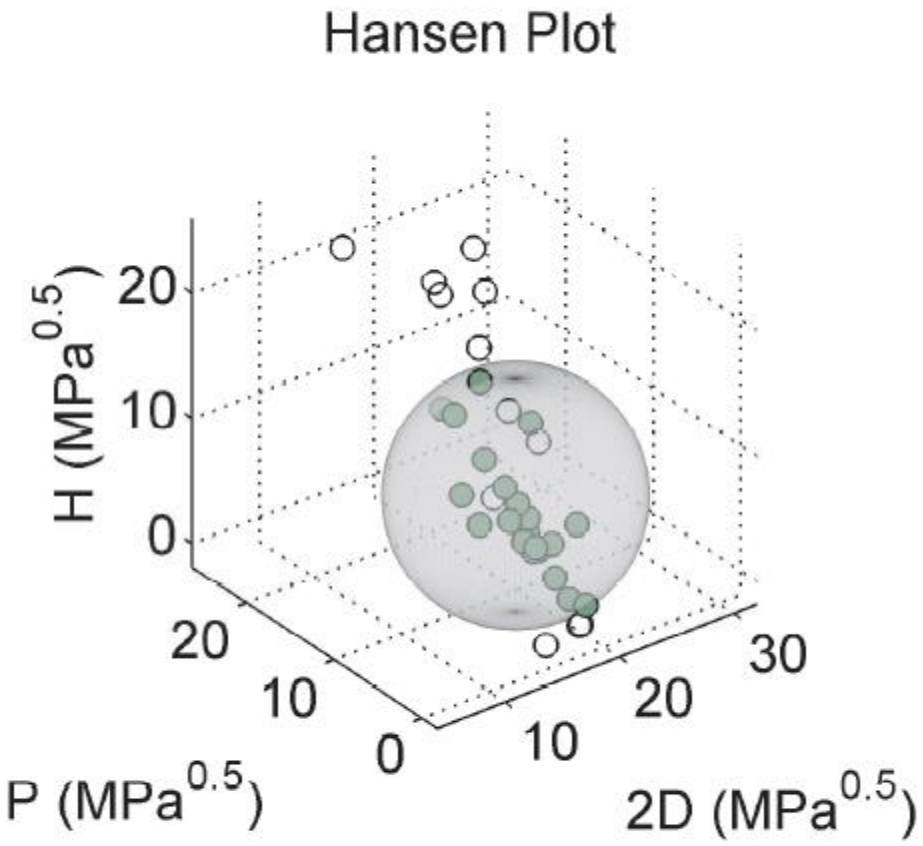


Figure 8: Good and bad solvents are denoted, also the good solvents are fitted within a sphere.

9. <filename>_2d.pdf – Solvents are shown in two-dimensional plot for better visualization.

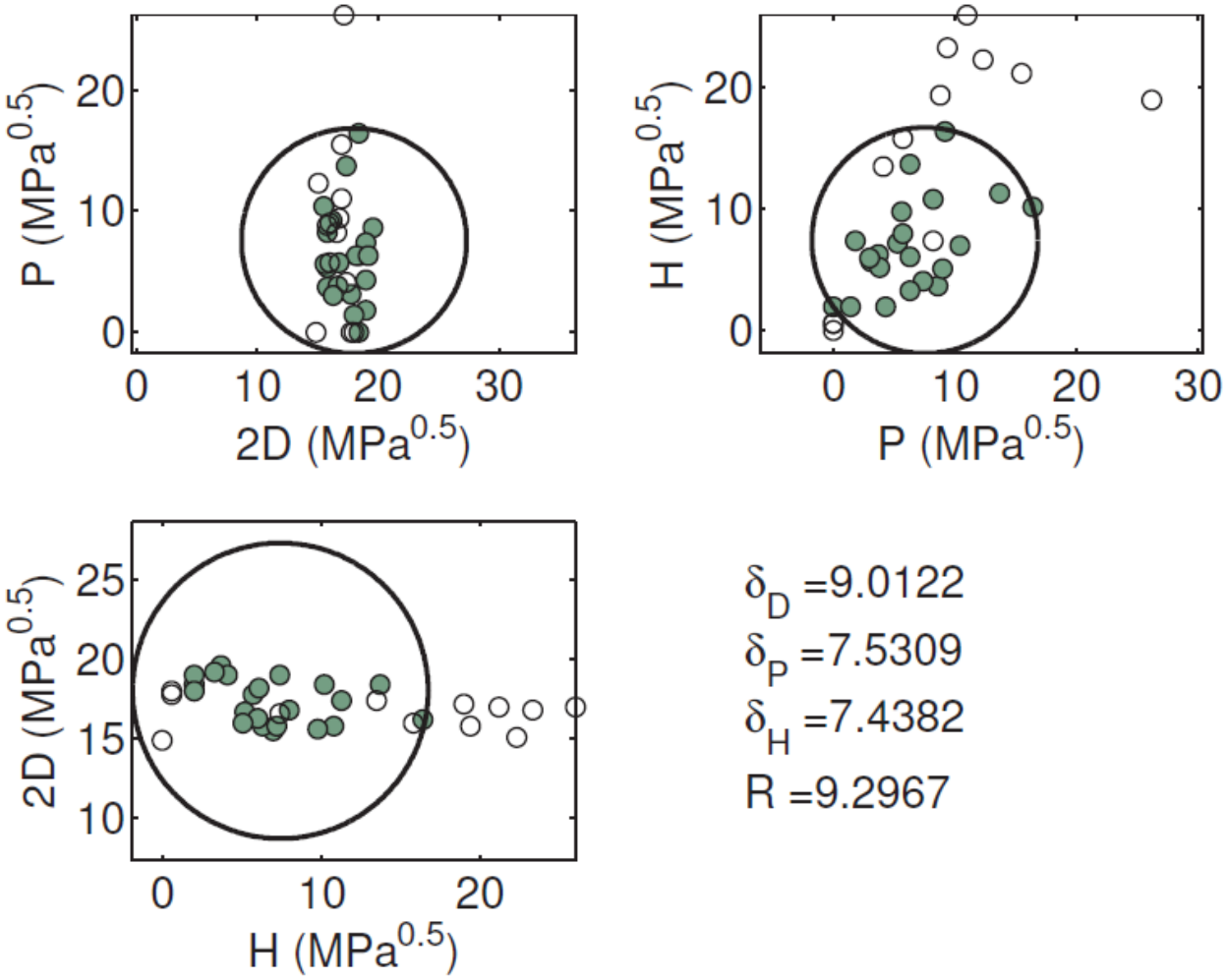


Figure 9: Two-dimensional plots where the good solvents (green circles) and bad solvents (empty circles) are shown. The sectional images of the hansen sphere are also shown.

10. <filename>_report.txt – Table listing the solvent names and corresponding T, δ_D, δ_P, δ_H, solubility, and RED values.

	A	B	C	D	E	F	G
1	Solvent	T	dd	dp	dh	Solubility	RED
2	1,4-dioxane	20.47	38	1.8	7.4	y	0.97
3	benzene	18.51	36.8	0	2	y	0.92
4	carbon tetrachloride	17.81	35.6	0	0.6	y	0.99
5	chlorobenzene	19.58	38	4.3	2	y	0.72
6	chloroform	18.95	35.6	3.1	5.7	y	0.41
7	cyclopentanone	17.9	33.4	3.8	5.2	y	0.32
8	Dichlorobenzene	NaN	37.2	6.2	3.2	y	0.63
9	isophorone	19.94	33.2	8.2	7.4	y	1
10	mesitylene	18.01	36	0	0.6	y	1
11	tetrahydrofuran	19.46	33.6	5.7	8	y	0.81
12	toluene	18.16	36	1.4	2	y	0.67
13	2-methoxy ethanol	24.82	32.4	9.2	16.4	n	2.47
14	acetone	19.94	31	10.4	7	n	1.43
15	benzyl alcohol	23.79	36.8	6.3	13.7	n	1.85
16	butyl acetate	17.41	31.6	3.7	6.3	n	0.7
17	cyclohexanol	22.4	34.8	4.1	13.5	n	1.73
18	diethyl carbonate	17.63	32.6	3	6	n	0.56
19	dimethyl formamide	24.86	34.8	13.7	11.3	n	2.2
20	dimethyl sulfoxide	26.68	36.8	16.4	10.2	n	2.54
21	ethanol	26.52	31.6	8.8	19.4	n	2.98
22	ethanolamine	31.28	34	15.5	21.2	n	3.75
23	ethyl acetate	18.15	31.6	5.3	7.2	n	0.83
24	ethylene glycol	32.95	34	11	26	n	4.19
25	formamide	36.65	34.4	26.2	19	n	4.86
26	hexane	14.9	29.8	0	0	n	1.36
27	methanol	29.61	30.2	12.3	22.3	n	3.73
28	o-dichlorobenzene	20.47	38.4	6.3	3.3	n	0.81
29	propylene glycol	30.22	33.6	9.4	23.3	n	3.64
30	propylene glycol mo	19.26	31.2	5.6	9.8	n	1.26

Table 1: Solvent names and corresponding T, δ_D, δ_P, δ_H, solubility, and RED values.