Basic properties of candidate solvents

The basic properties of the seven candidate solvents are listed in table 1.

Table 1 Basic properties of candidate solvents

Candidate solvents	Abbr.	Mole Weight g/mol	Normal boiling point T_{bp}℃	Specific gravity ρ	Solubility g/L
Benzene	Benz	78.11	80.09	0.8844	1.79
Toluene	Tol	92.14	110.63	0.8718	0.47
m-Xylene	Xyl	106.17	139.12	0.8687	0.2
Ethylbenzene	Eth	106.17	136.20	0.8718	0.15
135-Trimethylbenze	Tri	120.19	164.74	0.8696	0.05
Cyclohexane	CyH	84.16	80.72	0.7834	0.05
Octanol	Oct	130.23	195.20	0.8293	0.57

KOW values of the components

Ln(KOW) of the contaminants in wastewater are estimated in software EPI Suite, then the KOW value could be determined, as listed in table 2.

Table. 2 KOW values of the involved components.

Constituents	KOW Value
phenol	4.3060
3-methyl-phenol	7.0993
quinoline	7.6141
indole	8.4994
2,4 - dimethyl -phenol	9.9742
3, 5-dimethyl- phenol	10.4856
2, 6-dimethyl- phenol	10.5910

m-xylene	24.5325
naphthalene	27.1126

NRTL equation and binary interactive parameters

The calculation of activity coefficient in LLE is employed with NRTL equation, as expressed below:

$$\ln \gamma_i = \frac{\sum_j x_j \tau_{ji} G_{ji}}{\sum_k x_k G_{ki}} + \sum_j \frac{x_j G_{ij}}{\sum_k x_k G_{kj}} \left(\tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}} \right) \qquad (*)$$

Where

$$G_{ji} = \exp\left(-\alpha_{ij} \tau_{ij}\right) \qquad (a)$$

$$\tau_{ij} = a_{i,j} + \frac{b_{i,j}}{T} + e_{ij} lnT + f_{ij} T \qquad (b)$$

$$\alpha_{ij} = c_{ij} + d_{ij} \left(T - 273.15\right) \qquad (c)$$

All the binary interactive parameters of involved components in this paper are listed in table 3.

Table.3 Binary interactive parameters of involved components.

i	j	aij	aji	bij	bji	α	eij	eji
[a]								
PhOH	WW	205.9753	147.8374	-8352.64	-7315.47	0.2	-31.5614	-20.5607
MIBK	WW	282.1266	1.2587	-12671.5	-761.676	0.2	-41.9358	1.1267
PhOH	MIBK	0	0	-419.348	-335.283	0.2	0	0
[b]								
Benz	WW	45.1905	140.0874	591.3676	-5954.31	0.2	-7.5629	-20.0254
Tol	WW	-247.879	627.0528	14759.76	-27269.4	0.2	35.582	-92.7182

Xyl	WW	-50.0898	140.0831	5018.975	-5322.94	0.2	6.6123	-19.955
Eth	WW	-10.505	1.005837	4458.591	2260.014	0.2	0	0
Tri	WW	-3.7264	10.2521	2542.779	-66.0366	0.2	0	0
CyH	WW	-10.4585	13.1388	4954.897	-1066.98	0.2	0	0
Oct	WW	-5.3299	2.126	1690.022	2026.179	0.2	0	0
[c]								
PHOH	Benz	0	0	-186.417	859.605	0.3	0	0
MIBK	Benz	0	0	-303.002	422.1433	0.3	0	0
PHOH	Tol	0	0	-74.424	599.1280	0.3	0	0
MIBK	Tol	0	0	-329.6815	460.9119	0.3	0	0
MIBK	Xyl	0	0	-395.497	574.5596	0.3	0	0
PHOH	Xyl	0	0	31.39089	431.2643	0.3	0	0
PhOH	Eth	0	0	-6.6477	584.834	0.3	0	0
MIBK	Eth	0	0	-111.727	150.9951	0.3	0	0
PHOH	Tri	0	0	131.8239	303.8185	0.3	0	0
MIBK	Tri	0	0	-467.387	714.9152	0.3	0	0
PHOH	CyH	0	0	140.1814	727.6857	0.3	0	0
MIBK	CyH	0	0	-61.7705	495.5167	0.3	0	0
PHOH	Oct	0	0	-299.926	-279.415	0.3	0	0
MIBK	Oct	0	0	168.0731	30.5698	0.3	0	0
MIBK	DiOH	0	0	-186.34183	-360.567203	0.3		
PHOH	DiOH	0	0	209.435205	-164.972236	0.3		
WW	DiOH	0	0	1655.66251	-109.013912	0.3		
TOL	DiOH	0	0	691.667738	-229.871605	0.3		
QN	DiOH	0	0	-672.195664	156.444755	0.3		
DiOH	XYL	0	0	-155.725	558.1168	0.3		

Note: a- from literature(YANG Chu-fen, YANG Shi-ying, GUO Jian-wei, Simulation and design on phenol extraction process for coal-gasification wastewater, Modern Chemical Industry, 2012 7(32))；
b- from AspenPlus-APV71；
c- estimated in Aspen Plus with UNIFAC method.

MODEL STATISTICS

All the models were running under GAMS IDE X64 (GAMS 23.8/ CONOPT 3.0) environment in windows 7 X64.The main hardware configuration are:

Processor : Intel Xeon(R) CPU E3-1230

Memory(RAM) : 16G

Hard disk : Intel 120G SSD

Each of the 7 solvent blends are calculated with the same evaluation model (eq.1). MIBK and the designed solvent blend are applied to the operating optimization model. The model statics is listed in table 4.

Table 5. the model statics.

	Evaluation of solvent blend	Operating optimization
Blocks of equations	13	31
Single equations	381	1,071
Blocks of variables	10	13
Single variables	379	1,047
Non zero elements	2,027	8,444
Non linear n-z	1,408	6,556
Derivative pool	10	10
Constant pool	48	126
Code length	3,473	13,721
Execution time	0.786	2.874

The Properties of ABK and QH-1

Both ABK and QH-1 are the complex extractant developed by Tsinghua University. ABK is just the codename of the extractant and no further explanation about it is available in open literature. While QH-1 is also a codename where Q H are the abbreviations of Qing Hua, which is the name of the university. The properties of complex solvent(ABK and QH-1) available in the open literature are listed in table 5.

Table 5 The Properties of ABK and QH-1

	ABK	QH-1
manufacture	Tsinghua University	Tsinghua University
Chemical formula	Unpublished	Unpublished
Solubility (mg/L)	300	250
Density (kg/m3)	840	827
Dynamic viscosity (mPa•s)	5	9
Boiling point (℃)	185	191
Price (2002) ($)	4200	3200

This table is from literature (*Hong Jiang, Yong Tang & Qing-Xiang Guo (2003): Separation and Recycle of Phenol from Wastewater by Liquid–Liquid Extraction, Separation Science and Technology, 38:11, 2579-2596*)