Process Simulation – an efficient and capable tool in environmental technology

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General

Environmental processes want to clean air, water and soil. In many cases, however, pollution loading occurs even during a manufacturing process. In this case it is necessary to minimise loading firstly in manufacturing and secondly to reduce loading as much as possible..

This paper wants to talk about the treatment of the environmental process **waste water** by taking advantage of the process simulation software Chemcad,

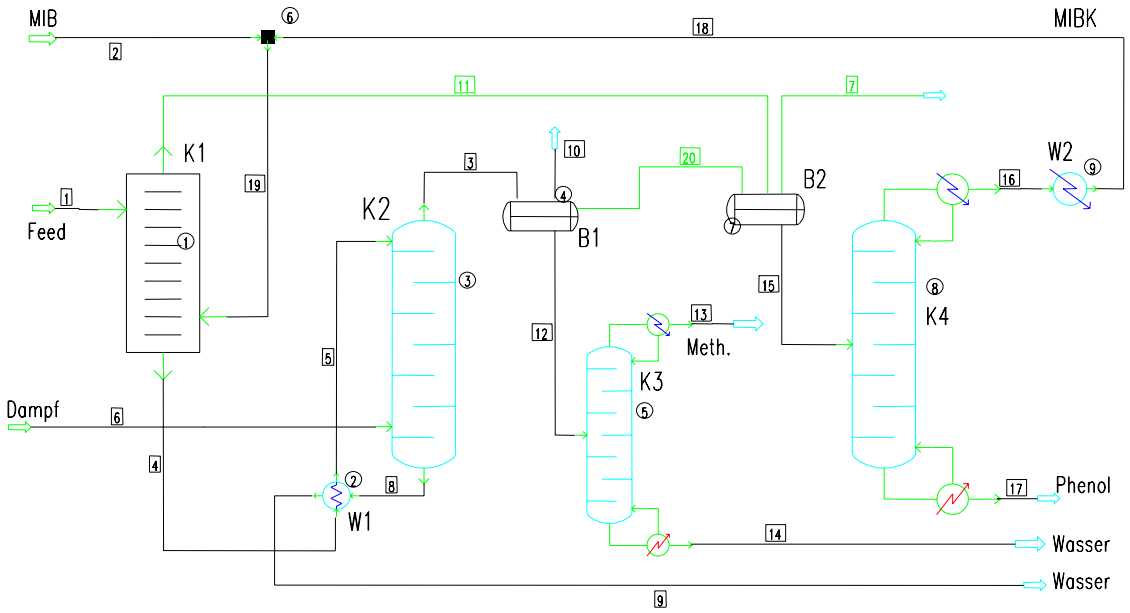
Waste Water Plant

A waste water charged with phenol and methanol had to be cleaned. In order to minimise the costs two questions had to be considered: Is it advisable to clean up the waste water before it is led into the river Emscher or should one take into account a modernisation of the existing plant in which the loading occurs.

A procedure described in Ullmann Chemical Encyclopaedia served as a model.. Due to some modifications during the simulation the following procedure was a first platform for cost calculation resulting in the statement that this plant would have become very spacious and expensive, thus leading to higher internal expenses compared with the saved fees to official authorities.

Therefore, it was decided to invest money into the plant where the problems were caused..

The process includes one extraction column, one stripping column as well as re-distillation columns. In this case cleaned up water with various residual loading is present 3 times. Also here it was not possible to obtain a 100 % cleaning up of water, but the residual loading is reduced considerably to such an extent that other procedures can be used.. As this preliminary study required only a rough cost calculation, no optimisation of the simulation was done.



Flow sheet of a waste water plant process simulation

Table of in- and output streams of the extraction columns in kg/h

Stream No.	1	19	11	4
Stream Name	Feed			
Temp C	20.0000*	20.0000*	20.0009	20.0006*
Pres bar	1.0000*	1.0000	1.0000	1.0000*
Enth MJ/h	-60899.	-4333.9	-4542.2	-60688.
Vapor mole fraction	0.00000	0.00000	0.00000	0.00000
Total kmol/h	213.8791	13.5823	15.1276	212.3255
Total kg/h	3999.9525	1074.3665	1219.9472	3853.6278
Total std L m3/h	4.0026	1.3231	1.4539	3.8709
Total std V m3/h	4793.81	304.43	339.06	4758.99
Flowrates in kg/h				
Water	3799.9014	58.5140	58.3155	800.0813
MIBK	0.0000	1006.8067	992.6320	13.4513
Phenol	160.0393	0.0000	160.0393	0.0000
Methanol	40.0118	9.0458	8.9605	40.0951

Stream no. 1 shows the composition of the loaded water which is led from below to extraction column K 1. Here phenol and methanol are contained.. The extraction medium is methyl isobutyl

ketene. (MIBK). Initially, the simulation was started with pure MIBK. By MIBK recovery slight amounts of water and methanol remained without having any significant influence on the process.

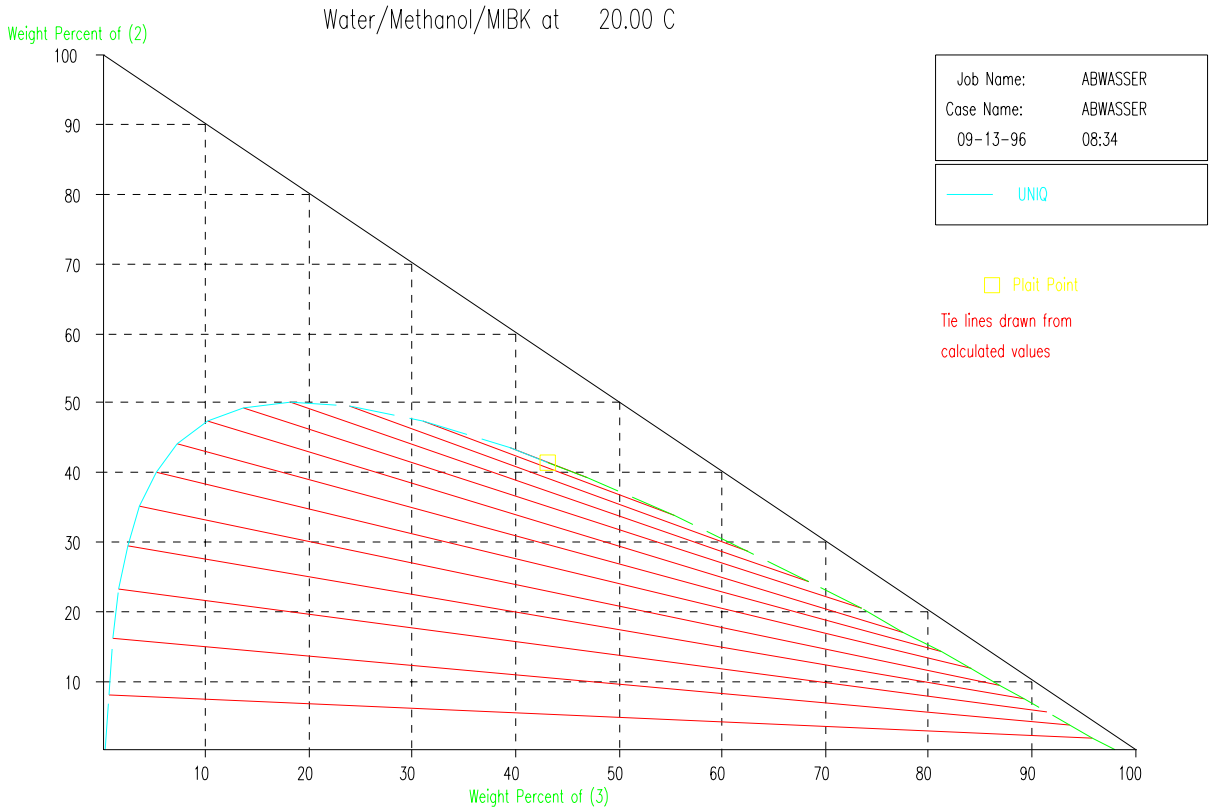
It easily can be recognised that in stream 11 the phenol is taken over quantitatively at the top of the column, whereas methanol remains in the water. Therefore, the water is pre-heated in a heat exchanger and afterwards stripped with vapour in column K2.

Table of In/Output Feeds of Stripper Columns in kg/h

Stream No.	5	6	3	8
Stream Name	vapour			
Temp C	94.9435*	120.2584	98.9885*	99.6186
Pres bar	1.0000*	2.0000*	1.0000*	1.0000
Enth MJ/h	-59467.	-13248.	-13158.	-59556.
Vapor mole fraction	0.00215450	1.0000*	1.0000	0.00000
Total kmol/h	212.3255	55.5086	55.1821	212.6524
Total kg/h	3853.6278	999.9876	1022.5527	3831.0624
Total std L m3/h	3.8709	1.0010	1.0369	3.8349
Total std V m3/h	4758.99	1244.15	1236.83	4766.32
Flowrates in kg/h				
Water	3800.0813	999.9876	969.3134	3830.7554
MIBK	13.4513	0.0000	13.4513	0.0000
Phenol	0.0000	0.0000	0.0000	0.0000
Methanol	40.0951	0.0000	39.7880	0.3070

Water coming in with stream 5 still contains methanol and some parts of MTBK. The stripping vapour in stream 6 comes towards this water and goes out quantitatively except a small part of methanol. By choosing other conditions probably the residual methanol can be reduced further. Thus it is possible to obtain the first part of cleaned u water in stream 8.

The next step is to condense occurring vapour resulting on top of stripping column K 2 as well as to treat components MTBK and methanol contained in the condensate.. The simulation shows that separation in two liquid phases at 20°C takes place.. The light phase, see stream 20, mainly contains MTBK whereas mostly water and methanol are contained in the heavy phase of stream 12 . Thus it is possible to regain MTBK in stream 20 by using a separator which needs no energy. The Chemcad simulation is able to predict such ratios, as on the one hand suitable models like UNIQUAC resp. NRTL or UNIFAC are available, on the other hand binary data, e.g. from Dechema publications, are available. The following equilibrium diagram shows the conodes of the system.



Liquid-liquid equilibrium of the mixture water/methanol/methyl-isobutyl-ketone in the separator in weight %

One can recognise that above of a 50 mol % methanol content no separation in two liquid phases is possible. The following table shows a methanol amount of the mixture in stream 3 of 40 weight % and approx. 14 weight %. of the MTBK. Thus a good separation is obtained for which no energy is required.

Table of In/Output Streams of the separator in kg/h.

Stream No.	3	10	20	12
Stream Name				
Temp C	98.9885*	20.0000	20.0000	20.0000
Pres bar	1.0000*	1.0000	1.0000	1.0000*
Enth MJ/h	-13158.	0.00000	-34.068	-15700.
Vapor mole fraction	1.0000	1.0000	0.00000	0.00000*
Total kmol/h	55.1821	0.0000	0.1049	55.0771
Total kg/h	1022.5527	0.0000	9.4190	1013.1338
Total std L m3/h	1.0369	0.0000	0.0117	1.0252
Total std V m3/h	1236.83	0.0000	2.35	1234.48
Flowrates in kg/h				
Water	969.3134	0.0000	0.1985	969.1149
MIBK	13.4513	0.0000	9.1352	4.3161
Phenol	0.0000	0.0000	0.0000	0.0000
Methanol	39.7880	0.0000	0.0853	39.7027

Table of In/Output streams of the methanol column in kg/h

Stream No.	12	13	14
Stream Name		Meth.	Water
Temp C	20.0000	73.0966	99.6289*
Pres bar	1.0000*	1.0000*	1.0000*
Enth MJ/h	-15700.	-760.62	-14613.
Vapor mole fraction	0.00000*	0.00000*	0.00000
Total kmol/h	55.0771	2.8984	52.1787
Total kg/h	1013.1338	73.1352	939.9986
Total std L m3/h	1.0252	0.0843	0.9409
Total std V m3/h	1234.48	64.96	1169.51
Flowrates in kg/h			
Water	969.1149	29.1164	939.9986
MIBK	4.3161	4.3161	0.0000
Phenol	0.0000	0.0000	0.0000
Methanol	39.7027	39.7027	0.0000

The methanol containing stream 12 is now led to column K3 for re-distillation in order to clean up the water. The composition of stream 14 proves that this has been achieved. In this simulation the water has no loading. The distillate amounts only consist of methanol and a rest of MTBK. If this process will be used in future times, decisions have to be made about the further use of this mixture.

Finally separation of MTBK/ methanol as well as re-distillation of MTBK have to be carried out..

Table of In/Output streams of MTBK re-distillation

Stream No.	15	16	17
Stream Name			Phenol
Temp C	20.0000*	86.4082*	180.7154*
Pres bar	1.0000*	1.0000*	1.0000*
Enth MJ/h	-4576.3	-4135.2	-213.40
Vapor mole fraction	0.00000	0.00000	0.00000
Total kmol/h	15.2325	13.4824	1.7500
Total kg/h	1229.3663	1064.3666	164.9998
Total std L m3/h	1.4656	1.3106	0.1550
Total std V m3/h	341.41	302.19	39.22
Flowrates in kg/h			
Water	58.5140	58.5140	0.0000
MIBK	1001.7673	996.8068	4.9605
Phenol	160.0393	0.0000	160.0393
Methanol	9.0458	9.0458	0.0000

After mixing all MTBK containing main streams a re-distillation in column K4 is done in order to clean MTBK to such an extent that it can be treated in a circle and then used again. Stream no.15 gives evidence about its realisation.. There is a rest of only small amounts of water and methanol without any influence at all.. The bottom of the column shows phenol in which, unfortunately, slight amount of MTBK are contained.

This process contains a recycle stream MTBK in which occurring losses have to be replenished.. This is done by feed stream 2. Also here the simulation time only takes some minutes.

The above study gives evidence about a successful simulation with Chemcad which even can be optimised further in case of final application. As the simulation only needs less than 2 minutes optimal parameters are obtained, even more as the programme offers the possibility of automatic parameter combination with subsequent graphical presentation of the results.