Supporting information

Process intensification for the recovery of hydrogen cyanide in the Andrussow Process

Luca Lehrich, Dr.-Ing. Chafika Adiche*

DOI: 10.1002/cite.202200059

Technische Universität Darmstadt, Department of mechanical engineering, Thermal Process Engineering Group, Otto-Berndt-Straße 2, D- 64287 Darmstadt, Germany.

* Corresponding author: Phone: + 49 (0) 6151 16 22520. Fax: + 49 (0) 6151 16 22548, E-mail: c.adiche@outlook.de

S1 Thermodynamic phase equilibrium of the system of hydrogen cyanide – water using the regressed NRTL model established in this work

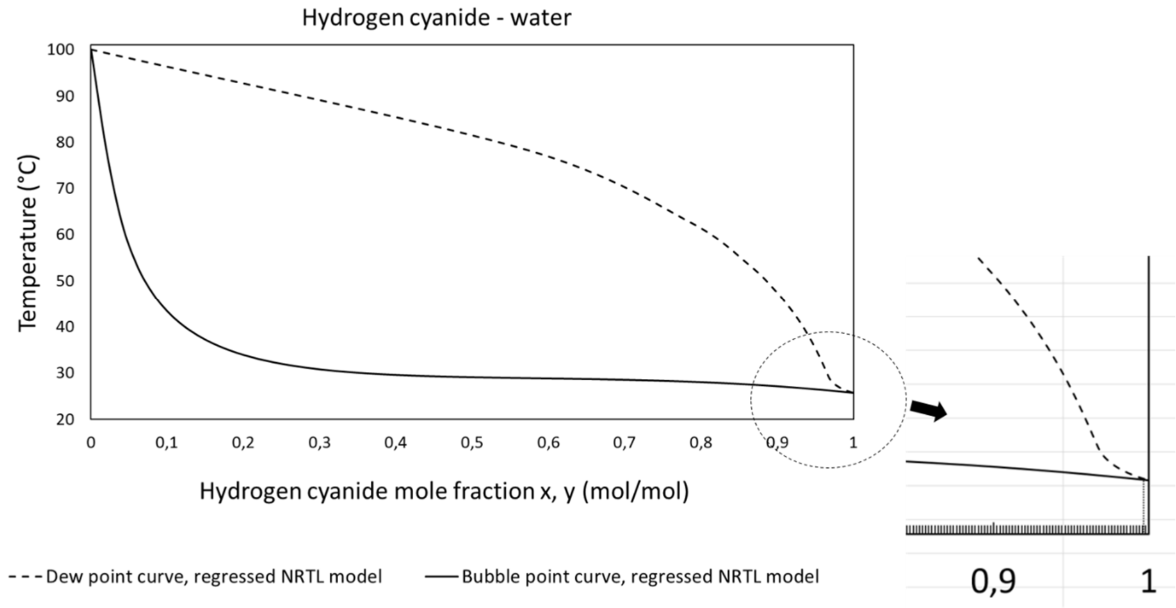

Figure S1. Binary mixture of hydrogen cyanide and water presents a tangent azeotrope for the regressed NRTL model.

S2 Data and correlations of the cost model of the distillation unit of the Andrussow process

Table S1. Prices and properties of heating and cooling media.

Low pressure steam 3.5 bar	
Price $C_{lps/j}$ (€ J^{-1})	$1.16 \cdot 10^{-8}$
Enthalpy of vaporization Δh_{lps} (kJ kg^{-1})	2147.4
Inlet / outlet temperature (°C)	140/138
Chilled water	
Price $C_{cw/j}$ (€ J^{-1})	$6.67 \cdot 10^{-9}$
Specific heat capacity $c_{p,cw}$ (J $kg^{-1}K^{-1}$) (temperature range: 5 – 20 °C)	4193
Inlet / outlet temperatures (°C)	5/15

Table S2. Purchased prices of the distillation column based on the cost correlations taken from reference 19.

Column vessel and sieve trays
$C_{col} = f_1 C_b + N_{stages} f_2 f_3 f_4 C_t + C_{pt}$ (in *1000 $*)
$C_b = 1.218\ exp\ [7.123 + 0.1478\ (lnW) + 0.02488 [lnW]^2]$, *W in lbs*
$C_t = 457.7$ exp $(0.1739D)$, *D in ft*
$C_{pt} = 249.6\ D^{0.6332}\ H^{0.8016}$ (cost for platforms and ladders), H in *ft*
$f_1 = 1.7$ (stainless steel 1.4301, AISI 304)
$f_2 = 1.189 + 0.0577D$ (stainless steel 1.4301, AISI 304)
$f_3 = 0.95$ (sieve trays)
$f_4 = 1 (N_T > 20)$
Column vessel and packing
$C_{col} = f_1 Cb + V_p C_P + C_{Pt}$ (in *1000 $*), V_p volume of packing in ft^3
$f_1 = 1.7$ (stainless steel 1.4301, AISI 304)
C_p *is the cost of packing* $\$/ft^3$
Heat exchanger (reboiler / condenser/ feed preheater)
$C_{Hex} = 1.218\ f_d f_m f_p C_b$ *(in $)*
$C_b = exp(8.821 - 0.30863\ (lnA_{hex}) + 0.0681\ (lnA_{Hex})^2)$, A_{Hex} in ft^2
Reboiler
$f_d = 1.35$ *(kettle reboiler)*
$f_m = 0.8193 + 0.15984\ (lnA_{hex})$ (stainless steel 1.4301, AISI 304)
$fp = 1.10$ *(pressure range: 4−6 bar)*
Condenser
$f_d = exp(-1.1156 + 0.0906 (lnA_{Hex}))$ *(fixed head)*
$f_m = 0.8193 + 0.15984\ (lnA_{hex})$ (stainless steel 1.4301, AISI 304)
$fp = 1.10$ *(pressure range: 4−6 bar)*
Heater (feed preheating)
$f_d = exp[-0.9816 + 0.0830 (lnA_{Hex})]$ *(U−tube)*
$f_m = 0.8193 + 0.15984\ (lnA_{hex})$ (stainless steel 1.4301, AISI 304)
$fp = 1.10$ *(pressure range: 4−6 bar)*

S3 Results of sensitivity analysis for the design optimization of the column with a side stripper

Table S3. Impact of increasing mass flow rate of the liquid side stream *Lss* on the reflux ratio *RR* in the main column, on the maximum composition of organonitriles in the main column and on the HCN loss in the whole distillation unit, NITRIWA = 500 kg/h.

L_{ss} (kg h^{-1})	RR [-]	Maximum liquid mass fraction of organonitriles in the main column	Maximum vapor mass fraction of organonitriles in the main column	HCN loss in the distillation unit (wt. %)
1000	1.85	0.0566	0.0590	0.50
1300	1.85	0.0358	0.0587	0.47
1500	1.85	0.02679	0.0552	0.46
1700	1.93	0.02338	0.0556	0.45
1900	2.05	0.02209	0.0584	0.43