Preliminary Design of a Polyurethane Recycle Plant

Appendix

January 1992

G-Groep '91-II-B

TU Delft

Delft University of Technology

Faculty of Mechanical Engineering and Marine Technology
Equipment for Process Industry

ERRATUM

REQUIRED ENERGY (Chapter 4 in report)

A mistake was made in chapter 4 of the report concerning the energy balance. In table 4.3 the duty of pump 1 (P1) was given to be 3500 kW. This should be 3.5 kW. Because of this error the total required work for pumping was incorrect. The time average work of P1 has to be calculated (as in the report): 3.5*(7.5/60)=0.44 kW. The total work (calculated by adding the duties of the remaining pumps in table 4.3) for pumping is then 9.0 kW.

The energy required for the two cutters is: 40.5 and 150 kW.

The high shear mixer will operate continuously, as discussed in the additional report about the PID, so the required energy is 33 kW.

The energy for mixing in V4, R1 and R2 is 6 kW in total. The energy required for the extractor (RDC) is 1.5 kW.

The total required work for the process is calculating by adding all these duties: 240 kW

ERRATUM REACTOR HARDWARE:

p. 6.20, line 7 - two filters in series should be
two filters in parallel

p. 6.20, line 14 - appendix A6.XV should be
appendix A6.XVI (data on filters)

ERRATUM SETTLER:

p. 6.24, line 17 - $_{l}$ = flow rate light phase should be
Q_{l} = flow rate light phase

p. 6.24, line 23 - x in eq. (6.32) is
θ in table A.3

p. 6.24, line 25 - Table 6.3 should be
Table A.3
p. 6.27, line 3 - add to results
$t_c = 105$ s
$dH_c = 0.039$ m

p. 6.27, line 9 - $t_s = 195$ m should be
$t_s = 195$ s

Appendix A6.XVI

p. s11, bottom - Hfl 8000,- should be
Hfl 7000,-

	Duty (kW)	Area(m^2)
H1 flash feed heater	924	385
H2 flash vapour condensor	71	1
H3 reactor feed preheater	235	37
H4 reactor feed heater	349	13
H5 reactor vapour condensor	5	0.3
H6 distillation top condensor	4596	
H7 distillation reboiler	4625	
H8 extractor feed cooler	6	0.2
H9 extractor feed/product exchanger	69	33
H10 extractor feed cooler	.5	0.2
H11 flash vapour condensor	30	0.3
H12 extractor feed/product exchanger	60	39
H13 flash feed heater	33	4
H14 flash bottom cooler	36	0.6

	volume (m^3)
V1 fresh MEG storage	37.5
V2 crude MEG storage	200
V3 KAc/MEG storage	5
V4 feed mixer	12.5
V5 cut PU storage	40
V6 prepared feed storage	250
V7 separator vessel	D=0.5, L=2.55
V8 water/HCL storage	
V9 water/HCL/DADPM storage	

	duty (kW)
cutter 1	40.5
cutter 2	150

	duty (kW)
high shear mixer	23

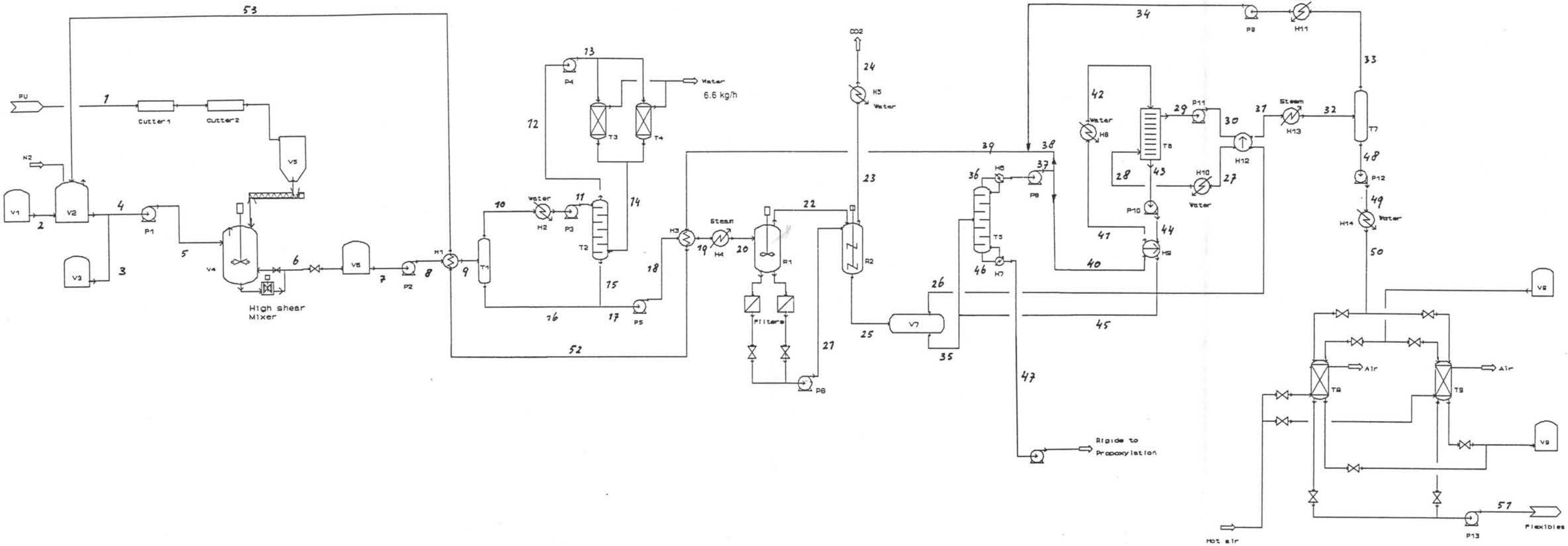
	Duty (W)
P1 MEG pump	450
P2 flash feed pump	950
P3 flash top pump	26
P4 N2 compressor	
P5 reactor feed pump	2300
P6 reactor 2 pump	230
P7 distillation bottom pump	20
P8 condensate pump	1200
P9 flash condensate pump	16
P10 extractor product pump	82
P11 flash feed pump	78
P12 flash bottom pump	95
P13 flexibles pump	50

	diameter, height (m)
T1 flash vessel, H_2O/feed	D=1.1, H=3.3
T2 MEG/H_2O stripper	D=0.2, H=8.5
T3 N_2 dryer	
T4 N_2 dryer	
T5 packed distillation column	D=1.5, H=10.0
T6 extractor column (RDC)	D=0.4, H=9.5
T7 flash column, flex/MEG	D=0.6, H=2.0
T8 ion-exchanger	D=0.3, H=2.0
T9 ion-exchanger	D=0.3, H=2.0
R1 reactor1	D=2.6, H=4.5
R2 reactor2	D=2.1, H=6.6

Appendix A.4.III. Process Flow diagram (corrected)

Poly Urethane Recycle Plant ICI
G-Groep '91-II-B

Note: operation upstream V5 is discontinuous, operation downstream V5 is continuous.



stream		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27
P	(bar)	1	1	1	1	1	1	1	2	1	0.10	1	1	2	1	1	1	0.10	5	4.4	3.0	3.0	3.0	3	2.5	3	2	1.2
T	(°C)	20	35	35	35	35	35	35	35	150	139	139	139	139	139	139	139	139	139	164	200	200	200	200	200	200	200	90
vapour fraction		-	-	-	-	-	-	-	-	-	1	0	1	1	1	1	-	-	-	-	2e-3	-	1	-	-	-	-	-
PU	(kg/h)	990	-	-	-	-	980	980	980	980	0	-	-	-	-	-	980	980	980	980	980	-	-	-	-	-	-	-
MEG	(kg/h)	-	254.6	20	10000	10000	10000	10000	10000	10000	378	378	–	-	–	378	9622	10000	10000	10000	10000	9883.5	10.6	-	-	9883.5	127.5	127.5
flexibles	(kg/h)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	714	-	-	-	714	714	714
rigids	(kg/h)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	351	-	-	-	351	-	-
DADPM	(kg/h)	-	-	-	0.35	0.35	0.35	0.35	0.35	0.35	-	-	-	-	-	-	0.35	0.35	0.35	0.35	0.35	31.85	-	-	-	31.85	8.6	8.6
KAc	(kg/h)	-	-	20	20	20	20	20	20	20	-	-	-	-	-	-	20	20	20	20	20	20	-	-	-	20	-	-
H_2O	(kg/h)	10	-	-	10	10	10	10	10	10	6.6	6.6	6.6	6.6	-	0.13	3.4	3.53	3.53	3.53	3.53	-	-	-	-	-	-	-
N_2	(kg/h)	–	–	–	–	–	–	–	–	–	–	-	44	44	44	-	-	–	-	-	-	–	-	–	–	-	–	–

stream		28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53
P	(bar)	1	1	3	2	1	0.15	3	2	1	3	3	3	3	1.2	1	1	3	2	1	1	0.15	3	2.5	2	2.5	1
T	(°C)	80	80	80	191	198	198	80	200	198	198	198	198	198	90	80	80	80	180	203	203	198	198	120	120	170	46
vapour fraction		-	-	-	-	0.14	1	-	-	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
PU	(kg/h)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
MEG	(kg/h)	127.5	127.5	127.5	127.5	127.5	126.8	126.8	9756	15660	10440	9598.6	9725.4	841.1	841.1	841.1	841.1	841.1	841.1	236.2	157.4	0.7	0.7	0.7	0.7	9725.4	9725.4
flexibles	(kg/h)	714	714	714	714	714	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	714	714	714	714	-	-
rigids	(kg/h)	-	-	-	-	-	-	-	351	-	-	-	-	-	-	-	-	-	-	351	351	-	-	-	-	-	-
DADPM	(kg/h)	8.6	0.29	0.29	0.29	0.29	0.16	0.16	23.3	0.21	0.21	0.20	0.35	0.01	0.01	0.01	8.33	8.33	8.33	47.1	31.38	0.13	0.13	0.13	0.13	0.35	0.35
KAc	(kg/h)	-	-	-	-	-	-	-	20	-	-	-	-	-	-	-	-	-	-	20	20	-	-	-	-	-	-
H_2O	(kg/h)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

```
======= Problem: A:\DADPMREC.EKA =======
{APPENDIX A.4.1

     THESE EQUATIONS ARE USED TO CALCULATE THE DADPM MASS BALANCE}


D5 = 31.5 + 0.35813                   {BALANCE REACTOR}
D5 = D8 + D4                          {BALANCE SETTLER}
D4*8.5 = D8*23                        {PERFORMANCE SETTLER}
D8-D15 = D9 + D16                     {BALANCE EXTRACTOR}
D6 = D16 + D4                         {BALANCE MIXPOINT IN FRONT OF DISTILLATION}
D14 = D15 + D17                       {BALANCE SPLIT POINT IN FRONT OF EXTRACTOR}
D17 + D12 = D13                       {BALANCE MIX POINT TO CRUDE MES STORAGE}
D9 = D12 + D10                        {BALANCE FLASH}
D6*0.21 = D14*30.3869                 {PERFORMANCE DISTILLATION}
D12 = 1.31*D10                        {PERFORMANCE FLASH}
D15/D17 = 841.12/(10440-841.12)       {RATIO OF DADPM STREAMS ON BASIS ACCORDING
                                       TO RATIO OF MES STREAMS FROM DISTILLATION}
D7 = D14 + D6

{PERFORMANCE EXTRACTOR}

E=2
K=2
F=(E-1)/(E^(5)-1)
(D9-D15/K)/(D8-D15/K)=F

======= Solution =======
Variables:
   D5            = +31.858
   D8            = +8.5966
   D4            = +23.261
   D15           = +0.017187
   D9            = +0.28563
   D16           = +8.2938
   D6            = +31.555
   D14           = +0.21333
   D17           = +0.19614
   D12           = +0.16198
   D13           = +0.35813
   D10           = +0.12365
   D7            = +31.768
   E             = +2.0000
   K             = +2.0000
   F             = +0.032258

Largest residual is [illegible]
Method: Iterative
Numeric processor: Emulator
```

```
===== Problem: A:\MEGREC.EKA =====
{APPENDIX A.4.II

    THESE EQUATIONS ARE UESD TO CALCULATE THE MEG MASS BALANCE}

m1=10000                    {feed}
mreg=116.5                  {reacting MEG}
m8=127.5                    {MEG in settler top to extractor}
m9 =127.5                   {MEG in settler top to flash through extractor}
m1=m3+mreg                  {balance reactor}
m3=m8+m4                    {balance settler}
m5=m4+m16                   {mix point in front of distillation}
m5=m14+m6                   {balance distillation}
m14=m17+m15                 {balance splitter in front of extractor}
m9=m12+m10                  {balance flash}
m13=m17+m12                 {balance mix point to crude MEG storage}
m8+m15=m16+m9               {balance extractor}
m14=m6*66.307               {performance distillation}
m14=m15*(10432/840.5)       {split ratio distillation top to extractor}
m12=m10*184.29              {performance flash}
mnw=m1-m13                  {calculation of required fresh MEG feed}

===== Solution =====
Variables:
  m1        = +10000.
  mreg      = +116.50
  m8        = +127.50
  m9        = +127.50
  m3        = +9883.5
  m4        = +9756.0
  m5        = +10597.
  m16       = +841.12
  m14       = +10440.
  m6        = +157.44
  m17       = +9598.6
  m15       = +841.12
  m12       = +126.81
  m10       = +0.68811
  m13       = +9725.4
  mnw       = +274.63

Largest residual is 2.5E-12
Method: Iterative
Numeric processor: Emulator
```

Appendix A.4.III. Process Flow diagram

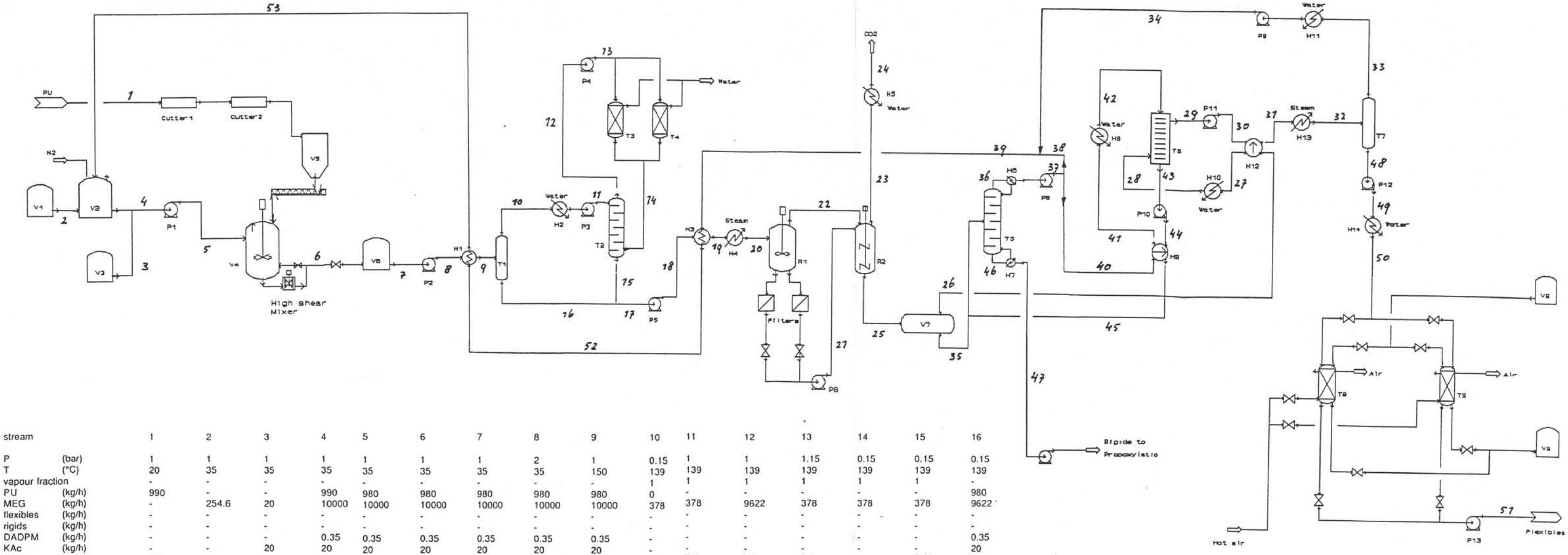
Poly Urethane Recycle Plant ICI
G-Groep '91-II-B
Note: operation upstream V5 is discontinuous,
operation downstream V5 is continuous.

	Duty (kW)	Area(m^2)
H1 flash feed heater	924	385
H2 flash vapour condensor	71	1
H3 reactor feed preheater	235	37
H4 reactor feed heater	349	13
H5 reactor vapour condensor	5	0.3
H6 distillation top condensor	4596	
H7 distillation reboiler	4625	
H8 extractor feed cooler	6	0.2
H9 extractor feed/product exchanger	69	33
H10 extractor feed cooler	5	0.2
H11 flash vapour condensor	30	0.3
H12 extractor feed/product exchanger	60	39
H13 flash feed heater	33	4
H14 flash bottom cooler	36	0.6

	Duty (W)
P1 MEG pump	450
P2 flash feed pump	950
P3 flash top pump	26
P4 pump	
P5 reactor feed pump	2300
P6 reactor 2 pump	230
P7 distillation bottom pump	20
P8 condensate pump	1200
P9 flash condensate pump	16
P10 extractor product pump	82
P11 flash feed pump	78
P12 flash bottom pump	95
P13 flexibles pump	50

	diameter, height (m)
T1 flash vessel, H_2O/feed	D=1.1, H=3.3
T2 MEG/H_2O stripper	D=0.2, H=8.5
T3 N_2 dryer	
T4 N_2 dryer	
T5 distillation column	D=1.5, H=10.0
T6 extractor column	D=0.4, H=9.5
T7 flash column, flex/MEG	D=0.6, H=2.0
T8 ion-exchanger	D=0.3, H=2.0
T9 ion-exchanger	D=0.3, H=2.0
R1 reactor1	D=2.6, H=4.5
R2 reactor2	D=2.1, H=6.6

	volume (m^3)
V1 fresh MEG storage	
V2 crude MEG storage	200
V3 KAc/MEG storage	
V4 feed mixer	50
V5 cut PU storage	40
V6 prepared feed storage	25
V7 separator vessel	D=0.5, L=2.55
V8 water/HCL storage	
V9 water/HCL/DADPM storage	



stream		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
P	(bar)	1	1	1	1	1	1	1	2	1	0.15	1	1	1.15	0.15	0.15	0.15
T	(°C)	20	35	35	35	35	35	35	35	150	139	139	139	139	139	139	139
vapour fraction		-	-	-	-	-	-	-	-	-	1	1	1	1	1	1	-
PU	(kg/h)	990	-	-	990	980	980	980	980	980	0	-	-	-	-	-	980
MEG	(kg/h)	-	254.6	20	10000	10000	10000	10000	10000	10000	378	378	9622	378	378	378	9622
flexibles	(kg/h)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
rigids	(kg/h)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
DADPM	(kg/h)	-	-	-	0.35	0.35	0.35	0.35	0.35	0.35	-	-	-	-	-	-	0.35
KAc	(kg/h)	-	-	20	20	20	20	20	20	20	-	-	-	-	-	-	20
H_2O	(kg/h)	10	-	-	10	10	10	10	10	10	6.6	6.6	6.6	6.6	-	0.13	3.4

stream		17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
P	(bar)	0.15	5	4.4	3.0	3.0	3.0	3	2.5	3	2	1.2	1	1	3	2	1	0.10	3
T	(°C)	139	139	164	200	200	200	200	200	200	200	90	80	80	80	191	198	198	80
vapour fraction		-	-	-	2e-3	-	1	-	-	-	-	-	-	-	-	-	0.14	1	-
PU	(kg/h)	980	980	980	980	-	-	-	-	-	-	-	-	-	-	-	-	-	-
MEG	(kg/h)	10000	10000	10000	10000	9823.5	60	127.5	127.5	127.5	127.5	127.5	127.5	127.5	127.5	127.5	127.5	126.8	126.8
flexibles	(kg/h)	-	-	-	-	714	-	714	714	714	714	714	714	714	714	714	714	-	-
rigids	(kg/h)	-	-	-	-	351	-	-	-	-	-	-	-	-	-	-	-	-	-
DADPM	(kg/h)	0.35	0.35	0.35	0.35	31.85	-	-	-	31.85	8.6	8.6	8.6	0.29	0.29	0.29	0.29	0.16	0.16
KAc	(kg/h)	20	20	20	20	20	-	-	-	-	-	-	-	-	-	-	-	-	-
H_2O	(kg/h)	3.53	3.53	3.53	3.53	-	-	-	-	-	-	-	-	-	-	-	-	-	-

stream		35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53
P	(bar)	2	1	3	3	3	3	1.2	1	1	3	2	1	1	0.15	3	2.5	2	2.5	1
T	(°C)	200	198	198	198	198	198	90	80	80	80	180	203	203	198	198	120	120	170	46
vapour fraction		-	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
PU	(kg/h)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
MEG	(kg/h)	9756	15660	10440	9598.6	9725.4	-	841.1	841.1	841.1	841.1	841.1	236.2	157.4	0.7	0.7	0.7	0.7	9725.4	9725.4
flexibles	(kg/h)	-	-	-	-	-	-	-	-	-	-	-	-	-	714	714	714	714	-	-
rigids	(kg/h)	351	351	351	351	351	351	-	-	-	-	-	-	351	-	-	-	-	-	-
DADPM	(kg/h)	23.3	0.21	0.21	0.20	0.35	0.01	0.01	0.01	8.33	8.33	8.33	47.1	31.4	0.1	0.1	0.1	0.1	0.35	0.35
KAc	(kg/h)	20	-	-	-	-	-	-	-	-	-	-	20	20	-	-	-	-	-	-
H_2O	(kg/h)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Heat exchanger

For cooling of liquid stream (MEG,DADPM) from distillation column to extractor, will be used cold liquid stream (MEG,DADPM) from extractor to feed of distillation column .

Hot liquid(MEG,DADPM) from distillation :

Flowrate liquid :

$Q_{meg} := 840.21$ [kg/hr]

$Q_{dadpm} := 0.01788$ [kg/hr]

$Q_{tot1} := Q_{meg} + Q_{dadpm}$

Temperature liquid :

$T_1 := 198$ --->---- $T_2 := 90$

$T_{1k} := T_1 + 273$ $T_{2k} := T_2 + 273$

Properties of hot liquid(MEG,DADPM) from distillation column :

Cp of MEG:

$$Cp_{meg1}(t) := 0.1148\cdot10^6 - 0.75\cdot10^2\cdot t + 0.8020\cdot t^2 - 0.57\cdot10^{-3}\cdot t^3$$

$$Cp_{meg1} := \int_{T_{2k}}^{T_{1k}} \frac{Cp_{meg1}(t)}{T_{1k} - T_{2k}}\,dt$$

$M_{meg} := 62.07$ [gram/mol]

$$Cp_{meg1} := \frac{Cp_{meg1}}{M_{meg}} \qquad Cp_{meg1} = 2.92796426\cdot10^3$$

Heat load :

$$H_1 := \frac{Q_{tot1}}{3600}\cdot Cp_{meg1}\cdot\left[T_{1k} - T_{2k}\right]$$

$$H_1 = 7.38047161\cdot10^4$$

Appendix A5.I

Cutter 1	Cutter 2	Transport	Drying	Transport	Dosing	Transport	Mixing	Advantages	Disadvantages
Granulator to reduce crude PU size to appx. 30 mm.	Granulator to further reduce PU particle size from 30 mm to 10 mm.		Expansion of N2 and evaporating of H2O after freezing and grinding in Cryogen-cutter.	Blowing with N2 to avoid dust explosion or use of force of gravity dependant on type of dosing unit.	Coriolis principle dosing unit.	Blowing with N2 to avoid dust explosion or use of force of gravity.	Continuous mixing with MEG.	Continuous, no intermediate storage necessary. Moisture content reduction to appx 0%.	Expensive due to high N2 consumption.
		Use force of gravity or blower in granulator to fill dryer. (Dependant on granulator design)	Use a Nauta-mixer with a N2 flow as drying agent. Use a Nauta-mixer under vacuum conditions.	Batchwise transport out of dryer to mixer with screw-conveyor.	Weighing of mixing vessel.	Dosing unit and mixing vessel are combined.	High shear in-line. Semi-batch mixing		HOSOKAWA-MICRON: - Volume too large - Very long drying time. - Vacuum very high
		Use screw-conveyor for PU transport from storage after cutter 2 to mixing/drying vessel.	Inject dry PU into MEG and use a N2 bubble flow during mixing to absorb H2O (ICI batch principle)	Transport to mixer is not necessary. Mixer and dryer are combined in one vessel.	Weighing of mixing vessel.	Dosing init and mixing vessel are combined.	High shear in-line	Mixer and dryer combined in a single vessel.	Complex process control. Only few experimental data available. Moisture content still relatively high after drying.
Granulator to reduce crude PU size to appx. 30 mm.	Granulator to further reduce PU particle size from 30 mm to 10 mm.	Use force of gravity or use blower in granulator to fill dryer. (Dependant on granulator design)	Batchwise drying under high vacuum conditions (without mixing with MEG).	Screw-conveyor for PU transport to mixer.	Weighing of mixing vessel.	Dosing unit and mixing vessel are combined.	High shear in-line		- Very high vacuum - Very long drying time
		Use force of gravity or use blower in granulator to fill dryer. (Dependant on granulator design)	Drying takes place in flash vessel after mixing. (Pre-flash storage necessary)	Use pump to fill pre-flash storage.	Weighing of mixing vessel (Before pre-flash storage).	Dosing unit and mixing vessel are combined.	High shear in-line	80% of moisture can be removed. No complex equipment necessary.	Lot of equipment necessary.
		Use force of gravity or use blower in granulator to fill dryer. (Dependant on granulator design)	PU is mixed with excess MEG (1:10). Slurry is filtered. Then H2O is stripped from MEG. MEG and filtrate are mixed again.		Weighing of mixing vessel.	Dosing unit and mixing vessel are combined.	High shear in-line.		Only 50% of moisture content reduction. Filtration is hard.
		Use force of gravity or use blower in granulator to fill dryer. (Dependant on granulator design)	Continuous drying in moving bed dryer. Use N2 or dry air as drying agent.	Use a screw conveyor for transport to mixer.	Weighing of mixing vessel.	Dosing unit and mixing vessel are combined	High shear in-line.	High moisture content reduction. Continuous drying.	No data available on PU behaviour in dryer.
		Use force of gravity or use blower in granulator to fill dryer. (Dependant on granulator design)	Batchwise drying in packed bed dryer. Use N2 or dry air as drying agent.	Use a screw conveyor for transport to mixer.	Weighing of mixing vessel.	Dosing unit and mixing vessel are combined.	High shear in-line.	High moisture content reducution.	No data available on PU behaviour in dryer.
		Use force of gravity or use blower in granulator to fill dryer. Conveyor dryer takes care of homogeneous particle distribution.	Continuous drying in conveyor dryer. Use dry air as drying agent.	Use a screw conveyor for transport to mixer.	Weighing of mixing vessel.	Dosing unit and mixing vessel are combined.	High shear in-line.	Continuous drying.	Expensive dryer. Large dryer.

Cold liquid(MEG,DADPM) from extractor :

Flowrate liquid :

$Q_{meg} := 840.21$ [kg/hr]

$Q_{dadpm} := 8.3282$ [kg/hr]

$Q_{tot2} := Q_{meg} + Q_{dadpm}$

take ; $Cp_{meg2} := Cp_{meg1}$

Temperature cold liquid :

$t_2 := 180$ [C] ----<---- $t_1 := 80$ [C]

$t_{2k} := t_2 + 273$ $t_{1k} := t_1 + 273$

Heat be needed to heating cold liquid : [Watt]

$$H_2 := \frac{Q_{tot2}}{3600} \cdot Cp_{meg2} \cdot \left[t_{2k} - t_{1k}\right]$$

$$H_2 = 6.90135978 \cdot 10^4$$

$T_1 = 198$ --->--- $T_2 = 90$

$t_2 = 180$ ---<--- $t_1 = 80$

$$R := \frac{T_1 - T_2}{t_2 - t_1} \qquad S := \frac{t_2 - t_1}{T_1 - t_1}$$

$R = 1.08$ $S = 0.84745763$

$$\delta T_{lm} := \frac{\left[T_1 - t_2\right] - \left[T_2 - t_1\right]}{\ln\left[\frac{T_1 - t_2}{T_2 - t_1}\right]} \quad [C]$$

$\delta T_{lm} = 13.61038022$

From Appendix A of "Apparaten voor warmteoverdracht"[st42/i20], choose heat exchanger : 6 shell passes 12 or more tube passes
The coefficient factor F :

$$F := 0.825$$

The correction logarithmic mean temperature :

$$\delta T_{lmc} := F \cdot \delta T_{lm}$$

$$\delta T_{lmc} = 11.22856368$$

From table 12.1 ["Chemical Engineering vol.6"] :

$U := 200$ [W/m^2 C] (organic - organic)

Provisional area :

$$A := \frac{H_1}{\delta T_{lmc} \cdot U} \quad [m^2]$$

$$A = 32.86471811$$

Appendix A5.II

Calculation of the diffusion coefficient with two estimation correlations given in Reid[1]

These correlations are: 1 Tyn and Calus method
2 Nakanishi correlation

For both correlations there are several parameter needed voor MEG and water these are:

$M_{meg} := 62.069 \cdot 10^{-3}$ kg/mol $\qquad M_{h20} := 18.015 \cdot 10^{-3}$

$Tb_{meg} := 470.5$ K $\qquad Tb_{h20} := 373.2$ K

$Tc_{meg} := 645$ K $\qquad Tc_{h20} := 647.3$ K

$Pc_{meg} := 77$ bar $\qquad Pc_{h20} := 57.1$ bar

$\rho tb_{meg} := 971.463$ kg/m3 density of MEG at Tb

1. Tyn and Calus method

Molair volume of MEG at normal boilingpoint

$$Vb_{meg} := \frac{M_{meg}}{\rho tb_{meg}} \qquad Vb_{meg} = 6.389 \cdot 10^{-5} \text{ m3/mol}$$

Molair volume of water at normal boilingpoint from Reid[1] table 3-9

$Vb_{h20} := 18.7 \cdot 10^{-6}$ m3/mol

Calculation of surface tension for water and MEG at Tb using Brock and Bird correlation

$$\alpha c_{meg} := 0.9076 \cdot \left[1 + \frac{\left[\frac{Tb_{meg}}{Tc_{meg}}\right] \cdot \ln\left[\frac{Pc_{meg}}{1.013}\right]}{1 - \frac{Tb_{meg}}{Tc_{meg}}} \right] \qquad \alpha c_{meg} = 11.506$$

$$\alpha c_{h20} := 0.9076 \cdot \left[1 + \frac{\left[\frac{Tb_{h20}}{Tc_{h20}} \right] \cdot \ln \left[\frac{Pc_{h20}}{1.013} \right]}{1 - \frac{Tb_{h20}}{Tc_{h20}}} \right] \qquad \alpha c_{h20} = 5.89$$

The surface tensions are

$$\sigma 1_{meg} := Pc_{meg}^{\frac{2}{3}} \cdot Tc_{meg}^{\frac{1}{3}} \cdot \left[0.132 \cdot \alpha c_{meg} - 0.278 \right] \cdot \left[1 - \frac{Tb_{meg}}{Tc_{meg}} \right]^{\frac{11}{9}} \qquad \text{dyne/cm}$$

$$\sigma_{meg} := \sigma 1_{meg} \cdot 10^{-3} \qquad \sigma_{meg} = 0.039 \qquad \text{N/m2}$$

$$\sigma 1_{h20} := Pc_{h20}^{\frac{2}{3}} \cdot Tc_{h20}^{\frac{1}{3}} \cdot \left[0.132 \cdot \alpha c_{h20} - 0.278 \right] \cdot \left[1 - \frac{Tb_{h20}}{Tc_{h20}} \right]^{\frac{11}{9}} \qquad \text{dyne/cm}$$

$$\sigma_{h20} := \sigma 1_{h20} \cdot 10^{-3} \qquad \sigma_{h20} = 0.022 \qquad \text{N/m2}$$

The viscosity of MEG as a function of temperature is:

$$\eta_{meg}(T) := \exp \left[-6.98 + \frac{2.894 \cdot 10^{3}}{T} \right] \qquad \text{cP}$$

When water is the solute a dimer value of should be used

$$Vbdim := 2 \cdot Vb_{h20}$$

$$Vbdim = 3.74 \cdot 10^{-5} \qquad \text{m3/mol}$$

The diffusion coefficient at a temperature of ... K is

$$D1(T) := 8.93\cdot 10^{-8}\cdot\frac{\left[Vb_{meg}\cdot 10^{6}\right]^{0.267}}{\left[Vbdim\cdot 10^{6}\right]^{0.433}}\cdot\frac{T}{\eta_{meg}(T)}\cdot\left[\frac{\sigma 1_{meg}}{\sigma 1_{h20}}\right]^{0.15} \qquad \text{cm2/s}$$

$D_{T.C}(T) := 10^{-4}\cdot D1(T)$ cm2/s $\qquad D_{T.C}(273 + 140) = 2.469\cdot 10^{-9}$ m2/s

2. Nakanishi correlation

For this correlation we needed the Nakanishi values voor MEG en water when water is the solute and MEG the solvent

$I_{h20} := 2.8 \qquad S_{h20} := 1$ water is the solute

$A_{meg} := 2.0 \qquad S_{meg} := 1$ meg is the solvent

density of meg and water as a function

$\rho_{meg}(T) := 1.348\cdot 10^{3} - 0.788\cdot T$ kg/m3

$\rho_{h20}(T) := 1.211\cdot 10^{3} - 0.692\cdot T$ kg/m3

Molar volumes of MEG and water as a function of temperature

$$V_{meg}(T) := \frac{M_{meg}}{\rho_{meg}(T)} \qquad V_{h20}(T) := \frac{M_{h20}}{\rho_{h20}(T)}$$

The diffusion coefficient of water in MEG at a temperature of .... K is

$$D2(T) := \left[\frac{9.97\cdot 10^{-8}}{\left[I_{h20}\cdot V_{h20}(T)\cdot 10^{6}\right]^{\frac{1}{3}}} + \frac{2.40\cdot 10^{-8}\cdot A_{meg}\cdot S_{meg}\cdot V_{meg}(T)\cdot 10^{6}}{I_{h20}\cdot S_{h20}\cdot V_{h20}(T)\cdot 10^{6}}\right]\cdot\frac{T}{\eta_{meg}(T)}$$

$D_N(T) := 10^{-4} \cdot D2(T)$ $D_N(273.15 + 140) = 3.214 \cdot 10^{-9}$ m2/s

The two correlation estimates these diffusion coefficients at T= 140 °C

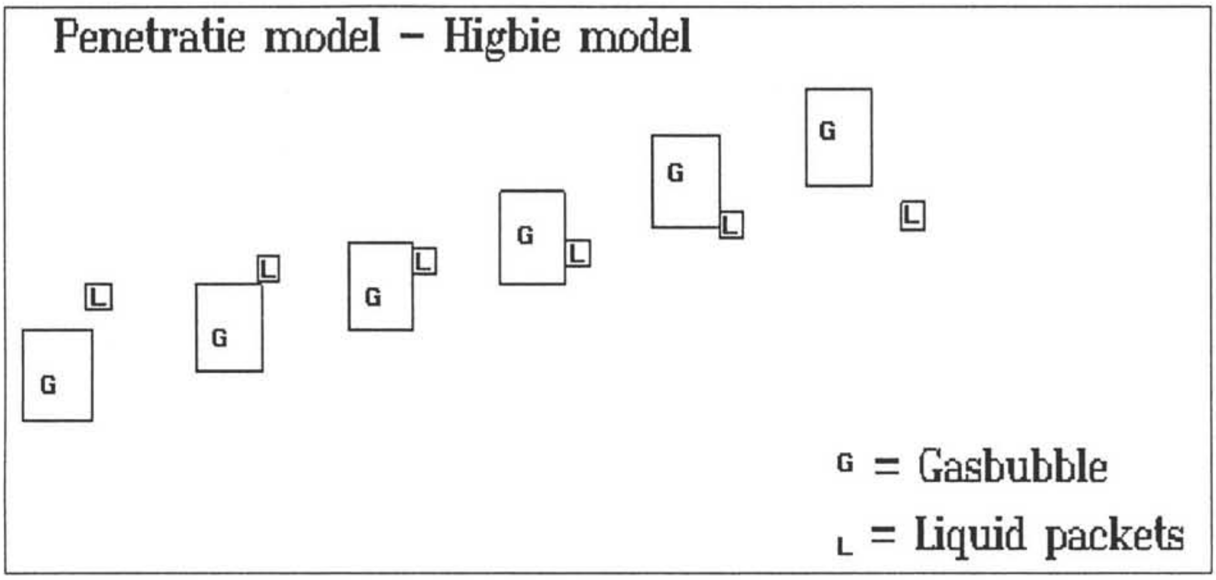
1. Tyn and Calus $D_{T.C}(273.15 + 140) = 2.476 \cdot 10^{-9}$ m2/s

2. Nakanishi $D_N(273.15 + 140) = 3.214 \cdot 10^{-9}$ m2/s

Appendix A5.III

```
** Structure and parameters of present model **
===============================================
Block     Type Input's/Comment                        Par1         Par2         Par3
===================================================================================
CO        CON                                         .0000
               ;[H20] in gasfeed
DB        CON                                        2.0000E-03
DIFF      CON                                        3.2140E-09
               ;diff.coeff at 140C
E         CON                                         .3000
FIV       CON                                         .8333
               ;gasflow m3/s
SPECS     CON                                         .5000
SURF      CON                                         .1000
               ;surface renewalrate
CGDANKWE  INT  FIV*(CO-CGDANKWE)/VG+KLDANKWE*S*(M*CLDANKWE-CGDANKWE)/VG
               ;gasphase Danckw mod                   .0000
CGFILM    INT  FIV*(CO-CGFILM)/VG+KLFILM*S*(M*CLFILM-CGFILM)/VG
               ;gasphase Filmmodel                    .0000
CGHIGBIE  INT  FIV*(CO-CGHIGBIE)/VG+KLHIGBIE*S*(M*CLHIGBIE-CGHIGBIE)/VG
               ;gasphase Higbie mod                   .0000
CLDANKWE  INT  -KLDANKWE*S*(M*CLDANKWE-CGDANKWE)/VL
               ;liq.phase danck mod                  1.000
CLFILM    INT  -KLFILM*S*(M*CLFILM-CGFILM)/VL
               ;liquidphase Filmmod                  1.000
CLHIGBIE  INT  -KLHIGBIE*S*(M*CLHIGBIE-CGHIGBIE)/VL
               ;liq.phase Higbi mod                  1.000
KLDANKWE  VAR  SQRT(DIFF*SURF)
               ;mtran.coef Danmode
KLFILM    VAR  DIFF/1E-04
               ;mtran.coef filmmode
KLHIGBIE  VAR  2*SQRT(DIFF/(PI*TET))
               ;mtran.coef higbmode
M         VAR  4*(106.122/28)*RHON2/(RHODEG)
               ;volum.distri.coeff
RHODEG    VAR  1.348E03-0.788*(273.15+140)
               ;density megphase
RHON2     VAR  28E-03*1E05/(8.3144*(273.15+140))
               ;density gasphase
S         VAR  6*VG/(DB)
               ;total bubble area
TET       VAR  DB/(4*FIV/(E*PI*2.3^2))
VG        VAR  E/(1-E)*VL
               ;volume of gas
VL        VAR  10000/RHODEG
               ;volume of liquid
PSI* cos
```

Appendix A5.IV



SURFACE RENEWAL MODEL [HIGBIE

- continuous refreshment of interface by packets of liquid
- all packets remain equal time θ at interface; e.g. $\theta = \frac{\text{length G-bubble}}{\text{rising velocity}}$
- during stay at interface transfer by "non stationary diffusion in semi-infinite mediu.

REALITY

- not all packets stay equally long at interface
- liquid moves
- liquid not infinite

Appendix A5.V

```
** Structure and parameters of present model **
================================================
Block     Type Inputs/Comment                         Par1          Par2          Par3
==========================================================================================
CO        CON                                         .0000
               ;[H20] in gasfeed
DB        CON                                        2.0000E-03
DIFF      CON                                        3.2140E-09
               ;diff.coeff at 140C
E         CON                                         .3000
FIV       CON                                         .2778
               ;gasflow m3/s
SPECS     CON                                         .5000
SURF      CON                                         .1000
               ;surface renewalrate
CGDANKWE  INT  FIV*(CO-CGDANKWE)/VG+KLDANKWE*S*(M*CLDANKWE-CGDANKWE)/VG
               ;gasphase Danckw mod                   .0000
CGFILM    INT  FIV*(CO-CGFILM)/VG+KLFILM*S*(M*CLFILM-CGFILM)/VG
               ;gasphase Filmmodel                    .0000
CGHIGBIE  INT  FIV*(CO-CGHIGBIE)/VG+KLHIGBIE*S*(M*CLHIGBIE-CGHIGBIE)/VG
               ;gasphase Higbie mod                   .0000
CLDANKWE  INT  -KLDANKWE*S*(M*CLDANKWE-CGDANKWE)/VL
               ;liq.phase danck mod                  1.000
CLFILM    INT  -KLFILM*S*(M*CLFILM-CGFILM)/VL
               ;liquidphase Filmmod                  1.000
CLHIGBIE  INT  -KLHIGBIE*S*(M*CLHIGBIE-CGHIGBIE)/VL
               ;liq.phase Higbi mod                  1.000
KLDANKWE  VAR  SQRT(DIFF*SURF)
               ;mtran.coef Danmode
KLFILM    VAR  DIFF/1E-04
               ;mtran.coef filmmode
KLHIGBIE  VAR  2*SQRT(DIFF/(PI*TET))
               ;mtran.coef higbmode
M         VAR  4*(106.122/28)*RHON2/(RHODEG)
               ;volum.distri.coeff
RHODEG    VAR  1.348E03-0.788*(273.15+140)
               ;density megphase
RHON2     VAR  28E-03*1E05/(8.3144*(273.15+140))
               ;density gasphase
S         VAR  6*VG/(DB)
               ;total bubble area
TET       VAR  DB/(4*FIV/(E*PI*2.3^2))
VG        VAR  E/(1-E)*VL
               ;volume of gas
VL        VAR  10000/RHODEG
               ;volume of liquid
PSI* cos
```

Appendix A5.VI

Calculation of the diffusion coefficient with two estimation correlations given in Reid, Prausnitz and Poling

These correlations are: 1 Tyn and Calus method
2 Nakanishi correlation

For both correlations there are several parameter needed voor DEG and water these are:

$M_{deg} := 106.122\cdot 10^{-3}$ kg/mol $M_{h20} := 18.015\cdot 10^{-3}$

$Tb_{deg} := 519.0$ K $Tb_{h20} := 373.2$ K

$Tc_{deg} := 681$ K $Tc_{h20} := 647.3$ K

$Pc_{deg} := 47$ bar $Pc_{h20} := 57.1$ bar

1. Tyn and Calus method

Molair volume of DEG at normal boilingpoint unknown an estimation is made with
1 Schroeder method :DEG = C4 H10 O3
C=7 H = 7 O = 7

$Vb_{deg1} := 4\cdot 7 + 10\cdot 7 + 3\cdot 7$ $Vb_{deg1} = 119$ cm3/mol

2 Le Bas method C = 14.8 H = 3.7 O =9.9 ether O =7.4 alcohol

$Vb_{deg2} := 4\cdot 14.8 + 10\cdot 3.7 + 9.9 + 2\cdot 7.4$ $Vb_{deg2} = 120.9$ cm3/mol

$$Vb_{deg} := \frac{Vb_{deg1} + Vb_{deg2}}{2}\cdot 10^{-6} \qquad Vb_{deg} = 1.2\cdot 10^{-4} \text{ m3/mol}$$

Molair volume of water at normal boilingpoint from Reid[1] table 3-9

$Vb_{h20} := 18.7\cdot 10^{-6}$ m3/mol

Calculation of surface tension for water and MEG at Tb using Brock and Bird correlation

$$\alpha c_{deg} := 0.9076\cdot\left[1 + \frac{\left[\frac{Tb_{deg}}{Tc_{deg}}\right]\cdot\ln\left[\frac{Pc_{deg}}{1.013}\right]}{1 - \frac{Tb_{deg}}{Tc_{deg}}}\right] \qquad \alpha c_{deg} = 12.065$$

$$\alpha c_{h20} := 0.9076\cdot\left[1+\frac{\left(\frac{Tb_{h20}}{Tc_{h20}}\right)\cdot\ln\left(\frac{Pc_{h20}}{1.013}\right)}{1-\frac{Tb_{h20}}{Tc_{h20}}}\right] \qquad \alpha c_{h20} = 5.89$$

The surface tensions are

$$\sigma 1_{deg} := Pc_{deg}^{\frac{2}{3}}\cdot Tc_{deg}^{\frac{1}{3}}\cdot\left(0.132\cdot\alpha c_{deg}-0.278\right)\cdot\left(1-\frac{Tb_{deg}}{Tc_{deg}}\right)^{\frac{11}{9}} \qquad \text{dyne/cm}$$

$$\sigma_{deg} := \sigma 1_{deg}\cdot 10^{-3} \qquad \sigma_{deg} = 0.026 \qquad \text{N/m2}$$

$$\sigma 1_{h20} := Pc_{h20}^{\frac{2}{3}}\cdot Tc_{h20}^{\frac{1}{3}}\cdot\left(0.132\cdot\alpha c_{h20}-0.278\right)\cdot\left(1-\frac{Tb_{h20}}{Tc_{h20}}\right)^{\frac{11}{9}} \qquad \text{dyne/cm}$$

$$\sigma_{h20} := \sigma 1_{h20}\cdot 10^{-3} \qquad \sigma_{h20} = 0.022 \qquad \text{N/m2}$$

The viscosity of DEG as a function of temperature using Lewis-Squire method:

viscosity known at 373 K $\quad nk := 1.25$ cp

$$\eta_{deg}(T) := \left(nk^{-0.2661}+\frac{T-373.15}{233}\right)^{\frac{-1}{0.2661}} \qquad \text{cp}$$

When water is the solute a dimer value of should be used

$$Vbdim := 2\cdot Vb_{h20}$$

$$Vbdim = 3.74\cdot 10^{-5} \qquad \text{m3/mol}$$

The diffusion coefficient at a temperature of 473.15 K is

$$D1(T) := 8.93\cdot 10^{-8}\cdot\frac{\left[Vb_{deg}\cdot 10^{6}\right]^{0.267}}{\left[Vbdim\cdot 10^{6}\right]^{0.433}}\cdot\frac{T}{\eta_{deg}(T)}\cdot\left[\frac{\sigma 1_{deg}}{\sigma 1_{h20}}\right]^{0.15} \qquad \text{cm2/s}$$

$D_{T.C}(T) := 10^{-4}\cdot D1(T)$ m2/s $\qquad D_{T.C}(273+200) = 1.058\cdot 10^{-8}$ m2/s

2. Nakanishi correlation

For this correlation we needed the Nakanishi values voor MEG en water when water is the solute and MEG the solvent

$I_{h20} := 2.8 \qquad S_{h20} := 1$ water is the solute

$A_{deg} := 2.0 \qquad S_{deg} := 1$ deg is the solvent

density of water as a function of temperature from Handbook

$\rho_{h20}(T) := 1.211\cdot 10^{3} - 0.692\cdot T$ kg/m3

$$V_{h20}(T) := \frac{M_{h20}}{\rho_{h20}(T)}$$ molaire volume of water in m3/mol

Molaire volume of deg with the Rackett technique using a known density at 293K ρ.293 = 1118 kg/m3

$$\phi(T) := \left[1-\frac{T}{Tc_{deg}}\right]^{\frac{2}{7}} - \left[1-\frac{293}{Tc_{deg}}\right]^{\frac{2}{7}} \qquad Vsr := \frac{M_{deg}}{1118}$$

$$V_{deg}(T) := Vsr\cdot 0.2489^{\phi(T)}$$

The diffusion coefficient of water in DEG at a temperature of 473 K is

$$D2(T) := \left[\frac{9.97\cdot 10^{-8}}{\left[I_{h20}\cdot V_{h20}(T)\cdot 10^{6}\right]^{\frac{1}{3}}} + \frac{2.40\cdot 10^{-8}\cdot A_{deg}\cdot S_{deg}\cdot V_{deg}(T)\cdot 10^{6}}{I_{h20}\cdot S_{h20}\cdot V_{h20}(T)\cdot 10^{6}}\right]\cdot\frac{T}{\eta_{deg}(T)}$$

$D_N(T) := 10^{-4}\cdot D2(T)$ $D_N(273.15 + 200) = 1.904\cdot 10^{-8}$ m2/s

The two correlation estimates these diffusion coefficients at T= 473 K

1. Tyn and Calus $D_{T.C}(273.15 + 200) = 1.06\cdot 10^{-8}$ m2/s

2. Nakanishi $D_N(273.15 + 200) = 1.904\cdot 10^{-8}$ m2/s

Appendix A5.VII

```
** Structure and parameters of present model **
===============================================
Block     Type Inputs/Comment               Par1        Par2        Par3
========================================================================
CO        CON                               .0000
               ;[H20] in gasfeed
DB        CON                              2.0000E-03
DIFF      CON                              1.5000E-08
               ;diff.coeff at 140C
E         CON                               .3000
FIV       CON                              2.7780E-04
               ;gasflow m3/s
SPECS     CON                                5.000
SURF      CON                               .1000
               ;surface renewalrate
CGDANKWE  INT  FIV*(CO-CGDANKWE)/VG+KLDANKWE*S*(M*CLDANKWE-CGDANKWE)/VG
               ;gasphase Danckw mod         .0000
CGFILM    INT  FIV*(CO-CGFILM)/VG+KLFILM*S*(M*CLFILM-CGFILM)/VG
               ;gasphase Filmmodel          .0000
CGHIGBIE  INT  FIV*(CO-CGHIGBIE)/VG+KLHIGBIE*S*(M*CLHIGBIE-CGHIGBIE)/VG
               ;gasphase Higbie mod         .0000
CLDANKWE  INT  -KLDANKWE*S*(M*CLDANKWE-CGDANKWE)/VL
               ;liq.phase danck mod         9.752
CLFILM    INT  -KLFILM*S*(M*CLFILM-CGFILM)/VL
               ;liquidphase Filmmod         9.752
CLHIGBIE  INT  -KLHIGBIE*S*(M*CLHIGBIE-CGHIGBIE)/VL
               ;liq.phase Higbi mod         9.752
KLDANKWE  VAR  SQRT(DIFF*SURF)
               ;mtran.coef Danmode
KLFILM    VAR  DIFF/1E-04
               ;mtran.coef filmmode
KLHIGBIE  VAR  2*SQRT(DIFF/(PI*TET))
               ;mtran.coef higbmode
M         VAR  40*(106.122/28)*RHON2/(RHODEG)
               ;volum.distri.coeff
RHODEG    VAR  1.348E03-0.788*(273.15+200)
               ;density megphase
RHON2     VAR  28E-03*1E05/(8.3144*(273.15+200))
               ;density gasphase
S         VAR  6*VG/(DB)
               ;total bubble area
TET       VAR  DB/(4*FIV/(E*PI*.45^2))
VG        VAR  E/(1-E)*VL
               ;volume of gas
VL        VAR  35/RHODEG
```

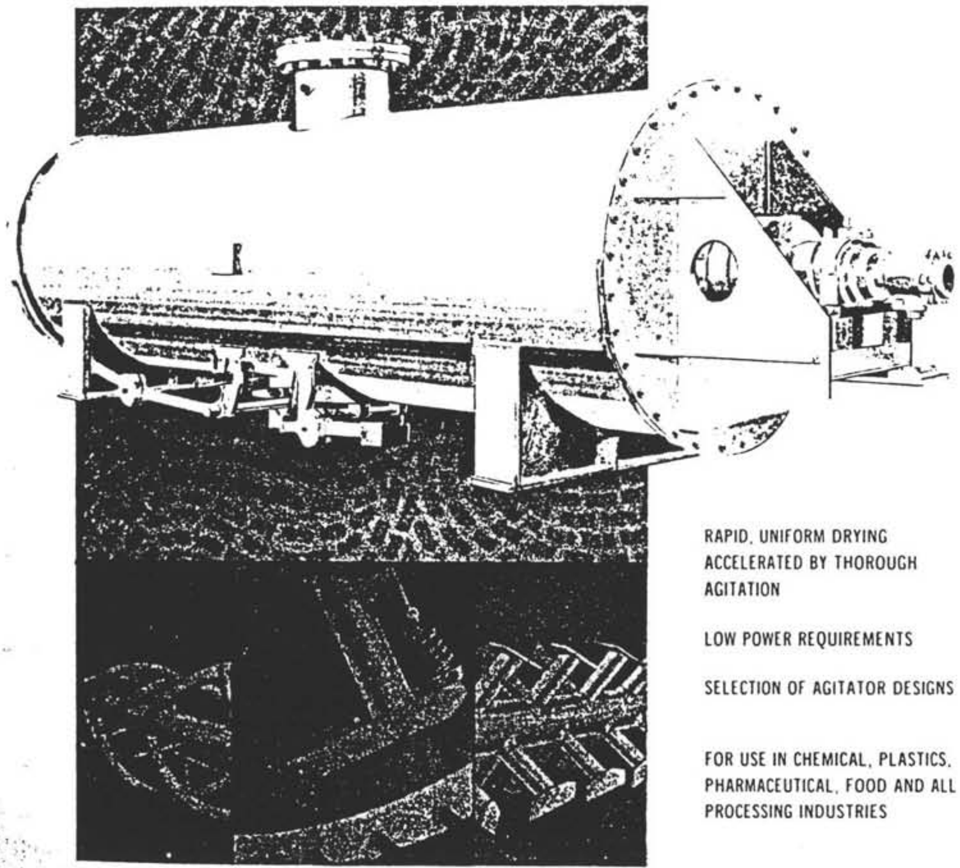
Appendix A5.VIII

TABLE OF SIZES . . . VACUUM ROTARY DRYERS

DRYER SIZE		TOTAL CAPACITY CU. FT.	WORKING CAPACITY 60% FULL CU. FT.	HEATING SURFACE 60% FULL SQ. FT.	*OVERALL DIMENSIONS			WEIGHT
FT. DIA.	LG.				WIDTH	LENGTH	HEIGHT	
2′	4′	12.2	7.3	10.6	3′	9′4″	4′	2800
2′	8′	24.2	14.5	21.2	3′	15′	4′	4300
3′	7′6″	49.1	29.4	47.4	4′	16′6″	7′	7400
3′	10′	65.6	39.3	63.0	4′	19′	7′	9500
3′	15′	98.2	58.9	96.5	4′	25′	7′	13,300
3′	20′	131.2	78.6	130.0	4′	30′	7′	16,000
4′	15′	167.6	100.6	139.6	5′	26′	8′3″	20,300
4′	20′	223.4	134.0	187.0	5′	31′	8′3″	25,100
5′	15′	246.2	147.7	183.7	6′	33′	8′	27,800
5′	20′	328.2	197.0	246.0	6′	38′	8′	34,500
5′	25′	400.2	240.1	307.2	6′	43′	8′	41,000
5′	30′	492.3	295.4	369.5	6′	48′	8′	49,000
6′4″	36′	893.6	536.2	584.4	7′	50′4″	11′	85,500

*Overall dimensions include drive, to these must be added foundation and operating space around dryer.

FIG. 3 Buflovak vacuum rotary dryers features and sizes. (From Blaw-Knox Buflovak Division Catalog 365-A.)



RAPID, UNIFORM DRYING ACCELERATED BY THOROUGH AGITATION

LOW POWER REQUIREMENTS

SELECTION OF AGITATOR DESIGNS

FOR USE IN CHEMICAL, PLASTICS, PHARMACEUTICAL, FOOD AND ALL PROCESSING INDUSTRIES

FIG. 4 Buflovak vacuum rotary dryers. (From Blaw-Knox Buflovak Division catalog 365-A.)

Appendix A5.IX

ADIABATIC FLASH P = 75 mm Hg T_{feed} = 150°C

```
 CHEMCAD 2 Version 2.4


 Filename : FLASH3.TLK

 FLOWSHEET SUMMARY

 Equipment             Stream Numbers

  1  FLAS            1  -2  -3

 Stream Connections

 Stream    Equipment
        From    To
    1            1
    2      1
    3      1

 COMPONENTS
   135   62         { Ethylene-Glycol    water }

 THERMODYNAMICS
 K-value model  :SRK
 Enthalpy model :SRK
 Water miscible

Adiabatic flash

                   Flash Summary

 Equipment name
         number            1
 Mode                      8    {adiabatic flash}
                       mmHg
 Parameter 1            75.0001    P_vessel

 Parameter 2            .000000
 Heat duty MJ   /hr      .000000
 K-values
  Ethylene-Glycol        .942510
```

```
 Water                   46.4204
```

ISOTHERMAL FLASH P = 75 mm Hg T_{feed} = 150°C ,T_{vessel}=140°C

CHEMCAD 2 Version 2.4

```
 Filename : FLASH3.TLK

 FLOWSHEET SUMMARY

 Equipment             Stream Numbers

  1  FLAS            1  -2  -3

 Stream Connections

 Stream    Equipment
        From    To
    1            1
    2       1
    3       1

 COMPONENTS
   135    62    { Ethylene-Glycol    water }

 THERMODYNAMICS
 K-value model  :SRK
 Enthalpy model :SRK
 Water miscible


Flash Summary

 Equipment name
        number             1
 Mode                      5    {isothermal flash}
                     deg C
 Parameter 1           140.000    Tvessel
                     mmHg
 Parameter 2           75.0001    Pvessel
 Heat duty MJ   /hr      730.866
 K-values
  Ethylene-Glycol        .971200
  Water                47.1568
```

Appendix A5.X

ADIABATIC FLASH WITH A FIXED PRESSURE OF P = 75 mmHG
variation of the input temperature

Feed contains: MEG	10000	kg/h	(161.111 kmol/h)
water	10	kg/h	(0.55494 kmol/h)
PU	1000	kg/h	

assume P = 75 mm HG

Tfeed łC	Tend łC	Top products V kmol/h	 MEG-Wat kmol/h	Bottom products B kmol/h	 MEG-Water kmol/h	removed waterfractio
151	139.51	6.9099	6.5353 0.37463	154.76	154.57 0.18031	0.675082
150	139.42	6.3739	6.0099 0.36404	155.29	155.1 0.1919	0.655999
149	139.39	5.8341	5.4908 0.35235	155.82	156.64 0.23011	0.634934
148	139.32	5.3147	4.9754 0.3393	156.35	156.13 0.21564	0.611417
147	139.24	4.7934	4.4695 0.32483	156.29	156.64 0.23011	0.585343
146	139.15	4.2419	3.9636 0.30836	157.4	157.15 0.24658	0.555664
145	139.05	3.7583	3.4684 0.28988	157.91	157.64 0.26506	0.522363

assume P = 76 mm HG

Tfeed łC	Tend łC	Top products V kmol/h	 MEG-Wat kmol/h	Bottom products B kmol/h	 MEG-Water kmol/h	removed waterfractio
151	139.73	6.5073	6.1413 0.366	155.16	154.97 0.18894	0.659531
150	139.66	5.9748	5.6203 0.35457	155.69	155.49 0.20037	0.638934
149	139.59	5.4445	5.1027 0.34183	156.22	156.01 0.21311	0.615977
148	139.52	4.9187	4.5911 0.32762	156.75	156.52 0.22732	0.59037
147	139.43	4.398	4.0863 0.31169	157.27	157.02 0.24325	0.561664

assume P = 74 mm HG

Tfeed łC	Tend łC	Top products		Bottom products		removed waterfractio
		V kmol/h	MEG-Wat kmol/h	B kmol/h	MEG-Water kmol/h	
151	139.24	6.776	6.4037 0.37287	154.89	154.71 0.18207	0.67191
150	139.18	6.2432	5.8812 0.36208	155.42	155.23 0.192886	0.652467
149	139.11	5.7111	5.361 0.35005	155.95	155.75 0.20489	0.630789

assume P = 50 mm HG

Tfeed łC	Tend łC	Top products		Bottom products		removed waterfractio
		V kmol/h	MEG-Wat kmol/h	B kmol/h	MEG-Water kmol/h	
151	132.16	10.605	10.161 0.44383	151.06	150.95 0.1111	0.79978
150	132.13	10.066	9.6272 0.43871	151.59	151.48 0.11623	0.790554
149	132.1	9.5317	9.0986 0.43319	152.13	152.01 0.12175	0.780607

At a fixed temperature T = 150 °C and changing the pressure in the vessel

P mmHg	Tend oC	Top products V kmol/h	 MEG-Wat kmol/h	Bottom products B kmol/h	 MEG-Water kmol/h	removed water- fraction	TOP H2O/MEG massratio
100	144.64	3.1674	2.9208 0.2466	158.5	158.19 0.30834	0.444372	0.024512
90	142.72	4.2542	3.9582 0.29596	157.41	157.15 0.25898	0.533319	0.021708
80	140.6	5.4554	5.4554 0.33891	156.21	155.99 0.21603	0.610715	0.018036
70	138.17	6.7985	6.422 0.37651	154.87	154.69 0.17843	0.67847	0.017021
60	135.39	8.3123	7.9029 0.40946	153.35	153.21 0.14548	0.737846	0.015042
50	132.13	10.066	9.6272 0.43871	151.59	151.48 0.11623	0.790554	0.01323
40	128.21	12.141	11.676 0.46474	149.52	149.43 0.090199	0.83746	0.011556

Appendix A5.XI

FLOW SUMMARIES CHEMCAD 2 - Version 2.4

Stream No.	1	2	3
Temp C	150.000	139.420	139.420
Pres mmHg	760.001	75.0001	75.0001
Enth MJ /hr	-4212.07	265.651	-4478.98
Vapor mole fraction	.000000	.997437	.000000
Total kgmol/hr	161.664	6.10565	155.556
Flowrates in kgmol/hr			
Ethylene-Glycol	161.109	5.74736	155.359
Water	.554936	.358288	.196649

FLOW SUMMARIES

Stream No.	1	2	3
Temp C	150.000	139.420	139.420
Pres mmHg	760.001	75.0001	75.0001
Enth MJ /hr	-4212.07	265.651	-4478.98
Vapor mass fraction	.000000	.997328	.000000
Total kg/hr	10009.7	363.184	9646.37
Flowrates in kg/hr			
Ethylene-Glycol	9999.71	356.727	9642.82
Water	9.99995	6.45634	3.54361

Appendix A5.XII

```
FLOW SUMMARIES                                   CHEMCAD 2 - Version 2.4

 Stream No.                1          2          3
 Temp C                150.000    140.000    140.000
 Pres mmHg              760.001    75.0001    75.0001
 Enth MJ   /hr        -4212.07    699.198   -4180.52
 Vapor mole fraction   .000000    .999922    .000000
 Total kgmol/hr        161.664    15.7748    145.890
 Flowrates in kgmol/hr
 Ethylene-Glycol        161.109    15.3109    145.799
 Water                .554936    .463947    .909884E-01
```

```
 FLOW SUMMARIES

 Stream No.                1          2          3
 Temp C                150.000    140.000    140.000
 Pres mmHg              760.001    75.0001    75.0001
 Enth MJ   /hr        -4212.07    699.198   -4180.52
 Vapor mass fraction   .000000    .989553    .000000
 Total kg/hr          10009.7    958.677    9051.10
 Flowrates in kg/hr
 Ethylene-Glycol        9999.71    950.317    9049.46
 Water                9.99995    8.36032    1.63961
```

Appendix A5.XIII

For the design of the flashvessel we used results from CHEMCAD

When the Feedtemperature is 150 o C and the vesselpressure is 75 mmHg (0.1 bar) The Top en bottomproducs are:

TOP			BOTTOM		
T_v	:= 139.24	oC	T_b	:= 139.24	oC
V	:= 6.3739	Kmol/h	B	:= 155.29	Kmol/h
MEG_v	:= 6.0099	Kmol/h	MEG_b	:= 155.1	Kmol/h
$H2O_v$	:= 0.32483	Kmol/h	$H2O_b$	:= 0.1909	Kmol/h

$Mmeg := 62$ kg/kmol $MH2O := 18$ kg/kmol $PU := 990$ kg/h

Total massflow of the gasphase en the liquidflow is

$Mgas := MEG_v \cdot Mmeg + H2O_v \cdot MH2O$ $Mliq := MEG_b \cdot Mmeg + H2O_b \cdot MH2O + PU$

$Mgas = 3.785 \cdot 10^2$ kg/h $Mliq = 1.061 \cdot 10^4$ kg/h

$Mg := \frac{Mgas}{3600}$ $Ml := \frac{Mliq}{3600}$

$Mg = 0.105$ kg/s $Ml = 2.947$ kg/s

At a temperature of 139 oC and a pressurre of 75 mmHg the densities are Assumed that the gas contains alone MEG

$\rho_{gas} := 0.238$ Kg/m3 $\rho_{liq} := 1024.49$ kg/m3

The design equtions for the vertical flash vessel are taken from CHEMICAL ENGINEERING VOLUME 6 page 364-365

The design gas velocity Uv

$$U_v := 0.035 \cdot \sqrt{\frac{\rho_{liq}}{\rho_{gas}}} \qquad U_v = 2.296 \text{ m/s}$$

Vapour volumetric flow- rate

$$\phi_v := \frac{Mg}{\rho_{gas}} \qquad \phi_v = 0.442 \text{ m3/s}$$

vessel Diameter $D := \sqrt{\frac{4 \cdot \phi_v}{\pi \cdot U_v}}$ $D = 0.495$ m

Liquid volumetric flow rate

$\phi l := \frac{Ml}{\rho_{liq}} \qquad \phi l = 2.877 \cdot 10^{-3}$ m3/s

Assume there is a liquid holdup of 600 s (10 minutes)

liquid height $\qquad H_{liq} := \phi l \cdot \frac{600}{\frac{\pi}{4} \cdot D^2} \qquad H_{liq} = 8.973$ m

The Feed liquid level distance is usely $H_f := 0.4$ m

The Height needed for the gas is

$H_{gas} := 1.5 \cdot D \quad H_{gas} = 0.742$ with a minimun of 1 m

Total height of the vessel $\quad Htot := H_{gas} + H_{liq}$

$Htot = 9.715$ m

$Par := \frac{Htot}{D} \qquad Par = 19.631$

For a good design the design parameter $\quad 3 < Par < 5$

To improve this design we take Par = 5 so Htot/D = 5

$H := 5 \quad Dnew := 1 \; Hl := 1$ guess values needed to solve the equations

Given

$$Dnew \approx \frac{H}{3}$$

$H \approx 1.3 \cdot Dnew + Hl$ $\qquad$ we take Hgas= 1.3 * Diameter

$$Hl \approx \phi l \cdot \frac{600}{\frac{\pi}{4} \cdot Dnew^2}$$

$$\begin{bmatrix} Dnew \\ H \\ Hl \end{bmatrix} := Find(Dnew, H, Hl) \qquad \begin{bmatrix} Dnew \\ H \\ Hl \end{bmatrix} = \begin{vmatrix} 1.089 \\ 3.268 \\ 1.852 \end{vmatrix}$$

$Ugas := \frac{\phi_v}{\frac{\pi}{4} \cdot Dnew^2} \qquad Ugas = 0.474$ m/s

$Hgas := H - Hl \quad Hgas = 1.416$

Appendix A5.XIV

The design of the horizontal flash vessel. There are no real design parameters for a horizontal flash vessel. A approximation is here given

$\phi_v = 0.442$ m3/s $\phi l = 2.877 \cdot 10^{-3}$ m3/s

again we assume a holdup of 10 minutes

Volume of the liquid in the vessel is

$V_{liq} := \phi l \cdot 600$ $V_{liq} = 1.726$ m3

Assume Height of the liquid is Hl=0.75*D $H(Dves) := 0.25 \cdot Dves$
with dves is diameter of the vessel

the cross area of the gas stream is

$$A_g(Dves) := \frac{\pi}{8} \cdot Dves^2 - H(Dves) \cdot \left[\frac{Dves^2}{4} - H(Dves)^2 \right]^{0.5} - \frac{Dves^2}{4} \cdot \mathrm{asin}\left[\frac{2 \cdot H(Dves)}{Dves} \right]$$

$$A_{liq}(Dves) := \frac{\pi}{4} \cdot Dves^2 - A_g(Dves)$$

For a good design is the ratio L/Dves = 5

$L(Dves) := 5 \cdot Dves$ with L is length of the vessel

$Vliq1(Dves) := A_{liq}(Dves) \cdot L(Dves)$

$Dves := 1$ a guess needed to solve the next equation

$Dves := \mathrm{root}\left[Vliq1(Dves) - V_{liq}, Dves \right]$ $Dves = 0.817$

The dimension of the horizontal flash vessel are

$Dves = 0.817$ m $L(Dves) = 4.087$ m

For the gas remains a volume of

$V_{gas} := \frac{\pi}{4} \cdot Dves^2 \cdot L(Dves) - V_{liq}$ $V_{gas} = 0.419$

$Vves := \frac{\pi}{4} \cdot Dves^2 \cdot L(Dves)$ $Vves = 2.145$

$V_{liq} = 1.726$

Appendix A5.XV

Calculation of the critical pressure to cause buckling Pc
Using the Brownell and Young correlation given in Coulson[17]

assuming : wall thickniss t is of the carbon steel vessel

$t := 15\cdot 10^{-3}$ m

Young modulus of carbon steel at 150 C is $E := 1\cdot 10^{11}$ N/m2
The assumed safty factor is 6 for external pressure vessels $S := 6$

Vertical vessel $D_v := 1.09$m $H := 3.3$ m

$Par1 := \frac{H}{D_v}$ $Par1 = 3.028$

$Par2 := \frac{D_v}{t}$ $Par2 = 72.667$ parameters needed for the graph of Collaps coefficient given here below

$Kc_{vertical} := 7$

$$Pc_{vertical} := \frac{Kc_{vertical}}{S}\cdot E\cdot\left[\frac{t}{D_v}\right]^3 \qquad Pc_{vertical} = 3.04\cdot 10^{5} \text{ N/m2}$$

With a safety factor of 6 is this critical pressure well above the design pessure of

$P_{design} := 1.10^{5}$

Horizontal vessel assume it is supported bij two ring with eff. length of L=3

$D_h := 0.8$ m $L_{eff} := 2.5$ m

$Par3 := \frac{L_{eff}}{D_h}$ $Par3 = 3.125$

$Kc_{horizontal} := 6$

$Par4 := \frac{D_h}{t}$ $Par4 = 53.333$

$$Pc_{horizontal} := \frac{Kc_{horizontal}}{S}\cdot E\cdot\left[\frac{t}{D_h}\right]^3 \qquad Pc_{horizontal} = 6.592\cdot 10^{5} \text{ N/m2}$$

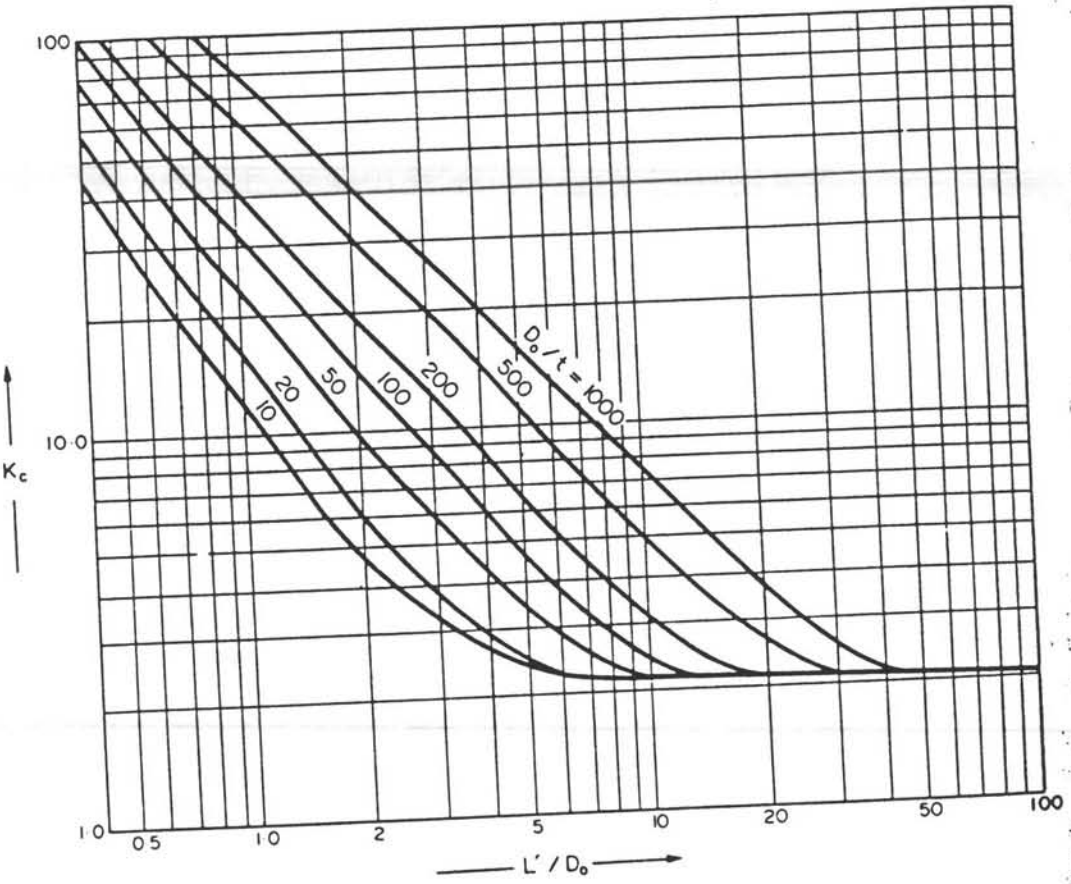
Also above the design pressure so a wall thickness of 15 mm is sufficient

!

F_{rp}

Packing type	Nominal size, mm	Wall thickness, mm	Outside diameter and length, mm	Approximate no. elements per m^3	Approximate weight per m^3, kg	Approximate surface area, m^2/m^3	Percent void space	Packing factor F_p, m^{-1}
Berl saddles, ceramic	6			3.78×10^6	900	900	60	2950
	13			590,000	865	465	62	790
	25			77,000	720	250	68	360
	38			22,800	640	150	71	215
	50			8,800	625	105	72	150
Intalox saddles, ceramic	6			4.15×10^6	865	984	75	2380
	13			730,000	720	625	78	660
	25			84,000	705	255	77	320
	38			25,000	670	195	80	170
	50			9,400	760	118	79	130
	75			1,870	590	92	80	70
Intalox saddles, metal	(No. 25)			168,400			97	135
	(No. 40)			50,100			97	82
	(No. 50)			14,700			98	52
	(No. 70)			4,630			98	43
Intalox saddles, plastic (polypropylene)	25			55,800	76	206	91	105
	50			7,760	64	108	93	69
	75			1,520	60	88	94	50
Pall rings, metal	16	26 gauge	16				92	230
	25	24	25	49,600	480	205	94	157
	38	22	38	13,000	415	130	95	92
	50	20	50	6,040	385	115	96	66
	90		90	1,170	270	92	97	53
Pall rings, plastic (polypropylene)	16		16	214,000	116	340	87	310
	25		25	50,100	88	205	90	170
	38		38	13,600	76	130	91	105
	50		50	6,360	72	100	92	82
	90		90	1,170	68	85	92	52
Raschig rings, ceramic	6	1.6	6	3.02×10^6	960	710	62	5250
	13	2.4	13	378,000	880	370	64	2000
	19	2.4	19	109,000	800	240	72	840
	25	3.2	25	47,700	670	190	74	510
	38	6.4	38	13,500	740	120	68	310
	50	6.4	50	5,800	660	92	74	215
	75	9.5	75	1,700	590	62	75	120
	100	9.5	100	700	580	46	80	
Raschig rings, steel	19	1.6	19	111,000	1500	245	80	730
	25	1.6	25	46,300	1140	185	86	450
	38	1.6	38	14,100	785	130	90	270
	50	1.6	50	5,900	590	95	92	187
	75	1.6	75	1,800	400	66	95	105
Hy-Pac, steel	(No. 1)		30	30,000	300	177	96	141
	(No. 2)		60	3,780	225	85	97	59
Levapacking†	(No. 1)			34,000	270	164		
	(No. 2)			10,500	210	118		
Low-density polyethylene Tellerettes	1			39,700	160	250	83	

Figure A5.XXVI.1


100
10·0
1·0
K_c
0·5
1·0
2
5
10
20
50
100
L' / D_o
10
20
50
100
200
500
$D_o / t = 1000$

Appendix A5.XVI

Packing Calculations

Strippers.

In 5.5.5.5 the calculation of a tray column is given in this appendix the calculations of random and structured packing column are given.

Random Packing column.

A packing with a nominal length of 25 mm gives the smallest HETP and therefor the smallest column. Raschig Rings can be used here.

The calculations for a random packing column are in the next tables:

Packing factor: $F_{\tau p}$ (see Fig.A5.XVI.1)	510
Pressure drop: $\Delta P \quad (mBar)$	300
Flow factor: F_{lg}	1.12
Capacity factor: $C_{\tau p}$ (see Figure A5.XVI.2)	0.24
Operating mass velocity of vapour: $m_g=\sqrt{\frac{C_{\gamma p}\rho_g(\rho_l-\rho_g)}{13F_{\gamma p}(\frac{\mu_l}{\rho_l})^{0.1}}}$	$\sqrt{\frac{0.24*0.82*(1100-0.82)}{13*510*(\frac{1.06}{1100})^{0.1}}}$
Diameter: $d=1.1284\sqrt{\frac{M_g}{m_g}}$	$1.1284\sqrt{\frac{44.4}{3600*0.26}}=0.25$

HETP	0.5
$H_p=N_{theoretisch}$ * HETP	0.5 * 43=21.5
$H_{column}=H_p+3.5$	25

So a random packing column will be 25 meters high with a diameter of 0.25 meter.

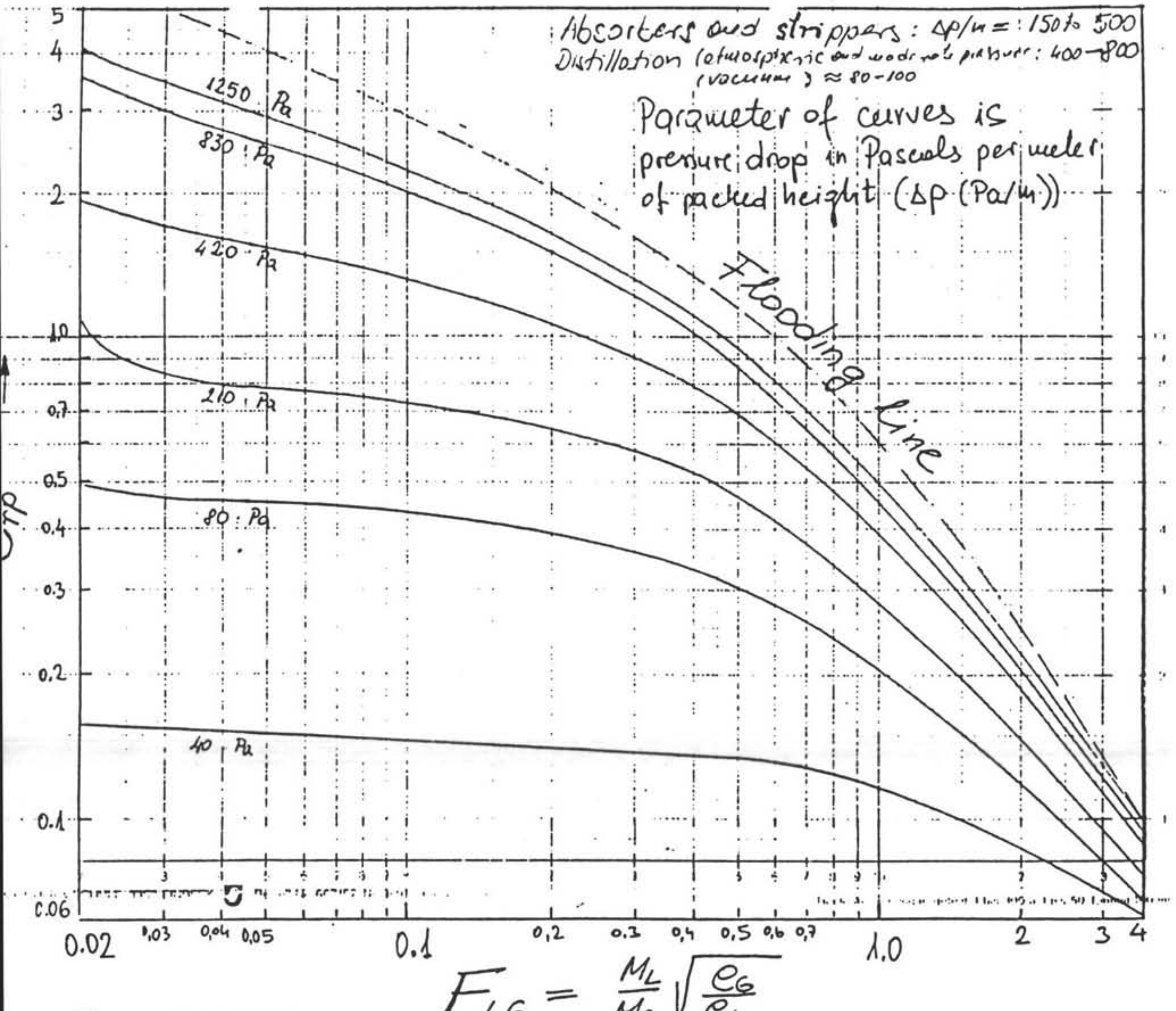


Figure A5.XXVI.2

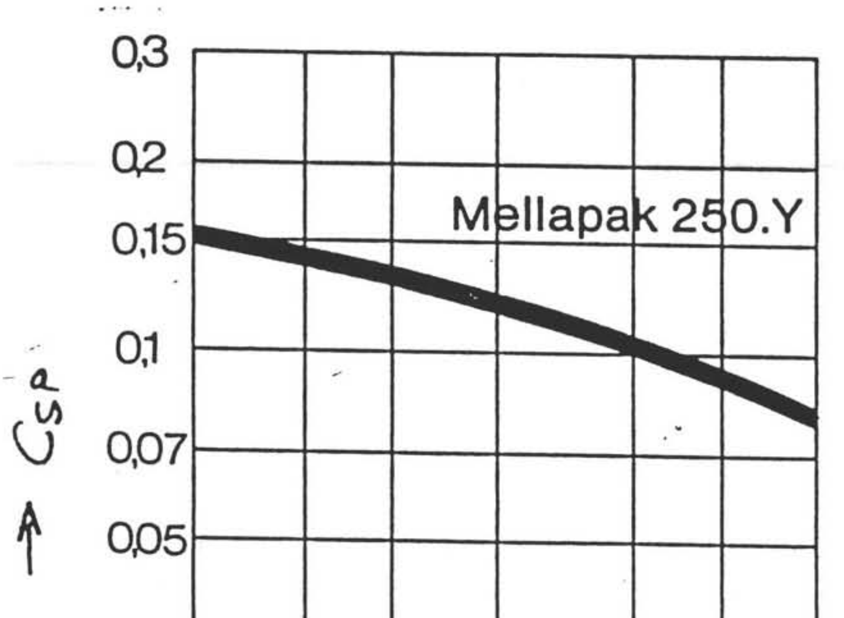


Figure A5.XXVI.3

Structured packing column.

The calculations for a structured packing column are in the next tables:

Flow factor:	0.12
Capacity factor: C_{sp} (see Figure A5.XVI.3)	0.01
Flooding velocity: $u_{g,\max}=C_{sp}\sqrt{\frac{\rho_l-\rho_g}{\rho_g}}$	$0.01\sqrt{\frac{1100-0.82}{0.82}}=0.37$
F-factor: $0.8\,u_{g,\max}\sqrt{\rho_g}$	$0.8*0.37\sqrt{0.82}=0.27$
<u>Diameter:</u> $d=1.1284\sqrt{\frac{M_g}{F\,(\rho_g)^{0.5}}}$	$1.1284\sqrt{\frac{44.4}{3600*0.27\,(0.82)^{0.5}}}=0.23$

HETP	0.33
$H_p=N_{theoretical}*$ HETP	43 * 0.33=14.3
$H_{column}=H_p+3.7$	18

So a structured packing column will be 18 meters high with a diameter of 0.23 meter.

Appendix A5.XVII

Cost Calculations

Costs of an apparat can be found in Webci[19] but not ever apparatus used in the plant is given in this book therefore cost calculations for these apparatus are given below:

Costs of the storage tanks.

For cost calculations of storage tanks the following formula is used:

$$C_{st}=C_{sto} * F_m * (I/336.2)$$

In which: $C_{sto}=\exp(7.483 + 0.6255 \ln V_{tank})$

F_m=material vessel=1 (carbon steel)

V_{tank}=tank volume

I=Chemical Engineering Plant Cost Index=

$$I=\frac{I_{equipment}+I_{tanks}}{2}=\frac{396.8+367.5}{2}=382.2$$

Calculations for each storage tank follow below:

-Crude MEG and MEG tank:

$C_{sto}=\exp(7.483 + 0.6255 \ln 37.5)=17{,}200$

$C_{st}=17{,}200 * 1 * (382.2/336.2)=19{,}500$ US$

So these 2 tanks together cost about Hfl.70,000.

-MEG with KAc tank:

For this tank the above mentioned formulas are not valid because it's volume is to small.

For this tank a assumed price is Hfl.2,000.

-Storage tank before the reactor:

$C_{sto}=\exp(7.483 + 0.6255 \ln 25)=13{,}300$

$C_{st}=13{,}300 * 1 * (382.2/336.2)=15{,}100$ US$

So this tank costs about Hfl.27,800.

All together these 4 storage tanks cost about Hfl.110,000.

Costs of the mixer unit.

For the mixer unit as mentioned in chapter 1 the following equipment is needed:

-Silverson's in line high shear mixer L700
-tank of 12.5 m^3 inclusive mixer
-about 5 m pipping

The cost calculation of the equipment follows below:

-High shear mixer L700 costs:Hfl.45,000

-Tank of 12.5 m^3 inclusive mixer:Hfl.56,000

-5 meter pipping with a diameter of 100 mm:about Hlf.150

So the total mixer unit will cost Hfl.101,000.

Costs of the heat exchanger.

For cost calculations of a heat exchanger the following formula is used:

$$C_{he}=C_{heo} * F_p * F_t * (I/336.2)$$

In which: $C_{heo}=\exp (a + b \ln A)$

a=7.085 (carbon steel)
b=0.656 (carbon steel)
A=heat transfer area=10
F_p=pressure factor=1.1 (10 bar < pressure < 20 bar)
F_t=heat exchanger type factor=0.8
I=Chemical Engineering Plant Cost Index=367.5

Filling in these formulas yields:

$$C_{heo}=\exp (7.085 + 0.656 \ln 10)=5408$$
$$C_{he}=5408 * 1.1 * 0.8 * (367.5/336.2)=5200 \text{ US\$}$$

So the heat exchanger costs about Hfl.9,600.

Costs of the flash vessel.

For cost calculations for a flash vessel the cost calculations of a pressure vessel is used.
For a pressure vessel the following formula is used:

$$C_{pv}=C_{pvo} * F_m * F_p * (I/336.2)$$

In which: C_{pvo}= (a + b * L) * $d^{1.1}$
a=1500
b=1100
L=hight of vessel=3.5 meter
D=diameter of vessel=1.2 meter
F_m=material factor=1 (carbon steel)
F_p=pressure factor=1.1 (0.1 bar under pressure)
I=Chemical Engineering Plant Cost Index=

$$I = \frac{I_{equipment} + I_{tanks}}{2} = \frac{396.8+367.5}{2} = 382.2$$

Filling in these formulas yields:

C_{pvo}= (1500 + 1100 * 3.5) * $1.2^{1.1}$=6538
C_{pv} = 6538 * 1 * 1.1 * (382.2/336.2)=8175 US$

So the flash vessel costs about Hfl.15,000.

Costs of the stripper.

For cost calculations of a stripper the following formula is used:

C_{co}=C_{pv} + C_{int}

In which: C_{pv}=C_{pvo} * F_m * F_p * (I_{pv}/336.2)
C_{pvo}= (a + b * H) * $D^{1.1}$
C_{int}=cost of column internals
a=1294
b=1141
H=hight of column
D=diameter of column
F_m=material factor=1 (carbon steel)
F_p=pressure factor=1 (1.0 bar)
I_{pv}=Chemical Engineering Plant Cost Index=382.2

Filling in these formulas for the Tray column yields:

C_{pvo}=(1294 +1141 * 8.5) * $0.22^{1.1}$=2080
C_{pv}=2080 * 1 * 1 * (382.2/336.2)=2360 US$

For a Tray column the next formula for C_{int} is used:

C_{int}=N_{tr} * C_{tr} * F_m * F_{nt} * F_{tt} * (I_{int}/336.2)

In which: C_{tr}=58.7 + 88.4 * D +52.9 * D^2
N_{tr}=number of trays=43

F_{nt}=number of trays factor=1
F_{tt}=tray type factor=1
I_{int}=Chemical Engineering Plant Cost Index=355.7

$C_{tr}=58.7 + 88.4 * 0.22 +52.9 * 0.22^2=81$
$C_{int}=43 * 81 * 1 * 1 * 1 * (355.7/336.2)=3685$ US$

And finally : $C_{co}=2360 + 3685=6000$ US$

So the Tray column costs about Hfl.11,000.

Similar calculations gave the costs of Random and structured Packing column:

Random Packing column : Hfl.25,000
Structured Packing column: Hfl.22,800

Appendix A5.XVIII

PU Drying Behaviour

To be able to set up models to describe drying behaviour of PU foam one first has to know how PU foam behaves. Unfortunately hardly any information on PU is available in the literature. The following assumptions have to be made:

- PU is non hygroscopic
- PU does not shrink during drying
- As can be seen in **Figure A5.XVIII.1** roughly drying takes place in two phases. First the constant drying rate period. In this period the surface of the PU is totally wet. Every time a molecule of moisture evaporates at the surfase it is replaced from within by another molecule. At a certain moment dry spots occur at the surface and the drying rate starts to decrease. It now depends on the speed of diffusion how fast the moisture is removed and evaporsted from the body. This is the falling rate period. Since the initial moisture content of the PU is very low ($x = 0.01$) drying take splace in the falling rate period.
- To describe the transfer of moisture from PU to gas the Fick's second law of diffusion is used.

Determination of Diffusivity Coefficient D:

No data are available on the diffusivity of PU foam. Since data are available on the diffusivity of plastics the D of PU is derived from these data.

$$D^{CO_2} = 2.5 x 10^{-7} e^{\left(-\frac{4378}{T}\right)}$$

$$D^{H_2O} \approx 10 \; x D^{CO_2}$$

$$D_{eff} = \frac{D_{H_2O} \rho_{plastic}}{\rho_{foam}} x E_{geo}$$

The geometry factor E_{geo} for closed foam is approximately 50. Assumed is that for open foam structures the geometry factor is 100.

To be able to use Fick's second law of diffusion Zuiderweg[10]:

$$N_a = K_g (c - c_g)$$

the mass transfer coefficient k_g has to be determined.
For a gas flow through a stack of spheres Zuiderweg[10] gives the following equation:

$$Sh = 1.25 \, Re^{0.59} \, Sc^{\frac{1}{3}}$$

From this equation k_g can be determined:

Sherwood number: $Sh = \frac{k_l d_p}{D}$

Reynolds number: $Re = \frac{\rho u d_p}{\eta}$

Schmidt number: $Sc = \frac{\eta}{\rho D}$

$$k_g = \frac{D}{d_c} (1.25 \, Re^{0.59} \, Sc^{\frac{1}{3}})$$

The amount of moisture contained by one sphere has to be estimated:

The initial moisture content of the PU: $X_0 = 0.01$ %
The volume of 1000 kg PU foam : V = 20.0 m^3
The volume of 1000 kg cut PU foam : V = 33.3 m^3
1 m^3 of cut PU foam contains 0.30 kg H_20.

Assumed is that 1 m^3 of PU theoretically contains 1.0 x 10e6 spheres with a 10 mm diameter: 1 sphere contains 3.0 x 10-7 kg H_2O.

Appendix A5.XIX

Program Moving Bed Dryer

```
{ start of TRKUSER.PAS  }
{ use with version 5.01 or 5.02 }

{$N+} { Change N+ into N- if you do NOT use double precision reals }

program TRKUser(input,output);

  {-------------------------------------------------------}
  { . All names of constants, variables, procedures etc. can  }
  {   be changed, except those starting with RK or TRK        }
  { . The user should change names like 'Robinson' into names }
  {   related with the problem to be solved!                  }
  {-------------------------------------------------------}

uses
  {$IFOPT N+} RKMath, TRKMath, {$ELSE} RKNorm, TRKNorm, {$ENDIF}
  crt; { add any other unit you want to use here }

const
  Comp    = 2;
  Tanks   = 10;
  AbsErr  = 1e-8;
  RelErr  = 1e-6;
  Spc     = ' ';

type
  ConcVector = array[1..Comp] of RKFloat;
  {------------------------------------------------------}
  { Above array MUST start with element 1 and end with Comp  }
  {------------------------------------------------------}

  ConcArray = array[0..Tanks] of ConcVector;
  {------------------------------------------------------}
  { Above array MUST start with element 0 and end with Tanks }
  {------------------------------------------------------}

var
  TimeStart, TimeEnd   : RKFloat;
  TimeFinal, TimeDelta : RKFloat;
  CStart, CEnd         : ConcArray;
  ErrCAbs, ErrCRel     : ConcVector;
```

```
  BEDROGRER              : TRKProblem;
{$F+} { This directive is a MUST for next procedure! }

procedure DerivatesTank(var CTankBef,CTank,dCdTime;
                        TankNumb : integer);

{$F-} { After the heading this directive is not needed anymore }

 var
   CBef : ConcVector absolute CTankBef;
   C    : ConcVector absolute CTank;
   dCdt : ConcVector absolute dCdTime;

   {-------------------------------------------------------}
   { Specify all 1..Comp differential equations in tank     }
   { numbered TankNumb, using:                              }
   { dCdt[i] := a function of (CBef[j], C[k], ..);          }
   { where  1 <= (i, j and k) <= Comp                       }
   { and C   [1..Comp] concentrations in tank  TankNumb      }
   {     CBef[1..Comp] concentrations in tank (TankNumb-1)  }
   {     dCdt[1..Comp] derivatives   in tank  TankNumb      }
   { N.B. TankNumb (value 1..Tanks) only added to enable    }
   {      intermediate output of results.                   }
   { ATTENTION: DO NOT CHANGE CBef OR C!                                }
   {-------------------------------------------------------}

 const

    rho = 1100;
     fi = 400/3600;          { m3/s gas debiet }
     D = 0.017;            { deeljes diameter}
   Avat = 5    ;          { vatdwarsoppervlak}
   Temp = 333 ;             {K gas temperatuur}
   Av   =500;            {totale grensvlak oppervlak}
   k3   = 0.05681818;         {((1-e)*(1-emf)*Rho)^-1}
   Tau  = 50/(fi*Tanks);      {s verblijjftijd in een tank}
 var
   ProdRate1, ProdRate2 : RKFloat;
   rhogas,v,Diff, Pvap, Re,Sc,kg, k1, k2,n : Real ;
 begin
    n:= (1.66+4.8e-03*(Temp-273.15))*1e-05;
    rhogas:=28*1e-3*1e05/(8.3144*Temp);
    v:=fi/(Avat);
    Diff:= 5.5e-03*exp(-4378/Temp);  { open cellen}
    Pvap:=exp(25.369-5152/Temp);
    re:= rhogas*v*D/n ;
    Sc:=n/(rhogas*Diff);
```

```
    kg:=(Diff/D)*(1.25*exp(0.59*ln(re))+exp(0.33*ln(Sc)));
    k1:= kg*Av;
    k2:=18*e-03*Pvap/(8.3144*Temp);

   ProdRate1  := +k1*(k2*C[1]-C[2]);     { water in PU}
   ProdRate2  :=ProdRate1 ;              {water in gas}
   dCdt[1] := -k3*ProdRate1;             {mbal water in pu}
   dCdt[2] := (CBef[2]-C[2])/(0.6*Tau)+ProdRate2/(0.6);  {mbal water in gas}
  end;

var
  Ti, Cj   : integer;
  FileName : string;
  OutFile  : text;
  Ready    : boolean;
begin
                                                  { main block }
  for Cj := 1 to Comp do begin
    ErrCAbs[Cj] := AbsErr;
    ErrCRel[Cj] := RelErr;
  end;
  TRKSetUpProblem(Comp, Tanks, DerivatesTank,
                 ErrCAbs, ErrCRel, Robinson);
  TimeStart := 0.0;
  CStart[0,1] := 0.01; CStart[0,2] := 0.0;
  for Ti := 1 to Tanks do  CStart[Ti,1] := 0.01;

   for Ti := 1 to Tanks do for Cj := 2 to Comp do CStart[Ti,Cj] := 0.0;
  TimeFinal := 1800; TimeDelta := 60; Ready := false;

  {-------------------------------------------------------}
  { The file created here can be used as input for RRGRAPH. }
  { If you only need output to the console delete all lines }
  { starting with   >>>                                     }
  {-------------------------------------------------------}

  {>>>} writeln('Hit RETURN for screen output only,'+
  {>>>}         ' use file name PRN for output to printer!');
  {>>>} write  ('File name for output to disk: ');
  {>>>} readln(FileName);
  {>>>} if FileName = '' then FileName := 'NUL';
  {>>>} assign(OutFile, FileName);
  {>>>} rewrite(OutFile);
  {>>>} writeln(OutFile,'Time':17,Spc,'C1':17,Spc,
                'C2':17);
   clrscr;
   repeat
```

```
    TimeEnd := TimeStart + TimeDelta;
    TRKFromToUsing(TimeStart, CStart, TimeEnd, CEnd, Robinson);
    writeln(’Time    : ’, TimeEnd);
    writeln(’C ’, Tanks:2, ’, 1 : ’, CEnd[Tanks,1]);
    writeln(’C ’, Tanks:2, ’, 2 : ’, CEnd[Tanks,2]);
    writeln;
    RKWriteSteps(output, Robinson);

    {>>>} { In next output values are separated by a space because }
    {>>>} { TURBO PASCAL has the nasty habit to concatenate values }
    {>>>} { if the last one of the two has a negative sign!        }
    {>>>} { e.g. 1.34E-0003-2.45E-0003                             }
    {>>>} { This causes programs like RRGRAPH to generate an error!}
    {>>>}   writeln(OutFile,TimeEnd:17,Spc,CEnd[Tanks,1]:17,Spc,
    {>>>}           CEnd[Tanks,2]:17); {,Spc,CEnd[Tanks,3]:17);}

    if abs(TimeFinal-TimeEnd)<0.5*abs(TimeDelta) then begin
      Ready := true;
    end else begin
      CStart    := CEnd;
      TimeStart := TimeEnd;
    end;
  until Ready or keypressed;

  {>>>} RKWriteSteps(OutFile, Robinson);
  {>>>} close(OutFile);
  repeat until keypressed
end.
{ end of TRKUSER.PAS }
```

Appendix A5.XX

```
{ start of TRKUSE2.PAS  }
{ use with version 5.01 or 5.02 }

{$N+} { Change N+ into N- if you do NOT use double precision reals }

program TRKUser(input,output);

  {---------------------------------------------------------}
  { . All names of constants, variables, procedures etc. can }
  {   be changed, except those starting with RK or TRK        }
  { . The user should change names like 'Robinson' into names }
  {   related with the problem to be solved!                  }
  {---------------------------------------------------------}

uses
  {$IFOPT N+} RKMath, TRKMath, {$ELSE} RKNorm, TRKNorm, {$ENDIF}
  crt; { add any other unit you want to use here }

const
  Comp    = 2;
  Tanks   = 10;
  AbsErr  = 1e-8;
  RelErr  = 1e-6;
  Spc     = ' ';

type
  ConcVector = array[1..Comp] of RKFloat;
  {--------------------------------------------------------}
  { Above array MUST start with element 1 and end with Comp  }
  {--------------------------------------------------------}

  ConcArray = array[0..Tanks] of ConcVector;
  {--------------------------------------------------------}
  { Above array MUST start with element 0 and end with Tanks }
  {--------------------------------------------------------}

var
  TimeStart, TimeEnd    : RKFloat;
  TimeFinal, TimeDelta : RKFloat;
  CStart, CEnd          : ConcArray;
  ErrCAbs, ErrCRel      : ConcVector;
  Robinson              : TRKProblem;

{$F+} { This directive is a MUST for next procedure! }

procedure DerivatesTank(var CTankBef,CTank,dCdTime;
```

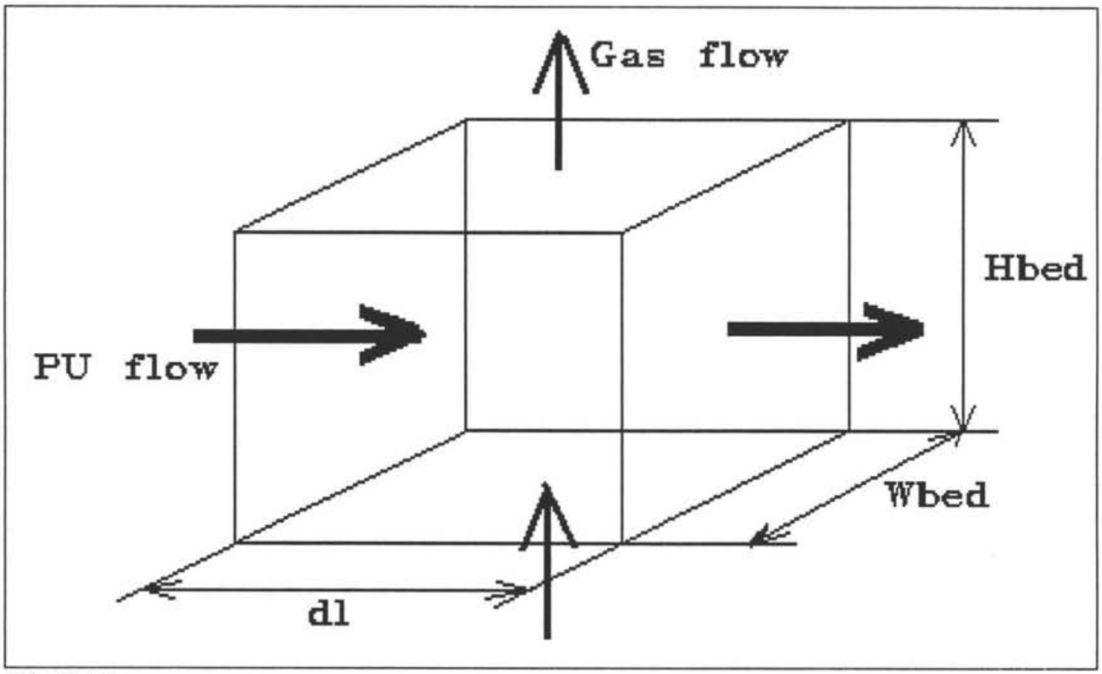
```
                          TankNumb : integer);

{$F-} { After the heading this directive is not needed anymore }

 var
   CBef : ConcVector absolute CTankBef;
   C    : ConcVector absolute CTank;
   dCdt : ConcVector absolute dCdTime;

   {----------------------------------------------------}
   { Specify all 1..Comp differential equations in tank     }
   { numbered TankNumb, using:                              }
   { dCdt[i] := a function of (CBef[j], C[k], ..);          }
   { where  1 <= (i, j and k) <= Comp                       }
   { and C    [1..Comp] concentrations in tank  TankNumb    }
   {      CBef[1..Comp] concentrations in tank (TankNumb-1) }
   {      dCdt[1..Comp] derivatives    in tank  TankNumb    }
   { N.B. TankNumb (value 1..Tanks) only added to enable    }
   {       intermediate output of results.                  }
   { ATTENTION: DO NOT CHANGE CBef OR C!                                }
   {----------------------------------------------------}

 const

    rho = 1100;
     fi = 250/3600;          { m3/s gas debiet }
     D = 0.017;            { deeljes diameter}
   Avat = 5    ;          { vatdwarsoppervlak}
   Temp = 333 ;             {K gas temperatuur}
   Av   =500;            {totale grensvlak oppervlak}
   k3   = 0.05681818;          {((1-e)*(1-emf)*Rho)^-1}
   Tau  = 32.129/(fi*Tanks);       {(Vreac/fi)/tanks  s}
 var
   ProdRate1, ProdRate2 : RKFloat;
   rhogas,v,Diff, Pvap, Re,Sc,kg, k1, k2,n : Real ;
 begin
    n:= (1.66+4.8e-03*(Temp-273.15))*1e-05;
    rhogas:=28*1e-3*1e05/(8.3144*Temp);
    v:=fi/(Avat);
    Diff:= 5.5e-03*exp(-4378/Temp);   { open cel}
    Pvap:=exp(25.369-5152/Temp);
    re:= rhogas*v*D/n ;
    Sc:=n/(rhogas*Diff);
    kg:=(Diff/D)*(1.25*exp(0.59*ln(re))+exp(0.33*ln(Sc)));
    k1:= kg*Av;
    k2:=18*e-3*Pvap/(8.3144*Temp);
```

```
    ProdRate1  := +k1*(k2*C[1]-C[2]);     { water in PU}
    ProdRate2  :=ProdRate1 ;              {water in gas}
    dCdt[1] := -k3*ProdRate1;              {mbal water in pu}
    dCdt[2] := (CBef[2]-C[2])/(0.6*Tau)+ProdRate2/(0.6);  {mbal water in gas}
  end;

var
  Ti, Cj   : integer;
  FileName : string;
  OutFile  : text;
  Ready    : boolean;
begin
                                                { main block }
  for Cj := 1 to Comp do begin
    ErrCAbs[Cj] := AbsErr;
    ErrCRel[Cj] := RelErr;
  end;
  TRKSetUpProblem(Comp, Tanks, DerivatesTank,
                  ErrCAbs, ErrCRel, Robinson);
  TimeStart := 0.0;
  CStart[0,1] := 0.01; CStart[0,2] := 0.0;
  for Ti := 1 to Tanks do  CStart[Ti,1] := 0.01;

   for Ti := 1 to Tanks do for Cj := 2 to Comp do CStart[Ti,Cj] := 0.0;
  TimeFinal := 1800; TimeDelta := 60; Ready := false;

  {--------------------------------------------------------}
  { The file created here can be used as input for RRGRAPH. }
  { If you only need output to the console delete all lines }
  { starting with   >>>                                    }
  {--------------------------------------------------------}

  {>>>} writeln(’Hit RETURN for screen output only,’+
  {>>>}         ’ use file name PRN for output to printer!’);
  {>>>} write  (’File name for output to disk: ’);
  {>>>} readln(FileName);
  {>>>} if FileName = ’’ then FileName := ’NUL’;
  {>>>} assign(OutFile, FileName);
  {>>>} rewrite(OutFile);
  {>>>} writeln(OutFile,’Time’:17,Spc,’C1’:17,Spc,
              ’C2’:17);
    clrscr;
    repeat
    TimeEnd := TimeStart + TimeDelta;
    TRKFromToUsing(TimeStart, CStart, TimeEnd, CEnd, Robinson);
    writeln(’Time     : ’, TimeEnd);
    writeln(’C ’, Tanks:2, ’, 1 : ’, CEnd[Tanks,1]);
```

```
    writeln(’C ’, Tanks:2, ’, 2 : ’, CEnd[Tanks,2]);
    writeln;

    RKWriteSteps(output, Robinson);

    {>>>} { In next output values are separated by a space because }
    {>>>} { TURBO PASCAL has the nasty habit to concatenate values }
    {>>>} { if the last one of the two has a negative sign!        }
    {>>>} { e.g. 1.34E-0003-2.45E-0003                             }
    {>>>} { This causes programs like RRGRAPH to generate an error!}
    {>>>}   writeln(OutFile,TimeEnd:17,Spc,CEnd[Tanks,1]:17,Spc,
    {>>>}             CEnd[Tanks,2]:17); {,Spc,CEnd[Tanks,3]:17);}

    if abs(TimeFinal-TimeEnd)<0.5*abs(TimeDelta) then begin
      Ready := true;
    end else begin
      CStart    := CEnd;
      TimeStart := TimeEnd;
    end;
  until Ready or keypressed;

  {>>>} RKWriteSteps(OutFile, Robinson);
  {>>>} close(OutFile);
  repeat until keypressed
end.

{ end of TRKUSER.PAS }
```

Appendix A5.XXI

Conveyor Dryer



Fig***

Before a model of the drying behaviour of the conveyor dryer can be derived a few assumptions have to be made:

- The moisture content of the drying agent is constant; $c_g = c$. Because the PU is constantly fed with fresh gas and the height of the PU bed (H_{bed}) is limited this assumption does not influence the outcome to a great extent.
- The PU throughput (PU flow) is constant; $\phi_m = c$.
- The mixture PU/H_2O behaves according to Raoult's Law; $yP = xP_{vap}$
- H_{2O} (g) behaves like an ideal gas; $PV = RT$.
- The PU mass flow is constant: 1000 kg/h = 0.278 kg/s.
- Gas flow should not exceed 0.30 m/s to avoid excessive whirling of the PU in the dryer.
- Width of the bed is the maximum width that is available on standard conveyor dryers. Other widths are 1.50 and 2.0 m.

Mass balance over volume:

$$\text{IN} \quad = \quad \text{OUT} \quad - \quad \text{TRANSFER}$$

$$\phi_m x_{l+\delta l} = \phi_m x_l - 1.0 x10^{-3} m_{wat} \; k_g (c_{H_2O} - c_g) \; A$$

No PU is in gas phase: $y_{PU} = 0$; $y_{H2O} = 1$
Combination of Raoult's law and the ideal gas law yields:

$$c_{H_2O} = \frac{xP_{vap}}{RT}$$

$$\phi_m \frac{\delta x}{\delta l} = -1.0 x10^{-3} m_{wat} \; k_g \left(\frac{xP_{vap}}{RT} - c_g \right) A_{spec}$$

$$\frac{\delta l}{\delta x} = - \frac{\phi_m RT}{1.0 x10^{-3} m_{wat} \; k_g (xP_{vap} - c_g RT) \; A_{spec}}$$

$$L_{bed} = \int_{x_o}^{x_e} \frac{-\phi_m RT}{1.0 x10^{-3} m_{wat} \; k_g A_{spec} \; H_{bed} \; W_{bed} \; (x P_{va}}$$

To determine D and kg the following Sherwood relationship is used Zuiderweg[10]:

$$Sh = 1.25 \, Re^{0.59} \, Sc^{\frac{1}{3}}$$

This relationship is applicable for stacks of spheres with a critical diameter of 1.77do. Therefore dPU = 0.017 m.

To meet the specifications (x0= 0.01 to xe =0.001) 9.0 kg/h H20 has to be removed from the PU. Once the length of the bed is known, together with gas velocity and bed width the gas flow and moisture concentration can be calculated. Since bed length also depends on moisture content of the gas this is an iterative process. In all calculations is assumed that the moisture content of the gas is constant over the control volume. Therefore this is a worst case analysis.

CALCULATION OF BED LENGTH OF CONVEYOR DRYER

GAS DATA

Drying agent: N2 gas

Gas temperature: $\mathrm{Temp} := 333.15$ (K)
Gas velocity: $\mathrm{Vgas} := 0.25$ (m/s)

Gas pressure: $\mathrm{Pgas} := 1.0 \cdot 10^{5}$ (N/m2)
Gas weight: $\mathrm{Mgas} := 28.0$ (kg/kmol)

Gas constant: $\mathrm{Rgas} := 8.3144$ (kJ/kmolK) (J/molK)

Gas density: $$\mathrm{rhogas} := \frac{\mathrm{Mgas} \cdot \mathrm{Pgas}}{\mathrm{Rgas} \cdot 1.0 \cdot 10^{3} \cdot \mathrm{Temp}} \quad \text{(kg/m3)}$$

$\mathrm{rhogas} = 1.01085136$

Gas viscosity: $$\mathrm{etha} := \left[1.66 + 4.8 \cdot 10^{-3} \cdot (\mathrm{Temp} - 273.15)\right] \cdot 1.0 \cdot 10^{-5}$$

$\mathrm{etha} = 1.948 \cdot 10^{-5}$

WATER DATA

Vapour pressure: $$\mathrm{Pvap} := \exp\left[25.369 - \frac{5152}{\mathrm{Temp}}\right] \quad \text{(N/m2)}$$

$\mathrm{Pvap} = 2.00201495 \cdot 10^{4}$

Moisture content PU: $\mathrm{x0} := 0.01$ (kg h20/kg PU)
$\mathrm{xe} := 0.001$

Water weight: $\mathrm{Mwat} := 18$ (kg/kmol)

PU DATA

PU throughput: $\mathrm{phi} := 0.278$ (kg/sec)

Specific PU area: $\mathrm{Aspec} := 500$ (m2/m3)

Diff. coeff. PU: $$\mathrm{Diff} := 5.5 \cdot 10^{-3} \cdot \exp\left[\frac{-4378}{\mathrm{Temp}}\right]$$

$\mathrm{Diff} = 1.07944377 \cdot 10^{-8}$

Height bed: $Hbed := 0.10$ (m)
Width bed: $Wbed := 3.0$ (m)

Particle diameter: $dPU := 0.017$ (m)

CALCULATIONS

Reynolds number: $$Re := \frac{rhogas \cdot Vgas \cdot dPU}{etha}$$

$$Re = 220.53995264$$

Schmidt number: $$Sc := \frac{etha}{rhogas \cdot Diff}$$

$$Sc = 1.78526063 \cdot 10^{3}$$

Transfer coeff.: $$kg := 1.25 \cdot \frac{Diff}{dPU} \cdot Re^{0.57} \cdot Sc^{\frac{1}{3}}$$

$$kg = 2.08616861 \cdot 10^{-4}$$

Moisture coeff gas: $cg := 11.05 \cdot 10^{-4}$ (mol/m3)

$$Lbed := \int_{x0}^{xe} \frac{-phi \cdot Rgas \cdot Temp}{1.0 \cdot 10^{-3} \cdot Mwat \cdot kg \cdot (x \cdot Pvap - cg \cdot Rgas \cdot Temp) \cdot Aspec \cdot Wbed \cdot Hbed} \, dx$$

$$Lbed = 167.51361786$$

$$cg := \frac{500}{Lbed \cdot Wbed \cdot Vgas \cdot 3600}$$

$$cg = 0.00110549$$

Appendix A5.XXII

Option 1 flashdrying

storage crude	36000
meg	18000
kac	18000
cutter 1	150000
cutter 2	250000
storage dry PU	27800
screw	13000
mixingvessel	56000
in line mixer	45000
weightunit	19000
pre reactor storage	27800
heat exchanger	9600
flash vessel	13500
condensor	10000
MEG stripper	11000
vacuum pomp	5000
gasdryer	40000
5 pumps	7000
total investment coast	756700

Option 2 cryogenic grounding

storage crude	36000
meg	18000
kac	18000
cutter 1	150000
cryogenic grounder	307800
expansion vessel	27800
screw	13000
mixingvessel	56000
in line mixer	45000
weightunit	19000
pre reactor storage	27800
heat exchanger	10000
N2 gas cooling installation	500000
total investment coast	1228400

Option 3 convey dryer

storage crude	36000
meg	18000
kac	18000
cutter 1	150000
cutter 2	250000
covey dryer	2500000
screw	13000
mixingvessel	56000
in line mixer	45000
weightunit	19000
pre reactor storage	27800
heat exchanger	10000
gas dryer	65000
4 pump	5400
total investment coast	3213200

Appendix A5.XXIII

List of companies

The next list provids the adresses of companies mentioned and/or recamended in preceding chapters.

Agglorex: Industriepark - Kerkhoven
B-3900 Lommel (Belgium)
Tel: (011) 54 25 32
Fax: (011) 54 57 92
Telex: 39206

Chris Heynen Systems B.V: Postbus 2050
8203 AB Lelystad (Netherlands)
Staalstraat 31
8211 AH Lelystad
Tel: +31 (0)3200 26849(33855)
Fax: +31 (0)3200 30844
Telex: (England)890511 oneone g
att: 38681001
Delair B.V: Etten-leur (Netherlands)
Tel: (01608) 85800

Dosco B.V: Postbus 102
3760 AC Soest (Netherlands)
Tel: (02155) 12734
Fax: (02155) 23206
Telex:43776

Hosokowa Micron: Haarlem (Netherlands)
Tel: (023) 311377/157511

Hydrochemie-Conhag B.V: Industrieweg 94
2651 BD Berkel en Rodenrijs (Netherlands)
Tel: (01891) 15822/15211
Fax: (01891) 15274

Kayser & Macky: Plaskylaan 144
B.8/9-1040 Brussel (Belgium)
Tel: (02) 735 40 72
Fax: (02) 734 76 00

Mica Machinery:
Mica House,Hyde Road,
Denton, Manchester, England M34 3AE
Tel: (061) 320 3356
Fax: (061) 320 3345
Telex:61556 caribag

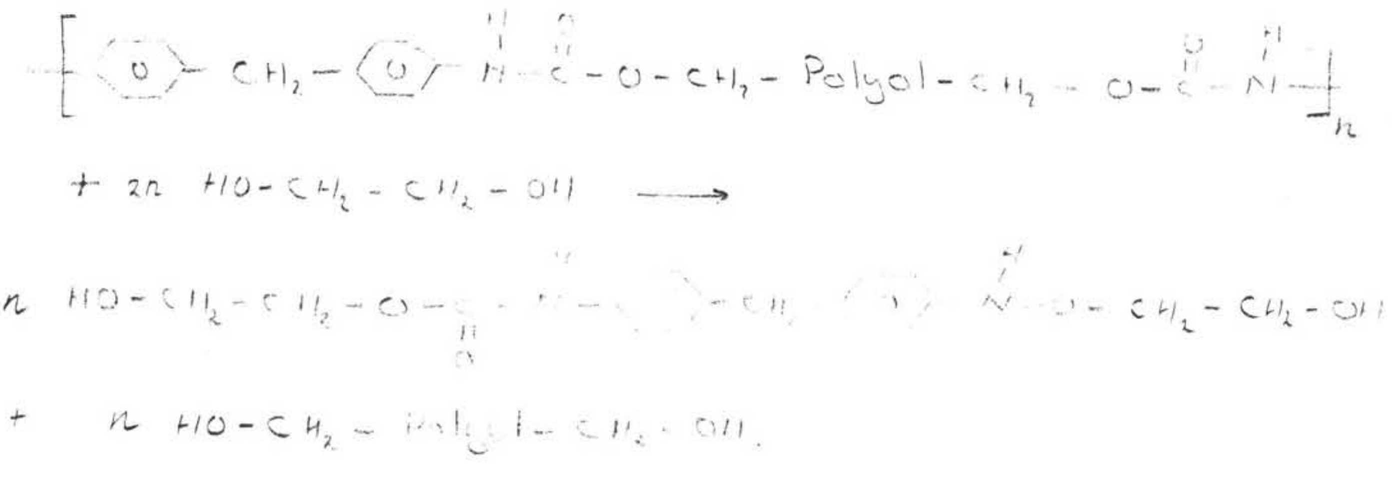
Silverson Machines Ltd:
Waterside, chesham, Bucks.,
England, HP5 1 PQ
Tel: (0494) 786331
Telex:837335 Silverson G.

UNTHA:
A.5431 Kuchl (austria)
Kellau 141
tel: (06244) 7770

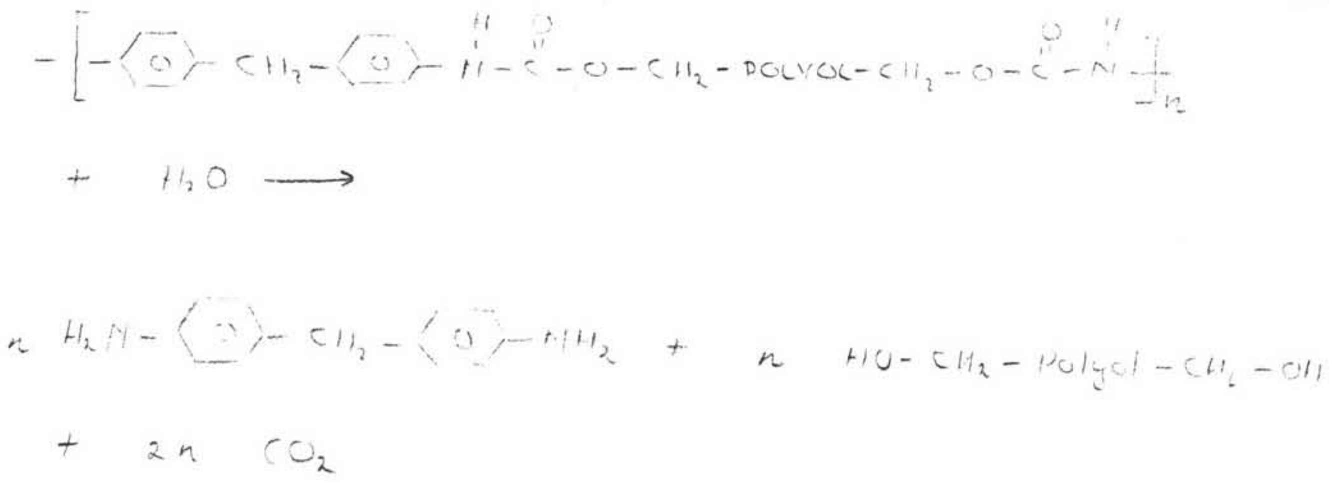
Van Vloten B.V:
Utrechtseweg 4a
3451 GG Vleuten (Netherlands)
Tel: (03407) 9299
Fax: (03407) 3904
Telex: 47.338

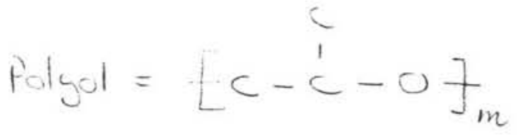
Appendix61: reactions in structure formula's.

Ⓐ GLYCOLYSIS: PU + MEG → RIGIDS + FLEXIBLES.



Ⓑ DADPM FORMATION: PU + H_2O → DADPM + CO_2 + FLEXIBLES





$$\text{Polyol} = \left[C - \overset{C}{\overset{|}{C}} - O \right]_m$$

Appendix 62: derivation of equation 4.

The mass of PU can be written as:

$$Mass\ PU = \rho\ \frac{1}{6}\ \pi\ d_p^3$$

the differential of PU is d(PU):

$$d(PU) = \rho\ \frac{1}{2}\ \pi\ d_p^2\ d(d_p)$$

this can be filled in in 1, and combined with 3 simultaniously, K_s and C_m are contracted to K_0:

$$\int_{d_0}^{d_p} d_p = \int_0^t 2*\frac{K_s}{\rho}\ d(t)$$

Solving this equation yields (4).

Appendix 63: determination of K_0.

According to ICI, a reaction time of 3 hours is required, at +/- 200 deg.C., for complete reaction of PU particles with initial diameter of 5E-4 m. These data are filled in (4) with d_p(3 h.)=0. K_0 is then readilly equated: 0.092 (kg/s m^2).

Appendix 64: derivation of equation 8.

A mass stream of PU particles as in (7) can be written as:

particle flux * mass of a particle * desity of a particle

mathematically:

$$\Phi_{mass,PU} = N^*\ (\frac{1}{6}\ \pi\ d_p^3)\ \rho$$

this can be filled in in the transport terms of (7) together with $N=N^*\tau$. This yields 8.

Appendix 5: derivation of equation 14.

As said in the text 11 is filled in in 9:

$$E(d_p) = \frac{-C\ A}{\tau} \exp(-\frac{A}{\tau}(d_p - d_0))$$

$$A = \frac{\rho}{2\ K_0}$$

Normalisation of E(d_p), with normalisation constant C, and d(d_p) from 12, means solving C from:

$$1 = \int_{-\infty}^{d_0} \frac{C\ (-A)}{\tau} \exp(-\frac{A}{\tau}\ (d_0 - d_p))\ d(d_p)$$

This yields C=-1, and (14) occurs.

Appendix 6: derivation of equation 16.

Again 11 is filled in, now in 15:

$$E(d_p) = C\ \frac{A\ (d_0 - d_p)}{\tau^2} \exp(\frac{-A\ (d_0 - d_p)}{\tau})$$

C is the normalisation constant to be calculated. Thus the next integral has to be solved:

$$1 = C \int_{-\infty}^{d_0} \frac{-A^2(d_0 - d_p)}{\tau^2} \exp(\frac{-A(d_0 - d_p)}{\tau})\ d(d_p)$$

C is -1, so 16 follows.

Appendix ~~6~~7: derivation of equation 17.

If a pulse of tracer is injected in the frist tank (resulting in a initial concentration C_0) of a two tanks in seris system the concentration in the effluent is:

$$C_1(t) = C_0 \exp(-\frac{t}{\tau_1})$$

So the mass balance across the second tank is:

$$\phi_v \, C_2(t) = \phi_v \, C_1(t) - V_{T,2} \frac{d(C_2(t)}{d(t)}$$

Combining the two above equations, and rewriting yields:

$$\frac{d(C_2(t))}{d(t)} = \frac{C_0}{\tau_2} \exp(-\frac{t}{\tau_1}) - \frac{C_2(t)}{\tau_2}$$

This can not be solved readilly, but Laplace transformation has to be applied:

$$s \, C_2(s) - C_2(0) = \frac{C_0}{\tau_2} (\frac{1}{s + \frac{1}{\tau_1}}) - (\frac{1}{\tau_2}) \, C_2(s)$$

rewriting this, thus solving, yields:

$$C_2(s) = (\frac{C_0}{\tau_2}) (\frac{1}{s + \frac{1}{\tau_1}}) (\frac{1}{s + \frac{1}{\tau_2}})$$

transforming this back to the t-domain yields:

$$E(t) = \frac{1}{\tau_1 - \tau_2} (\exp(\frac{-t}{\tau_1}) - \exp(\frac{-t}{\tau_2}))$$

Applying $C_0 = m/V_1$, and $C_2(t) = C_0 * E_2(t)$ yields 17.

Appendix 6.8: derivation of equation 18.

This is analogous to the derivation of 14 and 16. Again t and d(t) are taken from 11 and 12 and the same procedure is folloed. The value of the normalisation constant is again -1.

Appendix 6.9: determination of the volume flow.

The volume flow in the reactor, is determined by summing the volume flows of each relevant component (MEG, flexibles, rigids and PU). The pores of the MEG are assumed to be completly filed with MEG. As the conversion in the first reactor is approximately 100 %, the flow out consists of MEG, flexibles and rigids.

Volume flow in: PU: 980/1100 = 0.89
MEG: 10000/1110 = 9.01
Total volume flow in = 9.90, say 10 m_3/h.

Volume flow out: MEG: 9873/1110 = 8.89
flexibles: 714/1060 = 0.67
rigids: 351/1789 = 0.19
Total volume flow out = 9.76, say 10 m_3/h.

Although the volume flows are not completely constant, at this stage of design it can be assumed to be constant.

Appendix 6.10: derivation of equation 23.

Equation 16 is to be integrated according to 22. Filling in $E_2(d_p)$ yields:

$$\int_{10e-8}^{d_f} \frac{A_2}{\tau^2} (d_0 - d_p) \exp(\frac{-A}{\tau} d_0) \exp(\frac{A}{\tau} d_p) \, d(d_p) = 0.01$$

this can be rewritten, and solved:

$$\frac{0.01 \ \tau^2 \exp(\frac{A}{\tau} d_0)}{A^2} = \left[\frac{\tau \ d_0}{A} \exp(\frac{A}{\tau} d_p)\right]_{10e-8}^{d_0} - \left[\frac{\tau^2}{A^2} \exp(\frac{A}{\tau} d_p) \ (\frac{A}{\tau} d_p - 1\right]_{10e-8}^{d_0}$$

Filling in the boundaries and rewriting yields 23.

Appendix 11: Mercury file for tank volume and conversion calculation.

```
===== Problem: A:\TAU.BAK =====
{CALCULATION OF TANK VOLUMES}

o=0.092
0=5e-4
f=5e-5
hiv=10
ho=1100
=rho/(2*ko)

CALCULATION OF TAU TUBE AND TUBE VOLUME IN MODEL FOR 1-ST REAL REACTOR}
F=d0-(2*ko*tautube/rho)
autube=Vtube/phiv

CALCULATION OF (REAL) TANK VOLUMES, VOL1=VOL2}
 01=A*df/tau*(1-exp((A/tau)*(-df)))-((A*df/tau)-1)+exp((A/tau)*(-df))*(((A*(1e-
 )/tau)-1)
au=Vc/phiv


==== Solution =====
ariables:
 ko         = +0.092000  { = +23 / 250 }
 d0         = +0.00050000 { = +1 / 2000 }
 df         = +5.0000E-05 { = +1 / 20000 }
 phiv       = +10.000
 rho        = +1100.0
 A          = +5978.3     { = +137500 / 23 }
 tautube    = 0.1*Vtube
            = +2.6902
 Vtube      = +26.902     { = +2475 / 92 }
 tau        = 0.1*Vc
            = +2.0149
 Vc         = +20.149

rgest residual is 2.2E-11
thod: Iterative
meric processor: Emulator
```

```
==== Problem: C:\CALC\MERCURY\CONVERSI.EKA ====
CALCULATION OF CONVERSION IN (REAL) TANKS}

o=0.092
0=5e-4
f=5e-5
hiv=10
ho=1100
au=2.0149

CALCULATION OF AVERAGE DIAMETER IN EFFLUNET 1-ST REAL REACTOR}
av^3-df^3+(6*ko*tau/rho)*dav^2=0

CALCULATION OF CONVERSION IN (REAL) TANKS}
onv1=(d0^3-dav^3)/(d0^3)
onv2=1-conv1




==== Solution ====
ariables:
 ko        = +0.092000  { = +23 / 250 }
 d0        = +0.00050000 { = +1 / 2000 }
 df        = +5.0000E-05 { = +1 / 20000 }
 phiv      = +10.000
 rho       = +1100.0
 A         = +5978.3    { = +137500 / 23 }
 tau       = +2.0149    { = +20149 / 10000 }
 dav       = +1.1058E-05
 conv1     = +0.99999
 conv2     = +1.0817E-05

argest residual is 0
ethod: Exact
umeric processor: Emulator
```

Appendix 6.12: Calculation of the volume occupied by PU-particles

Determination of the particle flux:

N^*=phi,m/(rho*Vp)=1000*6/(1100*pi*(5e-4)^3)=1.4*10^{10}

Determination of the residence time in the tube:

Tau=(d_o-df)*rho/(2*k_o)=(5e^{-4}-5^{e-5})*1100/(2*0.092)=2.7 h
N, number of particles present: 2.7*1.4*10^{10}=3.78*10^{10}

Determination of the volume occupied by PU-particles:

V=pi/6*((do-df)/2)^3*N=pi/6*((5e^{-4}-4^{e-5})/2)^3*3,78*10^{10}=0.22 m^3

On the total volume of the first reactor of 22.6 m^3 this is about 1 vol%

Appendix 6.13: Calculation of the feed composition for the flash calculation for the reactor.

Basis is the mass balance, and reaction B.

DADPM formed: 31.5 kg/h, thus 0.161 kmol/h,
CO2 fomed: 2*0.161 kmol/h, thus 14.78 kg/h,
MEG fed to reactor: 10000 kg/h, thus 162 kmol/h.

Total moles/h: 161.483 kmol/h. So the mole fractions for the feed are:
zm = 162/162.483 = 0.99703
zc = 2*0.161/162.483 = 0.0019876
zd = 0.161/162.483 = 0.00099087

Appendix 6.14: MathCad file for determination of vapor fraction and composition

$$zd := 0.0009909$$

$$zc := 0.0019818$$

$$zm := 0.9970273$$

$$Pcs := 12203 \qquad Pms := 1.098 \qquad Pds := 0.003528$$

$$P := 3$$

$$Kc := \frac{Pcs}{P} \qquad Km := \frac{Pms}{P} \qquad Kd := \frac{Pds}{P}$$

$$yc(V) := \frac{zc \cdot Kc}{1 + V \cdot (Kc - 1)}$$

$$yd(V) := \frac{zd \cdot Kd}{1 + V \cdot (Kd - 1)}$$

$$ym(V) := \frac{zm \cdot Km}{1 + V \cdot (Km - 1)}$$

$$yt(V) := yc(V) + ym(V) + yd(V)$$

$$V := 0.00001$$

$$V := \mathrm{root}(yt(V) - 1, V)$$

$$yc(V) = 0.63473794 \qquad V = 0.0028771$$

$$yd(V) = 1.16865679 \cdot 10^{-6}$$

$$ym(V) = 0.36557884$$

$$yt(V) = 1.00031795$$

$$xc := \frac{yc(V)}{Kc} \qquad xd := \frac{yd(V)}{Kd} \qquad xm := \frac{ym(V)}{Km}$$

$$xc = 1.56044729 \cdot 10^{-4}$$

$$xd = 9.93755772 \cdot 10^{-4}$$

$$xm = 0.99884928$$

APPENDIX 6.1~~4~~5 Reactor Hardware:

Determination of the geometry for the reactors 1 and 2 :

$V_1 := 20$

$$T_1 := \left[\frac{4 \cdot V_1}{\pi \cdot 1.5}\right]^{\frac{1}{3}} \qquad T_1 = 2.57 \qquad Z_1 := 1.5 \cdot T_1 \qquad Z_1 = 3.855$$

$V_2 := 20$

$$T_2 := \left[\frac{4 \cdot V_2}{\pi \cdot 3}\right]^{\frac{1}{3}} \qquad T_2 = 2.04 \qquad Z_2 := 3 \cdot T_2 \qquad Z_2 = 6.12$$

$V_{1r} := V_1 + 0.5 \cdot \left[\frac{\pi}{4}\right] \cdot T_1^{\,2}$ $\qquad$ $V_{2r} := V_2 + 0.5 \cdot \left[\frac{\pi}{4}\right] \cdot T_2^{\,2}$

$V_{1r} = 22.594$ $\qquad$ $V_{2r} = 21.634$

$\eta_c := 0.15626 \cdot 10^{-3}$ Pas $\qquad$ $\eta_d := 1.3714 \cdot 10^{-3}$ Pas $\qquad$ $h := 0.083$

For the calculation of the viscosity of the mixture the following equation taken from Zuiderweg [2] is taken :

$$\eta_{mix} := \frac{\eta_c}{1 - h} \cdot \left[1 + \frac{1.5 \cdot \eta_d \cdot h}{\eta_c + \eta_d}\right] \qquad \eta_{mix} = 1.894 \cdot 10^{-4}$$

$\eta_{mix} := 0.19 \cdot 10^{-3}$ Pas $\qquad$ $\rho_{mix} := 1153$ kg/m3 $\qquad$ $t := 200$ c

$\phi_m := 11000$ kg/u $\qquad$ $Q_v := 26.5 \cdot 10^{-4}$ m3/s $\qquad$ $h := 0.083$

$P := 3$ bar (operating pressure for both vessels)

Reactor 1: propeller mixer with rotor speed N1=95 rpm. This is determined by the power equation with the power number taken from (1), see also figure 1.

$D_1 := \frac{T_1}{3}$ $D_1 = 0.857$ $N_1 := \frac{95}{60}$

$Re_1 := \frac{N_1 \cdot D_1^2 \cdot \rho_{mix}}{\eta_{mix}}$ $Re_1 = 7.052 \cdot 10^6 > 10^4$ (turbulent area)

power consumption : from figure 1 (1)) we find that Pv1=0.9.

$P_{v1} := 0.9$ $P_1 := P_{v1} \cdot \rho_{mix} \cdot N_1^3 \cdot D_1^5$ $P_1 = 1.901 \cdot 10^3$ Watts

R13

Reactor 2: here we wish to realize a dispersion with d3.2=1 mm,we use a turbine mixer with P2=0.1*V2 in Kw as a design rule for a turbine mixer the power number in the turbulent area Pv2=5. This is taken from figure 2 (1).

$D_2 := \frac{T_2}{4}$ $\quad D_2 = 0.51 \quad P_{v2} := 5 \quad \rho_c := 1160$

$N_2 := \frac{129}{60}$ (This implicates that a reduction of the number of revolutions from 129 rpm to 9 rpm is necessary in order to realize the required sauter diameter)

$N_3 := \frac{9}{60}$ (This number is found by iteration using the formula for the required sauter diameter)

$$\varepsilon := \frac{P_{v2} \cdot \rho_{mix} \cdot N_3^{\,3} \cdot D_2^{\,5}}{\rho_{mix} \cdot \left[\frac{\pi}{4}\right] \cdot T_2^{\,2} \cdot Z_2} \qquad \varepsilon = 2.91 \cdot 10^{-5} \qquad \sigma := 1.6 \cdot 10^{-3}$$

$$P_2 := P_{v2} \cdot \rho_{mix} \cdot N_2^{\,3} \cdot D_2^{\,5} \qquad P_2 = 1.976 \cdot 10^{3}$$

$$Re_2 := \frac{D_2^{\,2} \cdot N_3 \cdot \rho_{mix}}{\eta_{mix}} \qquad Re_2 = 2.367 \cdot 10^{5} \quad > \quad 10^{4} \quad \text{(turbulent area)}$$

For vessels with geometries other than standard the following correlation applies (taken from zuiderweg (2)), here we design the rotor on the required sauter diameter using the dissipated energy per unit mass which would follow from a number of revolutions of N3=9 rpm, which is the actual number of revolutions taking place in the second reactor:

$$d_{3.2} := 0.11 \cdot \left[\frac{\sigma^{0.6}}{\varepsilon^{0.4} \cdot \rho_c^{\,0.6}}\right] \cdot h^{0.5} \cdot \left[\frac{\eta_d}{\eta_c}\right]^{0.25} \qquad d_{3.2} = 0.001 \quad =1 \text{ mm}$$

With N3 = 9 rpm of a turbine mixer, the required sauter diameter is reached.

RAU

Determination of the necessary filter :

This determination is done on the basis of data handed out by Amafilter b.v., hereby expressing our gratitude towards this company for their cooperation and patience. Once the filter system was determined and belonging filters chosen, a check with Amafilter b.v. was made to see if the yielded results are applicable. The results have been found to be applicable.

The following filters have been chosen with the corresponding data given in table 1, 2 and 3 and figure 4 :

- Two basket wedge wired filters placed in duplo in order to make continouos operation possible, see table 3 for further details.
- Filter series type 72-S-I (S stands for screw on and I stands for carbon steel construction) with a connection measurement of 2 inch, see table 3 for further details.
- A mesh value of 325 corresponds with 50 micron meters (necessary filtering diameter), this data was supplied by phone.
- This mesh value corresponds with a correction factor for the pressure drop of c=3, this is found by iteration from the table in figure 3 where a mesh value of 100 corresponds with a correction factor of c=1.7.
- The corresponding pressure drop in meters water column (MWK) with 1 MWK=0.1 bar, is found from figure 3 for the serie nr. 72 with a flow rate of Qv=10 m3/hr (kapaciteit).
- The pressure drop read from figure 3 has to be corrected for the density. This is done by multiplying with the density of the mixture in kg/l.

The pressure drop is calculated as follows :

$\rho_m := 1.153$ kg/l $c := 3$ $dP_t := 0.29$ MWK $Q_v := 10$ m3/hr

$dP_r := \rho_m \cdot c \cdot dP_t \cdot 0.1$ $dP_r = 0.1$ bar

This answer is very small which is in accordance with the principle on which the reactor was designed, to reach a low value for the pressure drop for the filter system.

Approximate costing of the reactor hardware according to WEBCI/WUBO and offer by Amafilter b.v. and estimate by Gasequip b.v. for the extra costs for two turbines in serie in an agitated vessel:

Reactor1: agitated vessel with propellor	f 73,000
Reactor2: agitated column with two turbines and a motor reduction (1)	f 78,000
Isolation reactor1: for 200 C	f 12,650
Isolation reactor2: for 200 C	f 8,350
Filtersystem: 72-S-I in Duplo, includes 20 extra baskets for maintanance	f 9,500
1 pump: capacity 10 m3/hr	f 1,700
Total estimated costs reactor	f183,200

Material specification of reactor :

$P := 1.1 \cdot 3 \cdot 10^{-1}$ (operating pressure with a 10 percent safety margin)

$\sigma_d := 105$ (design stress at a temperature of 200 c for carbon steel)

$T_2 := 2.04 \cdot 10^3$ $T_1 := 2.57 \cdot 10^3$ (vessel diameter)

$e_2 := \dfrac{P \cdot T_2}{2 \cdot \sigma_d - P}$ $e_2 = 3.211$ (vessel thickness in mm according to BS 5500, British Standard for vessels subjected to internal pressure)

$e_1 := \dfrac{P \cdot T_1}{2 \cdot \sigma_d - P}$ $e_1 = 4.045$ (first reactor vessel thickness)

For practical design the minimum wall thickness for vessel diameters of 2-2.5 (m) is 9 mm, which is well above the calculated necessary wall thickness. This includes a corrosion allowance of 2 mm.

Appendix 6.16 Settler Calculation and Costs:

SETTLER CALCULATIONS AT T=200 c (473 K) AND P=2 bar :

$\rho_d := 1070$ kg/m3 $\rho_c := 1160$ kg/m3 (specific gravity)

$d\rho := \rho_c - \rho_d$ $d\rho = 90$ $T := 473$ K $P_{op} := 2$ bar

$\sigma_c := 0.0024$ N/m $\sigma_d := 0.0008$ N/m

$\sigma := \sigma_c - \sigma_d$ $\sigma = 0.0016$ (surface tension in N/m)

Calculation of viscosities with experimentally determined equations:

$$\eta_c := \exp\left[\left[\frac{6.69\cdot 10^3}{T}\right] - 16\right]\cdot 10^{-3} \qquad \eta_d := \exp\left[\left[\frac{5.92\cdot 10^3}{T}\right] - 12.2\right]\cdot 10^{-3}$$

$\eta_c = 1.56259563\cdot 10^{-4}$ Pas $\eta_d = 0.00137143$ Pas

$Q_c := 24.306\cdot 10^{-4}$ m3/s $Q_d := 2.207\cdot 10^{-4}$ m3/s

$Q_s := Q_d + Q_c$

$h := \left[\frac{Q_d}{Q_s}\right]$ m3/m3 (holdup)

$g := 9.8$ m/s2

minimum diameter :

$d_{min} := 150\cdot 10^{-6}$

sauter diameter :

$d_{3.2} := 1000\cdot 10^{-6}$

Calculation of the settler area with stokes-formula :

$$u_t := g\cdot d\rho\cdot\frac{d_{min}^{\,2}}{18\cdot\eta_c} \qquad u_t = 0.00705557$$

$$A_s := 4.96\cdot 10^{-5}\cdot\left[\frac{\eta_c}{d_{min}^{\,2}}\right] \qquad A_s = 0.34446553$$

Determination of the necessary height of the settler :

$$\theta_c := 31\cdot 10^3 \cdot \frac{\sigma^{0.24}\cdot \eta_d}{d\rho^{1.24}\cdot g^{1.24}\cdot d_{3.2}^{1.48}} \qquad \theta_c = 55.60886933$$

$A_c := 1.2$ $\quad$ $c := 0.025$ $\quad$ (m/s)^2/3 $\quad$ (for industrial systems)

$$dH1_c := \frac{Q_d\cdot \theta_c^{\frac{1}{3}}}{c\cdot h\cdot A_c} \qquad dH_c := \left[dH1_c\right]^3 \qquad dH_c = 0.03838459$$

$$H_s := 10\cdot dH_c \qquad H_s = 0.38384591$$

Decanter geometry :

$$D := \left[0.215\cdot A_c\right]^{0.5} \qquad D = 0.507937 \qquad r := \left[\frac{D}{2}\right]$$

$$L := 5\cdot D \qquad L = 2.53968502 \qquad t := \frac{D}{6} \qquad t = 0.08465617$$

$$I := 2\cdot\left[\left[\frac{D}{2}\right]^2 - t^2\right]^{0.5} \qquad A_r := I\cdot L \qquad A_s = 0.34446553$$

$$I = 0.4788876 \qquad A_r = 1.21622366$$

$$A_1 := 0.5\cdot\pi\cdot r^2 - t\cdot\left[r^2 - t^2\right]^{0.5} - r^2\cdot \operatorname{asin}\left[\frac{t}{r}\right] \qquad A_1 = 0.05912649$$

$$A_h := \pi\cdot r^2 - A_1 \qquad P := 2\cdot r\cdot \operatorname{acos}\left[\frac{t}{r}\right] \qquad V_s := \left[\frac{\pi}{4}\right]\cdot D^2\cdot L$$

$$A_h = 0.14350624 \qquad P = 0.62524984$$

$$D_l := \left[4 \cdot \frac{A_l}{I + P} \right] \qquad D_h := \left[4 \cdot \frac{A_h}{I + 2 \cdot \pi \cdot r - P} \right]$$

$$D_l = 0.21419974 \qquad D_h = 0.39605165$$

Check on coalescence time (to pass through dispersion-band):

$$t_c := 0.5 \cdot \left[dH_c \cdot \frac{A_c}{Q_d} \right] \qquad t_c = 104.35321491$$

Determination of residence time in settler :

$$V_s := \frac{\pi}{4} \cdot 5 \cdot D^3 \qquad V_s = 0.5146233$$

$$t_s := \frac{V_s}{Q_s} \qquad t_s = 194.1022514$$

Light phase (dispers) :

$$V_l := \frac{Q_d}{Q_s} \cdot V_s \qquad V_l = 0.04283837$$

$$t_{vl} := \frac{V_l}{Q_d} \qquad t_{vl} = 194.1022514$$

Heavy phase (continues) :

$$V_h := \frac{Q_c}{Q_s} \cdot V_s \qquad V_h = 0.47178493$$

$t_{vh} := \frac{V_h}{Q_c}$ $\qquad t_{vh} = 194.1022514$

Light phase outlet design :

velocity through outlet < 3m/s $\qquad v_l := 3$

$A_{ol} := \frac{Q_d}{v_l}$ $\qquad A_{ol} = 7.35666667 \cdot 10^{-5}$ $\qquad$ ϕ.ml=850 kg/u (mass flow rate light phase)

$d_{ol} := \left[4 \cdot \frac{A_{ol}}{\pi}\right]^{0.5}$ $\qquad d_{ol} = 0.00967822$ $\qquad$ ϕ.mh=10150 kg/u (mass flow rate heavy phase)

heavy phase outlet design : $v_h := 3$

$A_{oh} := \frac{Q_c}{v_h}$ $\qquad A_{oh} = 8.102 \cdot 10^{-4}$

$d_{oh} := \left[4 \cdot \frac{A_{oh}}{\pi}\right]^{0.5}$ $\qquad d_{oh} = 0.0321182$

Feed arrangement :

$\rho_c \cdot v_h^2 = 1.044 \cdot 10^4$ $\qquad \rho_d \cdot v_l^2 = 9.63 \cdot 10^3$

$N_{rel} := \frac{u_t \cdot D_l \cdot \rho_d}{\eta_d}$ $\qquad N_{rel} = 1.17912565 \cdot 10^3$

$N_{reh} := \frac{u_t \cdot D_h \cdot \rho_c}{\eta_c}$ $\qquad N_{reh} = 2.07441288 \cdot 10^4$

Results of the settler calculations :

$d_{min} = 1.5\cdot 10^{-4}$ $d_{3.2} = 1\cdot 10^{-3}$ $T = 473$ (t=180 c) $Q_d = 2.207\cdot 10^{-4}$ $\eta_d = 0.00137143$

$Q_c = 0.0024306$ $\eta_c = 1.56259563\cdot$

$u_t = 0.00705557$ (settling velocity, m/s)

$A_s = 0.34446553$ (necessary settler area, m2)

$A_c = 1.2$ (defined decanter cross section area, m2)

$A_r = 1.21622366$ (real settling area, m2)

$V_s = 0.5146233$ (decanter volume, m3)

$D = 0.507937$ (decanter diameter, m)

$L = 2.53968502$ (decanter length, m)

$t_s = 194.1022514$ (residence time in settler, seconds)

$\theta_c = 55.60886933$ (coalescence time, seconds)

$t_c = 104.35321491$ (time to pass through dispersion band, seconds)

$dH_c = 0.03838459$ (height of coalescence layer, m)

$D_l = 0.21419974$ (hydraulic diameter light phase, m)

$D_h = 0.39605165$ (hydraulic diameter heavy phase, m)

Cost calculation taken from WEBCI/WUBO, november 1989 :

Cilindrical tank with rounded fronts and a wall thickness off 8 mm, a volume of 1 m3, a lenght of 1,1 m and a diameter of 1 m cost f 11,000

In this case the volume Vs = 0.51 with a lenght of 2.5 m and a diameter of 0.5 m, meaning a correction of about 0.65 for the volume (based on extrapolion) and 1.1 for L/D.

This leads to a total estimate of f 8,000

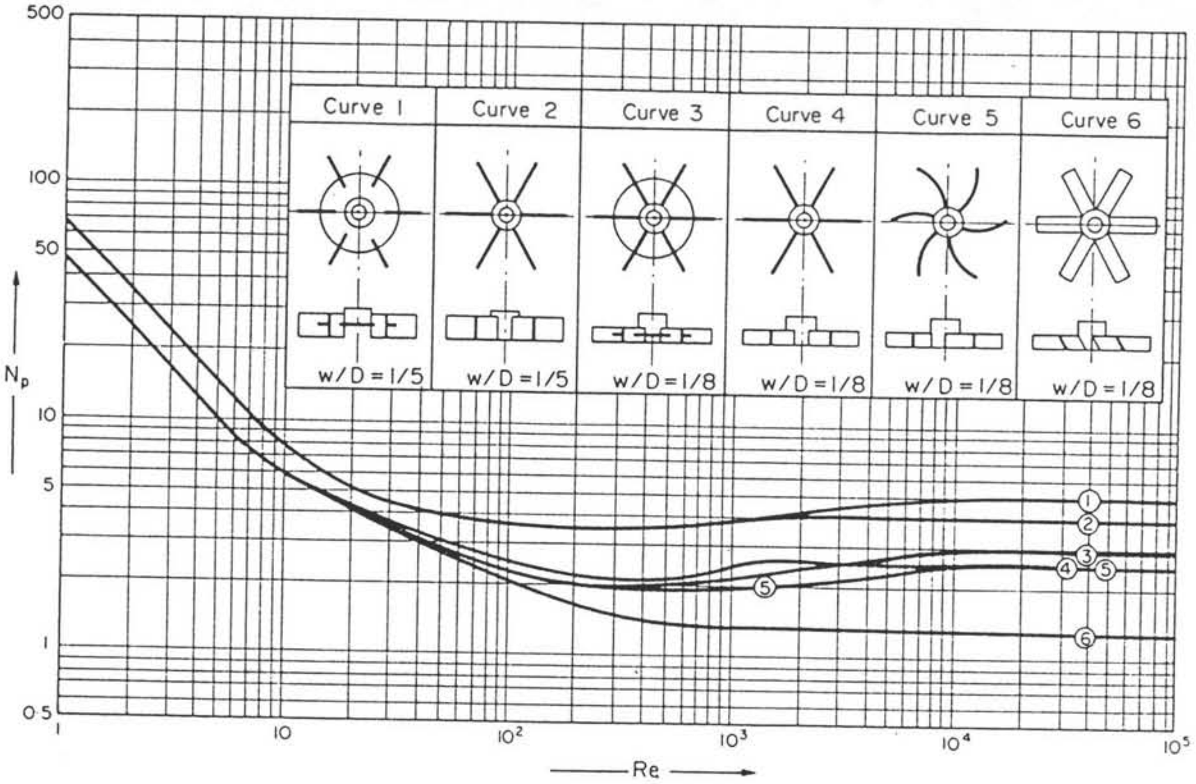


Fig 2. Power correlation for baffled turbine impellers. W = impeller width, D = impeller Diameter

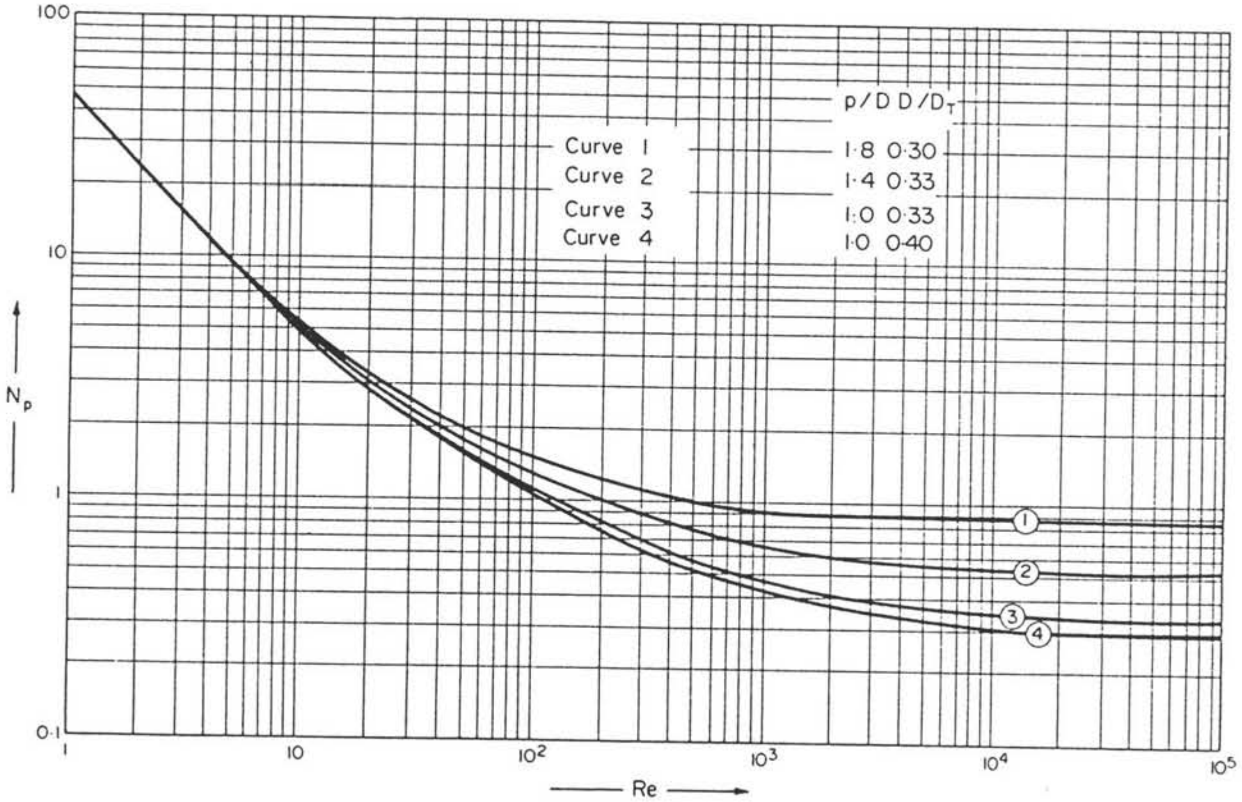


Fig 1 Power correlation for single three-bladed propellers, baffled
p = pitch blade
D = impeller Diameter
D_T = Tank Diameter

Type	Aansluit-maat (inch	Standaard perforatie mm	Opper-vlakte pijp cm²	Effektieve korflengte mm	Buiten-diameter korf mm	Filtrerend oppervlak cm²	Vrij oppervlak cm²	Verhouding vrij- tot pijp-oppervlak
50	¾	0.8	3.4	80	52	132	37	10.7
50	1	0.8	5.6	80	52	132	37	6.6
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
50	1½	1.2	13	120	68	263	97	7.4
50	2	2	22	150	90	428	197	9.1
50	2½	2	31	150	90	428	197	6.4
50	3	2.8	48	150	120	506	24[illegible]	5.1
50	4	3.6	82	260	120	947	483	5.9
50	5	3.6	129	300	150	1397	713	5.5
50	6	3.6	186	320	180	1830	933	5
50	8	3.6	323	415	263	3560	1742	5.3
72	⅜	0.8	1.2	70	36	84	23	18.9
72	½	0.8	2	70	38	84	23	11.8
72	¾	0.8	3.4	80	52	132	37	10.7
72	1	0.8	5.6	80	52	132	37	6.6
72	1¼	1.2	9.7	90	68	201	74	7.7
72	1½	1.2	13	120	68	263	97	7.4
72	2	2	22	120	90	330	152	7
72	2½	2	31	140	120	677	270	8.8
72	3	2.8	48	200	120	742	319	6
72	4	3.6	82	200	180	1091	556	6.8
72	5	3.6	129	310	180	1721	878	6
72	6	3.6	186	380	180	2100	1076	6
72	8	3.6	323	486	263	4030	2010	6.2
40	⅜	80 mesh	1.2	30	24	23	6	5.1
40	½	80 mesh	2	30	24	23	6	3.2
40	¾	80 mesh	3.4	36	32	46	12	3.6
40	1	0.8	5.6	58	40	72	19	3.5
40	1¼	0.8	9.7	81	52	134	37	3.8
40	1½	0.8	13	98	57	177	49	3.7
45	2	0.8	22	110	68	232	65	3
45	2½	0.8	31	130	81	339	94	3
45	3	0.8	48	170	100	536	148	3.1
30	1½	3.6	13	110	68	238	121	9.2
30	2	3.6	22	110	90	348	177	8.2
30	2½	3.6	31	180	100	563	287	9.3
30	3	3.6	48	180	100	563	287	6
30	4	3.6	82	200	120	740	377	4.6
30	5	3.6	129	240	130	1024	522	4.1
30	6	3.6	186	290	160	1463	727	4
30	8	3.6	323	370	220	2537	1294	4

Table 1 Filter specifications

Tabel voor de bepaling van het drukverlies

Deze tabellen zijn opgesteld uitgaande van schone korven, zonder bekleding met metaalgaas en met water als vloeistof. Voor eventuele afwijkingen, gelieve u de navolgende korrektiegegevens toe te passen.

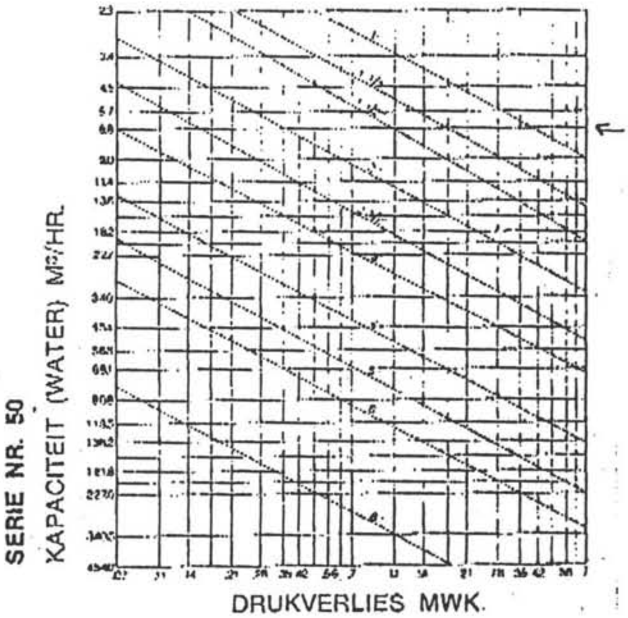
SOORTELIJK GEWICHT

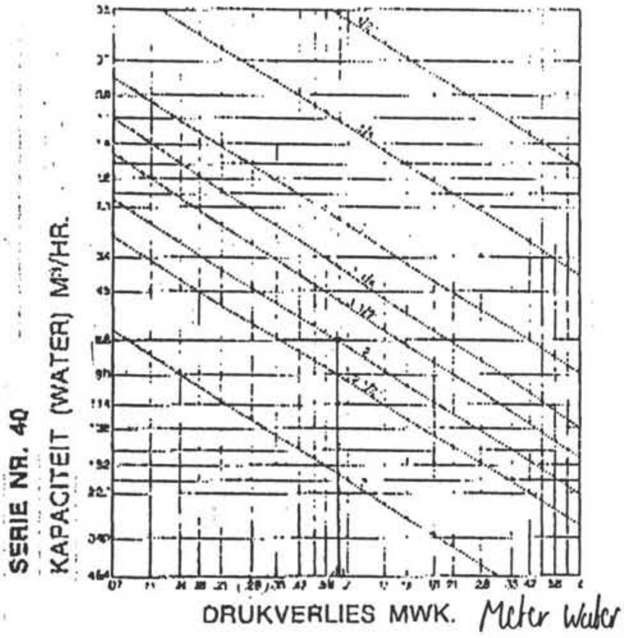
Vermenigvuldig het drukverlies voor water met het soortelijk gewicht van de in aanmerking komende vloeistof. (Water heeft een soortelijk gewicht van 1.0).

VISKOSITEIT

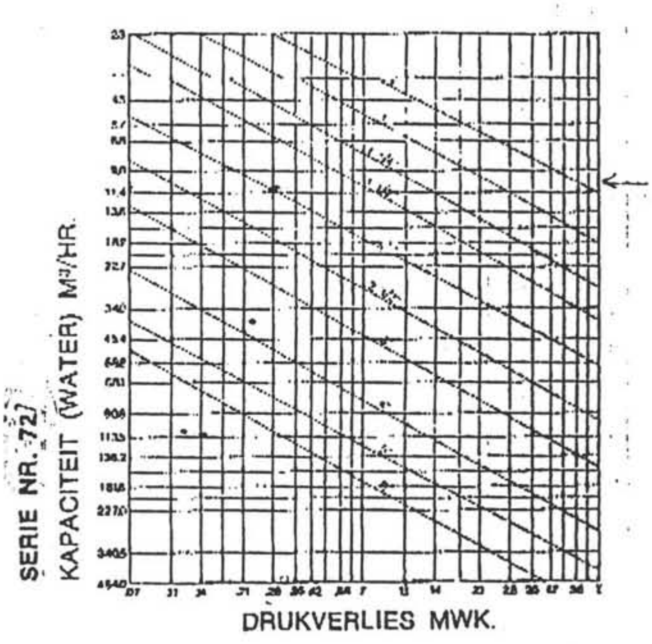
Vermenigvuldig de waterdrukverlies uitkomst met de onderstaande getallen indien vloeistoffen met een hogere viskositeit worden verwerkt. (Water heeft een viskositeit van 1 cps)

Viskositeit CPS	Geperforeerd metaal korf	40 Mesh Metaalgaas korfbekleding	60 Mesh Metaalgaas korfbekleding	80 Mesh Metaalgaas korfbekleding	100 Mesh Metaalgaas korfbekleding
1	1.0	1.2	1.4	1.6	1.7
105	1.6	1.9	2.1	2.4	2.6
210	1.7	2.2	2.4	2.6	2.8
425	1.9	2.4	2.7	2.9	3.2
625	2.0	2.6	2.9	3.2	3.5
1050	2.2	3.0	3.5	4.0	4.5
2150	2.5	3.5	4.2	5.0	6.0





Meter Water ko



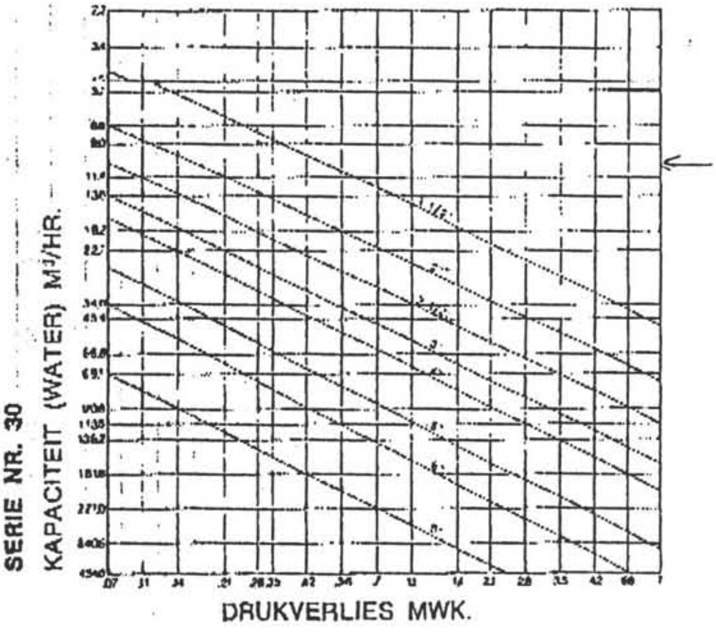


Fig. 3 Filter Pressure Drop

19

Tabel 2 Filter Specification

FELCO General Specification Sheet for WCS Filters and Screens

GSS 8-82

SCREEN SIZES

SCREEN O.D.		SUPPORT ROD SIZE (NO.)	TOTAL NO. OF SUPPORT RODS	PROFILE WIRE NORMALLY USED (NO.)	APPROX. WEIGHT	
INCHES	MM				LBS./FT.	KG/M
1 1/16	27	60	14	50,60,70	1	.5
1¼	32	60	18	"	1	.5
1.32	34	60	18	"	1	.5
1½	38	60	21	"	1¼	2
1.66	42	60	24	"	1¼	2
1¾	44	60	28	"	1½	2.25
1.9	48	60	24	"	1½	2.25
2	51	60	24	"	2	3
2⅜	60	60	26	"	2¼	3.3
2½	64	90	18	"	2¼	3.3
2⅞	73	60	32	"	2½	3.7
3	76	90	24	"	2½	3.7
3¼	83	90	28	"	2¾	4
3¼	83	60	39	"	2¾	4
3½	89	90	28	60,70	3	4.5
3⅝	92	90	24	"	4	6
4	102	90	34	"	5	7.5
4½	114	.1875	24	"	5½	8
4⅝	117	90	32	"	6	9
5¼	133	90	44	"	6	9
5⅝	143	90	36	"	7	10.5
6	152	.1875	36	60,70,90	8	12
8	203	.1875	40	"	10	15

NOTE 1. Above screens can be fabricated using the following materias:

(A) CARBON STEEL	(E) MONEL
(B) CARBON STEEL (GALVANIZED)	(F) HASTELOY
(C) STAINLESS STEEL (304/316)	(G) ALLOY 20
(D) INCONNEL	

2. Weights are approximate and will vary with different wire shapes and slot sizes.

3. For screen sizes not listed above, contact Felco Industries Ltd.

% OPEN AREA FOR WEDGE-WIRE PROFILES AND SELECTED SLOT OPENINGS

WRAP WIRE PROFILES	PROFILE WIDTH (W)	SLOT OPENINGS (INCHES)																	
		.004	.005	.006	.007	.008	.009	.010	.015	.020	.025	.030	.035	.040	.045	.050	.060	.070	.100
NO. 50	.050	7.4	9.0	10.7	12.2	13.8	15.3	16.7	23.0	28.6	33.6	37.5	41.2	44.4	47.5	50.0	54.5	58.3	66.6
NO. 60	.060	6.2	7.7	9.1	10.4	11.8	13.0	14.3	20.0	25.0	29.4	33.3	36.8	40.0	42.9	45.5	50.0	53.8	62.5
NO. 69	.069	5.5	6.7	7.9	9.1	10.3	11.4	12.6	17.8	22.4	26.6	30.3	33.5	36.5	39.4	41.8	46.4	50.2	59.1

$$\%\ \text{OPEN AREA} = \frac{\text{SLOT OPENING}}{\text{PROFILE WIDTH (W)} + \text{SLOT OPENINGS}}$$

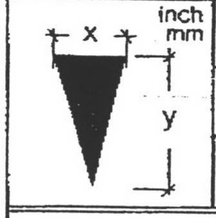
AREA OF TUBE

TUBE DIAMETER (INCHES)	1.00	1.50	2.00	2.50	3.00	3.50	4.00	4.50	5.00	5.50	6.00	6.50	7.00	7.50	8.00
AREA OF TUBE PER LINEAR FT. (IN²)	37.69	56.54	75.39	94.24	113.09	131.94	150.79	169.64	188.49	207.34	226.19	245.04	263.89	282.74	301.59

AREA OF TUBE = DIAMETER x 37.69 (SQ. INCHES) PER LINEAR FOOT

WIRE SIZES AVAILABLE

WEDGE-WIRE

inch mm	NO.	50	60	69	90
	x	.050 1.3	.060 1.5	.069 1.8	.090 2.3
	y	.090 2.3	.100 2.5	.130 3.3	.140 3.6

ROUND WIRE DIAMETER (D) mm

NO.	150	177	236	250	290	312
(D) mm	3.81	4.5	6	6.35	7.37	7.93

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IN CUSTOM
WEDGE-WIRE
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SYSTEMS

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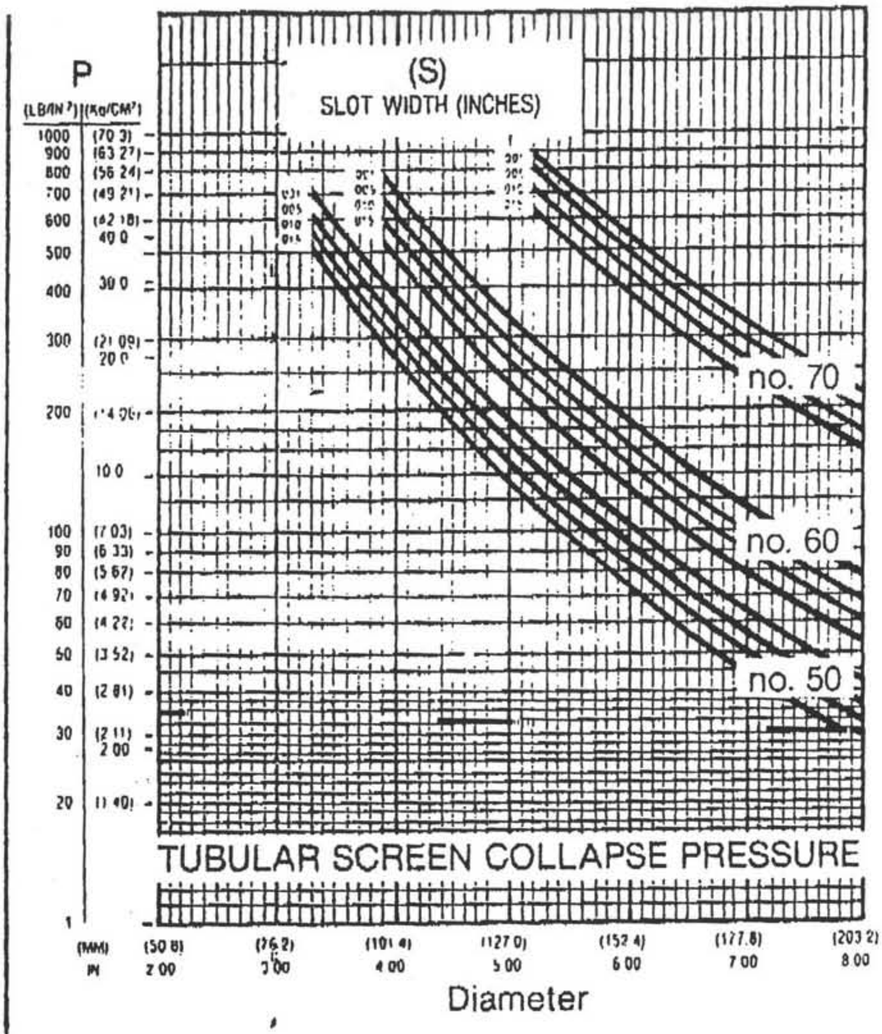
SEE OTHER SIDE

Specification Sheet (Cont.)

PARTICLE SIZE

U.S. MESH	INCHES	MICRONS*	MILLIMETERS
3	.265	6730	6.73
3½	.223	5660	5.66
4	.187	4760	4.76
5	.157	4000	4.00
6	.132	3360	3.36
7	.111	2830	2.83
8	.0937	2380	2.38
10	.0787	2000	2.00
12	.0661	1680	1.68
14	.0555	1410	1.41
16	.0469	1190	1.19
18	.0394	1000	1.00
20	.0331	841	.84
25	.0280	707	.71
30	.0232	595	.59
35	.0197	500	.50
40	.0165	420	.42
45	.0138	354	.35
50	.0117	297	.297
60	.0098	250	.250
70	.0083	210	.210
80	.0070	177	.177
100	.0059	149	.149
120	.0047	125	.125
140	.0041	105	.105
170	.0035	88	.088
200	.0029	74	.074
[illegible]	[illegible]	63	.063
270	.0021	53	.053
325	.0017	44	.044
400	.0015	37	.037

*PROPOSED ISO (INTERNATIONAL) STANDARDS



HOW TO ORDER FELCO FILTER AND STRAINER PARTS

Since all our screens are fabricated to customers' specifications, the following information is necessary:

OPERATING CONDITIONS:

- operating pressure
- operating temperature
- pressure loss
- slot opening
- flow rate
- open area needed

PHYSICAL SIZE:

- overall length
- outside diameter
- type of material
- special fittings

Felco screens are made from a large variety of wire sizes to meet your specifications.

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Tabel 3 Filter specification

Appendix A6.XVII

Determination of Psat of the Rigids

The Riedel Equation can be used to estimate the saturation pressure, when only the normal boiling point and critical temperature and pressure are known.

$$lnP_r^{sat} = D * (35 - \frac{36}{T_r} + (\frac{\alpha_c}{D} - 42) * lnT_r + T^6)$$

with

$$D = 0.0838 * (\alpha_c - 3.758)$$

and

$$\alpha_c = \frac{0.315 * (-35 + \frac{36}{T_{r,n}} + 42 * lnT_{r,n} - T_{r,n}^6) + lnP_c}{0.0838 * (-35 + \frac{36}{T_{r,n}} + 42 * lnT_{r,n} - T_{r,n}^6) - lnT_{r,n}}$$

The normal boiling point of the Rigids is about 450°C (= 723K), the critical temperature is about 928K and the critical pressure is about 24 bar. These values are obtained from group contribution methods.
This leads to:

$$lnP^{sat} = 143.87 - \frac{2.15 * 10^4}{T} - 15.60 * lnT + 1.0 * 10^8 * T^6$$

T is in Kelvin and P^{sat} is in Pa.

Appendix A6.XVIII

Calculations for isothermal flash

The gases are assumed to be ideal as well as the solutions. For a rough calculation this will be a reasonable assumption especially because the pressure won't that high. The temperature in the flash vessel shouldn't exceed 200°C because there is a danger of degeneration of the Rigids. This limits the pressure in the vessel to about 1 bar. The lower limit of the pressure is about 0.1 bar because else the capital costs for the vessel become to high. At 0.1 bar the temperature in the vessel is about 135°C. So the temperature range to be considered is 135-200°C and the pressure range is 0.1 to 1.0 bar.
The equations for the calculations are entered in Mercury (a computing programma) and the results are listed below.

1 For the mixture MEG-DADPM-Rigids:

Input data:
* P = 100 mbar (total pressure)
* Vapor fraction (mol) V = 0.9779 (required to satisfy specification)

```
====== Problem: C:\MERCURY\FLASH.EKA ======

ln(P1s)=20.53-6022.2/(T-28.25)
ln(P2s)=20.309-9009.7/T
ln(P3s)=ln(24312) + 0.6440*(35-36*928/T-24.23ln(T/928)+(T/928)^6)
Pb=z1*P1s + z2*P2s + z3*P3s
Pd=1/(z1/P1s + z2/P2s + z3/P3s)
K1=P1s/P
K2=P2s/P
K3=P3s/P
z1*K1/(1 + V*(K1-1)) + z2*K2/(1 + V*(K2-1)) +z3*K3/(1 + V*(K3-1))=1
z1=0.9936
z2=0.0055
z3=1-z1-z2
y1=z1*K1/(1 + V*(K1-1))
y2=z2*K2/(1 + V*(K2-1))
y3=z3*K3/(1 + V*(K3-1))
x1=y1/K1
x2=y2/K2
x3=y3/K3
L=1-V
V=0.9779
P=100
```

```
═════ Solution ═════
Variables:
  P1s      = EXP(20.53-6022.2/(T-28.25))
           = +136.23376931336958
  T        = 9009.7/(20.309-LN(P2s))
           = +413.90212468699201
  P2s      = +0.2325368498136327
  P3s      = EXP(10.09872533459663+0.644*(35-33408/(9009.7/(20.309-LN(P2s)))-
             24.23*LN(9009.7/(20.309-LN(P2s))/928)+(9009.7/(20.309-LN(P2s))/928)^-
6))
           = +0.0011853787026161718
  Pb       = 0.9936*P1s+0.0055*P2s+0.0009*P3s
           = +135.36315320927881
  z1       = +0.993600000000000   { = +621 / 625 }
  z2       = +0.00550000000000000 { = +11 / 2000 }
  z3       = +0.000900000000000 { = +9 / 10000 }
  Pd       = 1/(0.9936/P1s+0.0055/P2s+0.0009/P3s)
           = +1.2655079450555953
  K1       = 0.01*P1s
           = +1.3623376931336957
  P        = +100.00000000000000
  K2       = 0.01*P2s
           = +0.0023253684981363264
  K3       = 0.01*P3s
           = +1.1853787026161716E-05
  V        = +0.977900000000000   { = +9779 / 10000 }
  y1       = 0.009936*P1s/(1+0.9779*(0.01*P1s-1))
           = +0.99947479698302166
  y2       = 5.5E-05*P2s/(1+0.9779*(0.01*P2s-1))
           = +0.00052472053663899941
  y3       = 9E-06*P3s/(1+0.9779*(0.01*P3s-1))
           = +4.8248033932593264E-07
  x1       = 0.009936*P1s/(1+0.9779*(0.01*P1s-1))/(0.01*P1s)
           = +0.73364687919923555
  x2       = 5.5E-05*P2s/(1+0.9779*(0.01*P2s-1))/(0.01*P2s)
           = +0.22565048810953545
  x3       = 9E-06*P3s/(1+0.9779*(0.01*P3s-1))/(0.01*P3s)
           = +0.040702632691230395
  L        = +0.022100000000000  { = +221 / 10000 }

Largest residual is 2E-17
Method: Iterative
Numeric processor: 8087
```

The index 1,2 and 3 stands for MEG, DADPM and Rigids respectively

Pressure is in mbar and temp. in Kelvin.

P(index)s is the saturation pressure.

Z, y and x are molfractions in feed, top and bottom respectively.

V is the vapor fraction (mol) which will leave at the top and L is the liquid fraction (mol) which leaves the flash vessel at the bottom.

The main point is that y2 is about 100 times to high (it should be about 6.3*10^-6).

2 For the mixture MEG-DADPM

Input data:
* P is 100 mbar
* Vapor fraction (mol) V =0.9842 (required to satisfy the specification)

```
═════ Problem: C:\MERCURY\FLASH2.EKA ═════
ln(P1s)=20.53-6022.2/(T-28.25)
ln(P2s)=20.309-9009.7/T
Pb=z1*P1s + z2*P2s
Pd=1/(z1/P1s + z2/P2s)
K1=P1s/P
K2=P2s/P
z1*K1/(1 + V*(K1-1)) + z2*K2/(1 + V*(K2-1))=1
z1=0.999095
z2=1-z1
y1=z1*K1/(1 + V*(K1-1))
y2=z2*K2/(1 + V*(K2-1))
x1=y1/K1
x2=y2/K2
L=1-V
V=0.9842
P=100
```

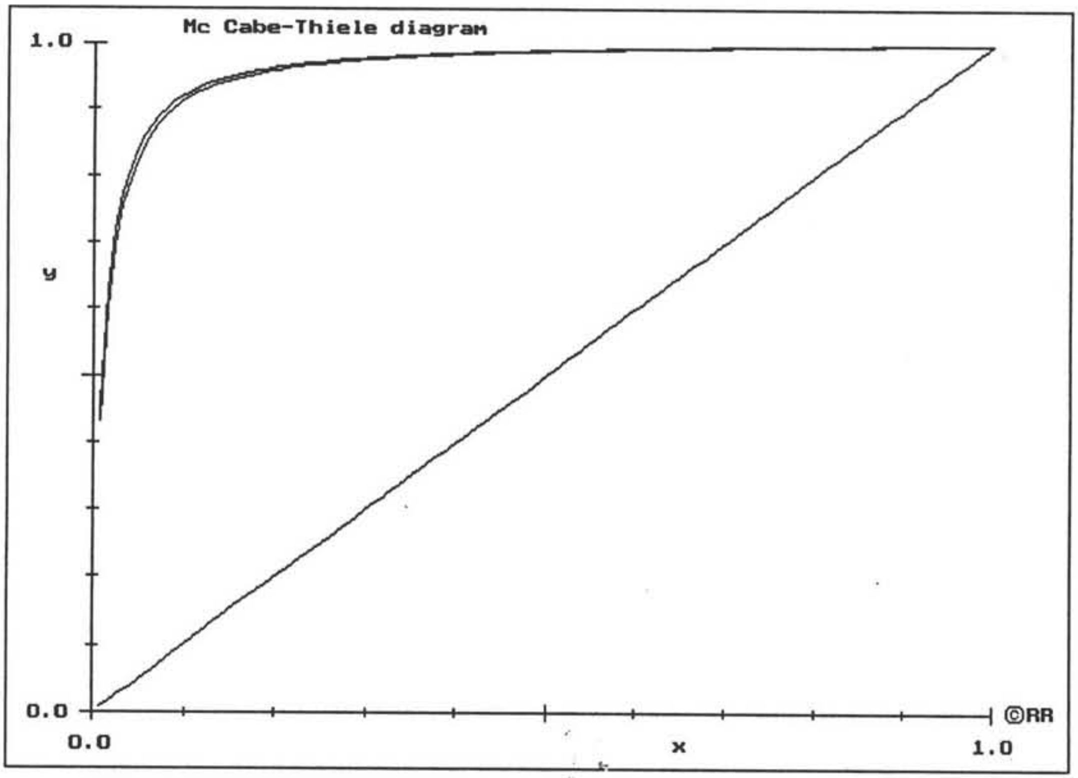
```
═══════ Solution ═══════
Variables:
  P1s      = EXP(20.53-6022.2/(T-28.25))
           = +105.46350172258235
  T        = 9009.7/(20.309-LN(P2s))
           = +407.68160716638931
  P2s      = +0.166819282016795
  Pb       = 0.999095*P1s+0.000905*P2s
           = +105.36820822497364
  z1       = +0.999095000000000
  z2       = +0.000905000000000
  Pd       = 1/(0.999095/P1s+0.000905/P2s)
           = +67.121281386869924
  K1       = 0.01*P1s
           = +1.0546350172258234
  P        = +100.00000000000000
  K2       = 0.01*P2s
           = +0.0016681928201679455
  V        = +0.984200000000000   { = +4921 / 5000 }
  y1       = 0.00999095*P1s/(1+0.9842*(0.01*P1s-1))
           = +0.99991344291068496
  y2       = 9.05E-06*P2s/(1+0.9842*(0.01*P2s-1))
           = +8.6557089315054367E-05
  x1       = 0.00999095*P1s/(1+0.9842*(0.01*P1s-1))/(0.01*P1s)
           = +0.94811325869011875
  x2       = 9.05E-06*P2s/(1+0.9842*(0.01*P2s-1))/(0.01*P2s)
           = +0.051886741309880607
  L        = +0.015800000000000  { = +79 / 5000 }


Largest residual is 7.8E-17
Method: Iterative
Numeric processor: 8087
```

Again y2 is much too high; it should be 6.3*10e-6 however it is 86.6*10e-6.

Appendix A6.XIX

Attempt to make a McCabe-Thiele diagram



At 200 °C the relative volatility (α) is 445.
The equilibrium equation then is: $y = \frac{445 \cdot x}{1 + 444 \cdot x}$

Appendix A6.XX

Chemcad listing

Mixture: MEG-Rigids-DADPM

```
                                                        Page  1
 CHEMCAD 2 Version 2.4


 Filename : DEST3.TLK
 Date: 13-Dec-91  Time:  5:16 pm



 FLOWSHEET SUMMARY

 Equipment            Stream Numbers

  1  SHOR          1  -2  -3


 COMPONENTS
  135 1002 1004

 THERMODYNAMICS
 K-value model  :SRK
 Enthalpy model :SRK
                                                         Page  2
                 Short-Cut Distillation Summary

Equipment name
       number             1
Mode                      2
Light key posn/name     1 Ethylene-
Frac. LK to overhead    .984230
Heavy key posn/name      2 DADPM
Frac. HK to overhead    .637750E-02
Condenser type           total
R/Rmin                100.000
No. of stages             2
Minimum no. of stages        2
Feed stage                2
Calculated duties
 Condenser MJ   /hr  -.1123E+05
 Reboiler MJ   /hr   .1110E+05
Column pres. bars     .999979
Rmin                .100000E-04
Reflux ratio        .100000E-02
```

```
                                                  Page  3
 FLOW SUMMARIES                                   CHEMCAD 2 - Version 2.4

Stream No.                 1          2          3
Temp C                 190.000    192.920    202.070
Pres bars             .999979    .999979    1.04998
Enth MJ   /hr         -2664.05   -2502.06   -33.6715
Vapor mole fraction    .000000    .000000    .000000
Total kgmol/hr         171.784    168.000    3.78600
Flowrates in kgmol/hr
Ethylene-Glycol        170.689    167.999    2.69178
DADPM                  .156799    .999984E-03  .155799
RIGIDS                .938494    .801465E-04  .938414


                                                  Page  4
 FLOW SUMMARIES                                   CHEMCAD 2 - Version 2.4

Stream No.                 1          2          3
Temp C                 190.000    192.920    202.070
Pres bars             .999979    .999979    1.04998
Enth MJ   /hr         -2664.05   -2502.06   -33.6715
Vapor mass fraction    .000000    .000000    .000000
Total kg/hr           10976.4    10427.6    548.935
Flowrates in kg/hr
Ethylene-Glycol        10594.3    10427.4    167.074
DADPM                  31.0932    .198297    30.8949
RIGIDS                350.997    .299748E-01  350.967


                                                  Page  5
 FLOW SUMMARIES                                   CHEMCAD 2 - Version 2.4

Stream No.                 1          2          3
Temp C                 190.000    192.920    202.070
Pres bars             .999979    .999979    1.04998
Enth MJ   /hr         -2664.05   -2502.06   -33.6715
Vapor mass fraction    .000000    .000000    .000000
Total kg/hr           10976.4    10427.6    548.935
Component mass fractions
Ethylene-Glycol        .965190    .999978    .304359
DADPM                  .283273E-02  .190166E-04  .562816E-01
RIGIDS                .319774E-01  .287457E-05  .639359
```

Mixture: MEG-DADPM

```
                                              Page  1
 CHEMCAD 2 Version 2.4


 Filename : DEST2.TLK
 Date: 13-Dec-91   Time:  5:18 pm


 FLOWSHEET SUMMARY

 Equipment              Stream Numbers

  1  SHOR            1  -2  -3


 COMPONENTS
   135 1002

 THERMODYNAMICS
 K-value model  :SRK
 Enthalpy model :SRK


                                              Page  2
                    Short-Cut Distillation Summary

Equipment name
        number             1
Mode                       2
Light key posn/name     1 Ethylene-
Frac. LK to overhead    .984230
Heavy key posn/name      2 DADPM
Frac. HK to overhead    .146080E-02
Condenser type           total
R/Rmin                100.000
No. of stages              3
Minimum no. of stages          2
Feed stage                 2
Calculated duties
  Condenser MJ   /hr  -.1665E+05
  Reboiler MJ   /hr    .1655E+05
Column pres. bars       .999979
Rmin                  .303150E-03
Reflux ratio          .303150E-01
```

```
                                         Page  3
 FLOW SUMMARIES                            CHEMCAD 2 - Version 2.4

Stream No.                 1          2          3
Temp C                190.000    192.920    202.420
Pres bars            .999979    .999979    1.04998
Enth MJ   /hr        -2657.48   -2502.06   -23.7739
Vapor mole fraction    .000000    .000000    .000000
Total kgmol/hr        171.784    168.001    3.78548
Flowrates in kgmol/hr
Ethylene-Glycol        170.689    167.999    2.69178
DADPM                  1.09529    .159999E-02  1.09369
```

```
                                         Page  4
 FLOW SUMMARIES                            CHEMCAD 2 - Version 2.4

Stream No.                 1          2          3
Temp C                190.000    192.920    202.420
Pres bars            .999979    .999979    1.04998
Enth MJ   /hr        -2657.48   -2502.06   -23.7739
Vapor mass fraction    .000000    .000000    .000000
Total kg/hr           10811.5    10427.7    383.953
Flowrates in kg/hr
Ethylene-Glycol        10594.3    10427.4    167.074
DADPM                  217.197    .317278    216.879
```

```
                                         Page  5
 FLOW SUMMARIES                            CHEMCAD 2 - Version 2.4

Stream No.                 1          2          3
Temp C                190.000    192.920    202.420
Pres bars            .999979    .999979    1.04998
Enth MJ   /hr        -2657.48   -2502.06   -23.7739
Vapor mass fraction    .000000    .000000    .000000
Total kg/hr           10811.5    10427.7    383.953
Component mass fractions
Ethylene-Glycol        .979911    .999970    .435141
DADPM                  .200894E-01  .304265E-04  .564859
```

Appendix A6.XXI

Other possible packed column

Packed column with Mellapak 125Y internals:

Top temperature	193°C
Bottom temperature	203°C
Column pressure	1 bar
Pressure drop	0.05 bar
Reflux ratio	0.5
Column diameter	1.24 m
HETP	0.87 m
Packing length	3.20
Total length	9.20
Superficial liq. velocity	4.4 m/h
Reboiler heat duty	4625 kW
Condensor heat duty	4595 kW

Appendix A6.XXII

Costing

A cost estimation was done for the two columns mentioned in paragraph 3.2.

1 The sieve trays column:

Shell: $C_{pv} = C_{pvo} * F_m * F_p * I/336.2$

with F_m: material-of-construction factor
F_p: design-pressure cost factor
I : Chemical Engineering Cost Index
C_{pvo}: $(a + b*l) * d^{1.1}$
with l: length of the vessel
d: internal diameter
a: 1294
b: 1141

The pressure in the column is 1 bar: $F_p = 1$
Material: stainless steel: $F_m = 3.7$
Chem. Eng. Cost Index: $I = 375$
Length of vessel: $l = 10$ m.
Internal diameter: $d = 1.48$ m.

This results in a total cost for the shell (C_{pv}): \$ 78,948.- (HFl 145,250.-)

Trays: $C_{int} = N_{tr} * C_{tr} * F_m * F_{nt} * F_{tt} * I/336.2$

with N_{tr}: number of trays
F_m : cost factor of construction material
F_{nt}: cost factor of number of trays
F_{tt}: cost factor of the tray type
I : CEPC Index
$C_{tr} = 58.7 + 88.4 * d + 52.9 * d^2$
with d: internal diameter

Number of trays is 10: $N_{tr} = 10$
Material: stainless steel: $F_m = 1.7$
$F_{nt} = 1.5$
$F_{tt} = 1$
$C_{tr} = \$ 306.-$

Total cost for internals (C_{int}): \$ 8,687.- (HFl 16,000.-)

So the total costs for the sieve trays column are: $ 87,635.- (HFl 161,250.-)

2 The packed column (with mellapak Y250)

Shell:

Same as the one above: $l = 7.60$ m.
$d = 1.36$ m.
$F\underline{m} = 3.7$ (again stainless steel)

This leads to C_{pv} = \$ 57,680.- (HFl 106,100.-)

Internals:

Mellapak Y250: HFl 10,000.-/m^3
Total packing volume: $0.25*\pi*1.36^2*1.65 = 2.40$ m^3
Internals cost: HFl 24,000.-

Total costs for the packed column: HFl 130,100.-

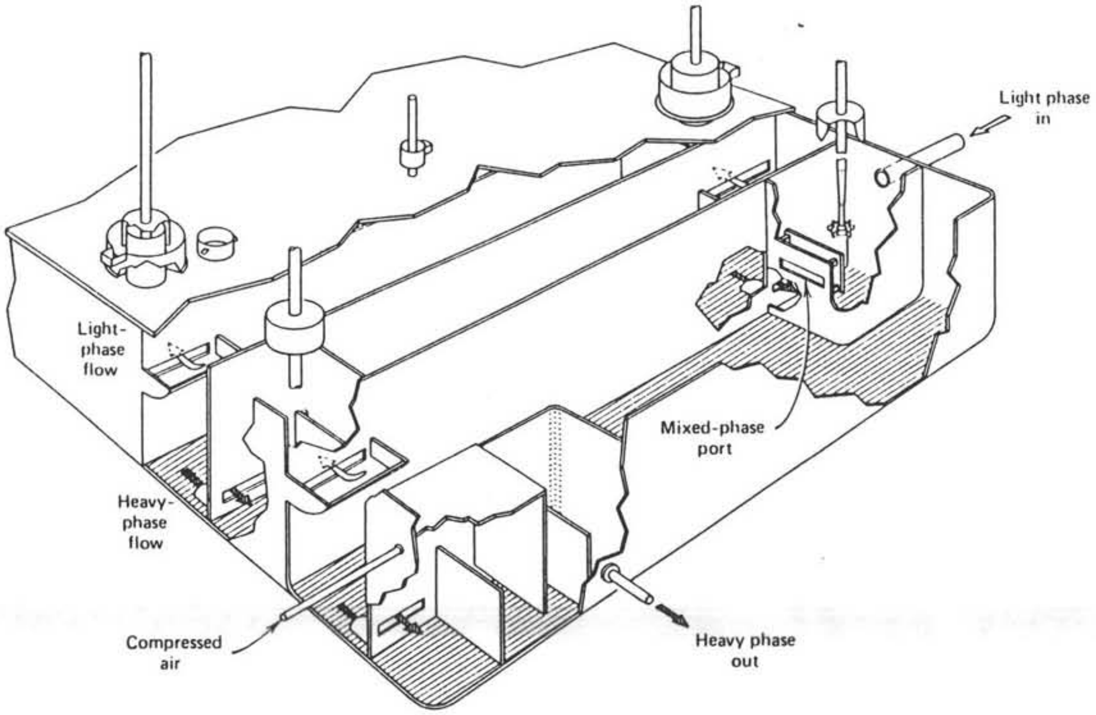


figure A.7.I.1 typical mixer-settler

Appendix A7.I EXTRACTION EQUIPMENT

1 MIXER-SETTLERS (figure A.7.I.1)

* the liquids are continuously contacted in the mixer under thorough agitation and then they flowout to another compartment of the same vessel or to another vessel where the phases seperate; these two vessels are often used in a cascade arrangement in order to obtain continuous operation,
* a cascade of mixer-settlers requires large floorarea which depends mostly on the settling characteristics of the liquid mixture,
* the intens agitation required for efficient extraction will have to be balanced against the possibility of forming a stable emulsion,
* the pumps and extensive piping system involved in mixer-settler installations increase the initial cost of the equipment,
* they are particularly practical and economical for the operations (washing and neutralization) that require high capacity and few stages (<3),
* very high flow rates prohibit the use of a column due to the large diameters,
* pilot testing is usually desired for proper design of mixer settlers,

useful features:

* flexibility and reliability,
* capacity to handle slurries,
* intensity of agitation can easily be varied independent of the liquid flow rates,
* high stage efficiency,
* good contacting,
* handles wide flow ratio,
* low headroom,
* many stages available,
* reliable scale up,
* relatively insensitive to interfacial debris and undissolved solids,

disadvantages:

* large holdup,
* high power costs,
* high investment,
* they require large floor or ground space (especially because of the typical settler),
* interstage pumping may be required,
* generally more complex than other devices and occupy a relatively large volume.
* large residence times (considerable time needed to achieve steady state) require large inventory of working solutions; they tie up a large amount of in-process material, which can be costly or hazardous,
* they can suffer large solvent losses; most commercial units are difficult to seal,

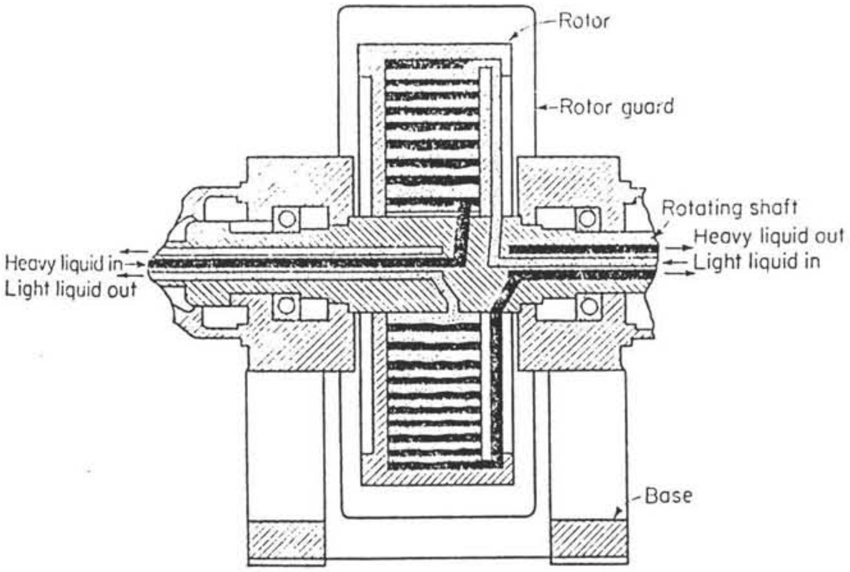


figure A.7.I.2 Podbielniak centrifugal extractor

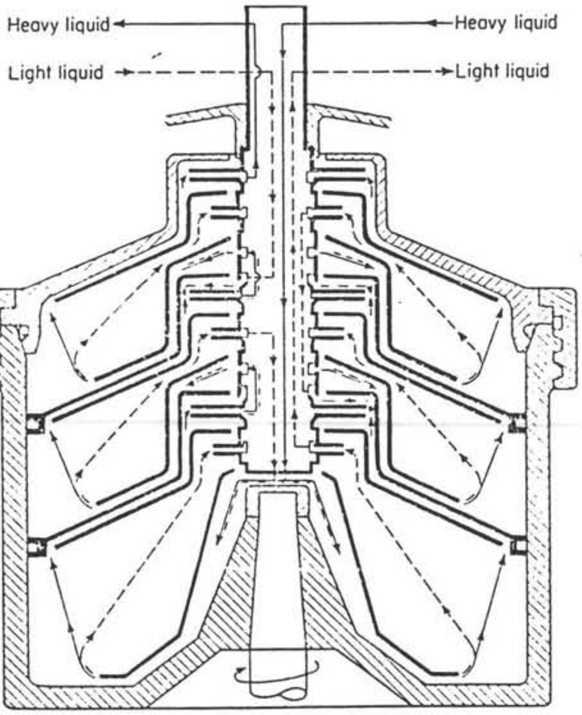


figure A.7.I.3 Luwesta centrifugal extractor

2 Centrifugal extractors (figures A.7.I.2 and A.7.I.3)

- Multi-stage countercurrent centrifugal extractors contain a series of perforated concentric cylinders. Heavy phase is fed into the center of the disc series, the light phase to its periphery. Interaction between the fluids is governed by a pressure balance. By setting the inlet pressure of the two phases and the outlet pressure of the light phase, one can shift the position of the interface and thus set which phase is dispersed and which is continuous.
- application of centrifugal force yields many times the force available under normal gravity conditions thereby enhancing the seperation of 'difficult settling' systems,
- by rapid rotation of the entire mass of liquids involved in extraction, as in a centrifuge, the pressure head available to force the liquids through the equipment could be greatly increased. This results in much higher liquid throughput with a shorter time of contact between the liquids,
- they can be advantageously used to process liquids with emulsifying tendencies or high viscosities or interfacial tensions which are difficult to handle in other extractors,
- Attractive for circumstances where the solute is particularly valuable (pharmaceuticals) or the requirements for product cleanliness are strict.
- ordinarily suitable only when three or fewer stages are required, although up to seven stages have been attained,

advantages:
- handles extremely low density difference between phases (less than 50 [kg/m^3],
- achieving steady state in a relatively short period, short residence time,
- low holdup volume, short holdup time, low space requirements,
- small inventory of equipment,
- small extractor volumes for high flow capacities,
- requires low inventories of the liquid-liquid phase,
- continuous extraction processes reach steady state quickly, with relatively little of the raffinate requiring reprocessing to bring it to its final specifications,

disadvantages:
- high initial and maintenance costs,
- high operating costs,
- limited number of stages in single unit.
- regular maintenance of the bearings and seals is required because they are relatively high speed machines with fast moving parts,
- if solids are present, plugging can be a problem,

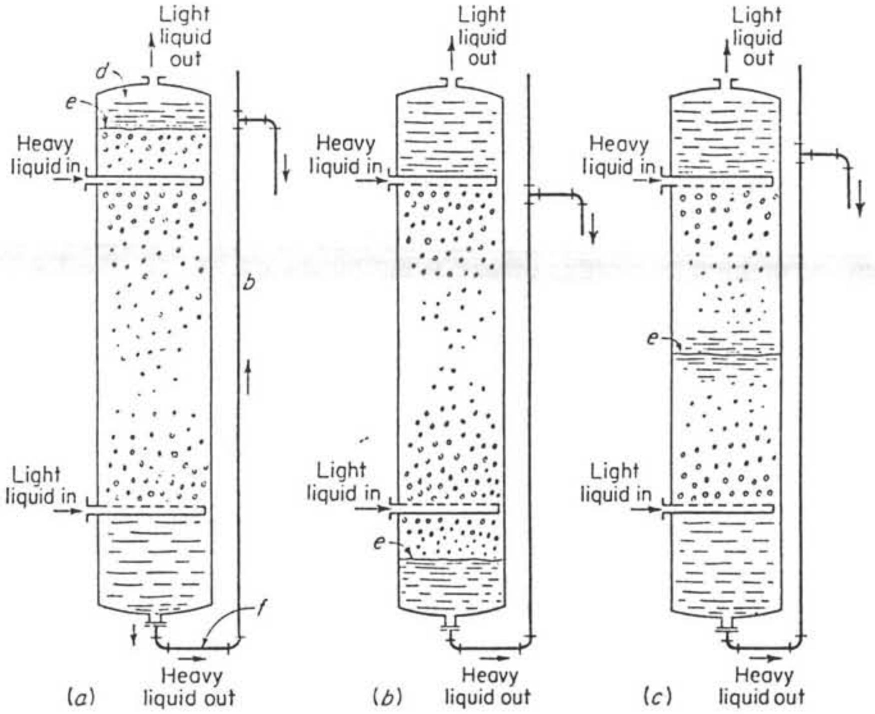


figure A.7.I.4 spray column

3 Unagitated columns

- * simplest type of contactors available for liquid- liquid-extraction,
- * they occupy small floor area, high headroom required,
- * low initial and operating costs,
- * relatively low efficiency,
- * most suitable for application where the number of stages required is low,
- * limited throughput with small density difference,
- * high headroom,
- * cannot handle high flow ratio,
- * not/less suitable for low density differences,
- * difficult scale up.

3.1 Spray column (figure A.7.I.4)

- * vertical column in which the dispersed phase is sprayed through the continuous phase,
- * capacity depends on the throughput rates of both the dispersed and the continuous phase and also on the size of the drops of the dispersed phase produced by the entrance nozzles,
- * axial mixing reduces the extraction rates because of the deviation from true countercurrent behaviour, therefore only used when the overall transferunits involved in the seperation process is relatively small,
- * only when the density ratio and viscosity ratio of the dispersed to the continuous phase are large, the continuous phase may approach perfect mixing. Such ideal conditions of flow behaviour are not normally met with in spray columns operated in commercial practice,
- * much axial mixing occurs, so theyseldom represent more than one theoretical stage,
- * they find their niche in the handling of fluids containing large amounts of suspended solids, because they lack internals to plug,
- * used for simple seperations like washing, treating and neutralization,

advantages:
- * simplest possible contactor in construction,
- * spraycolumns are inexpensive,
- * they have high flow capacity,

disadvantages:
- * very low efficiencies because of poor phase contact and excessive backmixing in the continuous phase,
- * it is ordinarily difficult to obtain an equivalent of more than a few theoretical stages in a single spray column,

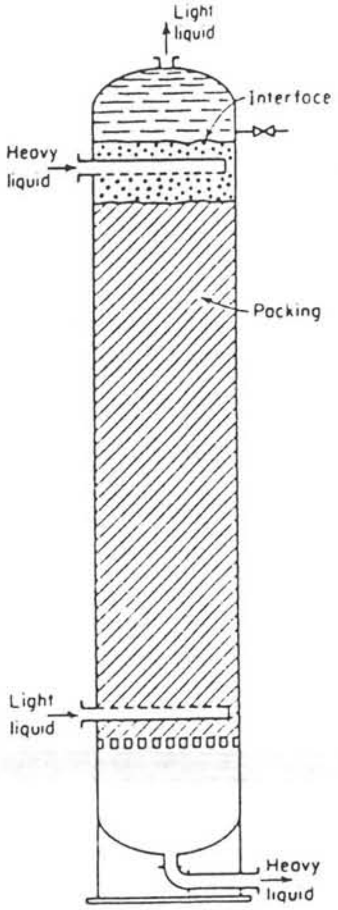


figure A.7.I.5 packed column

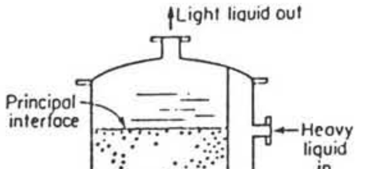


figure A.7.I.6 sieve-plate column

3.2 Packed column (figure A.7.I.5)

- the column is usually packed with packings such as Raschig rings, Lessing rings, Intallox and Bearl saddles, which promote coalescence and redispersion of the dispersed phase,
- to avoid coalescence of the dispersed phase it is essential that the continuous phase preferentially wets the packing and other column internals,
- columndiameter determined from desired flow capacity and flooding characteristics of the packing,
- more efficient than the spray extraction towers on account of increased efficiency brought about by the use of packings,
- the pair of liquid phases must have sufficient difference in density to induce and maintain traffic of the phases in the interstices of the packing,
- particularly used in cases where the number of transfer units is small,
- generally not suitable when the liquids contain suspended solids.
- they offer advantages when only a few stages (up to three, say) are required,
- should not be used if the ratio of flow rate is beyond the range 0.5 to 2.0 because of probable flooding when suitable hold-up and interfacial area were provided,
- packed column preferred over a spray column, as the reduced flow capacity is less significant than the improved mass transfer,

advantages:
- random packing aids the formation of drops, which helps the mass transfer; this leads to a better efficiency because of improved contacting and lessened axial mixing,
- the packing pieces in the column help to increase the local velocity of the continuous phase and restrict the circulation or backmixing in that phase,
- the packings improve the distribution and holdup of the dispersed phase by distorting and breaking up the bigger drops and hindering their free movement, thus yielding more surface for mass transport,

disadvantages:
- random packings restrict the free area for flow of the fluids and thus hinders throughput,
- can be difficult to scale up,
- they are subject to plugging when solids are present,
- effective initial distribution of liquid is critical for the performance of the extractor,

3.3 Sieve plate column (figure A.7.I.6)

- consists of multiorifice plates with or without downcomers,
- the dispersed phase travels up or down through the column depending upon the density of the phase dispersed,

- * they provide repeated coalescence and redispersion of the drop phase and offer the advantages of cross-flow of the continuous phase in addition to yielding high extraction efficiencies with practically no axial mixing,
- * essentially stagewise in operation but careful design can provide excellent flow capacities for this type of column,
- * they may be considered as a series of short spray columns arranged one above the other.
- * particularly used for processes requiring only a few thyeoretical stages and for corrosive systems where no mechanically moving parts are advantageous,
- * besides having a principle interface at either the top or the bottom of the column, the sieve plate extractor also has a number of intermediate interfaces, one for each tray,
- * because of simplicity and low costs, still used in many commercial ex tractions, despite their low efficiency,

advantages:
- * reasonably high throughput capacity, as they can be built in large dimensions,
- * simple scale-up, as there is little backmixing,
- * reasonably flexible and efficient,
- * the plates eliminate backmixing of the continuous phase almost completely,
- * the repeated coalescence and dispersion of the dispersed phase enhances the extraction rates considerably,

disadvantages:
- * they are very susceptible to solids plugging,
- * relatively narrow operating range in regard to throughput,
- * low efficiency,

4 Agitated columns

- * they receive mechanical energy via rotating or reciprotating elements or pulsation. This creates and maintains dispersion in the extractor over a wide range of operating conditions,
- * the degree of dispersion and consequently the performance of the column can be considerably enhanced by the introduction of some form of mechanical agitation,
- * they can generally attain a shorter height equivalent to a theoretical stage,

Rotary agitated

advantages:
- * good dispersion,
- * reasonable costs,
- * insensitive to silica contamination in the feed stream,
- * many stages possible,
- * relatively easy scale up,

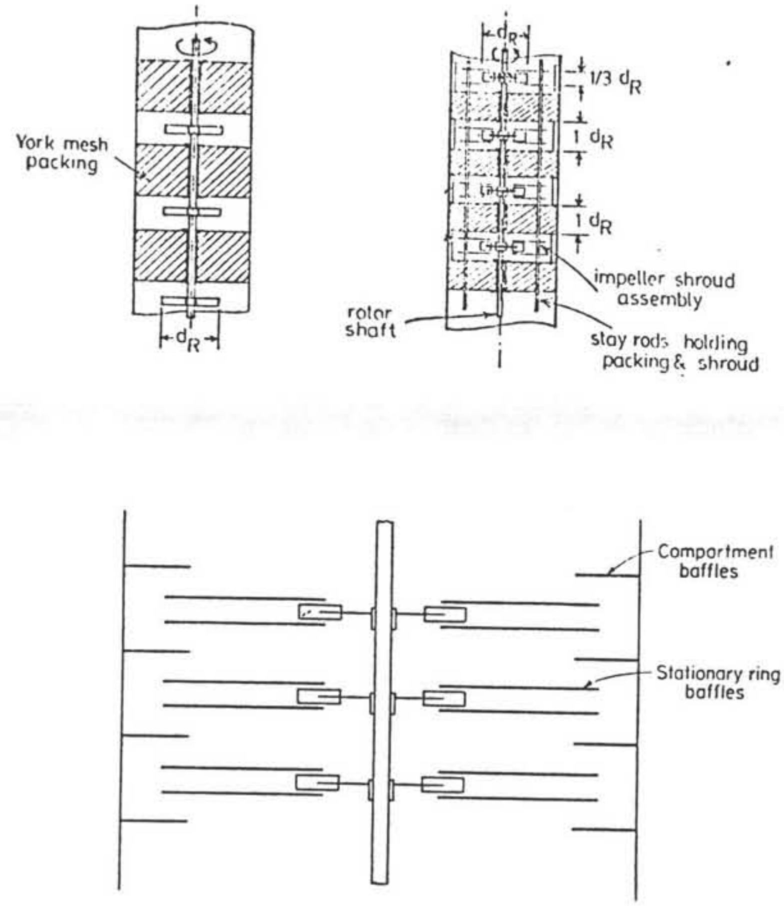


figure A.7.I.7 Scheibel column

- * they have a high efficiency (depends upon the geometry of the system and upon the power input to the impeller) and flexibility,

disadvantages:
- * limited throughput with small density difference,
- * cannot handle emulsifying systems,
- * cannot handle high flowratio.
- * since the force of gravity is used to produce countercurrent flow, mechanical agitation may also promote backmixing (this can be reduced by introducing suitable baffles),
- * these contactors have increased maintenance costs,

Pulse agitated

- * an oscillating pulse to the liquids in the extraction column (such as packed and Sieve-plate column) can appreciably increase the extraction efficiency (due to the increase in both turbulence and interfacial area caused by the breakup of dispersed phase),
- * high efficiency and the possibilaty of creating the pulse remotely have made such columns important in nuclear industry,
- * the performance of these column contactors indicates that they are more efficient and posess better operational flexibility than the conventional sieve-plate, packed and spray columns,
- * increases both turbulence and interfacial area,
- * low axial mixing and a relatively small increase in axial mixing with an increase in column diameter,

4.1 York Scheibel column (figure A.7.I.7)

- * extraction column with an impressive number of theoretical stages per unit of height,
- * replacement of the mesh not only solves the scale-up and solids problems but also raises the efficiency of the column.
- * first rotary agitated column to be introduced commercially,
- * earlier design: a cylindrical vessel with alternate packed (normally filled with York mesh packings) and unpacked sections serving as settling and mixing chambers with centrally spaced turbine blade impellers functioning within the unpacked, non-baffled sections,
- * later version: the impeller used is shrouded by keeping two stationary ring baffles on either side of the paddle in each rotor compartment. The ring baffles help the fluid to be thrown away radially to wards the wall. The wall forces the fluid to return to the central intake of the impeller before it passes through the next packed section,

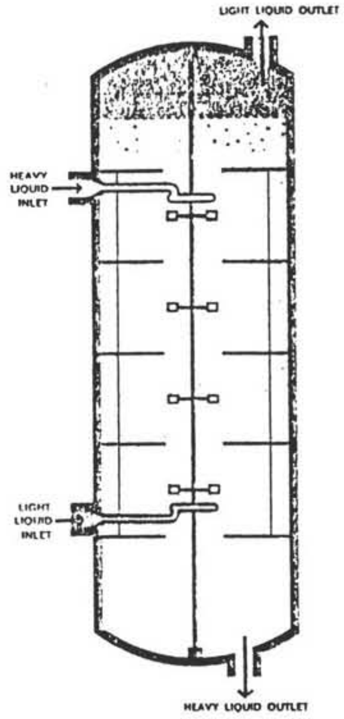


figure A.7.I.8
Oldshue-Rushton column

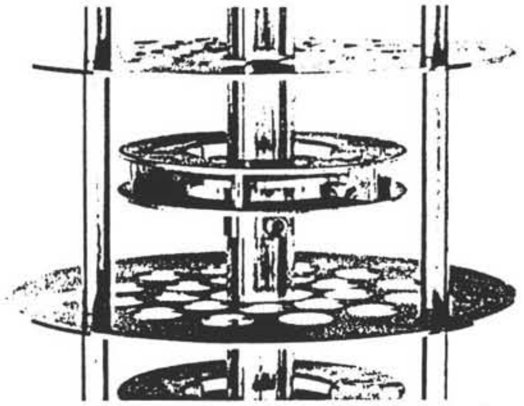


figure A.7.I.9 Kühni column

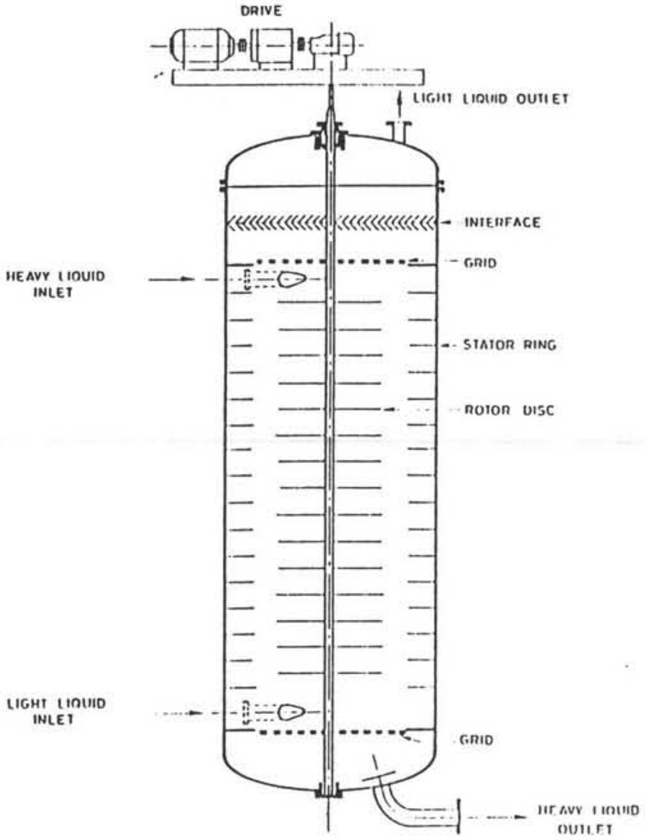


figure A.7.I.10 RDC

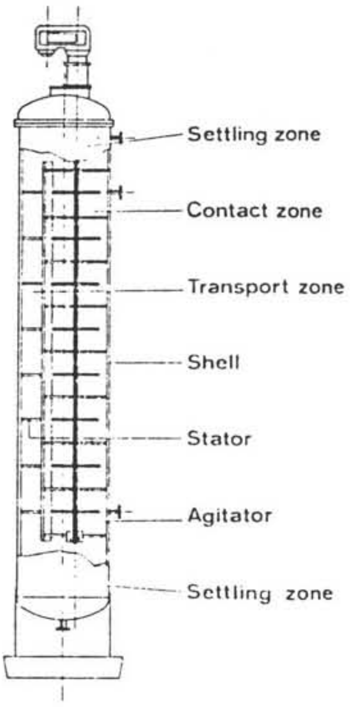


figure A.7.I.11 Asymmetric Rotating Disc column

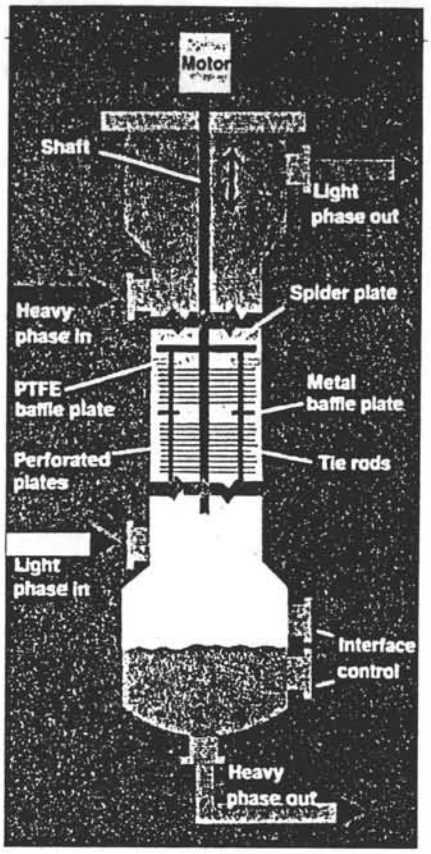


figure A.7.I.12 Karr column

figure A.7.I.13 vibrating plate extractor

The shell (1) of the column proper is connected at each end to settling sections of larger diameter. The upper settling section (2) is provided with a distributor for the heavy phase (3) and an overflow for the light phase (4). The lower settling section (5) contains an outlet for the heavy phase (6) and a distributor for the light phase (7). According to the choice of the phase being dispersed, either section may be equipped with an interface control. In the discussion that follows, the lighter phase is assumed to be dispersed.

A stack of perforated plates (8) is situated in the shell, fastened to a rod (9) connected to an eccentric (10) that imparts to the whole stack a vertical harmonic motion, the amplitude and frequency of which are among the important controlling variables. The geometry of the perforated plates is specific for the VPE. The plates are provided with a number of small circular holes for the dispersed phase (11) and with one or more large openings for the continuous phase (12). These openings may either be circular or have various forms suitable from the point of view of plate design. In columns of smaller diameter the passages for continuous phase of neighboring plates are placed on opposite sides of the column axis, so that a crossflow of phases between the plates can occur. On large plates, the distribution of passages is such that several parallel sections with a crossflow of phases are created. As a general rule, the plates are provided with a vertical cylindrical wall (13) on their circumference extending against the flow of the dispersed phase. A similar lining may be applied also to the passages for continuous phase.

* the stage efficiency in these columns increases with agitator speed until it reaches a maximum value and finally decreases at higher agitator speeds presumably because of the formation of emulsion which can not be broken even in the packed settling chamber.

4.2 Oldshue-Rushton Column (figure A.7.I.8)

* this is essentially a series of baffled mixing tanks stacked one atop another,
* the vertical baffles enhance the mixing characteristics of each compartment, and the horizontal baffles define the mixing stages and help to minimize axial mixing,

4.3 Kühni Column (figure A.7.I.9)

* consists of a series of mixing compartments (similar in principle to the Scheibel baffle column), each of which has a shrouded turbine impeller located between two perforated plates,
* the hole area of the plates depends on the flow rates and the process application.

4.4 Rotary Disc Contactor (figure A.7.I.10)

* one of the most widely used rotor-agitated columns for liquid-liquid extraction, especially in the petroleum and chemical industries,
* it uses shearing action of a rapidly rotating disc to interdisperse the liquids,
* the cylindrical column is seperated into compartments. A centrally mounted rotating shaft run by a variable speed gear unit carries a number of equally spaced discs such that each disc operates in the middle of a compartment formed by stator rings,
* the rotating discs offer a shearing action on larger drops and above a certain speed break them into smaller ones and therefore control the size of the dispersed drops,
* the stators limit axial mixing and define the mixing stages in the vessel,
* the intensity of turbulence is governed mainly by the rotor speed which also controls the size of the dispersed drops,
* severe backmixing of the phases at high speeds may produce drastic reduction in the concentration driving force, reducing the mass transfer efficiency,
* the equipment is more versatile in that its capacity can be varied at will and the scaling up is easier when compared to other contactors.

4.5 Asymmetric Rotating Disc Contactor (figure A.7.I.11)

- * a column having seperate mixing and settling compartments,
- * is asymmetric in that the shaft and rotors are not on the centerline of the vessel,
- * baffles between each stage direct the mixed liquids to a settling zone, from which they pass either upward or downward to the next stage,

4.6 Karr Column (figure A.7.I.12)

- * the droplets are formed by internals that reciprocate,
- * because it offers uniform shear mixing across the entire cross section, this column is particularly suitable for systems that tend to emulsify,
- * it offers very high throughput compared to other agitated extractors,
- * because of its uniform-shear-mixing characteristics it provides drops in a narrow size range,
- * has a relatively high volumetric efficiency ((throughput per unit area)* (stages per unit height))

4.7 Vibrating Plate Extractor (figure A.7.I.13)

- * similar to the reciprocating plate column;
    - smaller holes, less free area, employs downcomers or upcomers for the continuous phase (in this respect similar to the unagitated sieve plate column),
- * two seperate sets of plates, each set being supported by its own shaft,
- * the motion of the shaft is timed in such a way that each plate reciprocates 180 deg. out of place with the two adjecent plates,
- * thus the instantanuous velocities of neighbouring plates are of equal magnitude and opposite directions,
- * increases both capacity and efficiency.

4.8 Pulsed Sieve Plate Extractor

- * mechanical energy is provided by pulsing the liquid itself,
- * the liquids are cyclically pulsed in such a way that axial force is imposed on each of the phases,
- * during each cycle, first the light phase and then the heavy phase are accellerated through th plates. This action disperses one of the two phases into drops as it is forced through the plates, and agitates the continuous phase,
- * low axial mixing and high extraction efficiency because of:
    - uniform distribution of drops in the column,
    - uniform distribution of energy over a cross section of the column,

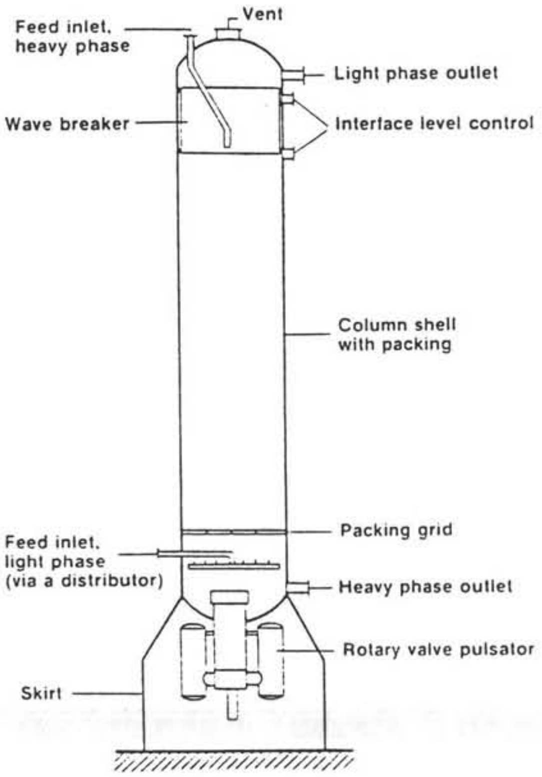


figure A.7.I.14 pulsed packed column

* at lower pulsed volume velocities (amplitude*frequency*column cross-sectional area) a discrete layer of liquid appears between plates during each reversal of the pulse cycle,
* with higher pulsed volume velocities no coalescence and fairly uniform dispersion occurs,
* this column acts as a stage-wise contactor, with coalescence and redispersion of the dispersed phaseat each plate,

4.9 Pulsed Packed Extractor (figure A.7.I.14)

* see : packed column
  columns agitated by pulsation

Appendix A7.II PHYSICAL PROPERTIES

MEG

$$C_p^{liq}(T(K)) = 0.1148\ 10^6 - 0.75\ 10^2\ T + 0.8020\ T^2 - 0.57\ 10^{-3}\ T^3 \qquad [J/kmol.K]$$

molecular weight	M_{MEG}	62.07 [g/mol]
viscosity (20°C)	η_{MEG}	$21\ 10^{-3}$ [Pa.s]
surface tension (20°C)	σ_{MEG}	$48.4\ 10^{-3}$ [N/m]
critical temperature	T_c	436.85 [°C]
critical pressure	P_c	77 [bar]

temp. [°C]	pressure [bar]	liq. visc. [cP]	liq.density [kg/m³]
25	0.000115	17.05294	1109.925
50	0.000906	7.06949	1092.448
75	0.005017	3.53366	1074.391
100	0.021117	2.01736	1055.666
125	0.071436	1.26939	1036.162
150	0.202678	0.85915	1015.745
175	0.498321	0.61475	994.249
200	1.089311	0.4592	971.463

surface tension $\sigma = A(1-T_r)^B$ with: $A = 0.069370$
$B = 0.59770$

FLEXIBLES

$$C_p^{liq}(T(K)) = C_p(25°C)\ (0.64 + 1.2\ 10^{-3}\ T) \qquad [J/kg.K]$$

specific heat (25°C)	$C_p(25°C)$	1930 [J/kg.K]
molecular weight	M_{MEG}	5000 [g/mol]

temp. [°C].	visc. [cP]	density [kg/l]
-1	53.0	-
4	30.0	-
5	24.0	-

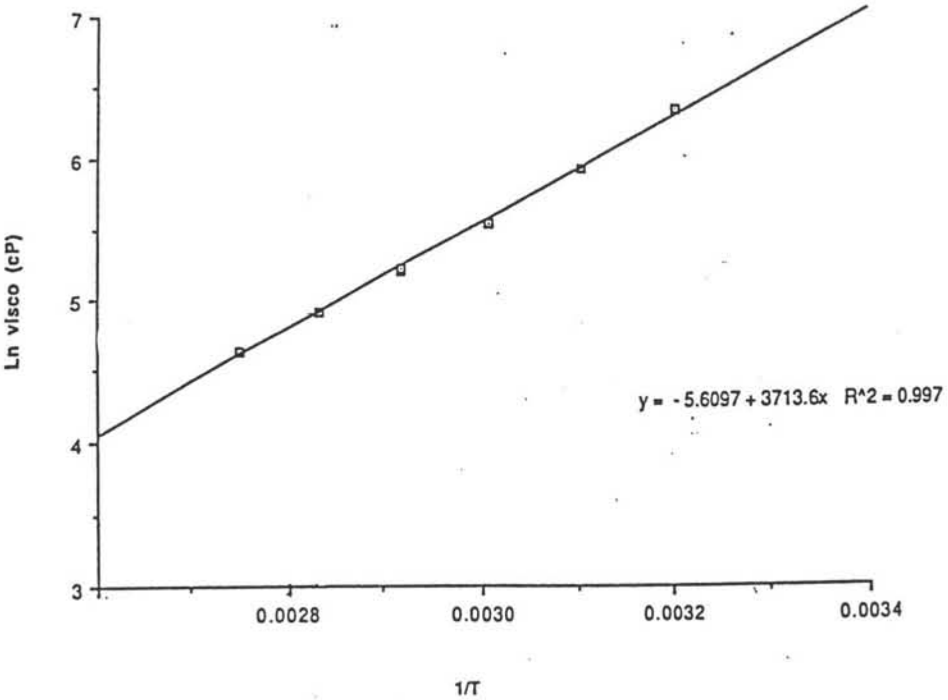


figure A.7.II.1 flexible viscosity as determined by MMK

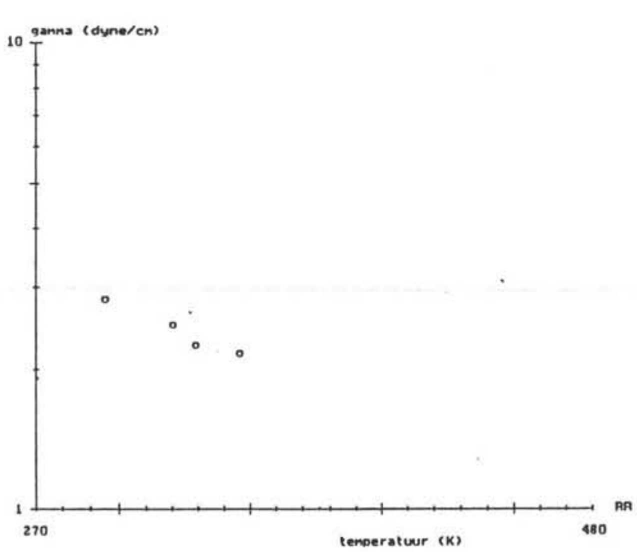


figure A.7.II.2 surface tension flexible-phase

10	22.0	-
15	19.0	-
16	15.0	-
21	12.5	-
24	-	1.060
25	11.0	-
40	6.0	1.007
45	-	1.003
50	-	0.999
55	-	0.996
60	-	0.992
65	-	0.988

Figure A.7.II.1: flexible viscosity as a function of temperature.

FLEXIBLE PHASE

density (24°C) ρ = 1070 [kg/m^3]

$$\ln(visc[cP]) = \frac{5.92\ 10^3}{T(K)} - 1.22\ 10^1$$

Figure A.7.II.2: flexible-phase surface tension as a function of temperature.

DADPM

molecular weight M_{DADPM} = 198.2 [g/mol]
density ρ_{DADPM} = 1100 [kg/m^3]

c_p(25°C)	366 [J/mol.K]
c_p(50°C]	410 [J/mol.K]
c_p(200°C)	540 [J/mol.K]

(*) $\rho_m = \Sigma\, x_i\, \rho_i$ ρ_m mixture density
x_i mass fraction component i

ρ_i density component i

(*) $\ln(\eta_m) = \Sigma x_i \ln(\eta_i)$ η_m mixture viscosity
x^i mole fraction component i
η_i viscosity component i

(*) molar weight of mixture
$M_m = \Sigma x_i M_i$ M_m molecular weight of mixture
x_i mole fraction component i
M_i molecular weight of component i

(*) diffusion coefficient

$$\delta = \frac{7.4\ 10^{-8}\ (\phi\ M_B)^{\frac{1}{2}}\ T}{\eta_B\ V_A^{0.6}}$$

δ = mutual diffusion coefficient of solute A at very low concentrations in solvent B, cm$_2$/s
ϕ = association factor of solvent B, dimensionless
M_B = molecular weight of solvent B, g/mol
η_B = viscosity of solvent B, cP
V_A = molar volume of solute A at its normal boiling temperature, cm^3/mol
T = temperature, K

(*) viscosity of mixture of continuous and dispersed phase in the column

$$\eta = \frac{\eta_c}{1-h}\left[1 + \frac{1.5\ \ \eta_d\ \ h}{\eta_d + \eta_c}\right]$$

η_m = mixture viscosity
η_c = viscosity continuous phase
η_d =viscosity dispersed phase
h = hold-up dispersed phase

(*) specific heat C_p of mixture
$C_{p,m} = \Sigma x_i C_{p,i}$ C_p = specific heat of mixture
x_i = concentration of component
$C_{p,i}$ = specific heat of component i

Appendix A7.III DESIGN OF ROTARY DISC CONTACTOR

The design of the Rotary Disc Contactor consists of two sections. In the capacity calculation the dimensions of stator, column, rotor and compartment will be calculated. In the seperation calculation the height of the column will be determined.

The design equations we used are from Zuiderweg [2]. Used properties calculated with Reid [7] and Perry [9].

A. Capacity calculation

1. Determine maximum hold-up h_{max} for the given $\alpha = Q_d/Q_c = V_d/V_c$ by iteration of:

$$\alpha = \frac{2\, h_{max}^{2} - h_{max}^{3}}{\left[1 - h_{max}\right]^{3}}$$

2. Choose operational hold-up h to be: $0.75 * h_{max}$.

3. Determine U_o with:

$$U_o \approx 0.9\, \frac{\left[\Delta\rho\; g\right]^{\frac{5}{21}}\, \sigma^{\frac{6}{21}}}{\rho_c^{\frac{10}{21}}\, \eta_c^{\frac{1}{21}}}$$

4. Determine d_m at this condition;

$$d_m = \left[\frac{\rho_c\, U_o^{2}}{\sigma}\right]^{-1}$$

5. Determine ε in case of $d_{3,2}$ between d_m (4.) and about 1 [mm],

$$d_{3,2} = 0.25 \left[\frac{\sigma}{\rho_c}\right]^{\frac{3}{5}} \epsilon^{-\frac{2}{5}}$$

6. Determine terminal velocity U_o ($d_{3,2}$ in this interval);

$$\frac{4}{3}\, \frac{\Delta\rho\; d_{3,2}\; g}{\rho_c\, U_o^{2}} = 2.35 \left[\frac{\eta_c}{U_o\, d_{3,2}\, \rho_c}\right]^{\frac{1}{5}}$$

This formula is valid in case Reynolds number Re is larger than 10 and smaller than a maximum value of 1360*$We^{-(6/5)}$.

Weber:

$$We = \frac{\rho_c U_o^2 d_{3,2}}{\sigma}$$

Reynolds:

$$Re = \frac{\rho_c U_o d_{3,2}}{\eta}$$

7. Use the hold-up correction to determine slip velocity U_s;

$$U_s = U_o e^{-h}$$

8. Use the known U_s, α and h to determine U_d and U_c;

$$U_s = \frac{U_d}{h} + \frac{U_c}{1-h}$$

$$\alpha = \frac{U_d}{U_c}$$

9. Determine stator diameter S and further column diameter D, height of compartment H and rotor diameter R;

$$\frac{\pi}{4} S^2 = \frac{Q_d + Q_c}{U_d + U_c}$$

Figure 7.4. gives us:

D [m]	0.06-0.3	0.3-1.0	> 1.0
S/D	0.7	0.7	0.7
R/D	0.5	0.5	0.5
H/D	0.3	0.2	0.1

B. Seperation calculation

1. Determine superficial velocities of dispersed (V_d) and continuous (V_c) phase;

$$V_d = U_d \left(\frac{S}{D}\right)^2$$

$$V_c = U_C \left(\frac{S}{D}\right)^2$$

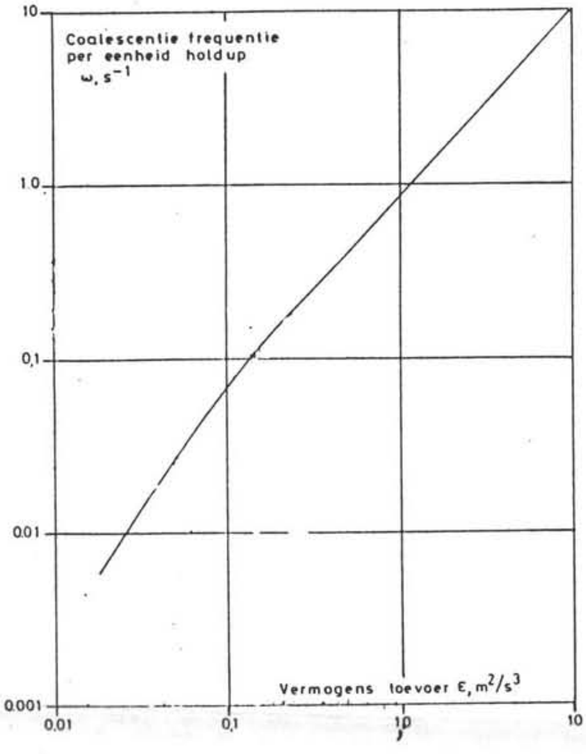


figure A.7.III.1 coalescence frequency ω

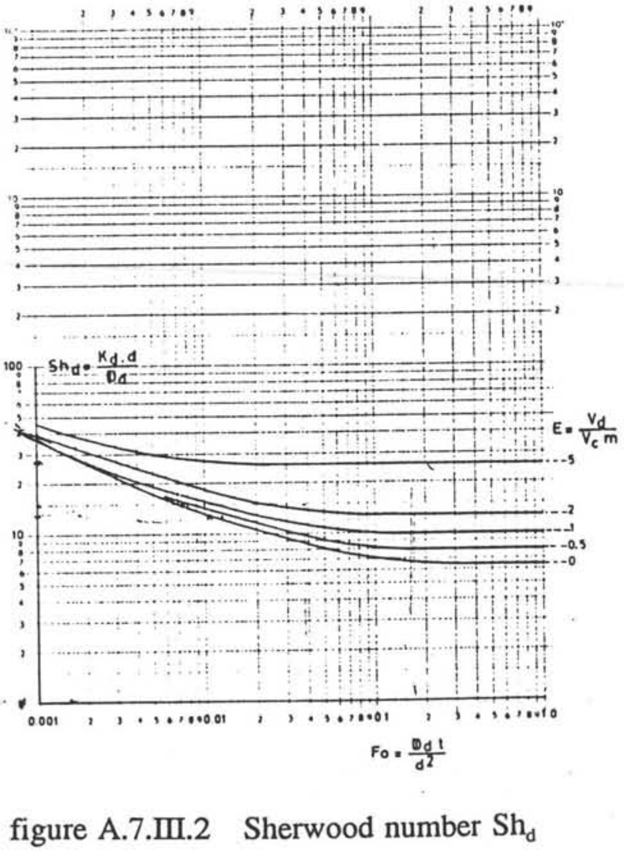


figure A.7.III.2 Sherwood number Sh_d

2. Determine extraction factor E;

$$E = K \frac{S}{F}$$

3. Determine interfacial area a, using the calculated values of h and $d_{3.2}$;

$$a = 6 \frac{h}{d_{3,2}}$$

4. Estimate contacting time t by determining coalescence constant ω from figure A.7.III.1 and knowing that t equals 3 to 5 times $(1/\omega)$.

5. Determine F_0, estimate Sherwood number of the dispersed phase Sh_d from figure A.7.III.2 and calculate the mass transfer coefficient of dispersed phase k_d ;

$$F_0 = \frac{t \ \delta_d}{{d_{3,2}}^2}$$

$$Sh_d = \frac{k_d \ d_{3,2}}{\delta_d}$$

6. Determine mass transfer coefficient of continuous phase k_c;

$$\frac{k_c \ d_{3.2}}{\delta_d} = 2 + 0.42 \left[\frac{d_{3,2}^{1.33} \ \varepsilon^{0.33} \ \rho_c}{\eta_c}\right]^{0.62} \left[\frac{\eta_c}{\delta_c \ \rho_c}\right]^{0.36}$$

7. Determine actual overall height of mass transfer unit HTU_{oc};

$$HTU_c = \frac{V_c}{a \ k_c}$$

$$HTU_d = \frac{V_d}{a \ k_d}$$

$$HTU_{oc} = HTU_C + HTU_d \ E$$

8. Determine number of revolutions of rotor;
9. Determine effective diffusion coefficients of dispersed ($\delta_{e,d}$) and continuous ($\delta_{e,c}$) phase;
10. Determine height of diffusion unit HDU_{oc} ;

$$\varepsilon = \frac{4}{\pi} c_p \frac{n^3 R^5}{H D^2}$$

$$\delta_{e,d} = \frac{V_d H}{h} + 0.024 R n H \left[\frac{S}{D}\right]^2$$

$$\delta_{e,c} = \frac{0.5 V_c H}{1-h} + 0.012 R n H \left[\frac{S}{D}\right]^2$$

In case of little axial mixing

$$\frac{(1-h) \delta_{e,c}}{V_c} + \frac{h \delta_{e,d}}{V_d} < HTU_{oc}$$

and

$$HDU_{oc} = \frac{(1-h) \delta_{e,c}}{V_c} + \frac{h \delta_{e,d} E}{V_d}$$

In case of much axial mixing

$$\frac{(1-h) \delta_{e,c}}{V_c} + \frac{h \delta_{e,d}}{V_d} > HTU_{oc}$$

and

$$HDU_{oc} = \frac{(1-h) \delta_{e,c} E}{V_c} + \frac{h \delta_{e,d}}{V_d}$$

11. Determine total height of effective overall mass transfer unit HTU_{oc}^*

$$HTU_{oc}^* = HTU_{oc} + HDU_{oc}$$

12. Determine height equivalent theoretical stages HETS;

$$HETS = \frac{\ln E}{E-1} HTU_{oc}^*$$

13. Determine length of extraction compartment (L) and total column length (L_{TOT});

$$L = N_{th}\ HETS$$

$$L_{TOT} = L + 0.3 + 0.5\ D$$

Calculations done with mathcad simulation program;

	$80_{o}C$	$100_{o}C$
α	1.088	1.090
h_{max}	0.391	0.391
h	0.293	0.293
U_o	0.083	0.085
d_m	0.0056	0.0053
$d_{3,2}$	0.0011	0.0010
ε	0.179	0.201
U_o	0.0265	0.0270
We	0.020	0.020
Re_{max}	$1.454\ 10^5$	$1.454\ 10^5$
Re	10.2	14.92
U_s	0.0198	0.0201
U_d	0.0042	0.0043
U_c	0.0039	0.0039
S	0.269	0.268
D	0.384	0.383
H	0.077	0.077
R	0.192	0.191
V_d	0.0021	0.0021
V_c	0.0019	0.0019
E	1.979	0.989
a	$1.577\ 10^3$	$1.6805\ 10^3$
ω	0.12	0.12
t	33.33	33.33
F_0	$5.92\ 10^{-4}$	$1.74\ 10^{-3}$
Sh_d	50	28
k_d	$9.899\ 10^{-7}$	$1.534\ 10^{-6}$
k_c	$1.670\ 10^{-6}$	$4.213\ 10^{-6}$

HTU_c	0.72	0.27
HTU_d	1.32	0.81
HTU_{oc}	3.32	1.07
n	0.135	0.134
$\delta_{e,d}$	$5.612\ 10^{-4}$	$5.699\ 10^{-4}$
$\delta_{e,c}$	$1.142\ 10^{-4}$	$1.157\ 10^{-4}$
HDU_{oc}	3.32	0.12
HTU_{oc}^*	3.52	1.19
HETS	2.46	1.20
L	9.83	27.67
L_{TOT}	10.32	28.17

Appendix A7.IV DESIGN OF PULSED PACKED COLUMN

The used design equations are from Ten Brink [4], Stemerding [5] and Lo [3]. Physical properties calculated with Reid [7] and Perry [9].

Choise of packing material;

The given calculation procedure is valid for packing materials with a void space up to 80%. We choose to use Raschig rings because they are largely applied in practice.

Raschig rings:
d_p = $19\ 10^{-3}$ [m]
S_p = 240 [m^2/m^3]
Ω = 0.8 [volume fraction]

A. Calculation of column diameter

Assume a pulsation velocity A_p*f of 0.0125 [m/s] and a pulsation frequency f of 5400 cycles/h.

1. Determine drop diameter d_o without pulsation and the Sauter mean drop diameter $d_{3,2}$;

$$d_o = 1.39 \left[\frac{\sigma}{\Delta\rho\ g}\right]^{0.5}$$

$$\frac{1}{d_{3,2}} - \frac{1}{d_0} = 6700 \left[\frac{1-\Omega}{\Omega}\right]^{0.95} \left[\frac{2\ \rho_c\ A_p\ f}{\eta_c\ S_p}\right] \left[\frac{\eta_c^2\ S_p}{\sigma\ \rho_c}\right]^{0.5} \left[\frac{\sigma\ S_p^2}{\Delta\rho\ g}\right]^{0.23}$$

2. Determination velocities of continuous (V_c) and dispersed (V_d) phase ;

First we need to calculate characteristic velocity V_o from

$$V_o = 6.23\ 10^{-3}\ d_{3,2}^{0.727}\ \Delta\rho^{0.815}$$

This equation is valid if R < 0.406, with

$$R = d_{3,2}^{0.787}\ \Delta\rho^{0.255}\ [2\ A_p\ f]^{-0.144}\ [S_p\ (1-\Omega)]^{0.426}$$

To calculate flooding velocities of continuous (V_{cf}) and dispersed (V_{df}) phase we solve the next equations by iteration;

$$V_{cf} = \Omega\ V_o\ [1-2\phi_f]\ [1-\phi_f]^2$$

$$V_{df} = 2\ \Omega\ V_o\ \phi_f^2\ [1-\phi_f]$$

$$\alpha = \frac{Q_d}{Q_c} = \frac{V_{df}}{V_{cf}}$$

To find the velocities of continuous and dispersed phase we use:

$$V_d = 0.75\ V_{df}$$

$$V_c = 0.75\ V_{cf}$$

3. Determine cross-sectional area A and diameter D of the column;

$$A = \frac{Q_d + Q_c}{V_c + V_d}$$

$$D = \left[\frac{4}{\pi}\ A\right]^{0.5}$$

B. Calculation of column height

1. Determine hold-up of dispersed phase ϕ_d by iteration of:

$$\frac{V_d}{\phi_d} + \frac{V_c}{1-\phi_d} = \Omega\ V_o\ (1-\phi_d)$$

2. Determine interfacial area a;

$$a = \frac{6\ \Omega\ \phi_d}{d_{3,2}}$$

3. First estimation height of overall diffusion unit HDU_o.

   Assume the axial diffusion coefficients of continuous ($\delta_{ax,c}$) and dispersed ($\delta_{ax,d}$) phase are 0.0015 and 0.001 respectively.

$$p_c = \frac{V_c}{\delta_{ax,c}}$$

$$p_d = \frac{V_d}{\delta_{ax,d}}$$

$$HDU_o = \frac{1}{p_c} + \frac{1}{p_d}$$

4. Determine overall mass transfer coefficient K_{oc}.

   Assume mass transfer coefficients of continuous (k_c) and dispersed (k_d) phase are the same as in case of RDC.

$$\frac{1}{K_{oc}} = \frac{1}{K_c} + \frac{m}{k_d}$$

5. Determine overall theoretical height of transfer unit HTU_{oc} based on continuous phase;

$$HTU_{oc} = \frac{V_d}{K_{oc}\ a}$$

6. Determine total height of effective overall mass transfer unit;

$$HTU^*_{oc} = HTU_{oc} + HDU_o$$

7. Determine height equivalent theoretical stages HETS;

$$HETS = \frac{\ln E}{E-1}\ HTU^*_{oc}$$

8. Estimation length of extraction equipment L;

$$L = N_{th}\ HETS$$

We can use the following equations to determine the actual extraction length L by iteration. By variation of L we can find a value at which the 'estimated' value (8.) equals the one found by iteration.

$$pl = \frac{1}{\frac{1}{E\ p_d} + \frac{1}{p_c}}$$

$$p2 = \frac{1}{\frac{1}{p_d} + \frac{1}{E\, p_d}}$$

$$p0 = \frac{\frac{0.1\, L}{HTU_{oc}} + 1}{\frac{0.1\, L}{HTU_{oc}} + \frac{p1}{p2}}\, p1$$

$$HDU_o = \frac{1}{p0 + \frac{0.8}{L} \frac{\ln E}{1 - \frac{1}{E}}}$$

$$HTU^*_{oc} = HTU_{oc} + HDU_o$$

$$HETS = \frac{\ln E}{E - 1}\, HTU^*_{oc}$$

$$L = N_{th}\, HETS$$

9. Determine total column length L_{TOT};

$$L_{TOT} = L + 6 + \left[\frac{L}{5\, D} - 1\right] 1.5$$

Calculations done with mathcad simulation program lead to:

	80$_o$C	100$_o$C
d_o	0.0103	0.0101
$d_{3,2}$	0.0014	0.0014
V_o	0.0018	0.0018
R	0.153	0.153
V_{cf}	$2.02\ 10^{-4}$	$2.03\ 10^{-4}$
V_{df}	$2.20\ 10^{-4}$	$2.21\ 10^{-4}$
V_d	$1.65\ 10^{-4}$	$1.66\ 10^{-4}$
V_c	$1.51\ 10^{-4}$	$1.52\ 10^{-4}$
A	1.08	1.09
D	1.17	1.18
ϕ_d	0.160	0.160
a	541.5	544.5
p_c	0.151	0.152
p_d	0.165	0.166
K_{oc}	$1.560\ 10^{-6}$	$1.579\ 10^{-6}$
HTU_{oc}	0.19	0.19
HDU_o	5.95	10.22
HTU_{oc}^*	0.14	10.42
HETS	4.28	10.47
L	17.14	41.89
L_{TOT}	25.06	54.00

Appendix A7.V DESIGN OF SIEVE PLATE COLUMN

Used equations are design equations from Krishna, college syllabus, subject: I21. Because design of RDC and PPC columns show that column dimensions become less easy for construction with increasing temperature (which leads to higher costs), and the different temperatures hardly effect the totally required energy of the total process that is designed, we choose the extraction to take place at 80°C. Design of the sieve plate column will only be done at a temperature of 80°C.

A. Determination of column area and diameter, downcomer area and perforated area.

1. choose a hole diameter d_h;

$$0.5 \sqrt{\frac{\sigma}{\Delta\rho\ g}} < d_h < \pi \sqrt{\frac{\sigma}{\Delta\rho\ g}}$$

in this case: $3.71 < d_h < 23.7$ [mm]

set a pitch; $12 < p < 20$ [mm]

2. Select hole velocity of dispersed phase (U_h);

$$Eo = (\Delta\rho)\ g\ \frac{d_h^2}{\sigma}$$

$$We = U_h^2\ \rho_d\ \frac{d_h^2}{\sigma}$$

From these two equations Uh can be determined by:

$$We = 4.33\ Eo^{-0.26}$$

The following guideline appeals:

$U_h > 0.15$ m/s

3. Predict Sauter mean drop diameter $d_{3.2}$;

$$Fr = \frac{U_h^2}{g\ d_h}$$

For Eö < 0.4:

$$\frac{d_{3.2}}{d_h} = Eo^{-0.4}\left[2.13\left(\frac{\Delta\rho}{\rho_d}\right)^{0.67} + \exp(-0.13\ Fr)\right]$$

For Eö ≥ 0.4:

$$\frac{d_{3.2}}{d_h} = Eo^{-0.42}\left[1.24 + \exp\left(-Fr^{0.42}\right)\right]$$

Generally $d_{3.2} \approx 0.003 - 0.007$ [m]

4. Determine active area of a tray or bubbling area A_b;

hole area (A_h);

$$A_h = \frac{Q_d}{U_h}$$

Number of holes (N_h);

$$N_h = \frac{A_h}{\frac{\pi}{4}\ d_h^2}$$

Bubling area A_b;

$$\frac{A_h}{A_b} = 0.907\left[\frac{d_h}{p}\right]^2$$

5. Determine active downcomer area A_d;

Assume $d_{min} = 0.1\ d_{3.2}$

$$U_{CD} = 0.249\ d_{\min}\left[\frac{g^2\ \Delta\rho^2}{\rho_c\ \eta_c}\right]^{\frac{1}{3}}$$

$$A_d = \frac{Q_c}{U_{CD}}$$

6. Determine tower diameter D;

$$A_T = A_b + 2\,A_d$$

$$D = \sqrt{\frac{4}{\pi}\,A_T}$$

B. Determination of number of plates and column height

1. Determine dispersed phase velocity (U_d) and dispersed phase hold-up (ϕ_d);

$$U_d = \frac{Q_d}{A_b + A_d}$$

$$V_{slip} = \frac{U_d}{\phi_d}$$

$$\frac{V_{slip}^2}{g\,d_p} = 2.725\,\frac{\Delta\rho}{\rho_c}\left[\frac{1 - \phi_d}{1 + \phi_d^{\frac{1}{3}}}\right]^{1.834}$$

2. Choose tray spacing;

   $T_s \approx 0.6$ [m]

3. Estimate overall tray efficiency E_o;

$$\frac{K_d}{\left[\dfrac{Ud}{\phi_d}\right]} = \frac{0.00375}{1 + \dfrac{\eta_d}{\eta_c}}$$

4. number of plates (N), extraction height (L) and column height (L_{TOT});

$$\frac{K_c}{\left[\frac{U_d}{\phi_d}\right]} = 0.725 \left[\frac{d_p \left[\frac{U_d}{\phi_d}\right] \rho_c}{\eta_c}\right]^{-0.43} \left[\frac{\eta_c}{\rho_c\, D_c}\right]^{-0.58} [1-\phi_d]$$

$$\frac{1}{K_{odr}} = \frac{1}{K_d} + \frac{m}{K_c}$$

$$a = \frac{6\ \phi_d}{d_p}$$

$$NTU_{odr} = \frac{K_{odr}\ a\ H_{dr}}{U_d}$$

$$Emd = 1-\exp(-NTUodr)$$

$$N = \frac{N_{th}}{E_o}$$

$$L = (N-1)\ T_s$$

$$L_{TOT} = L + 6$$

The results of optimizing the sieve plate column;
calculations done with mercury simulation program:

d_h	3.71 [mm]
p	12 [mm]
U_h	0.263 [m/s]
$d_{3.2}$	2.5 [mm]
A_b	0.016 [m^2]
A_d	0.0646 [m^2]

D	0.42 [m]
U_d	0.0032 [m/s]
ϕ_d	0.068 [volume fraction]
T_s	0.6 [m]
E_o	14.5 [%]
N	23 [-]
L	13.2 [m]
L_{tot}	19.2 [m]

Appendix A7.VI PRODUCT DATA SHEET

ROHM AND HAAS
EUROPEAN REGION

ION EXCHANGE
RESINS

AMBERLYST 15

STRONGLY ACIDIC CATALYST

PRODUCT DATA SHEET

Amberlyst 15 is a bead form, strongly acidic ion exchange resin developed particularly for heterogeneous acid catalysis of a wide variety of organic reactions.

It is also useful in non aqueous ion exchange systems for the removal of cationic impurities.

The macroreticular pore structure of Amberlyst 15 permits ready access of liquid or gaseous reactants to the hydrogen ion sites located throughout the bead, thus ensuring successful performance even in non swelling organic media.

APPLICATIONS

Alkylation, esterification, etherification, condensation, hydrolysis etc..

Physical and Chemical Properties

Type	Strong acid, macroreticular, cation exchanger
Ionic form (as supplied)	Hydrogen
Appearance	Opaque, spherical beads
Moisture content	1.5% maximum
Apparent density	Approximately 600g/litre
Particle size	0.3 to 1.2 mm
Fines content	1% maximum smaller than 0.3 mm
Concentration of acid sites	4.7 meq/g
Swelling	60–70% dry to water or ethanol wet form
Surface area	50 m^2/g
Porosity	0.40 ml/g
Average pore diameter	24 nm

Suggested Operating Conditions

pH range	0 to 14
Temperature limitation	120°C
Minimum bed depth	1000 mm
Service flow rate	1 to 10 BV/h
Regeneration conditions	
Concentration	1 to 3N HCl or H_2SO_4
Flow rate	1 to 4 BV/h
Rinse water requirements	4 to 10 BV

Appendix A7.VII DESIGN OF ION-EXCHANGER

Ion exchanger

Calculation of the ion exchanger column dimension :
Flow rate of liquid (Flexible, MEG, DADPM) :

$Q_{flex} := 714$ [kg/h]

$Q_{meg} := 0.6884$ [kg/h]

$Q_{dadpm} := 0.12365$ [kg/h]

$Q_{tot} := Q_{flex} + Q_{dadpm} + Q_{meg}$

The density of liquid at 120 C:

$\rho_{flex} := 948$ [kg/m^3]

$\rho_{dadpm} := 1100$ [kg/m^3]

$\rho_{meg} := 1036$ [kg/m^3]

$$\rho_{l} := \rho_{flex} \cdot \left[\frac{Q_{flex}}{Q_{tot}}\right] + \rho_{dadpm} \cdot \left[\frac{Q_{dadpm}}{Q_{tot}}\right] + \rho_{meg} \cdot \left[\frac{Q_{meg}}{Q_{tot}}\right]$$

$\rho_{l} = 948.111$

Molecular mass :

$M_{dadpm} := 198.3$ [gram/mol]

$$Qmol_{dadpm} := \frac{Q_{dadpm}}{M_{dadpm} \cdot 10^{-3}}$$ [mol/h]

$Qmol_{dadpm} = 0.624$

The resin capacity :

$C_{resin} := 4.7$ [meq/gram]

Adsorption :

DADPM + 2 (RESIN) ----> DADPM(RESIN)2

Density of resin :

$\rho_{resin} := 600$ [kg/m^3]

Fractional voidage of bed of particles :

$e := 0.4$

Volume of bed as function of adsorption time :
t in hours, take 24 hours for the adsorption proces

$$V_{bed}(t) := \frac{Qmol_{dadpm} \cdot 10^{3} \cdot t}{\frac{C_{resin}}{2} \cdot 10^{3} \cdot \rho_{resin}} \qquad [m^3]$$

$V_{bed}(24) = 0.011$

The thickness of bed in function of diameter and adsorption time :

$$l(D,t) := \frac{V_{bed}(t)}{\frac{\pi}{4} \cdot D^{2} \cdot (1 - e)} \qquad [m]$$

$l(0.1,24) = 2.252$

$l(0.2,24) = 0.563$ <----

$l(0.25,24) = 0.36$

$l(0.3,24) = 0.25$ $l(0.4,24) = 0.141$

The thickness of bed (with swelling 70 %) is equal to :

take diameter of 0.2 m, thus the thickness of bed :

$$\left[0.563 \cdot \frac{70}{100}\right] + 0.563 = 0.957 \qquad [\mathrm{m}]$$

$$l_s := 0.957 \quad [\mathrm{m}]$$

The fluid velocity through the bed :

$$u_1(D) := \frac{Q_{tot}}{\frac{\pi}{4} \cdot D^2 \cdot e \cdot 3600 \cdot \rho_1} \qquad [\mathrm{m/s}]$$

$u_1(0.1) = 0.067$

$u_1(0.2) = 0.017$ <---

$u_1(0.25) = 0.011$

$u_1(0.3) = 0.007$

$u_1(0.4) = 0.004$

The stay time of fluid over the bed :

$$T(D,t) := \frac{l(D,t)}{u_1(D)} \qquad [\mathrm{seconds}]$$

$T(0.1,24) = 33.786$
$T(0.2,24) = 33.786$
$T(0.3,24) = 33.786$

Calculation of pressure drop over the column :

The diameter of resin :
$d := 1.2$ [mm]

The fluid viscosity at 120 C :

$\mu := 0.0868$ [N s/m^2]

The surface area per unit volume of resin particle :

$$S := \frac{6}{d \cdot 10^{-3}} \qquad [m^2/m^3]$$

$$S = 5 \cdot 10^{3}$$

The flexible velocity in function of the diameter :

$$u(D) := u_1(D) \cdot e \qquad [m/s]$$

$u(0.1) = 0.027$

$u(0.2) = 0.007$ <---

$u(0.25) = 0.004$

$u(0.3) = 0.003$

$u(0.4) = 0.002$

The modified Reynolds number based on pore size :

$$Re_1(D) := \frac{u(D) \cdot \rho_1}{\mu \cdot S \cdot (1 - e)}$$

$Re_1(0.1) = 0.097$

$Re_1(0.2) = 0.024$

$Re_1(0.25) = 0.016$

$Re_1(0.3) = 0.011$

$Re_1(0.4) = 0.006$

The friction factor : $Wf = R1/(\rho.flex*V1^2)$

The friction factor in function of the diameter "

$$W_f(D) := \left[5 \cdot Re_1(D)^{-1} + 0.4 \cdot Re_1(D)^{-0.1}\right] \qquad \text{[Carman's formule]}$$

$W_f(0.1) = 52.006$

$W_f(0.2) = 206.582$

$W_f(0.25) = 322.485$

$W_f(0.3) = 464.134$

$W_f(0.4) = 824.675$

The pressure drop over the bed as function of diameter and adsorption time:

$$dP(D,t) := \frac{S\cdot(1 - e)\cdot l(D,t)\cdot \rho_l \cdot u(D)^2 \cdot W_f(D)}{e^3 \cdot 10^5} \qquad [\text{bar}]$$

$dP(0.1,24) = 37.013$

$dP(0.2,24) = 2.297$ <------

$dP(0.25,24) = 0.94$

$dP(0.3,24) = 0.453$

$dP(0.4,24) = 0.143$

The pressure drop over the column in the swollen condition :

$$dP(0.2,24)\cdot\frac{l_s}{l(0.2,24)} = 3.905 \qquad [\text{bar}]$$