MONASH UNIVERSITY

DEPARTMENT OF CHEMICAL ENGINEERING

APPENDIX TO CHAPTER 3

PROCESS SYNTHESIS AND FLOWSHEET DEVELOPMENT

Stream Number(s)	Description	Type	Hot/Cold	T_{IN} [°C]	H'_{IN} [kW]	T_{OUT} [°C]	H'_{OUT} [kW]	m' []	c_p [kJ.kg^{-1}]	m'_{cp}	ΔH'
									These are calculated		
11,12 (a)	Vaporiser recycle	Sink (sens)	Cold	62.10	-28959.8	86.5	-26970.4	**22.5059523**	4.07307596	91.6684534	2238.7
11,12 (b)	Vaporiser recycle	Sink (lat.)	Cold	86.5	-26970.4	86.5	-3706.6	22.5059523	#DIV/0!	#DIV/0!	0
14,15	Superheating	Sink	Cold	62.08	2976.8	158.3	3940.1	7.9159	1.26525728	10.0156501	963.2882
ex-RXN-1,16	Boiler	Source	Hot	700.0	10745.1	170.0	4430.0	7.9159	1.50522238	11.9151898	-6315.0506
16,17 (a)	Absorber feed	Source (sens	Hot	170.0	4430.0	90.0	3572.9	7.9159	1.35358993	10.7148825	-857.1906
16,17 (b)	Absorber feed	Source (lat.)	Hot	62.0	3572.9	62.0	3572.9	7.9159	0	0	0
16,17 (c)	Absorber feed	Source (lat.)	Hot	62.0	3572.9	62.0	3572.9	7.9159	#DIV/0!	#DIV/0!	0
19,20	Absorber, stage 1	Source	Hot	75.0	*-53691.3*	60.0	*-56946.9*	58.7193	1.232	72.34762	-1085.2143
28,29	Absorber, stage 2	Source	Hot	*65.0*	*-53691.3*	*50.0*	*-56946.9*	58.7193	1.232	72.34762	-1085.2143
31,32	Absorber, stage 3	Source	Hot	*55.0*	*-53691.3*	*40.0*	*-56946.9*	58.7193	1.232	72.34762	-1085.2143
38,40 ***FIX	Burner	Source	Hot	*907*	*6542*	*220*	*2550*	4.5937	1.266	5.81399228	-3992.0121
RCW	*Utility*	Sink		30.0		40			4.1899	0	0
TW	*Utility*	Sink		30.0		40			4.1899	0	0
DW	*Utility*	Sink		30.0		40			4.1899	0	0
LP Steam: 500bar(a)	*Utility*	Source		151.9		151			condensing	infinite	
HP Steam: 1200bar(a)	*Utility*	Source		188.0		187			condensing	infinite	

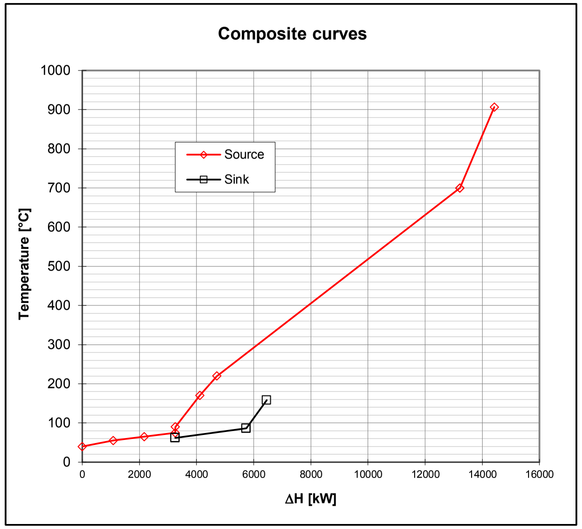
2238.6628
0.0

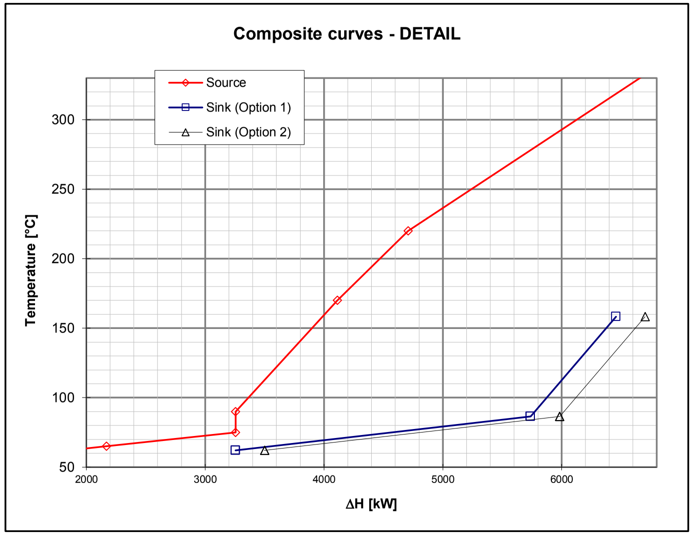
SOURCE STREAMS Composite Curve

Interval Number	Lower Temp	Upper Temp	Stream	m'_{cp}	ΔH'	Sub-Total ΔH'	Cumul-Total ΔH'
		40					*0*
1	40.0	55.0	31,32	72.34762	1085.2143	1085.2143	1085.2143
2	50.0	65.0	28,29	72.34762	1085.2143	1085.2143	2170.4286
3	60.0	75.0	19,20	72.34762	1085.2143	1085.2143	3255.6429
	75.0	90.0					3255.6429
4	90.0	170.0	16,17 (a)	10.7148825	857.1906	857.1906	4112.8335
5	170.0	220.0	ex-RXN-1,16	11.9151898	595.759491	595.759491	4708.59299
6	220.0	700.0	ex-RXN-1,16	11.9151898	5719.29111	8510.0074	13218.6004
		700.0	38,40	5.81399228	2790.71629		13218.6004
7	700.0	907	38,40	5.81399228	1201.29581	1201.29581	14419.8962

SINK STREAMS Composite Curves

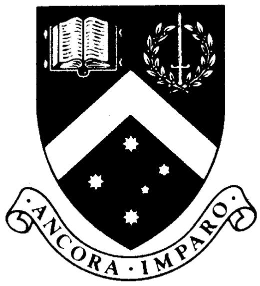
Interval Number	Lower Temp	Upper Temp	Stream	m'_{cp}	ΔH'	Sub-Total ΔH'	Cumulative Total ΔH'	
							OPTION 1	OPTION 2
		62.08				DATUM =	*3255.6429*	*3500*
1	62.08	62.10	14,15	10.0156501	0.13420971	0.13420971	3255.77711	3500.13421
2	62.10	86.5	14,15	10.0156501	244.595196	2483.258	5739.03511	5983.39221
		86.5	11,12(a)	91.6684534	2238.6628		*5739.0351*	*5983.3922*
3	86.5	158.3	14,15	10.0156501	718.558795	718.558795	6457.5939	6701.951





MONASH UNIVERSITY

DEPARTMENT OF CHEMICAL ENGINEERING



Appendix to Chapter 5

Mass and Energy Balances & Process Simulation

CALCULATION OF DESIGN "GRADE A" AND "GRADE B" CAPACITY

Total capacity: 80 $kt(54\%).y^{-1}$

Percentage of "Grade A": 90 %
Percentage of "Grade B": 10 %

Compositions [%]:

	HCHO	CH_3OH	H_2O
"Grade A"	54	1	45
"Grade B"	37	7	56

			350	$d_{op'n}.y^{-1}$	24	$h_{op'n}.d_{op'n}^{-1}$	3600	$s.h_{op'n}^{-1}$
Thus:								
Flow of "Grade A":	74.34034	$kt(54\%).y^{-1}$	212.401	$t(54\%).d_{op'n}^{-1}$	8.850041	$t(54\%).h_{op'n}^{-1}$	2.458345	$kg(54\%).s^{-1}$
Flow of "Grade B":	5.659656	$kt(54\%).y^{-1}$	16.17045	$t(54\%).d_{op'n}^{-1}$	0.673769	$t(54\%).h_{op'n}^{-1}$	0.187158	$kg(54\%).s^{-1}$
TOTAL flow	80	$kt(54\%).y^{-1}$	228.5714	$t(54\%).d_{op'n}^{-1}$	9.52381	$t(54\%).h_{op'n}^{-1}$	2.645503	$kg(54\%).s^{-1}$
Flow of "Grade A":	74.34034	$kt(54\%).y^{-1}$	212.401	$t(54\%).d_{op'n}^{-1}$	8.850041	$t(54\%).h_{op'n}^{-1}$	2.458345	$kg(54\%).s^{-1}$
Flow of "Grade B":	8.260038	$kt(37\%).y^{-1}$	23.60011	$t(37\%).d_{op'n}^{-1}$	0.983338	$t(37\%).h_{op'n}^{-1}$	0.273149	$kg(37\%).s^{-1}$
TOTAL flow	82.60038	$kt(solution).y^{-1}$	236.0011	$t(solution).d_{op'n}^{-1}$	9.833379	$t(solution).h_{op'n}^{-1}$	2.731494	$kg(solution).s^{-1}$

BASIC COMPLETE MATERIAL BALANCE

Assume:

About half of the methanol goes to each of the folowing reactions [Mechetta, p.358]:

$CH_3OH + 0.5O_2$ --> $HCHO + H_2O$	(1)	36%	of CH_3OH reacted
CH_3OH --> $HCHO + H_2$	(2)	60%	of CH_3OH reacted

The former is decreased by the presence of water [Catalyst Handbook, p. 493]

Dehydrogenation (2) is more prevalent for catalysis by silver [Formaldehyde (3), p. 9]

Atomic masses:		
C	12.011	$kg.kmol^{-1}$
H	1.0079	$kg.kmol^{-1}$
O	15.9994	$kg.kmol^{-1}$
N	14.0067	$kg.kmol^{-1}$

Sargent-Welch Sci. Co.

Molar masses:		
CH_3OH	0.032	$kg.mol^{-1}$
HCHO	0.030	$kg.mol^{-1}$
O_2	0.032	$kg.mol^{-1}$
N_2	0.028	$kg.mol^{-1}$
H_2O	0.018	$kg.mol^{-1}$
H_2	0.002	$kg.mol^{-1}$
CO_2	0.044	$kg.mol^{-1}$
CO	0.028	$kg.mol^{-1}$
HCOOH	0.046	$kg.mol^{-1}$

From Simon Farrar (Orica)

G.F.C Rogers & Y. R. Mayhew (5), p. 2

Assume: - other (side) reactions are **considered** (as follows):

- nitrogen is inert and approximates any argon present
- methanol is in excess
- oxygen (limiting) consumed to: 99.5% (once-through) *~~by analogy with Table 4 (p. 362) of McKetta~~*
- Off gases **released** contain all N_2, O_2 and H_2 and (nominal) 13.2% of H_2O exiting system *~~by simplification of Table 4 (p. 362) in McKetta~~*
- by-products form by: **Assume:** *Ullmann's(5), Vol. A11, p. 624.*

$H_2 + 0.5O_2$ --> H_2O	(3)	40.0%	of H_2 from (2) [WITHOUT recycled]
$HCHO$ --> $CO + H_2$	(4)	0.92%	of HCHO formed by (1) & (2) + recycled
$CH_3OH + 1.5O_2$ --> $CO_2 + 2H_2O$	(5)	4.0%	of CH_3OH reacted
$HCHO + O_2$ --> $CO_2 + H_2O$	(6)	6.5%	of HCHO formed by (1) & (2) + recycled **More complete combustion at the elevated temperature? - see Ullmann's (5), p. 626*

- the formation of formic acid (**during processing**!) is considered here: *Formaldehyde (3), p. 9*

$HCHO + 0.5O_2$ --> $HCOOH$	(7)	0.020%	of HCHO formed by (1) & (2) + recycled
cf. $HCHO + 0.5O_2$ --> $CO + H_2O$	(8)	0.020%	of HCHO formed by (1) & (2) + recycled

- the following are not considered: *cf. Catalyst Handbook, p. 493*
  - $CH_3OH + 0.5O_2$ --> $H_2O + H_2 + CO$ (9) *Essentially covered by other reactions*
  - $HCHO + HCHO$ --> CH_3OCHO (10) *Temperature is too high during processing - Simon Farrar.*
- Conversion of methanol is: 98.5% (once through) *(Ullmann)* Yield: 88.9%
- Ratio of total off-gas to that which is recycled is: **0.95** ==> Ratio of recycled off-gas to (100%) methanol fed: 157% *cf. US patent 4072717, col. 6*
- Percentage of fresh water entering the entire system on the process-side that enters the vaporiser (the rest entering the absorber): 50%
- Ambient air: Relative humididy = 80% Temperature = 37 °C hence Mole fraction = 0.049599 at 1atm(abs).

Mass fractions [-]:	HCHO	CH_3OH	H_2O	HCOOH
"Grade A"	0.54	0.01	< 0.45	< 0.001

Mole fraction of air [-]:	O_2	N_2	Ar	CO_2
	0.2095	0.7809	0.0093	0.0003

Approx.	O_2	N_2
	0.2095	0.7905

G.F.C Rogers & Y. R. Mayhew (5), p. 26

NOTE: Compared to a 50:50 split b/n rxn's (1) & (2) with no side reactions, the scheme outlined here requires:
- * less water [now also by (3); & more methanol compensate for red'n in (1)]
- * more methanol [due to "losses" in side-rxn's]
- & * more oxygen (in air) [due to extra methanol consumed]

as fresh feed.

NOTE: "Fresh Feed" is a hypothetical stream - in practice the components of this stream would be added variously at different points in the system.

NOTE (1): Absorber has not been properly modelled at all.

NOTE (2): Trace quantities of NO_x will be present in all gas/vapour process streams except for the fresh feed.

NOTE (3): Water in the incoming methanol has not been considered here. Formic acid in incoming methanol is negligible, and may be assumed to be completely combusted to "inert" CO_2

Water balance:

Note: Water in Absorber feed is already at a high mole fraction.

Total overhead/absorber feed = 0.22847389 if total pressure = 110 kPa(abs)

NOTE: p_{sat}(water @ 44°C) =	9.10 kPa(abs)	8.273%
NOTE: p_{sat}(water @ 50°C) =	12.33 kPa(abs)	11.209%
NOTE: p_{sat}(water @ 55°C) =	15.74 kPa(abs)	14.309%
NOTE: p_{sat}(water @ 60°C) =	19.92 kPa(abs)	18.109%
NOTE: p_{sat}(water @ 70°C) =	31.16 kPa(abs)	28.327%

FORMULAE:

$CH_3OH + 1.5O_2$ --> $CO_2 + 2H_2O$	(1)
$HCHO + O_2$ --> $CO_2 + H_2O$	(2)
$H_2 + 0.5O_2$ --> H_2O	(3)
$CO + 0.5O_2$ --> CO_2	(4)
$HCOOH + 0.5O_2$ --> $CO_2 + H_2O$	(5)

- Excess air supplied: 20%
- Assume **complete** combustion in off-gas burner (except N_2)

Using the spreadsheet's "iterate" function

Stream:	**Fresh feed**		**Recycled off-gas**		**Total reactor feed**	
MOLAR FLOWS [$mol.s^{-1}$]		FRACTION:		FRACTION:		FRACTION:
CH_3OH	54.35507	0.3008	0	0.0000	54.3551	0.1837
HCHO	0	0.0000	0	0.0000	0	0.0000
O_2	22.65455	0.1254	0.0553	0.0005	22.7099	0.0768
N_2	85.48174	0.4731	81.2076	0.7050	166.6894	0.5634
H_2O	18.18057	0.1006	9.5298	0.0827	27.7104	0.0937
H_2	0	0.0000	18.7581	0.1628	18.7581	0.0634
CO_2	0	0.0000	5.1838	0.0450	5.1838	0.0175
CO	0	0.0000	0.4608	0.0040	0.4608	0.0016
HCOOH	0	0.0000	0	0.0000	0	0.0000
TOTAL	180.6719	1.0000	115.1954	1.0000	295.8674	1.0000

REACTIONS:

51.3882561 51.3882561 51.3882561 =Total HCHO formed pre-degradation

(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	NETT	
-19.2706	-32.1177	0	0	-2.14118	0	0	0	-53.52943	CH_3OH
19.2706	32.11766	0	-0.47476	0	-3.31545	-0.01028	-0.01028	47.5775	HCHO
-9.6353	0	-6.423532	0	-3.21177	-3.31545	-0.00514	-0.00514	-22.59632	O_2
0	0	0	0	0	0	0	0	0	N_2
19.2706	0	12.84706	0	4.282355	3.315448	0	0.010278	39.72574	H_2O
0	32.11766	-12.84706	0.474756	0	0	0	0	19.74535	H_2
0	0	0	0	2.141177	3.315448	0	0	5.456626	CO_2
0	0	0	0.474756	0	0	0	0.010278	0.485033	CO
0	0	0	0	0	0	0.010278	0	0.010278	HCOOH
9.635298	32.11766	-6.423532	0.474756	1.070589	0	-0.00514	0.005139	36.87477	
	(N O T	Z E R O)			(N O T	Z E R O)		(NOT ZERO)	

	(Absorber feed) **Reactor effluent**		**Absorber water in**		**Off-gas**		**Product**	
		FRACTION:		FRACTION:		FRACTION:		FRACTION:
CH_3OH	0.8256	0.0025	0	0.0000	0	0.0000	0.8256	0.0072
HCHO	47.5775	0.1430	0	0.0000	0	0.0000	47.5775	0.4156
O_2	0.1135	0.0003	0	0.0000	0.0582	0.0005	0	0.0000
N_2	166.6894	0.5010	0	0.0000	85.4817	0.7050	0	0.0000
H_2O	67.4361	0.2027	18.18057	1.0000	10.0314	0.0827	66.0555	0.5771
H_2	38.5034	0.1157	0	0.0000	19.7454	0.1628	0	0.0000
CO_2	10.6404	0.0320	0	0.0000	5.4566	0.0450	0	0.0000
CO	0.9458	0.0028	0	0.0000	0.4850	0.0040	0	0.0000
HCOOH	0.0103	0.0000	0	0.0000	0	0.0000	0.0103	0.0001
	332.7421	1.0000	18.18057	1.0000	121.2584	1.0000	114.4689	1.0000
					Total out:	235.727267		

CHECK ! ACC = 0 = IN+GEN-OUT:			**Additional fuel/air**		**Combusted off-gas**		[$mol.s^{-1}$]
				FRACTION:		FRACTION:	
0.0000	0.0000	---	0	0.0000	0	0.0000	CH_3OH
0.0000	0.0000	---	0	0.0000	0	0.0000	HCHO
0.0000	*0.0000*	---	12.0800	0.1991	2.0230	0.0118	O_2
0.0000	0.0000	---	45.5811	0.7513	131.0628	0.7628	N_2
0.0000	0.0000	---	3.0092	0.0496	32.7859	0.1908	H_2O
0.0000	0.0000	---	0	0.0000	0	0.0000	H_2
0.0000	0.0000	---	0	0.0000	5.9417	0.0346	CO_2
0.0000	0.0000	---	0	0.0000	0	0.0000	CO
0.0000	0.0000	---	0	0.0000	0	0.0000	HCOOH
0.0000	0.0000	---	60.6703	1.0000	171.8134	1.0000	
(SHOULD BE ZERO)							

MASS FLOWS [$kg.s^{-1}$]	**Fresh feed**	FRACTION:	**Recycled off-gas**	FRACTION:	**Total reactor feed**	FRACTION:
CH_3OH	1.7416	0.3357	0	0.0000	1.7416	0.2200
HCHO	0	0.0000	0	0.0000	0	0.0000
O_2	0.7249	0.1397	0.0018	0.0006	0.7267	0.0918
N_2	2.3946	0.4615	2.2749	0.8341	4.6695	0.5899
H_2O	0.3275	0.0631	0.1717	0.0630	0.4992	0.0631
H_2	0	0.0000	0.0378	0.0139	0.0378	0.0048
CO_2	0	0.0000	0.2281	0.0837	0.2281	0.0288
CO	0	0.0000	0.0129	0.0047	0.0129	0.0016
HCOOH	0	0.0000	0	0.0000	0	0.0000
TOTAL	5.1887	1.0000	2.7272	1.0000	7.9159	1.0000

(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	NETT	
-0.61747	-1.02911	0	0	-0.06861	0	0	0	-1.71519	CH_3OH
0.578623	0.964371	0	-0.01426	0	-0.09955	-0.00031	-0.00031	1.428571	HCHO
-0.30832	0	-0.205545	0	-0.10277	-0.10609	-0.00016	-0.00016	-0.723055	O_2
0	0	0	0	0	0	0	0	0	N_2
0.347164	0	0.231442	0	0.077147	0.059728	0	0.000185	0.715667	H_2O
0	0.064743	-0.025897	0.000957	0	0	0	0	0.039803	H_2
0	0	0	0	0.094233	0.145912	0	0	0.240145	CO_2
0	0	0	0.013298	0	0	0	0.000288	0.013586	CO
0	0	0	0	0	0	0.000473	0	0.000473	HCOOH
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
(S H O U L D	B E	Z E R O)		(S H O U L D	B E	Z E R O)		(SHOULD BE ZERO)	
Actual reaction conversion: 35.453%	*59.089%*	25.02%	0.924%	3.939%	6.452%	0.0200%	0.0200%		
basis: CH_3OH	*CH_3OH*	H_2	HCHO	CH_3OH	HCHO	HCHO	HCHO		

^^^ Or 97.5% of the CH_3OH remaining after reactions (1) and (5) have proceeded

* Note: HCHO and H_2 calculated from total **generated**

	Reactor effluent	FRACTION:	**Absorber water in**	FRACTION:	**Off-gas**	FRACTION:	**Product**	FRACTION:
CH_3OH	0.0265	0.0033	0	0.0000	0	0.0000	0.026455	**0.0100**
HCHO	1.4286	0.1805	0	0.0000	0	0.0000	**1.428571**	**0.5400**
O_2	0.0036	0.0005	0	0.0000	0.0019	0.0006	0	0.0000
N_2	4.6695	0.5899	0	0.0000	2.3946	0.8341	0	0.0000
H_2O	1.2149	0.1535	0.3275	1.0000	0.1807	0.0630	1.190003	**0.4498**
H_2	0.0776	0.0098	0	0.0000	0.0398	0.0139	0	0.0000
CO_2	0.4683	0.0592	0	0.0000	0.2401	0.0837	0	0.0000
CO	0.0265	0.0033	0	0.0000	0.0136	0.0047	0	0.0000
HCOOH	0.0005	0.0001	0	0.0000	0	0.0000	0.000473	**0.00018**
	7.9159	1.0000	0.3275	1.0000	2.8707	1.0000	**2.645503**	1.0000
					Total out:	5.51625088		

			Additional fuel/air	FRACTION:	**Combusted off-gas**	FRACTION:	[$kg.s^{-1}$]
0.0000	0.0000	---	0	0.0000	0	0.0000	CH_3OH
0.0000	0.0000	---	0	0.0000	0	0.0000	HCHO
0.0000	*0.0000*	---	0.3865	0.2250	0.0647	0.0141	O_2
0.0000	0.0000	---	1.2769	0.7434	3.6715	0.8002	N_2
0.0000	0.0000	---	0.0542	0.0316	0.5906	0.1287	H_2O
0.0000	0.0000	---	0	0.0000	0	0.0000	H_2
0.0000	0.0000	---	0	0.0000	0.2615	0.0570	CO_2
0.0000	0.0000	---	0	0.0000	0	0.0000	CO
0.0000	0.0000	---	0	0.0000	0	0.0000	HCOOH
0.0000	0.0000	0.0000	1.7176	1.0000	4.5884	1.0000	
(SHOULD BE ZERO)							

NOTE: Some water enters with "fresh air"
= 5.643335 $mol.s^{-1}$
= 0.101666 $kg.s^{-1}$ ==> 0.225861 in MainsWater

MONASH

CLIENT: CHE4117		SHEET	1 of 1
PROJECT: MASS BALANCE		DATE	01/10/1999
		BY	DJV
DESIGN OF: ADDITIONAL GRADE "B" REQUIREMENTS		CHKD.	

① TOTAL FLOWS.

From the spreadsheet $\dot{m}_B = 0.273149 \, kg.s^{-1}$ — $\dot{m}_B = 0.273 kg.s^{-1}$

Equating formaldehyde content, this requires $\dot{m}_A = 0.187158 \, kg.s^{-1}$ — $\dot{m}_A = 0.187 kg.s^{-1}$

② ADDITIONAL METHANOL

The feed Grade A contains $(0.01 \dot{m}_A) \, kg.s^{-1}$ of methanol,

but the Grade B product $(0.07 \dot{m}_B) \, kg.s^{-1}$.

Thus a difference of $0.0172489 \, kg.s^{-1}$ of fresh methanol — $\dot{m}_M = 0.0172 kg.s^{-1}$

③ ADDITIONAL WATER

Likewise, additional water $\doteq \left[(0.45 - 0.0018)\dot{m}_A\right]$

$$+ \left[\left(0.56 - 0.0018 \times \frac{37}{54}\right)\dot{m}_B\right]$$

$$= 0.0687423 \, kg.s^{-1}$$

$\therefore \dot{m}_W = 0.0687 kg.s^{-1}$

Table 5a. Thermodynamic & Essential Data of Components

All data from Sinnott[2] unless otherwise stated

		Methanol (CH_3OH)	Air	Oxygen (O_2)	Nitrogen (N_2)	Formaldehyde (HCHO)	Carbon Dioxide (CO_2)	Carbon Monoxide (CO)	Water (H_2O)	Formic Acid (HCOOH)	Methyl Formate ($C_2H_4O_2$)	Hydrogen (H_2)	
MW	Molecular Weight [$g.mol^{-1}$]	32.042		32	28.013	30.026	44.01	28.01	18.015	46.025	60.052	2.016	**MW**
TFP	Normal Freezing Point [°C]	-97.7		-218.8	-209.9	-117.2	-56.6	-205.1	0	8.3	-99	-259.2	**TFP**
TBP	Normal Boiling Point [°C]	64.6		-183	-195.8	-19.2	-78.5	-191.5	100	100.6	31.7	-252.8	**TBP**
TC	Critical Temperature [K]	512.6		154.6	126.2	408	304.2	132.9	647.3	580	487.2	33.2	**TC**
PC	Critical Pressure [bar(abs)]	81		50.5	33.9	65.9	73.8	35	220.5		60	13	**PC**
VC	Critical Volume [$m^3.mol^{-1}$]	0.118		0.073	0.09		0.094	0.093	0.056		0.172	0.065	**VC**
LDEN	Liquid Density [$kg.m^{-3}$]	791		1149	805	815	777	803	998	1226	974	71	**LDEN**
TDEN	Ref. Temp for liquid density [°C]	20		-183	-195	-20	20	-192	20	15	20	-253	**TDEN**
HVAP	Heat of Vaporisation **at normal boiling point** [$J.mol^{-1}$]	35278		6824	5581	23027	17166	6046	40683	21939	28219	904	**HVAP**
VISA	Constants in the liquid viscosity eq.	555.3		85.68	90.3	319.83	578.08	94.06	658.25	729.35	363.19	13.82	**VISA**
VISB	Constants in the liquid viscosity eq.	260.64		51.5	46.14	171.35	185.24	48.9	283.16	325.72	212.7	5.39	**VISB**
DELHF	Standard Enthalpy of formation of of **vapour** at 298K [$kJ.mol^{-1}$]	-201.3		0	0	-115.97	-393.77	-110.62	-242	-378.86	-350.02	0	**DELHF**
	[$kJ.kg^{-1}$]	-6282.379		0	0	-3862.319323	-8947.284708	-3949.30382	-13433.2501	-8231.613254	-5828.6152	0	
DELGF	Standard Gibbs energy of formation of vapour at 298K [$kJ.mol^{-1}$]	-162.62				-109.99	-394.65	-137.37	-228.77	-351.23	-297.39		**DELGF**
CPVAPA	Constant in ideal gas heat capacity equation (see below)	21.152	28.94	28.106	31.15	23.475	19.795	30.869	32.243	11.715	1.432	27.143	**CPVAPA**
CPVAPB	Constant in ideal gas heat capacity equation (see below)	7.09E-02	4.15E-03	-3.68E-06	-1.36E-02	3.16E-02	7.34E-02	-1.29E-02	1.92E-03	1.36E-01	2.70E-01	9.27E-03	**CPVAPB**
CVPAPC	Constant in ideal gas heat capacity equation (see below)	2.59E-05	3.19E-06	1.75E-05	2.68E-05	2.99E-05	-5.60E-05	2.79E-05	1.06E-05	-8.41E-05	-1.95E-04	-1.38E-05	**CVPAPC**
CPVAPD	Constant in ideal gas heat capacity equation (see below)	-2.58E-08	-1.79E-09	-1.07E-08	-1.17E-08	-2.30E-08	1.72E-08	-1.27E-08	-3.60E-09	2.02E-08	5.70E-08	7.65E-09	**CPVAPD**
ANTA	Constant in Antoine equation	18.5875		15.4075	14.9502	16.4775	22.5898	14.3686	18.3036	16.9882	16.5104	13.6333	**ANTA**
ANTB	Constant in Antoine equation	3626.55		734.55	588.72	2204.13	3103.39	530.22	3816.44	3599.58	2590.87	164.9	**ANTB**
ANTC	Constant in Antoine equation	-34.29		-6.45	-6.6	-30.15	-0.16	-13.15	-46.13	-26.09	-42.6	3.19	**ANTC**
TMN	Minimum temperature for Antoine constant [°C]	-16		-210	-219	-88	-119	-210	11	-2	-48	-259	**TMN**
TMX	Maximum temperature for Antoine constant [°C]	91		-173	-183	**-2**	-69	-165	168	136	51	-248	**TMX**

$c_p[J.mol^{-1}.K^{-1}] = A + B.T + C.T^2 + D.T^3$; T in K

LOG(Viscosity[mPa.s]) = (VISA).{(1/T) - (1/VISB)}; T in K

LN($p_{vapour(sat'n)}$[mmHg(abs)]) = ANTA - (ANTB/(T + ANTC)); T in K

From Oxtoby & Nachtrieb [(2)]

Heat of formation of the **pure liquids** at 25°C:

Methanol	-238.66	-7448.349	*cf*. (aq)	-245.93	-7675.24
Water	-285.83	-15866.22			
Formic acid	-424.72	-9228.028	*cf*. (aq)	-425.43	-9243.45
	[kJ.mol^{-1}]	[kJ.kg^{-1}]		[kJ.mol^{-1}]	[kJ.kg^{-1}]

From Ullmann's [(5)]

Heat of solution at 23°C: **HCHO** 62 kJ.mol^{-1} = 1935.927 kJ.kg^{-1}

(T = 296.15 K)

Then with the mean specific heat of HCHO(g): 34.89326 J.mol^{-1}·K^{-1}

Mean specific heat of HCHO(l): 72.18094 J.mol^{-1}·K^{-1}

Mean specific heat of H_2O(l): 75.40113 J.mol^{-1}·K^{-1}

well might the mean c_p of 25%(mol.mol^{-1}) HCHO-H_2O(solution) be (approx.)

74.59608 J.mol^{-1}·K^{-1}

*Assuming additive specific heats of the pure liquid constituents (ideal), as per *Sinnott* [(2)], p. 284.

However, by the same token we would assume that the HCHO component of that mixture would have

mean c_p of HCHO(aq) = mean c_p of HCHO(l) = 72.18094 J.mol^{-1}·K^{-1} (they are very similar, in any case)

Heat of formation at 25°C: Gas -116.0 kJ.mol^{-1} = -3622.06 kJ.kg^{-1}

Hence: Aq -177.9254 kJ.mol^{-1} = -5555.66 kJ.kg^{-1}

(*cf.* -178.0 kJ.mol^{-1} if c_p's not considered.) = -5557.9841 kJ.kg^{-1}

From Perry [(7)]

Liquid Phase Heat Capacities

T in K, c_p in J.**k**mol^{-1}.K^{-1} $c_p = C1 + C2.T + C3.T^2 + C4.T^3 + C5.T^4$

	C1	C2	C3	C4	C5	T_min	T_max
Methanol	105800	-362.23	0.9379			175.47	400
Water	276370	-2090.1	8.125	-0.014116	9.3701E-06	273.16	533.15

From AIChE.S (Table 4)

Liquid Phase Heat Capacity

T in K, c_p in J.mol^{-1}.K^{-1} cp = A + B.T + C.T2 + D.T3

	A	B	C	D	T_min	T_max
HCHO	4.16E+02	-2.64E+00	4.98E-03	-	?	?

From Perry [(6)]

Liquid-phase heat capacity of formic acid:

0 °C :	0.436 cal.g^{-1}.°C^{-1},	1.824224 kJ.kg^{-1}.K^{-1},	83.95991 J.mol^{-1}.K^{-1},
15.5 °C :	0.509 cal.g^{-1}.°C^{-1},	2.129656 kJ.kg^{-1}.K^{-1},	98.01742 J.mol^{-1}.K^{-1},
20 to 100 °C :	0.524 cal.g^{-1}.°C^{-1},	2.192416 kJ.kg^{-1}.K^{-1},	100.9059 J.mol^{-1}.K^{-1},

This last row should be sufficiently accurate for the purposes of this report.

Energy Balance over Vaporiser (HX-1)

NOTE: Heat of solution of methanol [implicitly] considered.

Ideal vapour- [& liquid(?)]- phase assumed.

Recirc. liquid flow: 23.945 23.945 kg.s^{-1}

STREAMS IN:

No.	Description	HYSIM	Flow [kg.s^{-1}]	t [°C]	T [K]	Species	State	Mass frac. [-]	M_R [kg.mol^{-1}]	A / C1	B / C2	C / C3	D / C4	C5	$\bar{c}_p$ [kJ.kg^{-1}.K^{-1}]	$\Delta H^o_{f,298K}$ [kJ.kg^{-1}]	$\Delta H^o_{f,T}$ [kJ.kg^{-1}]	$\Delta H^o_{f,T}$ [kW]	
3	Demin'd water	WaterFeed	0.225861	37.05	310.20	H_2O	L	1	0.0180152	276370	-2090.1	8.125	-0.01412	9.37E-06	4.180306924	-15866.04645	-15815.69214	-3572.148043	H_2O
6	Methanol	MethanolFeed	1.7416	37.04	310.19	CH_3OH	L	1	0.032042	105800	-362.23	0.9379	0	0	2.571789791	-7448.349042	-7417.396266	-12918.13734	CH_3OH
9	Air & rec. off-gas	HPGas	5.948366	121.58	394.73	O_2	V	0.122168	0.0319988	28.11	-3.68E-06	1.75E-05	-1.07E-08		0.9302	0	89.8450	65.29035916	O_2
			5.948366		394.73	N_2	V	0.7850055	0.0280134	31.15	-0.01357	2.68E-05	-1.17E-08		1.042040847	0	100.6434311	469.9545017	N_2
			5.948366		394.73	H_2O	V	0.0459565	0.0180152	32.24	0.001924	1.06E-05	-3.60E-09		1.888880215	-13433.10094	-13250.66722	-3622.281895	H_2O
			5.948366		394.73	H_2	V	0.0063547	0.0020158	27.14	0.009274	-1.38E-05	7.65E-09		14.39067509	0	1389.894573	52.53801484	H_2
			5.948366		394.73	CO_2	V	0.0383467	0.0440098	19.8	0.07344	-5.60E-05	1.72E-08		0.890766635	-8948.007035	-8861.974121	-2021.416297	CO_2
			5.948366		394.73	CO	V	0.0021687	0.0280104	30.87	-0.01285	2.79E-05	-1.27E-08		1.0441883	-3948.533402	-3847.682563	-49.63510507	CO
13	Refluxed liquid	AAA	23.945	86.52	359.67	CH_3OH	Aq	0.3151	0.032042	105800	-362.23	0.9379	0	0	2.759445804	-7675.238749	-7505.483162	-56629.16116	CH_3OH
			23.945		359.67	H_2O	L	0.6849	0.0180152	276370	-2090.1	8.125	-0.01412	9.37E-06	4.183481453	-15866.04645	-15608.68704	-255980.3387	H_2O
															(average over 298K to T)		SUM =	-334205.3357	

Check mass balances: -7.3E-05

*Note: Aqueous c_p's taken as those for the pure liquid.

STREAMS OUT:

No.	Description	HYSIM	Flow [kg.s^{-1}]	t [°C]	T [K]	Species	State	Mass frac. [-]	M_R [kg.mol^{-1}]	A / C1	B / C2	C / C3	D / C4	C5	$\bar{c}_p$ [kJ.kg^{-1}.K^{-1}]	$\Delta H^o_{f,298K}$ [kJ.kg^{-1}]	$\Delta H^o_{f,T}$ [kJ.kg^{-1}]	$\Delta H^o_{f,T}$ [kW]			
14	Reactor feed	ProcessVap	7.9159	62.08	335.23	HCHO	V	0	0.0300262	23.48	3.16E-02	2.99E-05	-2.30E-08		1.1904	-3862.293597	-3818.1510	0	HCHO	minus feed:	0
			7.9159		335.23	CH_3OH	V	0.2200129	0.032042	21.15	7.09E-02	2.59E-05	-2.85E-08		1.4137	-6282.379377	-6229.9540	-10850.08793	CH_3OH	minus feed:	2068.0
			7.9159		335.23	O_2	V	0.0918026	0.0319988	28.11	-3.68E-06	1.75E-05	-1.07E-08		0.9226	0	34.2136	24.86299793	O_2	minus feed:	-40.4
			7.9159		335.23	H_2O	V	0.0630629	0.0180152	32.24	0.001924	1.06E-05	-3.60E-09		1.8759	-13433.10094	-13363.5378	-6671.078078	H_2O	minus feed:	523.4
			7.9159		335.23	H_2	V	0.0047752	0.0020158	27.14	0.009274	-1.38E-05	7.65E-09		14.353614	0	532.2793741	20.12016034	H_2	minus feed:	-32.4
			7.9159		335.23	CO_2	V	0.0288154	0.0440098	19.8	0.07344	-5.60E-05	1.72E-08		0.862979507	-8948.007035	-8916.004907	-2033.740719	CO_2	minus feed:	-12.3
			7.9159		335.23	CO	V	0.0016296	0.0280104	30.87	-0.01285	2.79E-05	-1.27E-08		1.042309198	-3948.533402	-3909.881137	-50.43746667	CO	minus feed:	-0.8
			7.9159		335.23	HCOOH	V	0	0.0460256	11.71	0.1358	-8.41E-05	2.02E-08		1.01930732	-8231.505945	-8193.706665	0	HCOOH	minus feed:	0
			7.9159		335.23	N_2	V	0.5898887	0.0280134	31.15	-0.01357	2.68E-05	-1.17E-08		1.041329524	0	38.61593515	180.3171092	N_2	minus feed:	-289.6
10	Liquid to heater	CCC	23.945	62.08	335.23	CH_3OH	Aq	0.3151	0.032042	105800	-362.23	0.9379	0	0	2.660808728	-7675.238749	-7576.567181	-57165.49283	CH_3OH	minus recirc:	-536.3
			23.945		335.23	H_2O	L	0.6849	0.0180152	276370	-2090.1	8.125	-0.01412	9.37E-06	4.178496813	-15866.04645	-15711.094	-257659.7989	H_2O	minus recirc:	-1679.5
															(average over 298K to T)		SUM =	-334205.3357		minus SUM:	0.0

Difference in enthalpy between Recirc. liquid in/out:	-2215.8	cf. HYSIM:	-1990.7995	"ERROR" =	-10%	recirc.	1.7814 pump	OUT - IN = 0
Difference in/out for others:	+ 2215.79	cf. HYSIM:	2238.6648	"ERROR" =	1.0%		1131.6109 H/Ex1	
			2238.6628				857.1907 H/Ex2	
							1990.583	
Recirc. liquid in/out, **but** HYSIM with "correct" flow:	-2215.79	cf. HYSIM:	-2383.474982	"ERROR" =	7.6%			
						nett proc.	2238.6628	

(Mass &) Energy Balance over Absorber (ABS-1)

NOTE: Heats of solution of methanol [implicitly] considered.

Ideal vapour- [& liquid(?)]- phase assumed.

Formic acid is treated as water for VLE.

Total pump-around flow: 56.750 $kg.s^{-1}$ (excluding product)

Total HEAT-EXCHANGED pump-around flow: 56.750 $kg.s^{-1}$ (excluding product)

STAGE 1 (BASE OF COLUMN)

Pump-around flow: 56.750 $kg.s^{-1}$

Mole fraction of HCHO in liquid from stage above: 0 GOAL SEEK!

STREAMS IN:

No.	Description	HYSIM	Flow $[kg.s^{-1}]$	t [°C]	T [K]	Species	State	Mass frac. [-]	Mass Flow $[kg.s^{-1}]$	M_R $[kg.mol^{-1}]$	Mole flow $[mol.s^{-1}]$	Mole frac. [-]	A / C1	B / C2	C / C3	D / C4	C5	$\bar{c}_p$ $[kJ.kg^{-1}.K^{-1}]$	$\Delta H^o_{f,\,298K}$ $[kJ.kg^{-1}]$	$\Delta H^o_{f,\,T}$ $[kJ.kg^{-1}]$	$\Delta H^o_{f,\,T}$ [kW]	
j	Fresh DMW fed	AbsWater	0.3275	37.00	310.15	HCHO	Aq	0	0	0.030026	0	0	416.31	-2.6391	0.004984	-		2.48927736	-5555.656	-5525.784	0	HCHO
			0.3275		310.15	CH_3OH	Aq	0	0	0.032042	0	0	105800	-362.23	0.9379	0	0	2.57167231	-7675.239	-7644.379	0	CH_3OH
	Combined liquid-IN temperature:		0.3275		310.15	H_2O	L	1	0.3275	0.018015	18.17909	1	276370	-2090.1	8.125	-0.01412	9.37E-06	4.1803182	-15866.05	-15815.88	-5179.7016	H_2O
	59.84 °C		0.3275		310.15	HCOOH	Aq	0	0	0.046026	0	0						2.192416	-9243.455	-9217.146	0	HCOOH
a	Reactor effluent	AbsFeed	7.916	90.00	363.15	HCHO	V	0.1804678	1.4285651	0.030026	47.57729	0.142986	23.48	0.03157	2.99E-05	-2.3E-08		1.2107	-3862.294	-3783.597	-5405.1149	HCHO
			7.9159		363.15	CH_3OH	V	0.003342	0.0264549	0.032042	0.825632	0.002481	21.15	0.07092	2.59E-05	-2.9E-08		1.4480	-6282.379	-6188.261	-163.70987	CH_3OH
			7.9159		363.15	O_2	V	0.000459	0.0036334	0.031999	0.113549	0.000341	28.11	-3.7E-06	1.75E-05	-1.1E-08		0.9261	0	60.1986	0.21872711	O_2
			7.9159		363.15	H_2O	V	0.1534721	1.2148697	0.018015	67.43581	0.202668	32.24	0.001924	1.06E-05	-3.6E-09		1.8819	-13433.1	-13310.78	-16170.863	H_2O
			7.9159		363.15	H_2	V	0.0098049	0.0776149	0.002016	38.50327	0.115716	27.14	0.009274	-1.4E-05	7.65E-09		14.3718531	0	934.17045	72.5055294	H_2
			7.9159		363.15	CO_2	V	0.059157	0.4682807	0.04401	10.64037	0.031978	19.8	0.07344	-5.6E-05	1.72E-08		0.87627156	-8948.007	-8891.049	-4163.5067	CO_2
			7.9159		363.15	CO	V	0.0033468	0.0264925	0.02801	0.945811	0.002842	30.87	-0.01285	2.79E-05	-1.3E-08		1.04303748	-3948.533	-3880.736	-102.81056	CO
			7.9159		363.15	HCOOH	V	5.976E-05	0.000473	0.046026	0.010278	3.09E-05	11.71	0.1358	-8.4E-05	2.02E-08		1.04557342	-8231.506	-8163.544	-3.8616253	HCOOH
			7.9159		363.15	N_2	V	0.5898907	4.6695157	0.028013	166.6886	0.500957	31.15	-0.01357	2.68E-05	-1.2E-08		1.04150997	0	67.698148	316.117566	N_2
m	Pump-around 1	-	56.750	60.00	333.15	HCHO	Aq	0.54	30.645	0.030026	1020.609	0.415637	416.31	-2.6391	0.004984	-		2.6765732	-5555.656	-5461.975	-167382.24	HCHO
			56.75		333.15	CH_3OH	Aq	0.01	0.5675	0.032042	17.71113	0.007213	105800	-362.23	0.9379	0	0	2.65293796	-7675.239	-7582.386	-4303.004	CH_3OH
			56.75		333.15	H_2O	L	0.44982	25.527285	0.018015	1416.986	0.57706	276370	-2090.1	8.125	-0.01412	9.37E-06	4.17834781	-15866.05	-15719.8	-401283.92	H_2O
			56.75		333.15	HCOOH	Aq	0.00018	0.010215	0.046026	0.221942	9.04E-05						2.192416	-9243.455	-9166.72	-93.638046	HCOOH

Mass fraction of HCHO in total liquid fed: 53.69% Mole fraction HCHO in total liquid fed: 0.41258272

(average over 298K to T) **SUM = -603863.53**

*Note: Aqueous c_p's taken as those for the pure liquid.

Check mass balances: 0

0

(given a total pressure of: 110 kPa(abs))

???

STREAMS OUT:

No.	Description	HYSIM	Flow $[kg.s^{-1}]$	t [°C]	T [K]	Species	State	Mass frac. [-]	Mass Flow $[kg.s^{-1}]$	M_R $[kg.mol^{-1}]$	Mole flow $[mol.s^{-1}]$	Mole frac. [-]	A / C1	B / C2	C / C3	D / C4	C5	$\bar{c}_p$ $[kJ.kg^{-1}.K^{-1}]$	$\Delta H^o_{f,\,298K}$ $[kJ.kg^{-1}]$	$\Delta H^o_{f,\,T}$ $[kJ.kg^{-1}]$	$\Delta H^o_{f,\,T}$ [kW]	
k	Product	-	2.645503	75.00	348.15	HCHO	Aq	0.54	1.4285716	0.030026	47.5775	0.415637	416.31	-2.6391	0.004984	-		2.83026044	-5555.656	-5414.143	-7734.4904	HCHO
	(pre-cooling)		2.645503		348.15	CH_3OH	Aq	0.01	0.026455	0.032042	0.825636	0.007213	105800	-362.23	0.9379	0	0	2.71149878	-7675.239	-7539.664	-199.46203	CH_3OH
			2.645503		348.15	H_2O	L	0.44982	1.1900002	0.018015	66.05534	0.57706	276370	-2090.1	8.125	-0.01412	9.37E-06	4.18043703	-15866.05	-15657.02	-18631.862	H_2O
			2.645503		348.15	HCOOH	Aq	0.00018	0.0004762	0.046026	0.010346	9.04E-05						2.192416	-9243.455	-9133.834	-4.3494453	HCOOH
b	V from stage 4	OHead_Total	5.598	50.00	323.15	HCHO	V	-1.17E-06	-6.53E-06	0.030026	-0.000217	-9.2E-07	23.48	0.03157	2.99E-05	-2.3E-08		1.1816	-3862.294	-3832.754	0.02502479	HCHO
			5.597897		323.15	CH_3OH	V	-2.16E-08	-1.21E-07	0.032042	-3.77E-06	-1.6E-08	21.15	0.07092	2.59E-05	-2.9E-08		1.3989	-6282.379	-6247.407	0.00075538	CH_3OH
			5.597897		323.15	O_2	V	0.0006491	0.0036334	0.031999	0.113549	0.00048	28.11	-3.7E-06	1.75E-05	-1.1E-08		0.9211	0	23.0281	0.0836711	O_2
			5.597897		323.15	H_2O	V	0.0629468	0.3523695	0.018015	19.55957	0.082721	32.24	0.001924	1.06E-05	-3.6E-09		1.8733	-13433.1	-13386.27	-4716.9129	H_2O
			5.597897		323.15	H_2	V	0.013865	0.0776149	0.002016	38.50327	0.162838	27.14	0.009274	-1.4E-05	7.65E-09		14.3452205	0	358.63051	27.8350649	H_2
			5.597897		323.15	CO_2	V	0.083653	0.4682807	0.04401	10.64037	0.045	19.8	0.07344	-5.6E-05	1.72E-08		0.85708331	-8948.007	-8926.58	-4180.145	CO_2
			5.597897		323.15	CO	V	0.0047326	0.0264925	0.02801	0.945811	0.004	30.87	-0.01285	2.79E-05	-1.3E-08		1.04208198	-3948.533	-3922.481	-103.9165	CO
			5.597897		323.15	HCOOH	V	-5.64E-07	-3.16E-06	0.046026	-6.86E-05	-2.9E-07	11.71	0.1358	-8.4E-05	2.02E-08		1.00771392	-8231.506	-8206.313	0.02591205	HCOOH
			5.597897		323.15	N_2	V	0.8341554	4.6695157	0.028013	166.6886	0.704961	31.15	-0.01357	2.68E-05	-1.2E-08		1.04133907	0	26.033477	121.563729	N_2
l	Pump-around 1	-	56.750	75.00	348.15	HCHO	Aq	0.54	30.645	0.030026	1020.609	0.415637	416.31	-2.6391	0.004984	-		2.83026044	-5555.656	-5414.143	-165916.4	HCHO
			56.75		348.15	CH_3OH	Aq	0.01	0.5675	0.032042	17.71113	0.007213	105800	-362.23	0.9379	0	0	2.71149878	-7675.239	-7539.664	-4278.7592	CH_3OH
			56.75		348.15	H_2O	L	0.44982	25.527285	0.018015	1416.986	0.57706	276370	-2090.1	8.125	-0.01412	9.37E-06	4.18043703	-15866.05	-15657.02	-399681.33	H_2O
			56.75		348.15	HCOOH	Aq	0.00018	0.010215	0.046026	0.221942	9.04E-05						2.192416	-9243.455	-9133.834	-93.302113	HCOOH

(average over 298K to T) **SUM = -605391.39**

Difference in enthalpy between Recirc. liquid in/out:	3093.02	cf. HYSIM:	3142.23	"ERROR" =	1.6%	recirc.	3.912	pump	**OUT - IN = -1527.8606**
Difference in in/out for others:	-4620.88	cf. HYSIM:	-3316.1539	"ERROR" =	-28%		-3146.101	H/Ex	NOT ADIABATIC HERE!
			-3316.1539				-3142.189		
Difference in/out for others AND heat loss:	-4620.9	cf. HYSIM:	-4844.014	"ERROR" =	4.8%				(Must recirculate
						nett proc.	-3316.154		84.782856 $kg.s^{-1}$
Overall:	-7713.9	cf. HYSIM:	-7986.245	"ERROR" =	3.5%				to be adiabatic.)

Energy Balance over Reactor (both RXN-1 and RXN-2)

Ideal vapour-phase assumed.

STREAMS IN:

No.	Description	HYSIM	Flow [kg.s^{-1}]	t [°C]	T [K]	Species	State	Mass frac. [-]	M_R [kg.mol^{-1}]	A / C1	B / C2	C / C3	D / C4	C5	$\bar{c}_p$ [kJ.kg^{-1}·K^{-1}]	$\Delta H_{f,298K}$ [kJ.kg^{-1}]	$\Delta H^o_{f,T}$ [kJ.kg^{-1}]	$\Delta H^o_{f,T}$ [kW]	
14	Reactor feed	Total_Feed	7.9159	158.26	431.41	HCHO	V	0	0.0300262	23.48	3.16E-02	2.99E-05	-2.30E-08		1.2609	-3862.293597	-3694.2703	0	HCHO
			7.9159		431.41	CH_3OH	V	0.2200129	0.032042	21.15	7.09E-02	2.59E-05	-2.85E-08		1.5314	-6282.379377	-6078.2973	-10585.9625	CH_3OH
			7.9159		431.41	O_2	V	0.0918026	0.0319988	28.11	-3.68E-06	1.75E-05	-1.07E-08		0.9351	0	124.6193	90.56087089	O_2
			7.9159		431.41	H_2O	V	0.0630629	0.0180152	32.24	0.001924	1.06E-05	-3.60E-09		1.8973	-13433.10094	-13180.2587	-6579.585144	H_2O
			7.9159		431.41	H_2	V	0.0047752	0.0020158	27.14	0.009274	-1.38E-05	7.65E-09		14.41034721	0	1920.345926	72.589076	H_2
			7.9159		431.41	CO_2	V	0.0288154	0.0440098	19.8	0.07344	-5.60E-05	1.72E-08		0.906900818	-8948.007035	-8827.151981	-2013.473367	CO_2
			7.9159		431.41	CO	V	0.0016296	0.0280104	30.87	-0.01285	2.79E-05	-1.27E-08		1.045932979	-3948.533402	-3809.1507	-49.13804402	CO
			7.9159		431.41	HCOOH	V	0	0.0460256	11.71	0.1358	-8.41E-05	2.02E-08		1.106826808	-8231.505945	-8084.008433	0	HCOOH
			7.9159		431.41	N_2	V	0.5898887	0.0280134	31.15	-0.01357	2.68E-05	-1.17E-08		1.043067619	0	139.0008598	649.0645146	N_2
															(average over 298K to T)		SUM =	-18415.9446	

Check mass balances: 0

STREAMS OUT:

No.	Description	HYSIM	Flow [kg.s^{-1}]	t [°C]	T [K]	Species	State	Mass frac. [-]	M_R [kg.mol^{-1}]	A / C1	B / C2	C / C3	D / C4	C5	$\bar{c}_p$ [kJ.kg^{-1}·K^{-1}]	$\Delta H_{f,298K}$ [kJ.kg^{-1}]	$\Delta H^o_{f,T}$ [kJ.kg^{-1}]	$\Delta H^o_{f,T}$ [kW]			
14	Reactor effluent	Convert_Eff	7.9159	700.00	973.15	HCHO	V	0.1804678	0.0300262	23.48	3.16E-02	2.99E-05	-2.30E-08		1.6375	-3862.293597	-2756.9508	-3938.483684	HCHO	minus feed:	-3938
			7.9159		973.15	CH_3OH	V	0.003342	0.032042	21.15	7.09E-02	2.59E-05	-2.85E-08		2.1308	-6282.379377	-4844.0821	-128.1497527	CH_3OH	minus feed:	10457.8
			7.9159		973.15	O_2	V	0.000459	0.0319988	28.11	-3.68E-06	1.75E-05	-1.07E-08		1.0100	0	681.7529	2.477099311	O_2	minus feed:	-88.1
			7.9159		973.15	H_2O	V	0.1534721	0.0180152	32.24	0.001924	1.06E-05	-3.60E-09		2.0506	-13433.10094	-12048.9316	-14637.88172	H_2O	minus feed:	-8058.3
			7.9159		973.15	H_2	V	0.0098049	0.0020158	27.14	0.009274	-1.38E-05	7.65E-09		14.60847417	0	9860.720061	765.3386233	H_2	minus feed:	692.7
			7.9159		973.15	CO_2	V	0.059157	0.0440098	19.8	0.07344	-5.60E-05	1.72E-08		1.076275079	-8948.007035	-8221.521356	-3849.979696	CO_2	minus feed:	-1836.5
			7.9159		973.15	CO	V	0.0033468	0.0280104	30.87	-0.01285	2.79E-05	-1.27E-08		1.101087454	-3948.533402	-3205.29937	-84.91653062	CO	minus feed:	-35.8
			7.9159		973.15	HCOOH	V	5.976E-05	0.0460256	11.71	0.1358	-8.41E-05	2.02E-08		1.466439451	-8231.505945	-7241.659315	-3.42554358	HCOOH	minus feed:	-3
			7.9159		973.15	N_2	V	0.5898907	0.0280134	31.15	-0.01357	2.68E-05	-1.17E-08		1.089651368	0	735.5146735	3434.497342	N_2	minus feed:	2785.4
															(average over 298K to T)		SUM =	-18440.52387		minus SUM:	-24.6

NOTE: For completely adiabatic operation the exit temperature would be: 975.049413 K, which is a difference of only -0.19%

cf. HYSIM: 6804.973

"ERROR" = -27786%

OUT - IN = -24.57927093

===> Approx. ADIABATIC

Energy Balance over Tail-gas Burner (RXN-3)

Ideal vapour-phase assumed.

STREAMS IN:

No.	Description	HYSIM	Flow [kg.s^{-1}]	t [°C]	T [K]	Species	State	Mass frac. [-]	M_R [kg.mol^{-1}]	A / C1	B / C2	C / C3	D / C4	C5	$\bar{c}_p$ [kJ.kg^{-1}.K^{-1}]	$\Delta H^o_{f,298K}$ [kJ.kg^{-1}]	$\Delta H^o_{f,T}$ [kJ.kg^{-1}]	$\Delta H^o_{f,T}$ [kW]	
39	Purged off-gas	Off-gas	2.870748	45.71	318.86	HCHO	V	0	0.0300262	23.48	3.16E-02	2.99E-05	-2.30E-08		1.1785	-3862.293597	-3837.8900	0	HCHO
			2.8707		318.86	CH_3OH	V	0	0.032042	21.15	7.09E-02	2.59E-05	-2.85E-08		1.3936	-6282.379377	-6253.5212	0	CH_3OH
			2.8707		318.86	O_2	V	0.0006491	0.0319988	28.11	-3.68E-06	1.75E-05	-1.07E-08		0.9206	0	19.0635	0.035521049	O_2
			2.8707		318.86	H_2O	V	0.0629512	0.0180152	32.24	0.001924	1.06E-05	-3.60E-09		1.8724	-13433.10094	-13394.3273	-2420.58511	H_2O
			2.8707		318.86	H_2	V	0.0138649	0.0020158	27.14	0.009274	-1.38E-05	7.65E-09		14.34216332	0	296.9917812	11.82106887	H_2
			2.87074824		318.86	CO_2	V	0.0836524	0.0440098	19.8	0.07344	-5.60E-05	1.72E-08		0.854967694	-8948.007035	-8930.302706	-2144.567625	CO_2
			2.87074824		318.86	CO	V	0.0047326	0.0280104	30.87	-0.01285	2.79E-05	-1.27E-08		1.04201441	-3948.533402	-3926.955784	-53.35154132	CO
			2.87074824		318.86	HCOOH	V	0	0.0460256	11.71	0.1358	-8.41E-05	2.02E-08		1.003562547	-8231.505945	-8210.724573	0	HCOOH
			2.87074824		318.86	N_2	V	0.8341498	0.0280134	31.15	-0.01357	2.68E-05	-1.17E-08		1.04135553	0	21.56397378	51.63782648	N_2
49	Extra air	ExtraAir	1.717638	45.71	318.86	HCHO	V	0	0.0300262	23.48	3.16E-02	2.99E-05	-2.30E-08		1.1785	-3862.293597	-3837.8900	0	HCHO
			1.7176		318.86	CH_3OH	V	0	0.032042	21.15	7.09E-02	2.59E-05	-2.85E-08		1.3936	-6282.379377	-6253.5212	0	CH_3OH
			1.7176		318.86	O_2	V	0.2250448	0.0319988	28.11	-3.68E-06	1.75E-05	-1.07E-08		0.9206	0	19.0635	7.368900182	O_2
			1.7176		318.86	H_2O	V	0.0315613	0.0180152	32.24	0.001924	1.06E-05	-3.60E-09		1.8724	-13433.10094	-13394.3273	-726.1181003	H_2O
			1.7176		318.86	H_2	V	0	0.0020158	27.14	0.009274	-1.38E-05	7.65E-09		14.34216332	0	296.9917812	0	H_2
			1.71763799		318.86	CO_2	V	0	0.0440098	19.8	0.07344	-5.60E-05	1.72E-08		0.854967694	-8948.007035	-8930.302706	0	CO_2
			1.71763799		318.86	CO	V	0	0.0280104	30.87	-0.01285	2.79E-05	-1.27E-08		1.04201441	-3948.533402	-3926.955784	0	CO
			1.71763799		318.86	HCOOH	V	0	0.0460256	11.71	0.1358	-8.41E-05	2.02E-08		1.003562547	-8231.505945	-8210.724573	0	HCOOH
			1.71763799		318.86	N_2	V	0.7433939	0.0280134	31.15	-0.01357	2.68E-05	-1.17E-08		1.04135553	0	21.56397378	27.5346413	N_2

(average over 298K to T) SUM = -5246.224418

Check mass balances: 0

STREAMS OUT:

No.	Description	HYSIM	Flow [kg.s^{-1}]	t [°C]	T [K]	Species	State	Mass frac. [-]	M_R [kg.mol^{-1}]	A / C1	B / C2	C / C3	D / C4	C5	$\bar{c}_p$ [kJ.kg^{-1}.K^{-1}]	$\Delta H^o_{f,298K}$ [kJ.kg^{-1}]	$\Delta H^o_{f,T}$ [kJ.kg^{-1}]	$\Delta H^o_{f,T}$ [kW]			
-	Tail-gas	Stack-gas	4.588386	907.69	1180.8	HCHO	V	0	0.0300262	23.48	3.16E-02	2.99E-05	-2.30E-08		1.7476	-3862.293597	-2319.7099	0	HCHO	minus feed:	0
			4.5884		1180.84	CH_3OH	V	0	0.032042	21.15	7.09E-02	2.59E-05	-2.85E-08		2.3026	-6282.379377	-4249.8801	0	CH_3OH	minus feed:	0.0
			4.5884		1180.84	O_2	V	0.0141084	0.0319988	28.11	-3.68E-06	1.75E-05	-1.07E-08		1.0297	0	908.8792	58.83611875	O_2	minus feed:	51.4
			4.5884		1180.84	H_2O	V	0.128726	0.0180152	32.24	0.001924	1.06E-05	-3.60E-09		2.1174	-13433.10094	-11564.1121	-6830.27937	H_2O	minus feed:	-3683.6
			4.5884		1180.84	H_2	V	0	0.0020158	27.14	0.009274	-1.38E-05	7.65E-09		14.75453281	0	13023.70807	0	H_2	minus feed:	-11.8
			4.58838623		1180.84	CO_2	V	0.0569898	0.0440098	19.8	0.07344	-5.60E-05	1.72E-08		1.118892788	-8948.007035	-7960.369322	-2081.566783	CO_2	minus feed:	63.0
			4.58838623		1180.84	CO	V	0	0.0280104	30.87	-0.01285	2.79E-05	-1.27E-08		1.122938148	-3948.533402	-2957.324883	0	CO	minus feed:	53.4
			4.58838623		1180.84	HCOOH	V	0	0.0460256	11.71	0.1358	-8.41E-05	2.02E-08		1.55866563	-8231.505945	-6855.684263	0	HCOOH	minus feed:	0
			4.58838623		1180.84	N_2	V	0.8001758	0.0280134	31.15	-0.01357	2.68E-05	-1.17E-08		1.110363036	0	980.1085692	3598.483976	N_2	minus feed:	3519.3

(average over 298K to T) SUM = -5254.526057 minus SUM: -8.3

NOTE: For completely adiabatic operation the exit temperature would be: 1182.1838 K, which is a difference of only -0.11%

cf. HYSIM: 4858.9326

"ERROR" = -58630%

OUT - IN = -8.301638695

===> Approx. ADIABATIC

Stream		**AAA**	**AbsFeed**	**AbsWater**	**AqMethanol**
Description					
Vapour frac.		0	1	0	0
Temperature	C	86.5180*	90.0000*	37.0000*	37.0368
Pressure	kPa	185	130	120.0000*	185
Molar Flow	mol/s*	957.0421	332.7419	18.1792	66.8933
Mass Flow	kg/s*	20.0000*	7.9159	0.3275*	1.9675
LiqVol Flow	L/s	21.6455	10.655	0.3282	2.4151
Enthalpy	kW	-26970.2295	3572.8516	-613.5226	-1896.8556
Density	kg/m3	876.7156	1.0243	998.2847	794.6892
Mole Wt.		20.8977	23.7898	18.0151	29.4125
Spec. Heat	kJ/kg-C	4.093	1.3378	4.1901	3.7051
Therm Cond	W/m-K	0.5255	0.0359	0.6277	0.2323
Viscosity	cP	0.3197	0.0157	0.6904	0.497
Z Factor		0.0015	1	0.0008	0.0027
Sur Tension	dyne/cm	52.6804	---	70.0165	35.611
Std Density	kg/m3	937.6828	---	1014.836	816.5136
Formaldehyde	mass frac.	0.0000*	0.1806	0.0000*	0
Methanol	mass frac.	0.3151*	0.0033	0.0000*	0.8852
Oxygen	mass frac.	0.0000*	0.0006	0.0000*	0
H2O	mass frac.	0.6849*	0.1534	1.0000*	0.1148
Hydrogen	mass frac.	0.0000*	0.0098	0.0000*	0
CO2	mass frac.	0.0000*	0.059	0.0000*	0
CO	mass frac.	0.0000*	0.0033	0.0000*	0
FormicAcid	mass frac.	0.0000*	0.0001	0.0000*	0
Nitrogen	mass frac.	0.0000*	0.5899	0.0000*	0
Argon	mass frac.	0.0000*	0	0.0000*	0

Stream		**BBB**	**BFWater1a**	**BFWater1b**	**BFWater1c**
Description					
Vapour frac.		0.2305	0	0	0
Temperature	C	62.0833	100.0000*	100.0153	151.8571
Pressure	kPa	185	400.0000*	500	500.0000*
Molar Flow	mol/s*	1252.9148	150.6514	150.6514	221.849
Mass Flow	kg/s*	27.9159	2.7140*	2.714	3.9966
LiqVol Flow	L/s	31.5978	2.7195	2.7195	4.0047
Enthalpy	kW	-25984.197	-4364.6093	-4364.2277	-5547.3923
Density	kg/m3	---	948.0489	948.0807	902.0124
Mole Wt.		22.2808	18.0151	18.0151	18.0151
Spec. Heat	kJ/kg-C	---	4.1965	4.1963	4.3193
Therm Cond	W/m-K	---	0.6807	0.6807	0.6863
Viscosity	cP	---	0.279	0.2789	0.1787
Z Factor		---	0.0024	0.0031	0.0028
Sur Tension	dyne/cm	---	58.6054	58.6025	48.2944
Std Density	kg/m3	---	1014.836	1014.836	1014.836
Formaldehyde	mass frac.	0	0.0000*	0	0
Methanol	mass frac.	0.2881	0.0000*	0	0
Oxygen	mass frac.	0.026	0.0000*	0	0
H2O	mass frac.	0.5086	1.0000*	1	1
Hydrogen	mass frac.	0.0014	0.0000*	0	0
CO2	mass frac.	0.0082	0.0000*	0	0
CO	mass frac.	0.0005	0.0000*	0	0
FormicAcid	mass frac.	0	0.0000*	0	0
Nitrogen	mass frac.	0.1673	0.0000*	0	0
Argon	mass frac.	0	0.0000*	0	0

Stream		**BFWater4a**	**BFWater4b**	**BFWater4c**	**BurnerFeed**
Description					
Vapour frac.		0	0	0.0000*	1
Temperature	C	100.0000*	100.1359	189.4517	45.7076
Pressure	kPa	400.0000*	1270	1240	110
Molar Flow	mol/s*	95.4755	95.4755	95.4755	182.0192
Mass Flow	kg/s*	1.7200*	1.72	1.72	4.59
LiqVol Flow	L/s	1.7235	1.7235	1.7235	6.0095
Enthalpy	kW	-2766.0752	-2763.9706	-2103.1497	1680.7712
Density	kg/m3	948.0489	948.3234	865.0236	1.0463
Mole Wt.		18.0151	18.0151	18.0151	25.2173
Spec. Heat	kJ/kg-C	4.1965	4.1946	4.4676	1.1762
Therm Cond	W/m-K	0.6807	0.6808	0.6714	0.034
Viscosity	cP	0.279	0.2786	0.1415	0.0176
Z Factor		0.0024	0.0078	0.0067	1
Sur Tension	dyne/cm	58.6054	58.5796	40.1818	---
Std Density	kg/m3	1014.836	1014.836	1014.836	---
Formaldehyde	mass frac.	0	0.0000*	0	0
Methanol	mass frac.	0	0.0000*	0	0
Oxygen	mass frac.	0	0.0000*	0	0.0847
H2O	mass frac.	1	1.0000*	1	0.0514
Hydrogen	mass frac.	0	0.0000*	0	0.0087
CO2	mass frac.	0	0.0000*	0	0.0522
CO	mass frac.	0	0.0000*	0	0.003
FormicAcid	mass frac.	0	0.0000*	0	0
Nitrogen	mass frac.	0	0.0000*	0	0.8001
Argon	mass frac.	0	0.0000*	0	0

Stream		**CCC**	**ColdFeed**	**Condens1**	**Condens4'**
Description					
Vapour frac.		0	0.8305	0.9417	0.0000*
Temperature	C	62.0833*	38.1968	100.1843	187.3985
Pressure	kPa	185	185	102.0000*	1185
Molar Flow	mol/s*	957.0473	295.8688	150.6551	31.5819
Mass Flow	kg/s*	20.0000*	7.9159	2.7141	0.569
LiqVol Flow	L/s	21.6455	9.9523	2.7195	0.5701
Enthalpy	kW	-28961.029	738.1688	1402.9055	-700.9128
Density	kg/m3	898.418	2.3013	0.6286	867.1453
Mole Wt.		20.8976	26.7547	18.0151	18.0151
Spec. Heat	kJ/kg-C	4.0504	1.5864	2.2474	4.4586
Therm Cond	W/m-K	0.5172	---	---	0.6726

Stream		**Q_Heat1b**	**Q_Heat2a**	**Q_Heat2b**	**Q_Super1'**
Description					
Vapour frac.		2.0000*	2.0000*	2.0000*	2.0000*
Temperature	C	0.0000*	0.0000*	0.0000*	0.0000*
Pressure	kPa	0.0000*	0.0000*	0.0000*	0.0000*
Molar Flow	mol/s*	0.0000*	0.0000*	0.0000*	0.0000*
Mass Flow	kg/s*	0.0000*	0.0000*	0.0000*	0.0000*
LiqVol Flow	L/s	0.0000*	0.0000*	0.0000*	0.0000*
Enthalpy	kW	1131.611	857.1907	857.1907	963.2883
Density	kg/m3	0	0	0	0
Mole Wt.		0	0	0	0
Spec. Heat	kJ/kg-C	---	---	---	---
Therm Cond	W/m-K	---	---	---	---
Viscosity	cP	---	---	---	---
Z Factor		---	---	---	---
Sur Tension	dyne/cm	---	---	---	---
Std Density	kg/m3	---	---	---	---
Formaldehyde	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
Methanol	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
Oxygen	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
H2O	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
Hydrogen	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
CO2	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
CO	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
FormicAcid	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
Nitrogen	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
Argon	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*

Stream		**Q_react**	**RCW1_in**	**RCW1_out**	**RecLiq1**
Description					
Vapour frac.		2.0000*	0	0	0
Temperature	C	0.0000*	30.0000*	45.0000*	75.0000*
Pressure	kPa	0.0000*	400.0000*	360	130.0000*
Molar Flow	mol/s*	0.0000*	2885.0285	2885.0285	2569.1488
Mass Flow	kg/s*	0.0000*	51.9741	51.9741	59.3941
LiqVol Flow	L/s	0.0000*	52.079	52.079	70.1631
Enthalpy	kW	0.0000*	-98890.026	-95597.3417	-54273.8546
Density	kg/m3	0	1003.6873	992.2268	773.2326
Mole Wt.		0	18.0151	18.0151	23.1182
Spec. Heat	kJ/kg-C	---	4.1894	4.1909	3.7574
Therm Cond	W/m-K	---	0.6182	0.6376	0.3688
Viscosity	cP	---	0.7972	0.5939	0.1746
Z Factor		---	0.0028	0.0025	0.0013
Sur Tension	dyne/cm	---	71.2338	68.6162	41.0466
Std Density	kg/m3	---	1014.836	1014.836	839.4352
Formaldehyde	mass frac.	0.0000*	0.0000*	0	0.5407
Methanol	mass frac.	0.0000*	0.0000*	0	0.01
Oxygen	mass frac.	0.0000*	0.0000*	0	0
H2O	mass frac.	0.0000*	1.0000*	1	0.4492
Hydrogen	mass frac.	0.0000*	0.0000*	0	0
CO2	mass frac.	0.0000*	0.0000*	0	0
CO	mass frac.	0.0000*	0.0000*	0	0
FormicAcid	mass frac.	0.0000*	0.0000*	0	0.0002
Nitrogen	mass frac.	0.0000*	0.0000*	0	0
Argon	mass frac.	0.0000*	0.0000*	0	0

Stream		**RecLiq2_a**	**RecLiq2_b**	**RecLiq3_a**	**RecLiq3_b**
Description					
Vapour frac.		0	0	0	0
Temperature	C	75.0145	60	60.0000*	60.0000*
Pressure	kPa	170.0000*	120	120	120.0000*
Molar Flow	mol/s*	2569.1488	2569.1488	2454.7765	2454.7776*
Mass Flow	kg/s*	59.3941	59.3941	56.7500*	56.75
LiqVol Flow	L/s	70.1631	70.1631	67.0396	67.0396
Enthalpy	kW	-54269.76	-57562.4443	-54999.9036	-54999.9279
Density	kg/m3	773.2152	790.785	790.785	790.7851
Mole Wt.		23.1182	23.1182	23.1182	23.1182
Spec. Heat	kJ/kg-C	3.7575	3.6248	3.6248	3.6248
Therm Cond	W/m-K	0.3688	0.3747	0.3747	0.3747
Viscosity	cP	0.1745	0.2115	0.2115	0.2115
Z Factor		0.0018	0.0013	0.0013	0.0013
Sur Tension	dyne/cm	41.0438	43.9075	43.9075	43.9075
Std Density	kg/m3	839.4352	839.4352	839.4352	839.4353
Formaldehyde	mass frac.	0.5407	0.5407	0.5407	0.5407*
Methanol	mass frac.	0.01	0.01	0.01	0.0100*
Oxygen	mass frac.	0	0	0	0.0000*
H2O	mass frac.	0.4492	0.4492	0.4492	0.4492*
Hydrogen	mass frac.	0	0	0	0.0000*
CO2	mass frac.	0	0	0	0.0000*
CO	mass frac.	0	0	0	0.0000*
FormicAcid	mass frac.	0.0002	0.0002	0.0002	0.0002*
Nitrogen	mass frac.	0	0	0	0.0000*
Argon	mass frac.	0	0	0	0.0000*

Stream		**RecOff-gas**	**RecVap_a**	**RecVap_b**	**Stack-gas**
Description					
Vapour frac.		1	1	1	0.9539
Temperature	C	50	49.9958	49.9954*	907.692
Pressure	kPa	110	101.0000*	101.0000*	110
Molar Flow	mol/s*	115.1998	115.1998	115.1954*	171.9008
Mass Flow	kg/s*	2.7268	2.7268	2.7272	4.59
LiqVol Flow	L/s	3.8276	3.8276	3.8286	5.5203
Enthalpy	kW	1074.1837	1074.1837	1074.1202	6539.7038
Density	kg/m3	0.9691	0.8898	0.89	0.3136
Mole Wt.		23.6706	23.6706	23.6744	26.7015
Spec. Heat	kJ/kg-C	1.26	1.26	1.2597	1.3624
Therm Cond	W/m-K	0.0382	0.0382	0.0382	---

Viscosity	cP	0.4463	---	---	0.1431
Z Factor		0.0015	---	---	0.0064
Sur Tension	dyne/cm	56.9883	---	---	40.6386
Std Density	kg/m3	937.6853	---	---	1014.836
Formaldehyde	mass frac.	0.0000*	0	0	0.0000*
Methanol	mass frac.	0.3151*	0.22	0	0.0000*
Oxygen	mass frac.	0.0000*	0.0918	0	0.0000*
H2O	mass frac.	0.6849*	0.0631	1	1.0000*
Hydrogen	mass frac.	0.0000*	0.0048	0	0.0000*
CO2	mass frac.	0.0000*	0.0288	0	0.0000*
CO	mass frac.	0.0000*	0.0016	0	0.0000*
FormicAcid	mass frac.	0.0000*	0	0	0.0000*
Nitrogen	mass frac.	0.0000*	0.5899	0	0.0000*
Argon	mass frac.	0.0000*	0	0	0.0000*

Stream		**Condens4b**	**Condens4c**	**Condens4c'**	**Convert_Eff**
Description					
Vapour frac.		0.0000*	0.0000*	0.0000*	0.9689
Temperature	C	187.3985	187.3985	187.3985	700.0000*
Pressure	kPa	1185	1185	1185	160
Molar Flow	mol/s*	31.5819	26.8842	26.8842	332.7419
Mass Flow	kg/s*	0.569	0.4843	0.4843	7.9159
LiqVol Flow	L/s	0.5701	0.4853	0.4853	10.655
Enthalpy	kW	-700.9128	-596.6548	-596.6548	10745.0928
Density	kg/m3	867.1453	867.1453	867.1453	0.4855
Mole Wt.		18.0151	18.0151	18.0151	23.7898
Spec. Heat	kJ/kg-C	4.4586	4.4586	4.4586	1.634
Therm Cond	W/m-K	0.6726	0.6726	0.6726	---
Viscosity	cP	0.1431	0.1431	0.1431	---
Z Factor		0.0064	0.0064	0.0064	---
Sur Tension	dyne/cm	40.6386	40.6386	40.6386	---
Std Density	kg/m3	1014.836	1014.836	1014.836	---
Formaldehyde	mass frac.	0	0	0	0.1806
Methanol	mass frac.	0	0	0	0.0033
Oxygen	mass frac.	0	0	0	0.0006
H2O	mass frac.	1	1	1	0.1534
Hydrogen	mass frac.	0	0	0	0.0098
CO2	mass frac.	0	0	0	0.059
CO	mass frac.	0	0	0	0.0033
FormicAcid	mass frac.	0	0	0	0.0001
Nitrogen	mass frac.	0	0	0	0.5899
Argon	mass frac.	0	0	0	0

Stream		**CoolEff**	**DDD**	**DrumFeed**	**EEE**
Description					
Vapour frac.		1	0	0.4044	0
Temperature	C	170.0000*	62.0967	151.8571	72.6444
Pressure	kPa	145	245	500	215
Molar Flow	mol/s*	332.7419	957.0473	372.5042	957.0473
Mass Flow	kg/s*	7.9159	20	6.7107	20
LiqVol Flow	L/s	10.655	21.6455	6.7242	21.6455
Enthalpy	kW	4430.0422	-28959.2476	-3596.7701	-28102.0568
Density	kg/m3	0.9362	898.4362	6.2766	889.1826
Mole Wt.		23.7898	20.8976	18.0151	20.8976
Spec. Heat	kJ/kg-C	1.372	4.0504	3.6221	4.0674
Therm Cond	W/m-K	0.043	0.5172	---	0.5215
Viscosity	cP	0.019	0.4462	---	0.3849
Z Factor		1	0.002	---	0.0018
Sur Tension	dyne/cm	---	56.986	---	55.1394
Std Density	kg/m3	---	937.6853	---	937.6853
Formaldehyde	mass frac.	0.1806	0	0	0
Methanol	mass frac.	0.0033	0.3151	0	0.3151
Oxygen	mass frac.	0.0006	0	0	0
H2O	mass frac.	0.1534	0.6849	1	0.6849
Hydrogen	mass frac.	0.0098	0	0	0
CO2	mass frac.	0.059	0	0	0
CO	mass frac.	0.0033	0	0	0
FormicAcid	mass frac.	0.0001	0	0	0
Nitrogen	mass frac.	0.5899	0	0	0
Argon	mass frac.	0	0	0	0

Stream		**Exhaust1**	**Exhaust2**	**ExtraAir**	**FFF**
Description					
Vapour frac.		1	1	1	0
Temperature	C	328.4914	206.3792	37.0000*	86.5180*
Pressure	kPa	106	101	110	185.0000*
Molar Flow	mol/s*	171.9008	171.9008	60.6691	957.0473
Mass Flow	kg/s*	4.59	4.59	1.7176*	20
LiqVol Flow	L/s	5.5203	5.5203	1.9775	21.6455
Enthalpy	kW	3134.5079	2473.6871	549.2388	-26970.4458
Density	kg/m3	0.5658	0.6764	1.2077	876.7184
Mole Wt.		26.7015	26.7015	28.3109	20.8976
Spec. Heat	kJ/kg-C	1.1953	1.1635	1.0368	4.0931
Therm Cond	W/m-K	0.0442	0.0362	0.0264	0.5255
Viscosity	cP	0.0273	0.0232	0.0187	0.3197
Z Factor		1	1	1	0.0015
Sur Tension	dyne/cm	---	---	---	52.6808
Std Density	kg/m3	---	---	---	937.6853
Formaldehyde	mass frac.	0	0	0.0000*	0
Methanol	mass frac.	0	0	0.0000*	0.3151
Oxygen	mass frac.	0.0142	0.0142	0.2250*	0
H2O	mass frac.	0.1289	0.1289	0.0316*	0.6849
Hydrogen	mass frac.	0	0	0.0000*	0
CO2	mass frac.	0.0568	0.0568	0.0000*	0
CO	mass frac.	0	0	0.0000*	0
FormicAcid	mass frac.	0	0	0.0000*	0
Nitrogen	mass frac.	0.8001	0.8001	0.7434*	0
Argon	mass frac.	0	0	0.0000*	0

Viscosity	cP	0.017	0.017	0.017	---
Z Factor		1	1	1	---
Sur Tension	dyne/cm	---	---	---	---
Std Density	kg/m3	---	---	---	---
Formaldehyde	mass frac.	0	0	0.0000*	0
Methanol	mass frac.	0	0	0.0000*	0
Oxygen	mass frac.	0.0008	0.0008	0.0006*	0.0142
H2O	mass frac.	0.0632	0.0632	0.0630*	0.1289
Hydrogen	mass frac.	0.0139	0.0139	0.0139*	0
CO2	mass frac.	0.0834	0.0834	0.0837*	0.0568
CO	mass frac.	0.0047	0.0047	0.0047*	0
FormicAcid	mass frac.	0	0	0.0000*	0
Nitrogen	mass frac.	0.8339	0.8339	0.8341*	0.8001
Argon	mass frac.	0	0	0.0000*	0

Stream		**Steam1a**	**Steam1b**	**Steam1c**	**Steam4a**
Description					
Vapour frac.		0.7500*	1	0.7500*	1.0000*
Temperature	C	151.8557	151.8571	151.8557*	187.9668
Pressure	kPa	500.0000*	500	500.0000*	1200.0000*
Molar Flow	mol/s*	221.849	150.6551	221.8528	95.4755
Mass Flow	kg/s*	3.9966	2.7141	3.9967*	1.72
LiqVol Flow	L/s	4.0047	2.7195	4.0048	1.7235
Enthalpy	kW	767.4445	1950.6219	767.4574	1302.046
Density	kg/m3	3.3956	2.5491	3.3956	5.6387
Mole Wt.		18.0151	18.0151	18.0151	18.0151
Spec. Heat	kJ/kg-C	3.0264	2.5954	3.0264	3.0477
Therm Cond	W/m-K	---	0.0288	---	0.032
Viscosity	cP	---	0.014	---	0.0152
Z Factor		---	1	---	1
Sur Tension	dyne/cm	---	---	---	---
Std Density	kg/m3	---	---	---	---
Formaldehyde	mass frac.	0.0000*	0	0.0000*	0
Methanol	mass frac.	0.0000*	0	0.0000*	0
Oxygen	mass frac.	0.0000*	0	0.0000*	0
H2O	mass frac.	1.0000*	1	1.0000*	1
Hydrogen	mass frac.	0.0000*	0	0.0000*	0
CO2	mass frac.	0.0000*	0	0.0000*	0
CO	mass frac.	0.0000*	0	0.0000*	0
FormicAcid	mass frac.	0.0000*	0	0.0000*	0
Nitrogen	mass frac.	0.0000*	0	0.0000*	0
Argon	mass frac.	0.0000*	0	0.0000*	0

Stream		**Steam4b**	**Steam4b'**	**Steam4c**	**Steam4c'**
Description					
Vapour frac.		1	1.0000*	1	1.0000*
Temperature	C	187.9668	187.9668	187.9668	187.9668
Pressure	kPa	1200	1200.0000*	1200	1200.0000*
Molar Flow	mol/s*	31.5819	31.5819	26.8842	26.8842
Mass Flow	kg/s*	0.569	0.569	0.4843	0.4843
LiqVol Flow	L/s	0.5701	0.5701	0.4853	0.4853
Enthalpy	kW	430.6981	430.6981	366.6335	366.6335
Density	kg/m3	5.6387	5.6387	5.6387	5.6387
Mole Wt.		18.0151	18.0151	18.0151	18.0151
Spec. Heat	kJ/kg-C	3.0477	3.0477	3.0477	3.0477
Therm Cond	W/m-K	0.032	0.032	0.032	0.032
Viscosity	cP	0.0152	0.0152	0.0152	0.0152
Z Factor		1	1	1	1
Sur Tension	dyne/cm	---	---	---	---
Std Density	kg/m3	---	---	---	---
Formaldehyde	mass frac.	0	0	0	0.0000*
Methanol	mass frac.	0	0	0	0.0000*
Oxygen	mass frac.	0	0	0	0.0000*
H2O	mass frac.	1	1	1	1.0000*
Hydrogen	mass frac.	0	0	0	0.0000*
CO2	mass frac.	0	0	0	0.0000*
CO	mass frac.	0	0	0	0.0000*
FormicAcid	mass frac.	0	0	0	0.0000*
Nitrogen	mass frac.	0	0	0	0.0000*
Argon	mass frac.	0	0	0	0.0000*

Stream		**Steam4d**	**Total_Feed**	**W_APump1**	**W_BPump1**
Description					
Vapour frac.		1	1	2.0000*	2.0000*
Temperature	C	187.9668	158.2616	0.0000*	0.0000*
Pressure	kPa	1200	170	0.0000*	0.0000*
Molar Flow	mol/s*	37.0093	295.8674	0.0000*	0.0000*
Mass Flow	kg/s*	0.6667	7.9159	0.0000*	0.0000*
LiqVol Flow	L/s	0.6681	9.9523	0.0000*	0.0000*
Enthalpy	kW	504.7143	3940.1198	4.0946	0.3816
Density	kg/m3	5.6387	1.268	0	0
Mole Wt.		18.0151	26.7549	0	0
Spec. Heat	kJ/kg-C	3.0477	1.2972	---	---
Therm Cond	W/m-K	0.032	0.037	---	---
Viscosity	cP	0.0152	0.0198	---	---
Z Factor		1	1	---	---
Sur Tension	dyne/cm	---	---	---	---
Std Density	kg/m3	---	---	---	---
Formaldehyde	mass frac.	0	0	0.0000*	0.0000*
Methanol	mass frac.	0	0.22	0.0000*	0.0000*
Oxygen	mass frac.	0	0.0918	0.0000*	0.0000*
H2O	mass frac.	1	0.0631	0.0000*	0.0000*
Hydrogen	mass frac.	0	0.0048	0.0000*	0.0000*
CO2	mass frac.	0	0.0288	0.0000*	0.0000*
CO	mass frac.	0	0.0016	0.0000*	0.0000*
FormicAcid	mass frac.	0	0	0.0000*	0.0000*
Nitrogen	mass frac.	0	0.5899	0.0000*	0.0000*
Argon	mass frac.	0	0	0.0000*	0.0000*

Stream		HPGas	LPAir	LPGas	MainsWater
Description					
Vapour frac.		1	1	1	0
Temperature	C	121.583	37.0000*	43.5838	37.0000*
Pressure	kPa	185.0000*	101.0000*	101	400.0000*
Molar Flow	mol/s*	228.9755	113.7801	228.9755	12.5395
Mass Flow	kg/s*	5.9484	3.2212*	5.9484	0.2259*
LiqVol Flow	L/s	7.5372	3.7087	7.5372	0.2264
Enthalpy	kW	2635.0243	1030.0533	2104.1736	-423.1333
Density	kg/m3	1.4644	1.1089	0.9963	998.3729
Mole Wt.		25.9782	28.3107	25.9782	18.0151
Spec. Heat	kJ/kg-C	1.1508	1.0368	1.1387	4.1901
Therm Cond	W/m-K	0.0382	0.0264	0.032	0.6277
Viscosity	cP	0.021	0.0187	0.0179	0.6904
Z Factor		1	1	1	0.0028
Sur Tension	dyne/cm	---	---	---	70.0165
Std Density	kg/m3	---	---	---	1014.836
Formaldehyde	mass frac.	0	0.0000*	0	0
Methanol	mass frac.	0	0.0000*	0	0
Oxygen	mass frac.	0.1222	0.2250*	0.1222	0
H2O	mass frac.	0.046	0.0316*	0.046	1
Hydrogen	mass frac.	0.0064	0.0000*	0.0064	0
CO2	mass frac.	0.0384	0.0000*	0.0384	0
CO	mass frac.	0.0022	0.0000*	0.0022	0
FormicAcid	mass frac.	0	0.0000*	0	0
Nitrogen	mass frac.	0.785	0.7434*	0.785	0
Argon	mass frac.	0	0.0000*	0	0

Stream		W_BPump4	W_Blower	W_MethPump	W_Turb2
Description					
Vapour frac.		2.0000*	2.0000*	2.0000*	2.0000*
Temperature	C	0.0000*	0.0000*	0.0000*	0.0000*
Pressure	kPa	0.0000*	0.0000*	0.0000*	0.0000*
Molar Flow	mol/s*	0.0000*	0.0000*	0.0000*	0.0000*
Mass Flow	kg/s*	0.0000*	0.0000*	0.0000*	0.0000*
LiqVol Flow	L/s	0.0000*	0.0000*	0.0000*	0.0000*
Enthalpy	kW	2.1046	530.8508	0.2252	547.7165
Density	kg/m3	0	0	0	0
Mole Wt.		0	0	0	0
Spec. Heat	kJ/kg-C	---	---	---	---
Therm Cond	W/m-K	---	---	---	---
Viscosity	cP	---	---	---	---
Z Factor		---	---	---	---
Sur Tension	dyne/cm	---	---	---	---
Std Density	kg/m3	---	---	---	---
Formaldehyde	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
Methanol	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
Oxygen	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
H2O	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
Hydrogen	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
CO2	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
CO	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
FormicAcid	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
Nitrogen	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*
Argon	mass frac.	0.0000*	0.0000*	0.0000*	0.0000*

Stream		MethanolFeed	MethanolPipe	OHead_Total	Off-gas
Description					
Vapour frac.		0	0	1	1
Temperature	C	37.0355	37.0000*	50.0000*	50
Pressure	kPa	185.0000*	110.0000*	110.0000*	110
Molar Flow	mol/s*	54.3538	54.3538	236.5498	121.3501
Mass Flow	kg/s*	1.7416	1.7416*	5.5993	2.8724
LiqVol Flow	L/s	2.1887	2.1887	7.8596	4.032
Enthalpy	kW	-1473.7222	-1473.9474	2205.7159	1131.5323
Density	kg/m3	773.4377	773.4186	0.9691	0.9691
Mole Wt.		32.0419	32.0419	23.6706	23.6706
Spec. Heat	kJ/kg-C	3.6422	3.642	1.26	1.26
Therm Cond	W/m-K	0.1747	0.1747	0.0382	0.0382
Viscosity	cP	0.4623	0.4625	0.017	0.017
Z Factor		0.003	0.0018	1	1
Sur Tension	dyne/cm	27.6753	27.6809	---	---
Std Density	kg/m3	796.4045	796.4045	---	---
Formaldehyde	mass frac.	0.0000*	0	0	0
Methanol	mass frac.	1.0000*	1	0	0
Oxygen	mass frac.	0.0000*	0	0.0008	0.0008
H2O	mass frac.	0.0000*	0	0.0632	0.0632
Hydrogen	mass frac.	0.0000*	0	0.0139	0.0139
CO2	mass frac.	0.0000*	0	0.0834	0.0834
CO	mass frac.	0.0000*	0	0.0047	0.0047
FormicAcid	mass frac.	0.0000*	0	0	0
Nitrogen	mass frac.	0.0000*	0	0.8339	0.8339
Argon	mass frac.	0.0000*	0	0	0

Stream		W_VapPump	WaterFeed
Description			
Vapour frac.		2.0000*	0
Temperature	C	0.0000*	37.0456
Pressure	kPa	0.0000*	185
Molar Flow	mol/s*	0.0000*	12.5395
Mass Flow	kg/s*	0.0000*	0.2259
LiqVol Flow	L/s	0.0000*	0.2264
Enthalpy	kW	1.7814	-423.1333
Density	kg/m3	0	998.2705
Mole Wt.		0	18.0151
Spec. Heat	kJ/kg-C	---	4.1901
Therm Cond	W/m-K	---	0.6277
Viscosity	cP	---	0.6898
Z Factor		---	0.0013
Sur Tension	dyne/cm	---	70.0085
Std Density	kg/m3	---	1014.836
Formaldehyde	mass frac.	0.0000*	0.0000*
Methanol	mass frac.	0.0000*	0.0000*
Oxygen	mass frac.	0.0000*	0.0000*
H2O	mass frac.	0.0000*	1.0000*
Hydrogen	mass frac.	0.0000*	0.0000*
CO2	mass frac.	0.0000*	0.0000*
CO	mass frac.	0.0000*	0.0000*
FormicAcid	mass frac.	0.0000*	0.0000*
Nitrogen	mass frac.	0.0000*	0.0000*
Argon	mass frac.	0.0000*	0.0000*

Stream		PRODUCT	ProcessVap	Q_Abs	Q_Burner
Description					
Vapour frac.		0	1	2.0000*	2.0000*
Temperature	C	60	62.0833	0.0000*	0.0000*
Pressure	kPa	120	185.0000*	0.0000*	0.0000*
Molar Flow	mol/s*	114.3723	295.8674*	0.0000*	0.0000*
Mass Flow	kg/s*	2.6441	7.9159	0.0000*	0.0000*
LiqVol Flow	L/s	3.1235	9.9523	0.0000*	0.0000*
Enthalpy	kW	-2562.5408	2976.8316	-27.5397	0.0000*
Density	kg/m3	790.785	1.7759	0	0
Mole Wt.		23.1182	26.7549	0	0
Spec. Heat	kJ/kg-C	3.6248	1.2336	---	---
Therm Cond	W/m-K	0.3747	0.0295	---	---
Viscosity	cP	0.2115	0.0154	---	---
Z Factor		0.0013	1	---	---
Sur Tension	dyne/cm	43.9075	---	---	---
Std Density	kg/m3	839.4352	---	---	---
Formaldehyde	mass frac.	0.5407	0.0000*	0.0000*	0.0000*
Methanol	mass frac.	0.01	0.2200*	0.0000*	0.0000*
Oxygen	mass frac.	0	0.0918*	0.0000*	0.0000*
H2O	mass frac.	0.4492	0.0631*	0.0000*	0.0000*
Hydrogen	mass frac.	0	0.0048*	0.0000*	0.0000*
CO2	mass frac.	0	0.0288*	0.0000*	0.0000*
CO	mass frac.	0	0.0016*	0.0000*	0.0000*
FormicAcid	mass frac.	0.0002	0.0000*	0.0000*	0.0000*
Nitrogen	mass frac.	0	0.5899*	0.0000*	0.0000*
Argon	mass frac.	0	0.0000*	0.0000*	0.0000*

STREAM MASS COMPOSITIONS

Stream name BBB

Mass Fraction

Component	**Total**	**Vapour**	**Light Liquid**	**Heavy Liquid**
Formaldehyde	0	0	0	---
Methanol	0.2881	0.1958	0.3232	---
Oxygen	0.026	0.0946	0	---
H2O	0.5086	0.0658	0.6768	---
Hydrogen	0.0014	0.0049	0	---
CO2	0.0082	0.0296	0	---
CO	0.0005	0.0017	0	---
FormicAcid	0	0	0	---
Nitrogen	0.1673	0.6077	0	---
Argon	0	0	0	---
---	---	---	---	---
<snip!>				
---	---	---	---	---

Mass Flows in kg/h

Formaldehyde	0	0	0	---
Methanol	28956.3262	5415.8833	23540.4434	---
Oxygen	2616.1794	2615.8643	0.3154	---
H2O	51110.7188	1819.2366	49291.4844	---
Hydrogen	136.1387	136.1146	0.0241	---
CO2	821.2947	819.3807	1.914	---
CO	46.4667	46.4565	0.0102	---
FormicAcid	0	0	0	---
Nitrogen	16810.0879	16809.3906	0.6961	---
Argon	0	0	0	---
---	---	---	---	---
<snip!>				
---	---	---	---	---
Total flow	27.9159	7.684	20.2319	0

STREAM MASS COMPOSITIONS

Stream name ColdFeed

Mass Fraction

Component	**Total**	**Vapour**	**Light Liquid**	**Heavy Liquid**
Formaldehyde	0	0	0	---
Methanol	0.22	0.13	0.6829	---
Oxygen	0.0918	0.1097	0	---
H2O	0.0631	0.0137	0.3171	---
Hydrogen	0.0048	0.0057	0	---
CO2	0.0288	0.0344	0	---
CO	0.0016	0.0019	0	---
FormicAcid	0	0	0	---
Nitrogen	0.5899	0.7046	0	---
Argon	0	0	0	---
---	---	---	---	---
<snip!>				
---	---	---	---	---

Mass Flows in kg/h

Formaldehyde	0	0	0	---
Methanol	6269.7598	3101.2915	3168.4683	---
Oxygen	2616.0107	2615.9941	0.0165	---
H2O	1797.4092	326.3094	1471.0997	---
Hydrogen	136.1388	136.1351	0.0037	---
CO2	821.295	821.1005	0.1945	---
CO	46.4667	46.4646	0.0021	---
FormicAcid	0	0	0	---
Nitrogen	16810.0859	16810.0605	0.0265	---
Argon	0	0	0	---
---	---	---	---	---
<snip!>				
---	---	---	---	---
Total flow	7.9159	6.627	1.2888	0

STREAM MASS COMPOSITIONS

Stream name Convert_Eff

Mass Fraction

Component	**Total**	**Vapour**	**Light Liquid**	**Heavy Liquid**
Formaldehyde	0.1806	0.1916	---	0
Methanol	0.0033	0.0035	---	0
Oxygen	0.0006	0.0006	---	0.0001
H2O	0.1534	0.1628	---	0.0001
Hydrogen	0.0098	0.0104	---	0
CO2	0.059	0.0018	---	0.9969
CO	0.0033	0.0034	---	0.0024
FormicAcid	0.0001	0.0001	---	0
Nitrogen	0.5899	0.6258	---	0.0005
Argon	0	0	---	0
---	---	---	---	---
<snip!>				
---	---	---	---	---

Mass Flows in kg/h

Formaldehyde	5146.2549	5146.1899	---	0.0651
Methanol	95.2399	95.2387	---	0.0012
Oxygen	16.6598	16.5632	---	0.0966
H2O	4371.5361	4371.4492	---	0.0869
Hydrogen	279.4381	279.4333	---	0.0049
CO2	1680.9608	48.5047	---	1632.4562
CO	95.3084	91.3722	---	3.9362
FormicAcid	1.5783	1.5782	---	0.0001
Nitrogen	16810.0879	16809.2734	---	0.8148
Argon	0	0	---	0
---	---	---	---	---
<snip!>				
---	---	---	---	---
Total flow	7.9159	7.461	0	0.4549

STREAM MASS COMPOSITIONS

Stream name Stack-gas

Mass Fraction

Component	**Total**	**Vapour**	**Light Liquid**	**Heavy Liquid**
Formaldehyde	0	0	0	---
Methanol	0	0	0	---
Oxygen	0.0142	0.0003	0.1968	---
H2O	0.1289	0.1387	0	---
Hydrogen	0	0	0	---
CO2	0.0568	0	0.8031	---
CO	0	0	0	---
FormicAcid	0	0	0	---
Nitrogen	0.8001	0.861	0.0001	---
Argon	0	0	0	---
---	---	---	---	---
<snip!>				
---	---	---	---	---

Mass Flows in kg/h

Formaldehyde	0	0	0	---
Methanol	0	0	0	---
Oxygen	234.4494	4.3651	230.0844	---
H2O	2129.9111	2129.8926	0.0185	---
Hydrogen	0	0	0	---
CO2	939.0356	0	939.0356	---
CO	0	0	0	---
FormicAcid	0	0	0	---
Nitrogen	13219.3457	13219.2148	0.1309	---
Argon	0	0	0	---
---	---	---	---	---
<snip!>				
---	---	---	---	---
Total flow	4.5897	4.2649	0.3248	0

Van Laar, IDEAL (DEFAULT)

```
+-------------------- Aij Interaction Parameters ---------------------+
¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices   A_UnifacVLE      ¦
¦            H_Henry's Coeff     L_UnifacLLE     C_UnifacLLE_All
¦            I_j immiscible in i           B_all immiscible in i      ¦
¦                Formaldehyde Methanol     Oxygen       H2O           ¦
¦Formaldehyde     ---          ---          ---           -5.7036     ¦
¦Methanol         ---          ---          ---            0.6257     ¦
¦Oxygen           ---          ---          ---           29.1896     ¦
¦H2O              62.9893       0.7643     -80.3697       ---         ¦
¦Hydrogen         ---           2.6055      ---            8.0175     ¦
¦CO2              ---          ---          ---          676.2780     ¦
¦CO               ---          -4.0521      ---       -12385.0000     ¦
¦FormicAcid       ---          ---          ---           -1.5362     ¦
¦Nitrogen         ---          ---          ---            7.0546
¦Argon            ---          ---          ---           33.2214     ¦
+---------------------------------------------------------------------+
```

```
+-------------------- Aij Interaction Parameters ---------------------+
¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices   A_UnifacVLE      ¦
             H_Henry's Coeff     L_UnifacLLE     C_UnifacLLE_All
¦            I_j immiscible in i           B_all immiscible in i      ¦
¦                Hydrogen     CO2          CO           FormicAcid    ¦
¦Formaldehyde     ---          ---          ---          ---          ¦
¦Methanol         24.7952      ---          13.8729      ---          ¦
¦Oxygen           ---          ---          ---          ---          ¦
¦H2O              -6.5127    -183.6914     266.3600      -0.7971      ¦
¦Hydrogen         ---          ---          ---          ---          ¦
¦CO2              ---          ---          ---          ---          ¦
¦CO               ---          ---          ---          ---          ¦
¦FormicAcid       ---          ---          ---          ---          ¦
 Nitrogen         ---          ---          ---          ---
¦Argon            ---          ---          ---          ---          ¦
+---------------------------------------------------------------------+
```

```
ameters ---------------------+
-Matrices   A_UnifacVLE      ¦
LLE     C_UnifacLLE_All      ¦
  B_all immiscible in i      ¦
  Nitrogen     Argon         ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   30.1561     -42.2753      ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
-----------------------------+
```

```
+-------------------- Bij Interaction Parameters ---------------------+
¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices                    ¦
¦
¦                                                                     ¦
¦                Formaldehyde Methanol     Oxygen       H2O           ¦
¦Formaldehyde     ---          ---          ---          ---          ¦
¦Methanol         ---          ---          ---          ---          ¦
¦Oxygen           ---          ---          ---          -0.0498      ¦
¦H2O              ---          ---          19.3401      ---          ¦
¦Hydrogen         ---          -0.0009      ---          -0.0100      ¦
¦CO2              ---          ---          ---          -0.0977      ¦
¦CO               ---          -0.0036      ---          ---          ¦
¦FormicAcid       ---          ---          ---          ---          ¦
¦Nitrogen         ---          ---          ---          -0.0004
¦Argon            ---          ---          ---          -0.0299      ¦
+---------------------------------------------------------------------+
```

```
+-------------------- Bij Interaction Parameters ---------------------+
¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices                    ¦

¦                                                                     ¦
¦                Hydrogen     CO2          CO           FormicAcid    ¦
¦Formaldehyde     ---          ---          ---          ---          ¦
¦Methanol         -1.9464      ---          -0.0294      ---          ¦
¦Oxygen           ---          ---          ---          ---          ¦
¦H2O              4.4304       39.0684     -36.7130      ---          ¦
¦Hydrogen         ---          ---          ---          ---          ¦
¦CO2              ---          ---          ---          ---          ¦
¦CO               ---          ---          ---          ---          ¦
¦FormicAcid       ---          ---          ---          ---          ¦
 Nitrogen         ---          ---          ---          ---
¦Argon            ---          ---          ---          ---          ¦
+---------------------------------------------------------------------+
```

```
ameters ---------------------+
-Matrices                    ¦
                             ¦
                             ¦
  Nitrogen     Argon         ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   -2.3370      11.6313      ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
-----------------------------+
```

Van Laar, IDEAL (DEFAULT *PLUS* UNIFAC VLE)

Unifac Groups Unavailable for Formaldehyde - Methanol   interaction pair

Unifac Groups Unavailable for Formaldehyde - FormicAcid   interaction pair

```
+-------------------- Aij Interaction Parameters ---------------------+
¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices   A_UnifacVLE      ¦
¦            H_Henry's Coeff     L_UnifacLLE     C_UnifacLLE_All
¦            I_j immiscible in i           B_all immiscible in i      ¦
¦                Formaldehyde Methanol     Oxygen       H2O           ¦
¦Formaldehyde     ---          ---        -12.1627      -5.7036       ¦
¦Methanol         ---          ---        -12.1627       0.6257       ¦
¦Oxygen         1480.4229    2570.1833     ---          29.1896       ¦
¦H2O              62.9893       0.7643    -80.3697      ---           ¦
¦Hydrogen        693.7556       2.6055     ---           8.0175       ¦
¦CO2           -3918.1270   -3094.8086     ---         676.2780       ¦
¦CO             1192.2665      -4.0521     ---      -12385.0000       ¦
¦FormicAcid       ---           0.2458    -12.1627      -1.5362       ¦
¦Nitrogen       -124.3227    1518.7225     ---           7.0546
¦Argon          1356.6383    2893.7578     ---          33.2214       ¦
+---------------------------------------------------------------------+
```

```
+-------------------- Aij Interaction Parameters ---------------------+
¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices   A_UnifacVLE      ¦
             H_Henry's Coeff     L_UnifacLLE     C_UnifacLLE_All
¦            I_j immiscible in i           B_all immiscible in i      ¦
¦                Hydrogen     CO2          CO           FormicAcid    ¦
¦Formaldehyde     11.5578      69.6759     -2.0741       ---          ¦
¦Methanol         24.7952      69.6759     13.8729        0.0257      ¦
¦Oxygen          ---          ---          ---         1792.9489      ¦
¦H2O              -6.5127    -183.6914    266.3600       -0.7971      ¦
¦Hydrogen        ---          ---          ---         1025.6306      ¦
¦CO2             ---          ---          ---        -3727.8840      ¦
¦CO              ---          ---          ---         1542.3230      ¦
¦FormicAcid       11.5578      69.6759     -2.0741       ---          ¦
 Nitrogen        ---          ---          ---          339.0691
¦Argon           ---          ---          ---         1772.0728      ¦
+---------------------------------------------------------------------+
```

```
eters ---------------------+
atrices   A_UnifacVLE      ¦
E     C_UnifacLLE_All      ¦
B_all immiscible in i      ¦
Nitrogen     Argon         ¦
 20.0324      -9.9439      ¦
 20.0324      -9.9439      ¦
 ---          ---          ¦
 30.1561     -42.2753      ¦
 ---          ---          ¦
 ---          ---          ¦
 ---          ---          ¦
 20.0324      -9.9439      ¦
 ---          ---          ¦
 ---          ---          ¦
---------------------------+
```

```
+-------------------- Bij Interaction Parameters ---------------------+
¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices                    ¦
¦
¦                                                                     ¦
¦                Formaldehyde Methanol     Oxygen       H2O           ¦
¦Formaldehyde     ---          ---          3.6612      ---           ¦
¦Methanol         ---          ---          3.6612      ---           ¦
¦Oxygen          -0.0043      -0.0043      ---          -0.0498       ¦
¦H2O              ---          ---         19.3401      ---           ¦
¦Hydrogen        -0.0010      -0.0009      ---          -0.0100       ¦
¦CO2              0.0011       0.0011      ---          -0.0977       ¦
¦CO              -0.0024      -0.0036      ---          ---           ¦
¦FormicAcid       ---          0.0000       3.6612      ---           ¦
¦Nitrogen        -0.0037      -0.0037      ---          -0.0004
¦Argon           -0.0039      -0.0039      ---          -0.0299       ¦
+---------------------------------------------------------------------+
```

```
+-------------------- Bij Interaction Parameters ---------------------+
¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices                    ¦

¦                                                                     ¦
¦                Hydrogen     CO2          CO           FormicAcid    ¦
¦Formaldehyde    -0.1687      -8.4077       1.9472       ---          ¦
¦Methanol        -1.9464      -8.4077      -0.0294        0.0000      ¦
¦Oxygen          ---          ---          ---           -0.0043      ¦
¦H2O              4.4304      39.0684     -36.7130       ---          ¦
¦Hydrogen        ---          ---          ---           -0.0010      ¦
¦CO2             ---          ---          ---            0.0011      ¦
¦CO              ---          ---          ---           -0.0024      ¦
¦FormicAcid      -0.1687      -8.4077       1.9472       ---          ¦
 Nitrogen        ---          ---          ---           -0.0037
¦Argon           ---          ---          ---           -0.0039      ¦
+---------------------------------------------------------------------+
```

```
eters ---------------------+
atrices                    ¦
                           ¦
                           ¦
Nitrogen     Argon         ¦
 -1.1520       3.2910      ¦
 -1.1520       3.2910      ¦
 ---          ---          ¦
 -2.3370      11.6313      ¦
 ---          ---          ¦
 ---          ---          ¦
 ---          ---          ¦
 -1.1520       3.2910      ¦
 ---          ---          ¦
 ---          ---          ¦
---------------------------+
```

NRTL, IDEAL (DEFAULT)

```
+------------------------------ A:\DP_0080.SIM -------------------------
¦ +-------------------- Aij Interaction Parameters ---------------------+
¦ ¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices   A_UnifacVLE      ¦
¦ ¦           H_Henry's Coeff     L_UnifacLLE     C_UnifacLLE_All       
¦ ¦           I_j immiscible in i           B_all immiscible in i      ¦
¦ ¦               Formaldehyde Methanol     Oxygen       H2O             ¦
¦ ¦Formaldehyde     ---       -2642.7380      ---         321.3200      ¦
¦ ¦Methanol       -79.2009      ---           ---         610.4030      ¦
¦ ¦Oxygen           ---         ---           ---          29.1896      ¦
¦ ¦H2O          -2806.8950     -48.6725     -80.3697       ---          ¦
¦ ¦Hydrogen         ---          2.6055       ---           8.0175      ¦
¦ ¦CO2              ---         ---           ---         676.2780      ¦
¦ ¦CO               ---         -4.0521       ---      -12385.0000      ¦
¦ ¦FormicAcid       ---         ---           ---        -250.2830      ¦
¦ ¦Nitrogen         ---         ---           ---           7.0546       
¦ ¦Argon            ---         ---           ---          33.2214      ¦
¦ +---------------------------------------------------------------------+
```

```
+------------------------------ A:\DP_0080.SIM -------------------------
¦ +-------------------- Aij Interaction Parameters ---------------------+
¦ ¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices   A_UnifacVLE      ¦
¦           H_Henry's Coeff     L_UnifacLLE     C_UnifacLLE_All         
¦ ¦           I_j immiscible in i           B_all immiscible in i      ¦
¦ ¦               Hydrogen     CO2          CO           FormicAcid     ¦
¦ ¦Formaldehyde     ---         ---          ---          ---           ¦
¦ ¦Methanol        24.7952      ---          13.8729      ---           ¦
¦ ¦Oxygen           ---         ---          ---          ---           ¦
¦ ¦H2O             -6.5127    -183.6914     266.3600     248.8916       ¦
¦ ¦Hydrogen         ---         ---          ---          ---           ¦
¦ ¦CO2              ---         ---          ---          ---           ¦
¦ ¦CO               ---         ---          ---          ---           ¦
¦ ¦FormicAcid       ---         ---          ---          ---           ¦
¦  Nitrogen         ---         ---          ---          ---            
¦ ¦Argon            ---         ---          ---          ---           ¦
¦ +---------------------------------------------------------------------+
```

```
SIM -------------------------
meters ---------------------+
Matrices   A_UnifacVLE      ¦
LE     C_UnifacLLE_All      ¦
 B_all immiscible in i      ¦
 Nitrogen     Argon         ¦
  ---          ---          ¦
  ---          ---          ¦
  ---          ---          ¦
  30.1561     -42.2753      ¦
  ---          ---          ¦
  ---          ---          ¦
  ---          ---          ¦
  ---          ---          ¦
  ---          ---          ¦
  ---          ---          ¦
----------------------------+
```

```
+------------------------------ A:\DP_0080.SIM -------------------------
¦ +-------------------- Bij Interaction Parameters ---------------------+
¦ ¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices                    ¦
¦ ¦
¦ ¦                                                                     ¦
¦ ¦               Formaldehyde Methanol     Oxygen       H2O             ¦
¦ ¦Formaldehyde     ---         ---          ---          ---           ¦
¦ ¦Methanol         ---         ---          ---          ---           ¦
¦ ¦Oxygen           ---         ---          ---         -0.0498        ¦
¦ ¦H2O              ---         ---         19.3401       ---           ¦
¦ ¦Hydrogen         ---        -0.0009       ---         -0.0100        ¦
¦ ¦CO2              ---         ---          ---         -0.0977        ¦
¦ ¦CO               ---        -0.0036       ---          ---           ¦
¦ ¦FormicAcid       ---         ---          ---          ---           ¦
¦ ¦Nitrogen         ---         ---          ---         -0.0004         
¦ ¦Argon            ---         ---          ---         -0.0299        ¦
¦ +---------------------------------------------------------------------+
```

```
+------------------------------ A:\DP_0080.SIM -------------------------
¦ +-------------------- Bij Interaction Parameters ---------------------+
¦ ¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices                    ¦
¦
¦ ¦                                                                     ¦
¦ ¦               Hydrogen     CO2          CO           FormicAcid     ¦
¦ ¦Formaldehyde     ---         ---          ---          ---           ¦
¦ ¦Methanol        -1.9464      ---          -0.0294      ---           ¦
¦ ¦Oxygen           ---         ---          ---          ---           ¦
¦ ¦H2O              4.4304     39.0684      -36.7130      ---           ¦
¦ ¦Hydrogen         ---         ---          ---          ---           ¦
¦ ¦CO2              ---         ---          ---          ---           ¦
¦ ¦CO               ---         ---          ---          ---           ¦
¦ ¦FormicAcid       ---         ---          ---          ---           ¦
¦  Nitrogen         ---         ---          ---          ---            
¦ ¦Argon            ---         ---          ---          ---           ¦
¦ +---------------------------------------------------------------------+
```

```
.SIM -------------------------
ameters ---------------------+
-Matrices                    ¦
                             ¦
                             ¦
  Nitrogen     Argon         ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   -2.3370      11.6313      ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
-----------------------------+
```

```
+------------------------------ A:\DP_0080.SIM -------------------------
¦ +--------------- NRTL Alpha(i,j) Interaction Parameter ---------------+
¦ ¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices   A_UnifacVLE      ¦
¦ ¦           H_Henry's Coeff     L_UnifacLLE     C_UnifacLLE_All       ¦
¦ ¦           I_j immiscible in i           B_all immiscible in i      ¦
¦ ¦               Formaldehyde Methanol     Oxygen       H2O             ¦
¦ ¦Formaldehyde     ---          2.4335      ---          1.4582        ¦
¦ ¦Methanol         2.4335      ---          ---          0.3001        ¦
¦ ¦Oxygen           ---         ---          ---          ---           ¦
¦ ¦H2O              1.4582      0.3001       ---          ---           ¦
¦ ¦Hydrogen         ---         ---          ---          ---           ¦
¦ ¦CO2              ---         ---          ---          ---           ¦
¦ ¦CO               ---         ---          ---          ---           ¦
¦ ¦FormicAcid       ---         ---          ---          4.3935        ¦
¦ ¦Nitrogen         ---         ---          ---          ---            
¦ ¦Argon            ---         ---          ---          ---           ¦
¦ +---------------------------------------------------------------------+
```

```
+------------------------------ A:\DP_0080.SIM -------------------------
¦ +--------------- NRTL Alpha(i,j) Interaction Parameter ---------------+
¦ ¦ HOT KEYS   F1_Help   F2_Menu   S_Switch-Matrices   A_UnifacVLE      ¦
¦           H_Henry's Coeff     L_UnifacLLE     C_UnifacLLE_All         
¦ ¦           I_j immiscible in i           B_all immiscible in i      ¦
¦ ¦               Hydrogen     CO2          CO           FormicAcid     ¦
¦ ¦Formaldehyde     ---         ---          ---          ---           ¦
¦ ¦Methanol         ---         ---          ---          ---           ¦
¦ ¦Oxygen           ---         ---          ---          ---           ¦
¦ ¦H2O              ---         ---          ---          4.3935        ¦
¦ ¦Hydrogen         ---         ---          ---          ---           ¦
¦ ¦CO2              ---         ---          ---          ---           ¦
¦ ¦CO               ---         ---          ---          ---           ¦
¦ ¦FormicAcid       ---         ---          ---          ---           ¦
¦  Nitrogen         ---         ---          ---          ---            
¦ ¦Argon            ---         ---          ---          ---           ¦
¦ +---------------------------------------------------------------------+
```

```
.SIM -------------------------
ion Parameter ---------------+
-Matrices   A_UnifacVLE      ¦
LLE     C_UnifacLLE_All      ¦
  B_all immiscible in i      ¦
  Nitrogen     Argon         ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
   ---          ---          ¦
-----------------------------+
```

```
++---------------------- Binary Interaction Parameters ----------------------+-+
¦¦                                                                          ¦ ¦
¦¦   HYSIM displays all binary interaction parameters in the form of two    ¦ ¦
¦¦   corresponding matrices. Any blanks in the matrix correspond to         ¦ ¦
¦¦   a stored value of zero. Any element in the matrix may be overwritten   ¦ ¦
¦¦   by using the cursor to move to that position and either pressing <F2>  ¦ ¦
¦¦   for a menu or entering the number directly. There are also a series of ¦ ¦
¦¦   Hot Keys available in the form.                                        ¦ ¦
¦¦                                                                          ¦ ¦
¦¦   If you are entering data the components across the top of the menu     ¦ ¦
¦¦   represent the "i" and the components down the side represent the "j".  ¦ ¦
¦¦                                                                          ¦ ¦
¦¦                              a(i,j)                                      ¦ ¦
¦¦                           1    2    3    4                               ¦ ¦
¦¦                 j  i-->   ic4  nc4  ic5  nc5                             ¦ ¦
¦¦                 |     ic4  ---  2,1  3,1  4,1                            ¦ ¦
¦¦                 v     nc4  1,2  ---  3,2  4,2                            ¦ ¦
¦¦                       ic5  1,3  2,3  ---  4,3                            ¦ ¦
¦¦                       nc5  1,4  2,4  3,4  ---                            ¦ ¦
¦¦                                                                          ¦ ¦
¦¦                                                                          ¦ ¦
¦¦                                                   more                   ¦ ¦
```

```
+---------------------- Binary Interaction Parameters ----------------------+
¦                                                                           ¦
¦  Each activity model, with the exception of NRTL and Chien-Null has       ¦
¦  two such matrices, you may use the "S" key to switch between the two. The ¦
¦  second matrix corresponds to the bij matrix and is filled in exactly the ¦
¦  same manner as the aij matrix. All of the activity models follow this    ¦
¦  format where                                                             ¦
¦                                                                           ¦
¦          Aij = aij + bij * T   ( T = temperature in Kelvin deg)           ¦
¦                                                                           ¦
¦  The NRTL model is different in that it contains a third matrix           ¦
¦  corresponding to the "alpha(i,j)" term. In this case "S" acts as a       ¦
¦  three way switch, pressing from the Bij matrix will give you the alpha   ¦
¦  matrix. The units of Aij are different for each activity model and are   ¦
¦  explained in their corresponding section. If Aijs are not available for  ¦
¦  all binary parameters you may use the various UNIFAC estimation          ¦
¦  methods. You have the choice of using the <F2> menu to regress a specific ¦
¦  binary pair, or utilize the Hot Keys available in the form.              ¦
¦                                                                           ¦
¦                                                 more                      ¦
+---------------------------------------------------------------------------+
```

```
+-------------------- Binary Interaction Parameters --------------------+
¦                                                                      ¦
¦  The LLE option is not available for the Wilson model since it is    ¦
¦  not capable of predicting three phase equilibria. HYSIM's imple-     ¦
¦  mentation of the NRTL equation contains temperature dependent        ¦
¦  energy parameters as well as the alpha parameter. After selecting    ¦
¦  the NRTL equation, the second matrix accessed using the "S" command  ¦
```

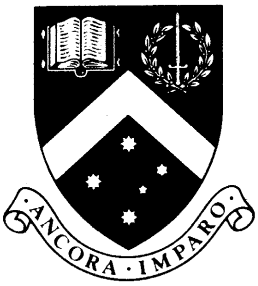
```
¦  is the B(i,j) parameter matrix. Pressing the "S" key a second time  ¦
¦  will result in HYSIM displaying the Alpha(i,j) matrix, it is         ¦
¦  important to note that Alpha(i,j) = Alpha(j,i). In order to toggle  ¦
¦  back to the A(i,j) matrix you must press the "S" key a third time.  ¦
¦  As with the other activity models, only the aij parameter is         ¦
¦  regressed, the alpha parameter is set equal to 0.3.                  ¦
+----------------------------------------------------------------------+
```

```
+-------------------- Paramater Estimation Using Unifac ---------------------+
¦                                                                            ¦
¦ HYSIM uses Unifac to generate Aijs or energy parameters for all of         ¦
¦ the available activity models. Only Aij and Aji are regressed for          ¦
¦ each activity model, Bij and Bji are set to zero and the Alpha term        ¦
¦ for the NRTL is set equal to 0.3. Given a binary HYSIM, will calculate     ¦
¦ the Unifac activitys at the two infinite dilution points, and three        ¦
¦ intermediate compositions, at a temperature of 298 K and 1 atm pressure.   ¦
¦ All of the library components in HYSIM carry Unifac structure information, ¦
¦ any Hypothetical components should have these groups assigned if the       ¦
¦ Unifac option is being used. The calculated activities are then used       ¦
¦ in the internal regression routines to produce the Aijs. There are two     ¦
¦ important things to note;                                                  ¦
¦                                                                            ¦
¦ First, the parameters are regressed at atmospheric pressure, this will     ¦
¦ produce better results when using the ideal model for the vapour phase.    ¦
¦ Second, Unifac is a generalized method and is only going to produce        ¦
¦ approximate results +/- (10 - 15 )%. The method will work quite well as    ¦
¦ long as the given binary components are NOT the primary constitients       ¦
¦ being separated in a fractionation system. If no other source of Aij       ¦
¦ data is available this option should be used as opposed to using zero     ¦
¦ for the energy parameters.                                                 ¦
¦                                          Hot Keys                          ¦
+----------------------------------------------------------------------------+
```

```
+----------------------------------------------------------------------------+
¦Wilson             UNIQUAC            NRTL               VanLaar            ¦
¦Margules           Chien-Null                                               ¦
¦VanLaar two or four parameter VanLaar equation [Aij = aij + bij*T]          ¦
¦ Which activity model do you require                                        ¦
¦>                                                                           ¦
+----------------------------------------------------------------------------+
```

MONASH UNIVERSITY

DEPARTMENT OF CHEMICAL ENGINEERING



APPENDIX TO CHAPTER 6

SPECIFICATION OF EQUIPMENT ITEMS

MONASH

CLIENT: CHE4117		SHEET	1 of 2
PROJECT: SPECIFICATION OF ITEMS		DATE	22/09/1999
		BY	DIV.
DESIGN OF: HX-6 : STAGE 3 RECIRCULATION COOLER		CHKD.	DIV

① DUTY

From worksheet "Abs'r" of spreadsheet Dp_eb-09.xls : (↱ Detailed Design section.)

Energy of incoming fluid =

$$\begin{array}{r} -161\,48.8 \\ -210.4 \\ -171\,101.7 \\ -12.7 \\ \hline -187\,473.6 \end{array} \text{ kW}$$

similarly
Energy of outgoing fluid = −188061.1 kW

$\Rightarrow \Delta\dot{H} = 587.5$ kW

$\Delta\dot{H} \doteqdot 590$ kW

② TEMPERATURE DRIVING FORCE.

$(\Delta T)_{LM} = 10°C$

$(\Delta T)_{LM} = 10°C$

Perry⁽⁶⁾ : $S \equiv \dfrac{t_2 - t_1}{T_1 - t_1} = \dfrac{41-30}{51-30} = \dfrac{11}{21} = 0.52$

$R \equiv \dfrac{T_1 - T_2}{t_2 - t_1} = \dfrac{51-40}{41-30} = \dfrac{11}{11} = 1.$

$\Rightarrow F_T \doteqdot 0.8$ → OKAY ↙ two tube passes.

↳ better : $F_T = 1$ (one tube pass).

$F_T = 1$

③ AREA

$\Delta\dot{H} = UA(\Delta T)_{LM} \cdot F_T$

From Sinnott⁽²⁾ take $U \simeq 800\ \mathrm{W.m^{-2}.K^{-1}}$
↖ Aqueous solution

→ $A =$ ~~117.5~~ 73.4 m² → OKAY.

$A \doteqdot$ ~~110~~ 75 m²

④ BRANCH NOMINAL SIZES

Process : $\dot{V}_p \simeq (13.830\ \mathrm{kg.s^{-1}}) \div (1050\ \mathrm{kg.m^{-3}}) = 0.0132\ \mathrm{m^3.s^{-1}}$

Take $v \leq$ ~~1~~ 2 m.s⁻¹ ⇒ $A_p \geq$ ~~0.0168~~ 0.00659 m²

~~GRAVITY FLOW~~

⇒ $D_p \geq$ ~~0.130~~ 0.092 m = ~~130~~ 92 mm

→ Take $D_p =$ ~~152~~ 102 mm [Perry⁽⁶⁾]

$D_p =$ ~~152~~ 102 mm

Utility : $\dot{m}_u = \dfrac{\Delta\dot{H}}{c_{p_u}\Delta T_u} = \dfrac{587.5\ \mathrm{kW}}{(4.18)(11)\ \mathrm{kJ.kg.K^{-1}.K}} = 12.8\ \mathrm{kg.s^{-1}}$

$\dot{m}_u = 12.8\ \mathrm{kg.s^{-1}}$

$\therefore \dot{V}_u \simeq 0.0128\ \mathrm{m^3.s^{-1}}$ ⇒ $A_u \geq$ ~~0.0163~~ 0.0064 m² ($v \leq 2\ \mathrm{m.s^{-1}}$)

⇒ $D_u \geq$ ~~0.128~~ 0.090 m → Take $D_u =$ ~~152~~ 102 mm

$D_u =$ ~~152~~ 102 mm.

CLIENT: CHE4117	SHEET	2 of 2
PROJECT: SPECIFICATION OF ITEMS	DATE	22/09/1999
	BY	DJV
DESIGN OF: HX-6: STAGE 3 RECIRCULATION COOLER	CHKD.	DJV

⑤ PRESSURE

As the exchanger is at the base of the tall column, pressure will be affected.

Nominal operating pressure for stage 3 = 124 kPa (abs) at the top; 126 kPa (abs) at the bottom.

The height above the exchanger : 11.6 m (bottom)
14.1 m (top)

$\Delta H \simeq 14.1\,m$

With $\rho_L \simeq 995\ kg.m^{-3}$
& $g = 9.78\ m s^{-2}$ [Giancoli(2)]

$\rightarrow \Delta p = (995)(9.78)(14.1) = 137 \times 10^3$ Pa (abs)

$\Rightarrow$ P exiting HX-6 $\geq 137 + 124 = 261$ Pa (abs)

$P_{EXIT} \simeq 265\ kPa\ (abs)$

$\Rightarrow$ Take 265 kPa (abs)
[consider nozzles, 'tortuosity', ...]

↳ for $(-\Delta p)$ across the exchange = 40 kPa (abs) [Sinnott(2)]

$P_{IN} \doteqdot 305$ kPa (abs)

$P_{IN} = 305\ kPa\ (abs)$

⑥ DESIGN VALUES

Sinnott(2) recommends adding 5 to 10% to pressure:

take $P_{DESIGN} = 450$ kPa (abs)

$P_{DESIGN} = 450\ kPa\ (abs)$

Take $T_{DESIGN} = 150°C$

$T_{DESIGN} = 150°C$

MONASH

CLIENT: CHE4117		SHEET	1 of 1
PROJECT: SPECIFICATION OF ITEMS		DATE	22/09/1999
		BY	DJV
DESIGN OF: HX-7 : STAGE 2 RECIRCULATION COOLER		CHKD.	DJV

① NOTE

See specification of HX-6 for method.

② DUTY

$\Delta\dot{H} = (+525189.8) - (+522840.7) = 2349\ \mathrm{kW}$

$\Delta\dot{H} = 2349\ \mathrm{kW}$

③ TEMPERATURE DRIVING FORCE

$(\Delta T)_{LM} = 18\,°\mathrm{C}$

$S = \frac{45-30}{63-30} = \frac{15}{33} = 0.45\ ,\ R = \frac{63-48}{45-30} = \frac{15}{15} = 1.00$

$\Rightarrow F_T \doteqdot 0.88$

for 2 tube passes (or 4, ...)

⇒ CHOOSE THIS.

$(\Delta T)_{LM} = 18\,°\mathrm{C}$

$F_T = 0.88$

④ AREA

$A = \frac{2349 \times 10^3}{700 \times 0.88 \times 18} = \cancel{297}\ \cancel{356}\ 212\ \mathrm{m}^2$ ⇒ OKAY [Garnett]

$A = \cancel{300}\ \cancel{360}\ 210\ \mathrm{m}^2$

⑤ BRANCHES

Process: $\dot{V}_p = (41.2\ \mathrm{kg\cdot s^{-1}}) \div (1100\ \mathrm{kg\cdot m^{-3}}) = 0.037\ \mathrm{m^3\cdot s^{-1}}$

Then for $v \leq 2\ \mathrm{m\cdot s^{-1}}$

$\Rightarrow D_p \geq \cancel{0.217}\ 0.153\ \mathrm{m} \Rightarrow$ take $D_p = \cancel{227}\ 178\ \mathrm{mm}$

$D_p = \cancel{229}\ 178\ \mathrm{mm}$

Utility: $\dot{m}_u = \frac{\Delta\dot{H}}{c_{p_u}\Delta t_u} = \frac{2349}{(4.18)(15)} = 37.5\ \mathrm{kg\cdot s^{-1}} \rightarrow \dot{V}_u = 0.0375\ \mathrm{m^3\cdot s^{-1}}$

$\therefore v \leq 2\ \mathrm{m\,s^{-1}} \Rightarrow D_u \geq \cancel{219}\ 155\ \mathrm{mm} \Rightarrow D_u = \cancel{229}\ 178\ \mathrm{mm}$

$\dot{m}_u = 37.5\ \mathrm{kg\cdot s^{-1}}$

$D_u = \cancel{229}\ 178\ \mathrm{mm}$

⑥ PRESSURE

$\Delta p = \rho g \Delta H = (1100)(9.78)(10.1) = 108.7\ \mathrm{kPa}$

$\Rightarrow p_{EXIT} \simeq 109 + 126 = 235\ \mathrm{kPa} \rightarrow \sim 240\ \mathrm{kPa\ (abs)}$

$\therefore p_{IN} = 240 + 40 = 280\ \mathrm{kPa\ (abs)}$

$p_{EXIT} = 240\ \mathrm{kPa\ (abs)}$

$p_{IN} = 280\ \mathrm{kPa\ (abs)}$

⑦ DESIGN VALUES

$P_{DESIGN} \simeq 450\ \mathrm{kPa\ (abs)}$

$T_{DESIGN} = 150\,°\mathrm{C}$

$P_{DESIGN} = 450\ \mathrm{kPa\ (abs)}$

$T_{DESIGN} = 150\,°\mathrm{C}$.

MONASH

CLIENT: CHE4117		SHEET	1 of 1
PROJECT: SPECIFICATION OF ITEMS		DATE	23/09/1999
		BY	DJV
DESIGN OF: HX-8 : STAGE 1 RECIRCULATION COOLER		CHKD.	

① NOTE

See specification of HX-6 for method

② DUTY

$\Delta\dot{H} = (-298663.8) - (-300284.5) = 1620.7\ kW$

$\Delta\dot{H} \simeq 1621\ kW$

③ TEMPERATURE DRIVING FORCE

$(\Delta T)_{LM} = 30°C$

$(\Delta T)_{LM} = 30°C$

Alternatively, for co-current exchange: $(\Delta T)_{LM,cc} = \dfrac{(75-30)-(60-45)}{\ln\left(\frac{45}{15}\right)}$

$\therefore (\Delta T)_{LM,cc} = 27.3°C$

$\rightarrow$ equivalent to $F_T = \dfrac{27.3}{30} = 0.91 \rightarrow$ OKAY

Compare: $S = \dfrac{45-30}{75-30} = \dfrac{15}{45} = 0.33$, $R = 1.00$

$\rightarrow$ For a 1-2 exchanger, Perry(6) says $F_T \simeq 0.96$

Counter-current $\Rightarrow T_{WALL,MIN} \simeq \dfrac{60+30}{2} = 45°C$

$\rightarrow$ too low for 54% HCHO (by mass) [Kirk-Othmer(4)]

Co-current: $T_{WALL,MIN} \simeq \dfrac{60+45}{2} = 52.5°C$

$\rightarrow$ better!

$\Rightarrow$ CHOOSE CO-CURRENT ARRANGEMENT.

Record $(\Delta T)_{LM} = 30°C$, $F_T = 0.91$

$F_T = 0.91$

④ AREA

$A = \dfrac{1621 \times 10^3}{600 \times 27.3} = 98.96\ m^2$

$A = 100\ m^2$

⑤ BRANCHES

Process: $\dot{V}_P = (29.7\ kg.s^{-1}) \div (1150\ kg.m^{-3}) = 0.0258\ m^3.s^{-1}$

$V \leq 2\ ms^{-1} \Rightarrow D_P \geq 128\ mm$ Take $D_P = 152\ mm$

$D_P = 152\ mm$

Utility: $\dot{m}_u = \dfrac{1621\ kW}{(4.18)(15)} = 25.9\ kg.s^{-1} \rightarrow \dot{V}_u \simeq 0.0259\ m^3.s^{-1}$

$\therefore V \leq 2\ ms^{-1} \rightarrow D_u \geq 128\ mm \Rightarrow D_u = 152\ mm$

$\dot{m}_u = 25.9\ kg.s^{-1}$

$D_u = 152\ mm$

⑥ PRESSURE

$\Delta p = \rho g \Delta h \simeq (1150\ kg.m^{-3})(9.78\ m.s^{-2})(6.4\ m) = 72\ kPa$

$\Rightarrow p_{EXIT} \simeq 72 + 128 = 200\ kPa\ (abs)$

$\therefore p_{IN} \doteqdot p_{EXIT} + 40 = 240\ kPa\ (abs)$

$p_{EXIT} = 200\ kPa\ (abs)$

$p_{IN} = 240\ kPa\ (abs)$

⑦ DESIGN VALUES

Take $p_{DESIGN} = 450\ kPa\ (abs)$, as before, but increase T_{DESIGN} to 170°C to cope with absorber feed cooler failure

$p_{DESIGN} = 450\ kPa\ (abs)$

$T_{DESIGN} = 170°C$

MONASH

CLIENT: CHE4117
PROJECT: SPECIFICATION OF ITEMS
DESIGN OF: HX-11: SERPENTINE COOLING COILS

SHEET 1 of 1.
DATE 01/10/1999
BY DJV
CHKD. DJV.

① DUTY

From the specification of P-8, $\Delta\dot{H} = 153\,kW$

$\Delta\dot{H} = 153\,kW.$

② TEMPERATURE

$(\Delta T)_{lm} = 7\,^{\circ}C$ — minimum

37 — 42
30 — 35

Counter-current flow can be assumed.

$\Delta T_{lm} = 7\,^{\circ}c.$

③ AREA

$$A = \frac{153\times10^3}{1000\times7} = 21.8\,m^2$$

where $U = 1000\,W.m^{-2}.K^{-1}$, after Sinnott(2), due to the vigorous agitation, and water on both sides (essentially).

→ If the coil is one inch in diameter (outer)
→ circumference = 79.8 mm
→ Total length = 273 m

At 21 trays, length = 13 m per tray.

$A = 21.m^2$

Total length = 273 m

Length = 13 m per tray.

④ PRESSURE

See P-8

$P_{IN} = 143$ kPa (abs) } minimum (at top)
$P_{OUT} = 103$ kPa (abs)

$P_{IN} = 143$ kPa (abs)
$P_{OUT} = 103$ kPa (abs)

There is room for 254 mm coil between trays, with room for 8 lengths of tubing of various lengths on either side of the baffle.
Recall: column diameter = 1.8 m.

MONASH

CLIENT: CHE4117		SHEET	1 of 1.
PROJECT: SPECIFICATION OF ITEMS		DATE	24/09/1994
		BY	DJV
DESIGN OF: P-4A : STAGE 1 RECIRCULATION PUMP		CHKD.	

① NOTE :

Refer also to specification of HX-8

② VOLUMETRIC FLOWRATE

$\dot{m} = 29.7 \text{kg}\cdot\text{s}^{-1}$, $\rho = 1150 \text{ m}^3\cdot\text{kg}^{-1}$

$\Rightarrow \dot{V} = 29.8 \div 1150 \times 3600 = 93.3 \text{ m}^3.\text{h}^{-1}$

$\dot{V} = 93 \text{ m}^3.\text{h}^{-1}$

④ PUMP MODEL

From <u>CHE3108</u>, two models cope with $\dot{V} \geqslant 100 \text{ m}^3.\text{h}^{-1}$

Take the smaller, with higher efficiency, η : DR-816 (Worthington)

Model = DR-816

⑤ POWER

From the manufacturers graph, taking $\varnothing = 168$ mm

$\varnothing = 168$mm

$\Rightarrow \eta \doteq 67\%$, Power $\simeq$ 14 BHP = 10.4kW

Alternatively: $\text{Power}^{r} = \Delta p . \dot{V} = (40\text{kPa})(0.0259 \text{m}^3.\text{s}^{-1}) = 1036 \text{ W}$

③ HEAD

Total delivered head $\doteq \dfrac{40 \times 10^3 \text{Pa}}{(9.78 \text{ms}^{-2})(1150 \text{ kg}.\text{m}^{-3})} = 3.56 \text{ m}$

TDH = 3.56m

Whereas the selected pump delivers $\simeq$ 25m of head (hence the extra power).

<u>Perry</u>(6) indicates that the combination of TDH and $\dot{V}$ given here is suitable for a single-stage centrifugal pump.

However, there is concern that pumps capable of handling the relatively large $\dot{V}$ are often designed with a relatively large TDH (design), which must then be let down through a valve — while still consuming the higher power.

$\Rightarrow$ "Arbitrarily" take $\eta = 0.5$ [Else typically ~ 80%. — <u>Sinnott</u>(2)]

$\hookrightarrow$ Power = $\dfrac{1.036 \text{ kW}}{0.5} = 2.07 \text{ kW}$

$\eta_p = 50\%$

$\text{Power}_p = 2.07\text{kW}$ (required)

⑥ MOTOR

From Siemen's 1980 catalogue [<u>CHE4109</u>], typical drive efficiency is 80%.

Take motor power (round up) as 3kW.

$\eta_m = 80\%$

$\text{Power}_m = 3\text{kW}$

⑦ BRANCH.

As the suction is under gravity flow, take $V_s \leqslant 1 \text{m}.\text{s}^{-1}$ here.

$\therefore A_s \geqslant 0.0259 \text{ m}^2 \Rightarrow D_s \geqslant 181 \text{ mm} \Rightarrow$ take $D_s = 203$mm

$D_s = 203$mm

MONASH

CLIENT: CHE4117

PROJECT: SPECIFICATION OF ITEMS

DESIGN OF: P-6 : STAGE 2 RECIRCULATION PUMP.

SHEET 1 of 1

DATE 24/09/1999

BY DJV

CHKD.

① NOTE

Refer to specifications of P-4A & HX-7

② VOLUMETRIC FLOWRATE

$\dot{m} = 41.2\ kg.s^{-1} \rightarrow \dot{V} = \frac{41.2}{1100} = 0.0375\ m^3.s^{-1}$

$\dot{V} = 135\ m^3.h^{-1}$

③ HEAD

$TDH = \frac{40\times10^3}{(9.78)(1100)} = 3.718 m$

$TDH = 3.72 m$

④ POWER

$Power = \frac{\Delta p . \dot{V}}{\eta} = \frac{(40\times10^3)(0.0375)}{0.5} = 3000 W$

$Power_p = 3.0 kW$ (req'd)

⑤ MOTOR

$\eta_M = 80\%$ Take $Power_m = 4.5 kW$

$\eta_m = 80\%$

$Power_m = 4.5 kW$

⑥ BRANCH

$A_s \geqslant 0.0375\ m^2 \rightarrow D_s \geqslant 218\ mm \rightarrow D_s = 229\ mm$

$D_s = 229\ mm$

MONASH

CLIENT: CHE4117
PROJECT: SPECIFICATION OF ITEMS
DESIGN OF: P-7 : STAGE 3 RECIRCULATION PUMP

SHEET 1 of 1
DATE 24/09/1999
BY DJV
CHKD.

① NOTE

Refer to specification of HX-6 and P-6.

② VOLUMETRIC FLOWRATE

$\dot{m} = 13.7\ kg.s^{-1} \Rightarrow \dot{V} = \frac{13.7}{1050} = 0.0130\ m^3.s^{-1}$

$\dot{V} = 47\ m^3.h^{-1}$

③ HEAD

$TDH = \frac{40\times10^3}{(9.78)(1050)} = 3.90\ m$

$TDH = 3.90\ m$

④ POWER

$Power = \frac{\Delta p.\dot{V}}{\eta} = \frac{(40\times10^3)(0.0130)}{0.50} = 1040\ W$

$Power_p = 1.0\ kW$

⑤ MOTOR

$\eta_M = 80\%$. Take $Power_m = 1.5\ kW$

$\eta_m = 80\%$.
$Power_m = 1.5\ kW$

⑥ BRANCH

$V \le 1\ ms^{-1} \rightarrow A_s \geq 0.0130\ m^2 \rightarrow D_s \geq 129\ mm \rightarrow D_s = 152\ mm$

$D_s = 152\ mm$

MONASH

CLIENT: CHE4117
PROJECT: SPECIFICATION OF ITEMS
DESIGN OF: P-8 : STAGE 4 COOLANT PUMP
SHEET 1 of 2
DATE 24/09/1999
BY DJV
CHKD. DJV

① PRESSURE DROP :

Assume a pressure drop of 40kPa due to valves and frictional losses, etc. — both in the coils and in the pipework to and from the coils.

Suppose the exit pressure at the base of the column is $\geq$ 150kPa (abs), to get back to the cooling tower.

The top coil is at a height of $33.57 + 1.5 \doteq 35$m
[See Detailed Design of Absorber]

$\Rightarrow (\Delta p)_{STATIC} \doteq (35m)(9.78 m s^{-2})(1000 kg.m^{-3}) \doteq 342$ kPa
$\Rightarrow$ Exit pressure requirement satisfied.

Thus, to exit the coil, the water undergoes a $(-\Delta p)$ of $\simeq 382$kPa

However the water is "only" supplied at 400kPa (abs), and at no time must the water in the tubes be at a pressure lower than 101 kPa (abs)

$\Rightarrow$ Inlet p at base of column (after pump) $\geq$ ~~487~~ 523 kPa (abs)

Take Inlet p = ~~485~~ 525 kPa (abs)

$\therefore p_{IN} = 400$ kPa (abs) , $p_{OUT} =$ ~~485~~ 525 kPa (abs) w.r.t. P-8

$p_{IN} = 400$ kPa(abs)
$p_{OUT} =$ ~~485~~ 525 kPa(abs)

② TEMPERATURE
T = 30°C (assumed const.) for RCW.

T = 30°C

③ FLOW
From the Detailed Design of the Absorber, $\Delta\dot{H} = 153.0$kW

$$\Rightarrow \dot{m} = \frac{153.0}{(4.18)(35-30)} = 7.32\ kg.s^{-1}$$

$\therefore \dot{V} = 0.0073\ m^3.s^{-1}$

$\Delta\dot{H} = 153.0$kW (HX-11)
$\dot{m} = 7.32\ kg.s^{-1}$

$\dot{V} = 26.4\ m^3.h^{-1}$

④ HEAD
$$TDH = \frac{\overset{125}{\cancel{85}} \times 10^3}{(1000)(9.78)} = \overset{12.78}{\cancel{8.69}}\ m$$

TDH = ~~8.69~~ 12.78 m

⑤ POWER
$Power' = \dot{V}.\Delta p =$ ~~622~~ 913 W

From Sinnott², $\eta \simeq 70\%$

$\therefore Power_p =$ ~~889~~ 1304 W

$\eta \simeq 70\%$

$Power_p =$ ~~0.90~~ 1.30 kW

MONASH

CLIENT: CHE4117
PROJECT: SPECIFICATION OF ITEMS
DESIGN OF: P-8: STAGE 4 COOLANT PUMP
SHEET 2 of 2
DATE 24/09/1999
BY DIV
CHKD. DIV

⑥ MOTOR

Taking $\eta_m = 80\%$ ⇒ say $Power_m =$ ~~1.5~~ 2.0 kW

$\eta_m = 80\%$
$Power_m =$ ~~1.5~~ 2.0 kW

⑦ BRANCHES.

Suction: Take $V \leq 1.5\,ms^{-1}$
$\Rightarrow D_s \geq 79$ mm ⇒ $D_s = 102$ mm

$D_s = 102$ mm

Delivery: Take $V \leq 2.0\,ms^{-1}$
$\Rightarrow D_D \geq 68$ mm ⇒ $D_D = 76$ mm

$D_D = 76$ mm

MONASH

CLIENT: CHE4117
PROJECT: SPECIFICATION OF ITEMS
DESIGN OF: P-10 : Absorber water pump.

SHEET 1
DATE 24/09/1999
BY DJV
CHKD.

① NOTES

Refer also to specification of P-8

② VOLUMETRIC FLOWRATE

$\dot{m} = 0.3275 \text{ kg.s}^{-1}$

$\therefore \dot{V} = 0.00033 \text{ m}^3.\text{s}^{-1}$

$\dot{m} = 0.3275 \text{kg.s}^{-1}$
$\dot{V} = 1.18 \text{ m}^3.\text{h}^{-1}$

③ HEAD

If $\Delta p = 382$ kPa as for P-8, and the column pressure is 110 kPa (abs)

$\Rightarrow$ Pressure at base of column $\doteqdot 495$ kPa (abs)

cf. $p_{in} = 400$ kPa (abs)

$$TDH = \frac{95\times10^3}{(1000)(9.78)} = 9.71 \text{ m}$$

$p_{exit} = 495$ kPa(abs)
$p_{IN} = 400$ kPa (abs)

$TDH = 9.71$m

④ POWER

$$Power_p = \frac{(95\times10^3)(0.000328)}{\eta_p} = 51.9 \text{ W}$$

for $\eta_p = 0.60$ [Sinnott(2)]

$Power_p = 52$W
$\eta_p = 60\%$

⑤ MOTOR

$\eta_M = 80\%$. Take $Power_m = 0.10$ kW — small motors not in a great range of sizes

$\hookrightarrow$ Note : this is small enough for flange-mounting.

$\eta_m = 80\%$
$Power_m = 0.10$kW

⑥ BRANCHES

Suction : Take $v \leq 1.5 \text{ms}^{-1}$
$\rightarrow D_s \geqslant 16.7$mm $\Rightarrow D_s = 19$ mm $(\frac{3}{4}")$

$D_s = 19$mm

Delivery : Take $v \leq 2 \text{ ms}^{-1}$
$\rightarrow D_D = 14.4$ mm $\Rightarrow D_D = 19$mm $(\frac{3}{4}")$

$D_D = 19$mm

MONASH UNIVERSITY

DEPARTMENT OF CHEMICAL ENGINEERING

Appendix to Chapter 7

Part 1: Vapour–Liquid Equilibria

Vapour pressures over solutions, by the van Laar equation(s)

From R, P & P$^{(4)}$, Chapter 8, Table 8-3

$$g^E = A.x_1.x_2 / \{x_1.(A/B) + x_2\}$$

$$R.T.\ln(\gamma_1) = A.\{1 + (A/B).(x_1/x_2)\}^{-2}$$
$$R.T.\ln(\gamma_2) = B.\{1 + (B/A).(x_2/x_1)\}^{-2}$$

For the binary system methanol(1)-water(2):

From HYSIM:

a_{12} =	0.7643	b_{12} =	0
a_{21} =	0.6257	b_{21} =	0

T [°C] = 60 ∴ T [K] = 333.15

hence: A_{12} = 0.7643 = A ?

A_{21} = 0.6257 = B ?

By estimation from <u>*typical*</u> *activity coefficients at infinite dilution:*
(*From R, P & P$^{(4)}$, Chapter 8, Table 8-17*)

Note: species (1) is the solute, at inifinite dilution

For *n*-primary alcohols(1)-water(2):

T [°C]	α	ε	ζ	η	θ	Equation		γ1∞		**A**
25	-0.995	0.622	0.558	…	0	(a)	⇒	1.531087	⇒	1055.988
60	-0.755	0.583	0.460	…	0	(a)	⇒	1.940886	⇒	1836.896
100	-0.420	0.517	0.230	…	0	(a)	⇒	2.123244	⇒	2336.058

∴ A = T[K] × 16.95899 -3935.17

Equations:

(a) $\log(\gamma_1^{\infty}) = \alpha + \varepsilon.N_1 + \zeta/N_1 + \theta/N_2$

where N_i is the number of carbon atoms in molecule *i*

N_1 = 1 N_2 = 0

where A and B may be found by observing that for the van Laar equation:

for $x_1 \rightarrow 0$ R.T.ln(g1¥) = A

for $x_2 \rightarrow 0$ R.T.ln(g2¥) = B

where R = 8.31451 $J.mol^{-1}.K^{-1}$

For water(1)-*n*-primary alcohols(2):

T [°C]	α	ε	ζ	η	θ	Equation		γ1∞		**B**
25	0.760	0	0	…	-0.630	(a)	⇒	1.348963	⇒	742.0455
60	0.680	0	0	…	-0.440	(a)	⇒	1.737801	⇒	1530.747
100	0.617	0	0	…	-0.280	(a)	⇒	2.172701	⇒	2407.497

where N_i is the number of carbon atoms in molecule *i*

N_1 = 0 N_2 = 1

∴ B = T[K] × 22.19922 -5872.57

NOTE:
DECHEMA Chemistry Data Series, Vol. I, Part 1b (VLE …, Aq systems, Supp.2) gives:

A12 = 0.8509 γ_1^{∞} = 2.34 This is not very similar to the values estimated.

A21 = 0.5291 γ_2^{∞} = 1.70 This is similar to the value at 60°C.

Where these have been correlated for atmospheric pressure (**101.325kPa(abs)**).
It is to be assumed that the constants listed here are A/(R.T) and B/(R.T), respectively.
Thus, at 60°C:

A12 ⇒ 2356.975 = A γ_1^{∞} ⇒ 2354.9 = A

A21 ⇒ 1465.596 = B γ_2^{∞} ⇒ 1469.829 = B

Plotting VLE data based on these parameters:

methanol(1)-water(2), T[°C] = **60**

∴ T [K] = 333.15

From Antoine data, at 60°C:

$p_{vap,1}$ [kPa(abs)] = 84.65408 $p_{vap,2}$ [kPa(abs)] = 19.94065

A = 1836.896   0

B = 1530.747   0

Substance	A	B	C	D	eq'n	T_c [K]	p_c [bar]
	Constant (Reid, Prausnitz & Poling[(4)])						
Formaldehyde	-7.29343	1.08395	-1.63882	-2.30677	1	408	65.9
Water	-7.76451	1.45838	-2.7758	-1.23303	1	647.3	221.2
Methanol	-8.54796	0.76982	-3.1085	1.54481	1	512.6	80.9

$$(1)\ \ln(p_{vap}/p_c) = \{A(1 - T/T_c) + B(1 - T/T_c)^{1.5} + C(1 - T/T_c)^3 + D(1 - T/T_c)^6\}.(T_c/T)$$

Total pressure = 101.325 kPa(abs) $p_1 + p_2 = y_1P + y_2P = P = \gamma_1.x_1.p_{vap,1} + \gamma_2.x_2.p_{vap,2}$

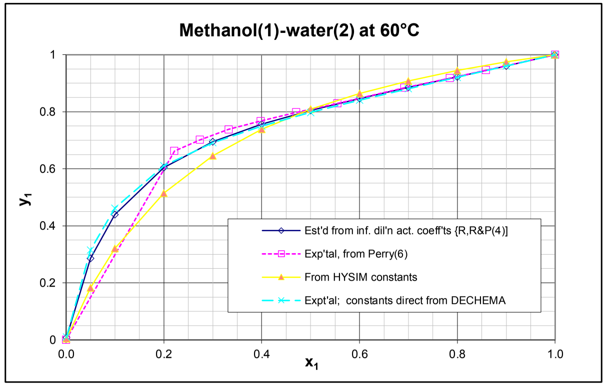
x_1	x_2	$\gamma 1$	γ_2	p_1 [kPa(a)]	p_2 [kPa(a)]	P [kPa(a)]	y_1	y_2	y_1	*From HYSIM*		y_1	*From DECHEMA*	
0.001	0.999	1.937802	1.000001	0.164043	19.92073	20.08477	0.008168	0.991832	0.004232729	A =	0.7643	0.0098267	A =	2356.97514
0.05	0.95	1.798037	1.001952	7.610557	18.9806	26.59116	0.286206	0.713794	0.182666758	B =	0.6257	0.3146282	B =	1465.59589
0.1	0.9	1.675797	1.007678	14.18631	18.08438	32.27069	0.439603	0.560397	0.320559648			0.4622945		
0.2	0.8	1.48052	1.029867	25.06641	16.42897	41.49538	0.604077	0.395923	0.514912578			0.6103714		
0.3	0.7	1.335354	1.065817	33.91294	14.87715	48.79009	0.695078	0.304922	0.64533758			0.6918171		
0.4	0.6	1.227125	1.11534	41.55246	13.34437	54.89683	0.756919	0.243081	0.738924481			0.7496741		
0.5	0.5	1.146843	1.178705	48.54249	11.75207	60.29455	0.805089	0.194911	0.809351274			0.7973377		
0.6	0.4	1.088265	1.256561	55.27565	10.02266	65.29831	0.84651	0.15349	0.864270021			0.8402283		
0.7	0.3	1.046995	1.34991	62.04268	8.075424	70.1181	0.884831	0.115169	0.908296098			0.8808938		
0.8	0.2	1.019909	1.460077	69.07153	5.822977	74.89451	0.922251	0.077749	0.944378619			0.9206492		
0.9	0.1	1.004774	1.588714	76.55239	3.167999	79.72039	0.960261	0.039739	0.974490144			0.960215		
0.999	0.001	1	1.736201	84.56946	0.034621	84.60408	0.999591	0.000409	0.999764212			0.9996002		

Experimental data from Perry[(6)], p. 3-73 (Table 3-26)

Note: Evaluated at 59.4°C

x_1	p_1 [mmHg]	p_2 [mmHg]	P [kPa(a)]	y_1
0.0000	0	145.4	19.38507	0
0.2217	210.1	106.9	42.26319	0.662776
0.2740	240.2	102.2	45.64958	0.701519
0.3324	272.1	96.6	49.15596	0.737998
0.3980	301.9	91.7	52.47568	0.767022
0.4708	335.6	84.8	56.04872	0.798287
0.555	373.7	76.9	60.07506	0.829339
0.692	439.4	57.8	66.28788	0.883749
0.785	486.6	43.8	70.71418	0.917421
0.859	526.9	30.1	74.26056	0.945961
1.000	609.3	0	81.23332	1

Note also the error in the original: they actually quote mole PERCENT



For the binary system formaldehyde(1)-water(2):

From HYSIM:

a_{12} = 62.9893 b_{12} = 0

a_{21} = -5.7036 b_{21} = 0

T [°C] = 60 ∴ T [K] = 333.15

hence: A_{12} = 62.9893 = A ?

A_{21} = -5.7036 = B ?

By estimation from *<u>typical</u>* *activity coefficients at infinite dilution:*
(From R, P & P[(4)], Chapter 8, Table 8-17)

Note: species (1) is the solute, at inifinite dilution

For *n*-aldehydes(1)-water(2):

T [°C]	α	ε	ζ	η	θ	Equation		$\gamma 1\infty$		**A**
25	-0.780	0.622	0.320	…	0	(a)	⇒	1.452112	⇒	924.7028
60	-0.400	0.583	0.210	…	0	(a)	⇒	2.471724	⇒	2506.598
100	-0.03	0.517	0	…	0	(a)	⇒	3.069022	⇒	3479.083

^^^Note: SAME AS previous

Equations:

(a) $\log(\gamma_1^{\infty}) = \alpha + \varepsilon.N_1 + \zeta/N_1 + \theta/N_2$

where N_i is the number of carbon atoms in molecule *i*

N_1 = 1 N_2 = 0

$\therefore$ A = T[K] × 33.82772 -9022.62

where A and B may be found by observing that for the van Laar equation:

for $x_1 \to 0$ R.T.ln(g1¥) = A

for $x_2 \to 0$ R.T.ln(g2¥) = B

where R = 8.31451 $J.mol^{-1}.K^{-1}$

NOTE: No data is given by R, P & P[4] for a water(1)-aldehyde(2) system
However information is available for water(1)-ketone(2) systems
It has been assumed that methanal (*i.e.* formaldehyde) can be modeled as
a HYPOTHETICAL single-carbon ketone (*i.e.* *methanone).
This is based on the statement, "aldehydes and ketones behave similarly and
undergo many of the same reactions," in John McMURRY; Organic Chemistry[3];
Brooks/Cole Publishing; Pacific Grove, California; 1992; p. 697.

This may be COMPARED with the case for a hypothetical single-carbon ketone:

For *n*-ketones(1)-water(2):

T [°C]	α	ε	ζ	η	θ	Equation		γ1∞		A
25	-1.475	0.622	0.500	0	…	(b)	⇒	1.402814	⇒	839.0822
60	-1.040	0.583	0.330	0	…	(b)	⇒	1.595879	⇒	1294.757
100	-0.621	0.517	0.200	0	…	(b)	⇒	1.97697	⇒	2114.596

^^^Note: SAME AS previous

Equations:

(b) $\log(\gamma_1^{\infty}) = \alpha + \varepsilon.N_1 + \zeta.(1/N'_1 + 1/N''_1) + \eta.(N_1 - N_2)^2$

$\therefore$ A = T[K] × 17.08944 -4305.68

where N_i is the number of carbon atoms in molecule *i*

N_1 = 1 N_2 = 0

N', N" are the number of carbon atoms in respective branches of branched compounds, INCLUDING the "polar grouping."

Thus

N'_1 = 1 N''_1 = 1

We observe that this approximation was acceptable for the lowest temperature (25°C), but quite inaccurate for larger deviations from ideality.

For water(1)-*n*-ketones(2):

T [°C]	α	ε	ζ	η	θ	Equation		γ1∞		B
25	1.857	0	0	…	-1.019	(c)	⇒	0.659174	⇒	-1033.16
60	1.493	0	0	…	-0.73	(c)	⇒	1.078947	⇒	210.4777
100	1.231	0	0	…	-0.557	(c)	⇒	1.309182	⇒	835.8371

Equations:

(c) $\log(\gamma_1^{\infty}) = \alpha + \varepsilon.N_1 + \zeta.(1/N'_1 + 1/N''_1 + 1/N'''_1) + \theta.(1/N'_2 + 1/N''_2)$

$\therefore$ B = T[K] × 24.70012 -8265.62

where N_i is the number of carbon atoms in molecule *i*

N_1 = 0 N_2 = 1

N', N" are the number of carbon atoms in respective branches of branched compounds, INCLUDING the "polar grouping."

Thus

N'_1 = 0 N''_1 = 0 N'''_1 = 0 N'_2 = 1 N''_2 = 1

Plotting VLE data based on these parameters:

formaldehyde(1)-water(2), T = 60 °C A = 2506.598

$\therefore$ T [K] = 333.15 B = 210.4777

From Antoine data, at 60°C:

$p_{vap,1}$ [kPa(abs)] = 1403.154 $p_{vap,2}$ [kPa(abs)] = 19.94065

Substance	A	B	C	D	eq'n	T_c [K]	p_c [bar]
	Constant (Reid, Prausnitz & Poling[4])						
Formaldehyde	-7.29343	1.08395	-1.63882	-2.30677	1	408	65.9
Water	-7.76451	1.45838	-2.7758	-1.23303	1	647.3	221.2
Methanol	-8.54796	0.76982	-3.1085	1.54481	1	512.6	80.9

(1) $\ln(p_{vap}/p_c) = \{A(1 - T/T_c) + B(1 - T/T_c)^{1.5} + C(1 - T/T_c)^3 + D(1 - T/T_c)^6\}.(T_c/T)$

Total pressure = 101.325 kPa(abs) $p_1 + p_2 = y_1P + y_2P = P = \gamma_1.x_1.p_{vap,1} + \gamma_2.x_2.p_{vap,2}$

x_1	x_2	γ1	γ_2	p_1 [kPa(a)]	p_2 [kPa(a)]	P [kPa(a)]	y_1	y_2
0.0001	0.9999	2.466411	1	0.346076	19.93866	20.28474	0.017061	0.982939
0.001	0.999	2.419887	1.000011	3.395474	19.92092	23.3164	0.145626	0.854374
0.02	0.98	1.796153	1.002909	50.40561	19.59869	70.00429	0.720036	0.279964
0.05	0.95	1.407668	1.011344	98.75878	19.15852	117.9173	0.837526	0.162474
0.1	0.9	1.182532	1.024956	165.9274	18.39447	184.3219	0.900205	0.099795
0.2	0.8	1.058873	1.043499	297.1525	16.64643	313.799	0.946952	0.053048
0.3	0.7	1.024585	1.054564	431.2955	14.72009	446.0156	0.966996	0.033004
0.4	0.6	1.011388	1.061769	567.6535	12.70342	580.3569	0.978111	0.021889
0.5	0.5	1.005445	1.066806	705.3973	10.6364	716.0337	0.985145	0.014855
0.6	0.4	1.002546	1.070518	844.0363	8.53873	852.5751	0.989985	0.010015

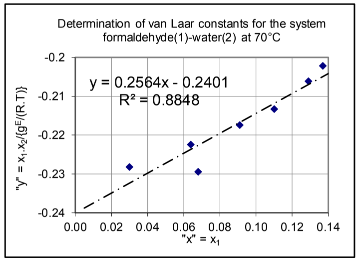
0.7	0.3	1.001093	1.073364	983.2811	6.421076	989.7022	0.993512	0.006488
0.8	0.2	1.000383	1.075615	1122.953	4.289694	1127.243	0.996195	0.003805
0.9	0.1	1.000077	1.077439	1262.937	2.148484	1265.085	0.998302	0.001698
0.999	0.001	1	1.078933	1401.751	0.021515	1401.773	0.999985	1.53E-05

Experimental data from M. Albert, L. Hahnenstein, H. Hasse & G. Maurer, AIChE.J, p. 1743 (Table 1)
&, also, hence recalculated van Laar data
Note: Evaluated at t[°C] = 70 , **as T[K] = 343.15** (approx.) ⇒

x_1	p [kPa(a)]	y_1		$\gamma_1 = y_1/y_{Raoult\ 1}$	$\gamma_{1\ Recalc.}$	ERROR^2	⇓	but also: $\gamma_2 = y_2/y_{Raoult\ 2}$	$\gamma_{2\ Recalc.}$	ERROR^2
0.030	31	0.029	⇒	0.016761	0.013832	8.583E-06	$p_{vap,1}$= 1787.843	0.995006	1	2.494E-05
0.064	30.9	0.054	⇒	0.014583	0.013832	5.642E-07	$p_{vap,2}$= 31.18772	1.00136	1	1.849E-06
0.068	31.2	0.056	⇒	0.014372	0.013832	2.914E-07	[kPa(abs)]	1.013274	1	0.0001762
0.091	30.9	0.071	⇒	0.013485	0.013832	1.204E-07		1.012574	1	0.0001581
0.110	30.9	0.083	⇒	0.013041	0.013832	6.251E-07	A = -12213.6	1.020832	1	0.000434
0.129	30.7	0.093	⇒	0.012379	0.013832	2.109E-06	B = -1.1E+10	1.025047	1	0.0006274
0.137	30.5	0.098	⇒	0.012203	0.013832	2.652E-06		1.022144	1	0.0004904
				0.086517	1000 × SUM =	0.014945	(least-squares regression)		SUM =	0.001913

TOTAL SUM = 0.016857599

Alternative correlation:
Linearised van Laar equation: *[see R.P.&P., Example 8-1]*
$x_1.x_2/\{g^E/(R.T)\} = D + C.(2x_1 - 1)$
where: $A = R.T/(D - C)$ $B = R.T/(D + C)$
and by definition: $g^E/(R.T) \equiv x_1.\ln(\gamma_1) + x_2.\ln(\gamma_2)$



$\gamma_1 = p_1/(x_1.p_{vap\ 1})$	$\gamma_2 = p_2/(x_2.p_{vap\ 2})$	$x_1.x_2/\{g^E/(R.T)\}$
0.016761	0.995006	-0.2282
0.014583	1.00136	-0.22243
0.014372	1.013274	-0.22946
0.013485	1.012574	-0.21739
0.013041	1.020832	-0.21328
0.012379	1.025047	-0.20617
0.012203	1.022144	-0.2022

From the graph:

2C	(D - C)
0.256391	-0.24006

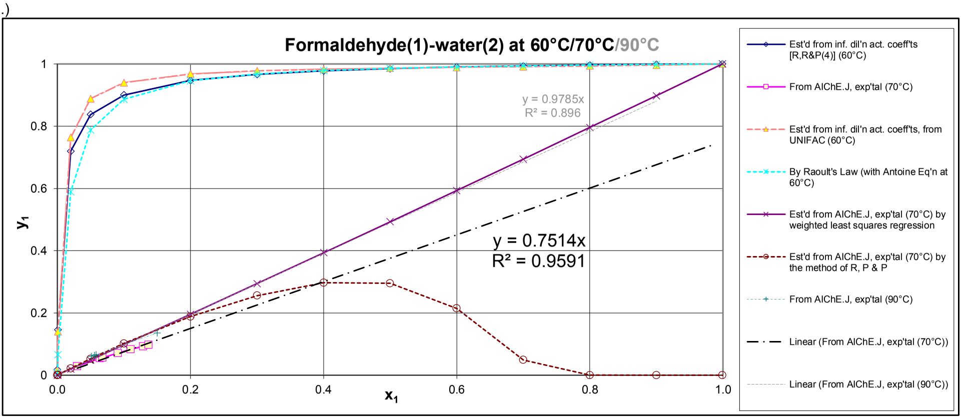
Hence:

A = -11885.1
B = 174684.3

However observe that the sensitivity in B is very great,
as it is found by dividing by the SUM of 2C and (D - C),
which are both of very similar magnitude, but opposite sign.
From the graph (below) it is not physically realistic at large x_1,
and it "probably" does not satisfy the Gibbs-Duhem equation.

Experimental data from M. Albert, L. Hahnenstein,
H. Hasse & G. Maurer, AIChE.J, p. 1743 (Table 1)
Note: Evaluated at t[°C] = 90 ,
as T[K] = 363.15 (approx.)

x_1	p [kPa(a)]	y_1
0.051	71.4	0.061
0.056	71.4	0.064
0.058	70.6	0.066
0.150	71.6	0.136



Recalculated van Laar constants:

T = 70 °C
∴ T [K] = 343.15
From Antoine data, at 70°C:
$p_{vap,1}$ [kPa(abs)] = 1787.843 $p_{vap,2}$ [kPa(abs)] = 31.18772

A = -12213.6
B = -1.1E+10

-9273.5879 -29317.985 -12262.41228 -11885.138
-6805.042 -4113.3916 -1009975.48 174684.34
(previous "guesses")

Total pressure = 101.325 kPa(abs) $p_1 + p_2 = y_1P + y_2P = P = \gamma_1.x_1.p_{vap,1} + \gamma_2.x_2.p_{vap,2}$

x_1	x_2	γ1	γ_2	p_1 [kPa(a)]	p_2 [kPa(a)]	P [kPa(a)]	y_1	y_2	y_1
0.0001	0.9999	0.013832	1	0.001941	19.93866	19.9406	9.73E-05	0.999903	0.000109199
0.001	0.999	0.013832	1	0.019408	19.92071	19.94012	0.000973	0.999027	0.00109134
0.02	0.98	0.013832	1	0.388164	19.54184	19.93	0.019476	0.980524	0.0215527
0.05	0.95	0.013832	1	0.97041	18.94362	19.91403	0.04873	0.95127	0.052791981
0.1	0.9	0.013832	1	1.940821	17.94659	19.88741	0.09759	0.90241	0.101888421
0.2	0.8	0.013832	1	3.881648	15.95252	19.83416	0.195705	0.804295	0.188165947
0.3	0.7	0.013832	0.999999	5.822482	13.95844	19.78093	0.294348	0.705652	0.255697777
0.4	0.6	0.013832	0.999998	7.763327	11.96437	19.72769	0.393524	0.606476	0.297156603
0.5	0.5	0.013832	0.999995	9.704189	9.970278	19.67447	0.493238	0.506762	0.295529612
0.6	0.4	0.013832	0.999989	11.64508	7.976175	19.62126	0.593493	0.406507	0.214488827
0.7	0.3	0.013832	0.999974	13.58604	5.98204	19.56808	0.694296	0.305704	0.049001975
0.8	0.2	0.013832	0.999924	15.52715	3.987826	19.51497	0.795653	0.204347	2.07456E-05
0.9	0.1	0.013833	0.999614	17.46887	1.993295	19.46217	0.897581	0.102419	2.62656E-76
0.999	0.001	0.013964	0.008681	19.57402	0.000173	19.57419	0.999991	8.84E-06	2.86146E-23

[Est'd from AIChE.J, exp'tal (70°C) by the method of R, P & P]
A = -11885.1377
B = 11128.0122

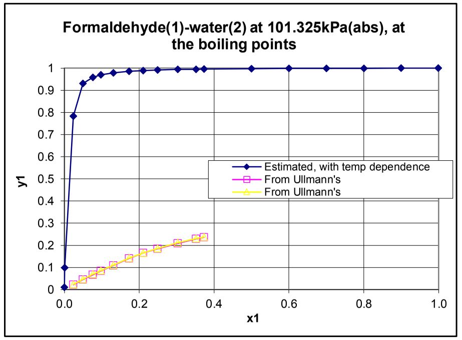
From UNIFAC estimation of activity coefficients at infinitite dilution [R,P&P and AIChE.J]

T = 60 °C
∴ T [K] = 333.15
From Antoine data, at 60°C:
$p_{vap,1}$ [kPa(abs)] = 1403.154 $p_{vap,2}$ [kPa(abs)] = 19.94065

A = 2319.507
B = 2851.515
NOTE: The previous (initial) estimation was close to this value for A

Total pressure = 101.325 kPa(abs) $p_1 + p_2 = y_1P + y_2P = P = \gamma_1.x_1.p_{vap,1} + \gamma_2.x_2.p_{vap,2}$

x_1	x_2	γ1	γ_2	p_1 [kPa(a)]	p_2 [kPa(a)]	P [kPa(a)]	y_1	y_2	*cf.* $y_{Raoult\ 1}$
0.0001	0.9999	2.309974	1	0.324125	19.93866	20.26278	0.015996	0.984004	0.006988178
0.001	0.999	2.307144	1.000001	3.237279	19.92072	23.158	0.139791	0.860209	0.065802063
0.02	0.98	2.248465	1.000275	63.09888	19.5472	82.64608	0.763483	0.236517	0.589499648
0.05	0.95	2.159827	1.001737	151.5285	18.97652	170.505	0.888704	0.111296	0.787392424
0.1	0.9	2.022445	1.007098	283.7802	18.07397	301.8542	0.940124	0.059876	0.886602064
0.2	0.8	1.782948	1.029835	500.3503	16.42847	516.7788	0.96821	0.03179	0.946212357
0.3	0.7	1.584723	1.071209	667.0831	14.95242	682.0355	0.978077	0.021923	0.967904568
0.4	0.6	1.421961	1.135724	798.0925	13.58824	811.6808	0.983259	0.016741	0.979127973
0.5	0.5	1.28999	1.230139	905.0276	12.26489	917.2925	0.986629	0.013371	0.985987828
0.6	0.4	1.185169	1.36469	997.7851	10.88512	1008.67	0.989208	0.010792	0.990614716
0.7	0.3	1.104846	1.555139	1085.189	9.303147	1094.492	0.9915	0.0085	0.993946312
0.8	0.2	1.047366	1.826335	1175.693	7.283664	1182.977	0.993843	0.006157	0.996459752
0.9	0.1	1.012168	2.218582	1278.205	4.423997	1282.629	0.996551	0.003449	0.998423456
0.999	0.001	1.000001	2.792411	1401.753	0.055682	1401.809	0.99996	3.97E-05	0.999985775



Plotting VLE data based on these parameters:
formaldehyde(1)-water(2)
Total pressure = **101.325** **kPa(abs)**
T[K] = 273.15 + t[°C]
From Antoine data, at T[K]:

A = 33.82772 × T[K] + -9022.62
B = 24.70012 × T[K] + -8265.62

$p_1 + p_2 = y_1P + y_2P = P = \gamma_1.x_1.p_{vap,1} + \gamma_2.x_2.p_{vap,2}$

x_1	x_2	guess T [K]	A	B	$p_{vap,1}$	$p_{vap,2}$	γ1	γ_2	p_1 [kPa(a)]	p_2 [kPa(a)]	P [kPa(a)]	y_1	y_2
0.0001	0.9999	372.84	3589.601	943.4921	3409.471	100.2506	3.180605	1	1.084417841	100.2406	101.325	0.010702	0.989298
0.001	0.999	370.28	3502.945	880.2182	3236.943	91.40732	3.091958	1.000005	10.00849006	91.31633	101.3248	0.098776	0.901224
0.02408	0.97592	335.74	2334.751	2000.0000	1496.138	22.45697	2.203823	1.000562	79.39647307	21.92853	101.325	0.783582	0.216418
0.049585	0.950415	313.04	1566.757	-533.5355	822.2511	7.342221	2.315175	0.993312	94.39352083	6.931486	101.325	0.931592	0.068408
0.076291	0.923709	304.51	1278.299	-744.1603	641.2998	4.59191	1.985022	0.991998	97.11739686	4.20765	101.325	0.958474	0.041526
0.097782	0.902218	299.54	1109.996	-867.0508	550.9453	3.443021	1.823689	0.991005	98.24659106	3.078416	101.325	0.969618	0.030382
0.131141	0.868859	293.73	913.4836	-1010.539	458.2639	2.425547	1.651316	0.989724	99.2391977	2.085803	101.325	0.979415	0.020585
0.172983	0.827017	288.39	732.8137	-1142.46	384.192	1.73293	1.503317	0.988625	99.90830338	1.416861	101.3252	0.986017	0.013983

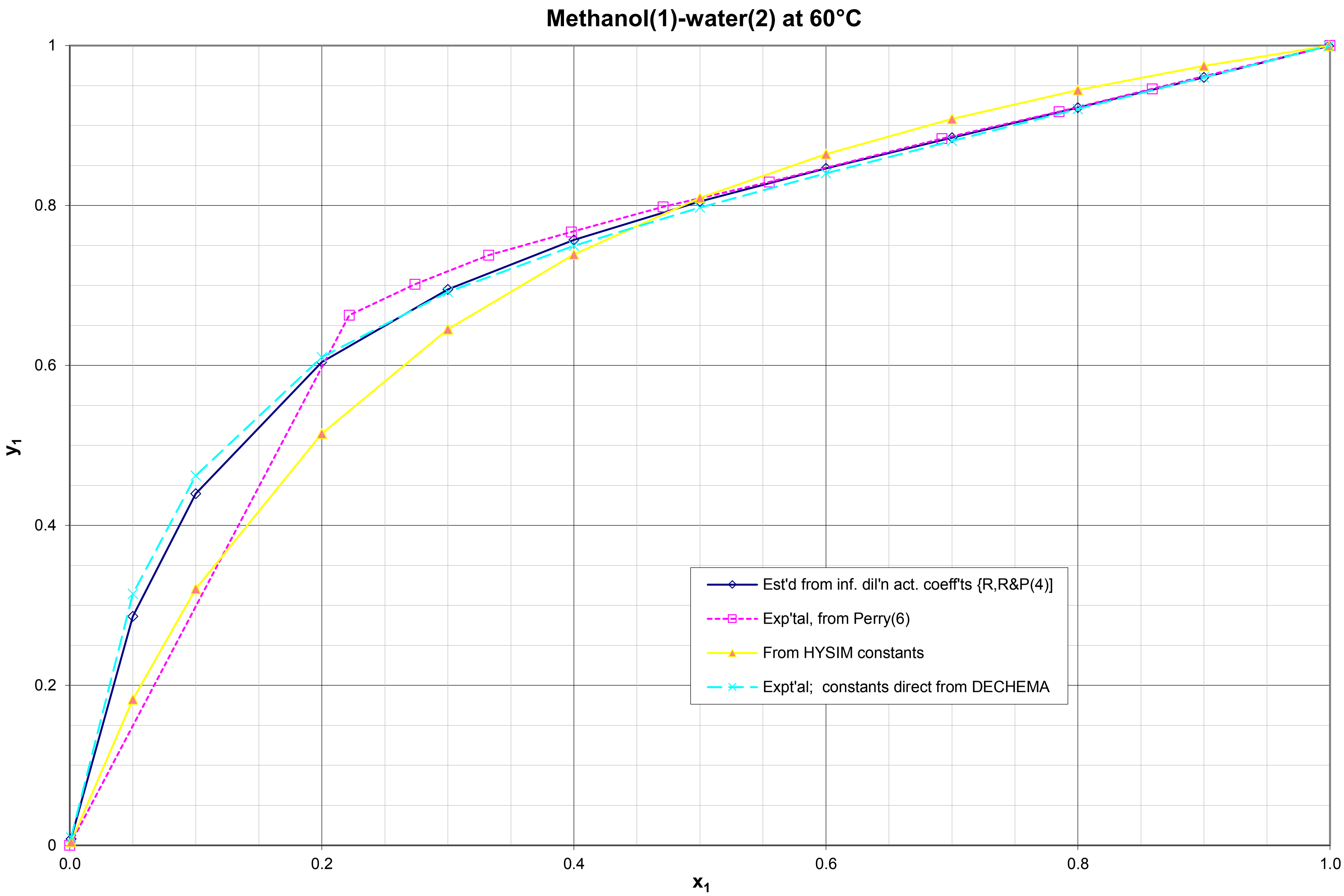
0.210371	0.789629	284.71	608.6011	-1233.156	338.942	1.363857	1.406109	0.988132	100.2608535	1.064159	101.325	0.989498	0.010502
0.24947	0.75053	281.59	502.8934	-1310.341	303.8154	1.106178	1.326047	0.988105	100.5047291	0.820344	101.3251	0.991904	0.008096
0.302879	0.697121	278.11	385.3565	-1396.164	268.1794	0.870923	1.240057	0.988853	100.7246077	0.600371	101.325	0.994075	0.005925
0.351845	0.648155	275.48	296.3584	-1461.148	243.4523	0.72339	1.177487	0.990282	100.8606203	0.464312	101.3249	0.995418	0.004582
0.37312	0.62688	274.46	261.8400	-1486.352	234.3607	0.672415	1.153954	0.991103	100.9071454	0.417773	101.3249	0.995877	0.004123
0.5	0.5	269.41	90.8153	-1611.23	193.188	0.463859	1.046583	0.997437	101.0936494	0.231335	101.325	0.997717	0.002283
0.6	0.4	266.17	-18.5966	-1691.12	170.0118	0.362735	0.991901	0.999799	101.1808733	0.145065	101.3259	0.998568	0.001432
0.7	0.3	263.19	-119.5476	-1764.831	150.6419	0.287356	0.960083	0.985089	101.2400513	0.084921	101.325	0.999162	0.000838
0.8	0.2	260.13	-222.9547	-1840.337	132.6669	0.224942	0.954307	0.913329	101.2839122	0.041089	101.325	0.999594	0.000406
0.9	0.1	256.84	-334.2593	-1921.608	115.2788	0.171557	0.9765	0.71529	101.3127295	0.012271	101.325	0.999879	0.000121
0.999	0.001	253.92	-433.0178	-1993.719	101.4268	0.134009	0.999996	0.392314	101.3249457	5.26E-05	101.325	0.999999	5.19E-07

Experimental data from Ullmann's [(5)] *, Vol. A11, p. 622 (Table 3)*

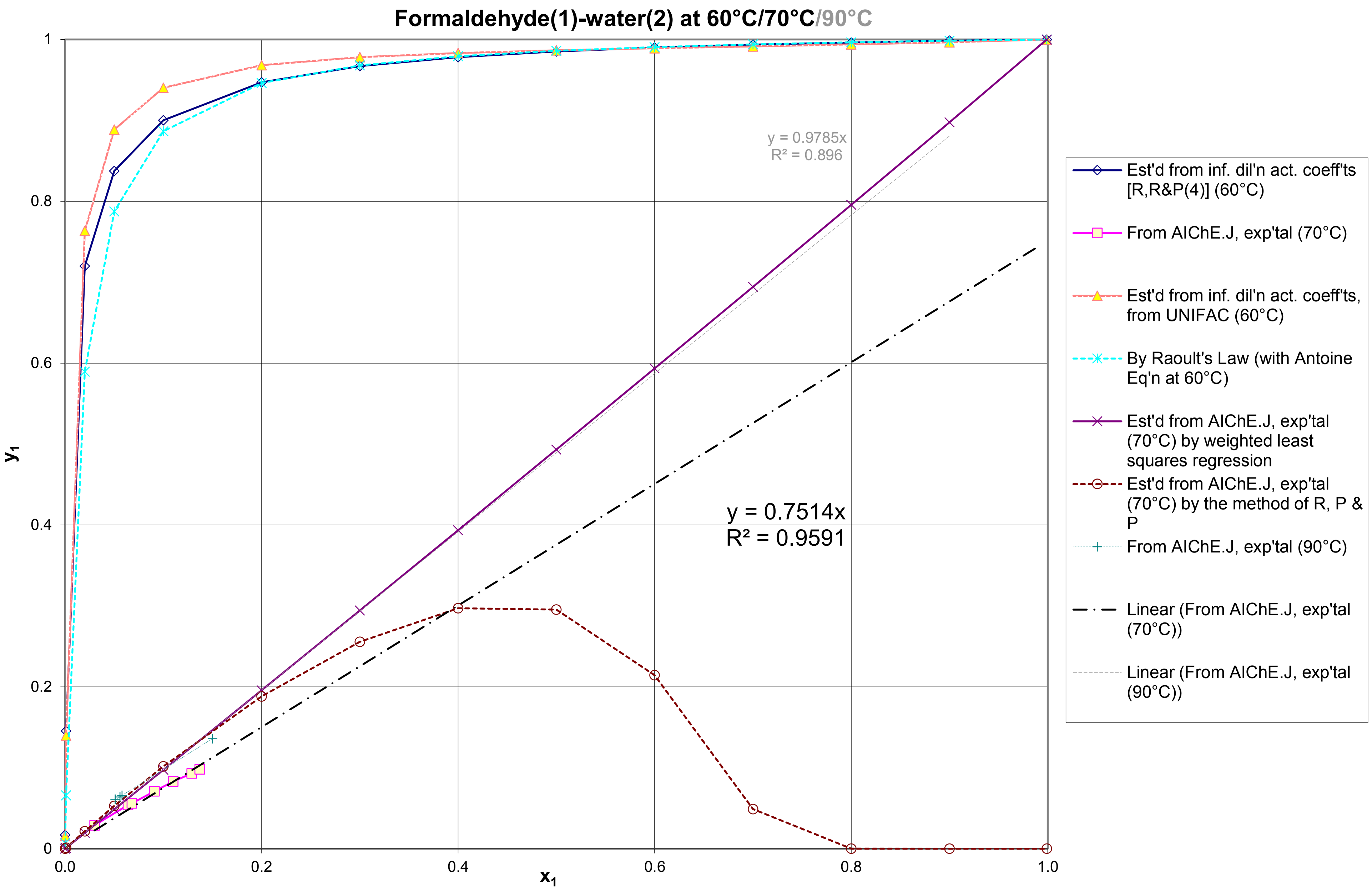
CH_3OH 0.032 kg.mol^{-1} HCHO 0.030 kg.mol^{-1} H_2O 0.018 kg.mol^{-1}

Note: Evaluated at the boiling points, at P [kPa(abs)] = 101.325

$x_{Mass\ 1}$	x_1	$y_{Mass\ 1}$	y_1	p_1 [kPa(a)]	∴ y_1	*cf.* y_1 above	ERROR^2
0.0395	0.02408	0.0368	0.0224	2.35	0.0232	0.7835823	0.5787882
0.08	0.049585	0.073	0.0451	4.75	0.0469	0.9315916	0.7842768
0.121	0.076291	0.106	0.0664	7	0.0691	0.9584737	0.7933898
0.153	0.097782	0.132	0.0836	8.65	0.0854	0.9696184	0.7834509
0.201	0.131141	0.1695	0.1091	11.2	0.1105	0.9794147	0.7562042
0.2585	0.172983	0.2145	0.1408	14.45	0.1426	0.9860167	0.7128827
0.3075	0.210371	0.249	0.1659	16.8	0.1658	0.9894976	0.6783744
0.3565	0.24947	0.274	0.1846	18.8	0.1855	0.9919038	0.6509539
0.420	0.302879	0.305	0.2084	21.4	0.2112	0.9940748	0.6150673
0.475	0.351845	0.331	0.2289	23.4	0.2309	0.9954176	0.5859848
0.498	0.37312	0.340	0.2361	24.1	0.2378	0.9958769	0.5759287
					(a check)		



Methanol(1)-water(2) at 60°C


Formaldehyde(1)-water(2) at 60°C/70°C/90°C
y₁
1
0.8
0.6
0.4
0.2
0
x₁
0.0
0.2
0.4
0.6
0.8
1.0
y = 0.9785x
R² = 0.896
y = 0.7514x
R² = 0.9591
Est'd from inf. dil'n act. coeff'ts [R,R&P(4)] (60°C)
From AIChE.J, exp'tal (70°C)
Est'd from inf. dil'n act. coeff'ts, from UNIFAC (60°C)
By Raoult's Law (with Antoine Eq'n at 60°C)
Est'd from AIChE.J, exp'tal (70°C) by weighted least squares regression
Est'd from AIChE.J, exp'tal (70°C) by the method of R, P & P
From AIChE.J, exp'tal (90°C)
Linear (From AIChE.J, exp'tal (70°C))
Linear (From AIChE.J, exp'tal (90°C))

Formaldehyde(1)		**Water(2)**
0.9183	r_i	0.9200
0.780	q_i	1.400
-149.00	u_ij	240.00
0.0001	x_i	0.9999
60	T [°C]	60
333.15	T [K]	333.15
9.98E-05	ϕ_i	0.9999
5.57E-05	θ_i	0.999944
1.055264	τ_ij	0.917004
10	z	10
0.7732	l_i	-2.32
2.310288	γ_i	1

Refer to:
R,P&P; T8-21, T8-3
AIChE.J; T6, T7

⇒ 1.93E-05 = B (van Laar)

⇒ 2319.50663 = A (van Laar)

Similarly:

t [°C]	T [K]	γ_1^∞	**A**	γ_2^∞	**B**
60	333.15	2.310288	2319.507	2.799482	2851.515
25	298.15	2.316579	2082.565	2.811124	2562.229
100	373.15	2.304493	2590.208	2.78857	3181.768
0	273.15	2.32201	1913.26	2.821003	2355.352
45	318.15	2.312822	2217.971	2.804196	2727.577
80	353.15	2.307233	2454.867	2.79375	3016.682
120	393.15	2.302023	2725.532	2.783866	3346.785

Hence:

A = T[K] × 6.76855 +64.54

B = T[K] × 8.26043 +2355.78

DECHEMA DATA 23/09/1998
Megat Ahmad
David Verrelli
CHE3117

TUTORIAL 4 Question 1

DECHEMA experimental data

x_meth	x_w	T [ºC]
0.0000	1.0000	100.00
0.0089	0.9911	98.43
0.0204	0.9796	96.65
0.0306	0.9694	95.12
0.0419	0.9581	93.32
0.0516	0.9484	92.13
0.0616	0.9384	91.05
0.0689	0.9311	90.21
0.0759	0.9241	89.54
0.0954	0.9046	87.86
0.1242	0.8758	85.72
0.1672	0.8328	83.10
0.1990	0.8010	81.57
0.2348	0.7652	80.01
0.3458	0.6542	76.62
0.3934	0.6066	75.43
0.4654	0.5346	73.89
0.6469	0.3531	70.46
0.7463	0.2537	68.69
0.7601	0.2399	68.50
0.8423	0.1577	67.04
0.8708	0.1292	66.61
0.9001	0.0999	66.11
0.9163	0.0837	65.87
0.9529	0.0471	65.24
0.9750	0.0250	64.88
1.0000	0.0000	64.51

PART (a)

	Methanol	Water
Methanol	---	-0.1800
Water	-0.1800	---

Case	Mole_Frac Liq Methanol [---]	Mole_Frac Vap Methanol [---]	Temp. Feed [ºC]
29	0.0000	0	99.7769
30	0.0089	0.0088543	99.5691
31	0.0204	0.0377609	99.2843
32	0.0306	0.0572935	99.0172
33	0.0419	0.0793334	98.7061
34	0.0516	0.0985251	98.4268
35	0.0616	0.118515	98.1279
36	0.0689	0.133208	97.9028
37	0.0759	0.147354	97.682
38	0.0954	0.186918	97.042
39	0.1242	0.245192	96.0386
40	0.1672	0.330091	94.4389
41	0.1990	0.390082	93.2002
42	0.2348	0.453905	91.7707
44	0.3458	0.345798	87.2917
45	0.3934	0.681376	85.4199
46	0.4654	0.756025	82.7067
47	0.6469	0.884807	76.6777
57	0.7463	0.929978	73.8892
49	0.7601	0.935239	73.5291
50	0.8423	0.842281	71.5108
51	0.8708	0.870711	70.8587
52	0.9001	0.900062	70.2122
53	0.9163	0.916278	69.8648
54	0.9529	0.952897	69.1048
55	0.9750	0.975021	68.6619
56	1.0000	1	68.1744

PART (b)

	Methanol	Water
Methanol	---	0.6207
Water	0.7611	---

Case	Mole_Frac Liq Methanol [---]	Mole_Frac Vap Methanol [---]	Temp. Feed [ºC]
2	0	0	99.9909
3	0.0089	0.0623018	98.4445
4	0.0204	0.132037	96.6251
5	0.0306	0.185592	95.1575
6	0.0419	0.237506	93.6702
7	0.0516	0.276896	92.5002
8	0.0616	0.313306	91.3789
9	0.0689	0.337556	90.611
10	0.0759	0.359181	89.9113
11	0.0954	0.412283	88.1297
12	0.1242	0.475731	85.874
13	0.1672	0.547657	83.1338
14	0.199	0.589006	81.4654
15	0.2348	0.627343	79.8584
16	0.3458	0.713103	76.0809
17	0.3934	0.740849	74.8243
18	0.4654	0.777213	73.1764
19	0.6469	0.854333	69.8027
20	0.7463	0.893798	68.2046
21	0.7601	0.899298	67.9907
22	0.8423	0.932493	66.748
23	0.8708	0.944261	66.3276
24	0.9001	0.956535	65.9003
25	0.9163	0.963407	65.666
26	0.9529	0.979173	65.1417
27	0.975	0.988866	64.8285
28	1	1	64.4755

PART (c)

	Methanol	Water
Methanol	---	0.4742
Water	0.8316	---

Case	Mole_Frac Liq Methanol [---]	Mole_Frac Vap Methanol [---]	Temp. Feed [ºC]
1	0	0	99.9909
2	0.0089	0.066269	98.3262
3	0.0204	0.139071	96.3987
4	0.0306	0.194016	94.8657
5	0.0419	0.246495	93.3407
6	0.0516	0.285818	92.1495
7	0.0616	0.321791	91.0227
8	0.0689	0.345556	90.2579
9	0.0759	0.36662	89.5657
10	0.0954	0.417862	87.8234
11	0.1242	0.478261	85.6575
12	0.1672	0.545874	83.0814
13	0.199	0.584522	81.5376
14	0.2348	0.620376	80.0628
15	0.3458	0.702127	76.5904
16	0.3934	0.729571	75.4113
17	0.4654	0.766751	73.8243
18	0.6469	0.850301	70.3692
19	0.7463	0.893959	68.6345
20	0.7601	0.899963	68.3987
21	0.8423	0.935368	67.0169
22	0.8708	0.947448	66.5465
23	0.9001	0.959722	66.0677
24	0.9163	0.966433	65.8052
25	0.9529	0.981362	65.2183
26	0.975	0.990196	64.8683
27	1	1	64.4755

ERRORS

	Part (a) Diff T		Part (b) Diff T		Part (c) Diff T	
	-0.22	0.22	-0.01	0.01	-0.01	0.01
	1.14	1.14	0.01	0.01	-0.10	0.1
	2.63	2.63	-0.02	0.02	-0.25	0.25
	3.90	3.9	0.04	0.04	-0.25	0.25
	5.39	5.39	0.35	0.35	0.02	0.02
	6.30	6.3	0.37	0.37	0.02	0.02
	7.08	7.08	0.33	0.33	-0.03	0.03
	7.69	7.69	0.40	0.4	0.05	0.05
	8.14	8.14	0.37	0.37	0.03	0.03
	9.18	9.18	0.27	0.27	-0.04	0.04
	10.32	10.3	0.15	0.15	-0.06	0.06
	11.34	11.3	0.03	0.03	-0.02	0.02
	11.63	11.6	-0.10	0.1	-0.03	0.03
	11.76	11.8	-0.15	0.15	0.05	0.05
	10.67	10.7	-0.54	0.54	-0.03	0.03
	11.86	11.9	-0.61	0.61	-0.02	0.02
	11.53	11.5	-0.71	0.71	-0.07	0.07
	12.25	12.2	-0.66	0.66	-0.09	0.09
	7.99	7.99	-0.49	0.49	-0.06	0.06
	5.39	5.39	-0.51	0.51	-0.10	0.1
	6.49	6.49	-0.29	0.29	-0.02	0.02
	4.90	4.9	-0.28	0.28	-0.06	0.06
	4.75	4.75	-0.21	0.21	-0.04	0.04
	4.34	4.34	-0.20	0.2	-0.06	0.06
	4.62	4.62	-0.10	0.1	-0.02	0.02
	4.22	4.22	-0.05	0.05	-0.01	0.01
	4.15	4.15	-0.03	0.03	-0.03	0.03
Mean Deviation	7.03		0.27		0.06	
Maximum Deviation	12.25		0.71		0.25	

Antoine constants from "VLE of Formaldehyde Mixtures: New Data and Model Revision" in AIChEJ, 42(6), p. 1745.

Substance	**Constant** A_2	B_2	C_2	**Constant (Sinnott[(2)])** A_2	B_2	C_2	**Constant (Reid, Prausnitz & Poling[(4)])** A	B	C	D	eq'n	T_c [K]	p_c [bar]
Formaldehyde	14.4625	-2204.13	-30.15	16.4775	-2204.13	-30.15	-7.29343	1.08395	-1.63882	-2.30677	1	408	65.9
Water	16.2886	-3816.44	-46.13	18.3036	-3816.44	-46.13	-7.76451	1.45838	-2.7758	-1.23303	1	647.3	221.2
Methanol	16.5725	-3626.55	-34.29	18.5875	-3626.55	-34.29	-8.54796	0.76982	-3.1085	1.54481	1	512.6	80.9
				(sign altered)	**TO GIVE [mmHg]**								

(1) $\ln(p_{vap}/p_c) = \{A(1 - T/T_c) + B(1 - T/T_c)^{1.5} + C(1 - T/T_c)^3 + D(1 - T/T_c)^6\}.(T_c/T)$

(2) $\ln(p_{vap}) = A - B/T + C.\ln(T) + D(p_{vap}/T^2)$

Equation: $\ln(\, p^o[\text{kPa}]\,) = A_2 + B_2 / (T[\text{K}] + C_2)$

NOTE: All pressures are absolute

Check pure-component boiling points at atmospheric pressure

==> p° = 101.325 kPa

		t[°C] = - 273.15	+ T[K]
254.0521 K	=	-19.0979 °C	-19.0982
373.1525 K	=	100.0025 °C	100.0021
337.6612 K	=	64.51121 °C	64.51083

Now for Raoult's Law:

Composition:	
Formaldehyde	0.54
Water	0.45
Methanol	0.01
SUM	1

		p° [kPa]	p [kPa]
t[°C] =	-20	97.36911	52.57932
T[K] =	253.15	0.116889	0.0526
		1.002321	0.010023
			52.64194

		p° [kPa]	p [kPa]
t[°C] =	0	219.6436	118.6075
T[K] =	273.15	0.593078	0.266885
		4.013874	0.040139
			118.9146

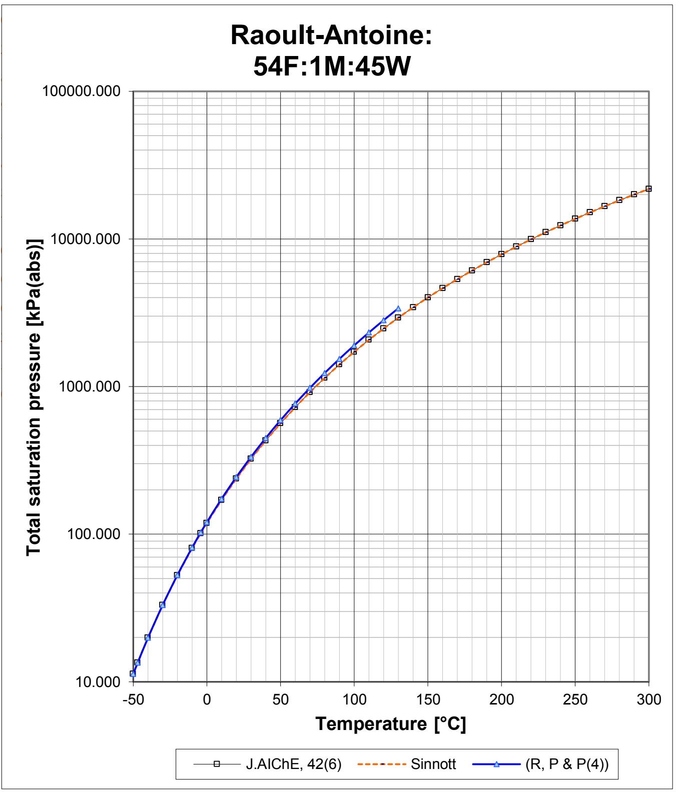
		p° [kPa]	p [kPa]
t[°C] =	20	437.8067	236.4156
T[K] =	293.15	2.313304	1.040987
		12.97214	0.129721
			237.5863

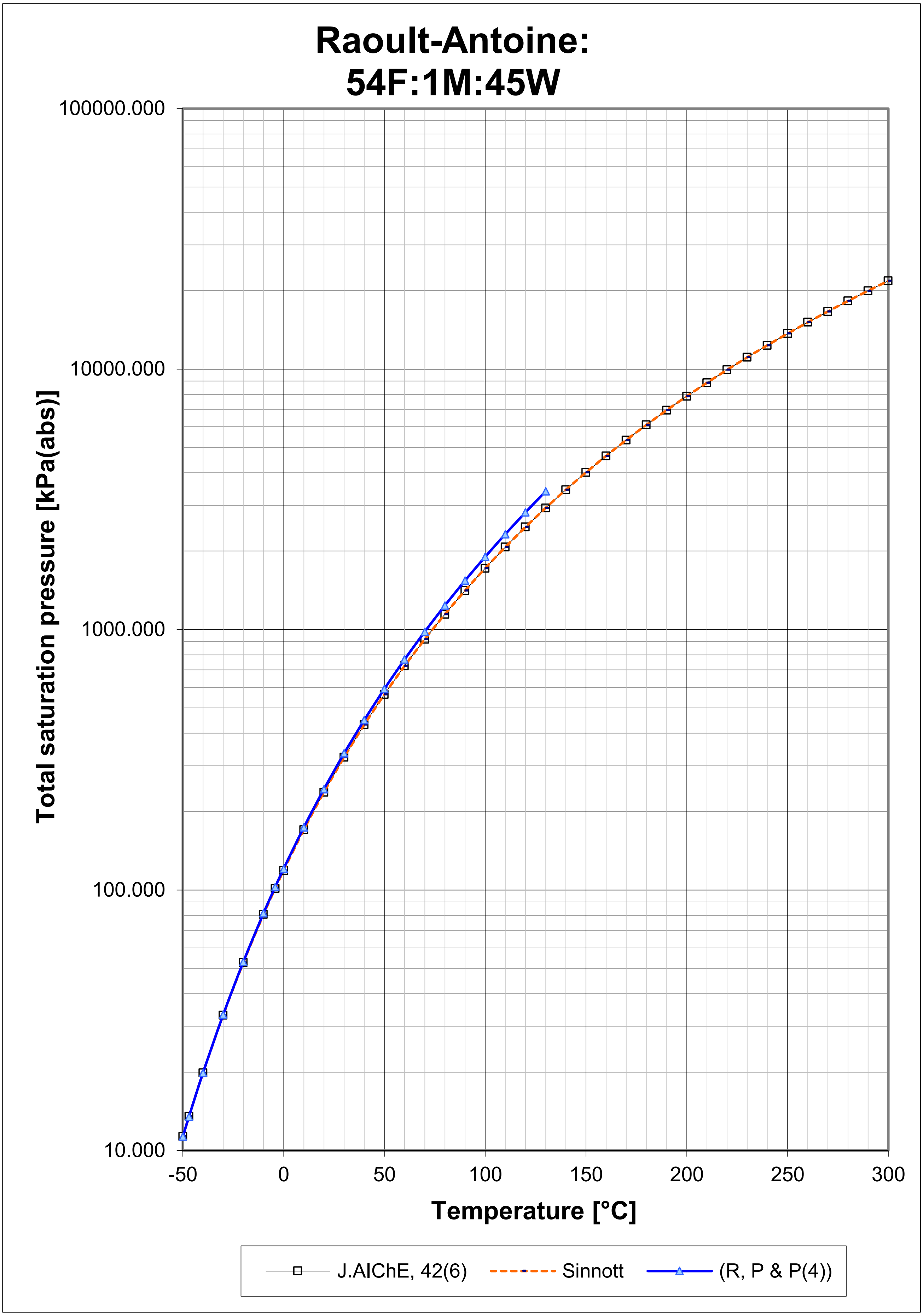
t[°C] =		T[K] =		p_{TOTAL} =	(Sinnott[(2)])	(R, P & P[(4)])	
t[°C] =	-50	T[K] =	223.15	p_{TOTAL} = 11.316 kPa(abs)	11.316	11.303	-0.1%
t[°C] =	**-46.9606**	T[K] =	226.1894	p_{TOTAL} = 13.509 kPa(abs)	**13.509**	13.498	= ERROR
t[°C] =	-40	T[K] =	233.15	p_{TOTAL} = 19.866 kPa(abs)	19.866	19.874	
t[°C] =	-30	T[K] =	243.15	p_{TOTAL} = 33.084 kPa(abs)	33.084	33.185	
t[°C] =	-20	T[K] =	253.15	p_{TOTAL} = 52.642 kPa(abs)	52.643	52.985	
t[°C] =	-10	T[K] =	263.15	p_{TOTAL} = 80.505 kPa(abs)	80.506	81.367	1.1%
t[°C] =	**-4.2046**	T[K] =	268.9454	p_{TOTAL} = **101.325** kPa(abs)	101.326	102.688	= ERROR
t[°C] =	0	T[K] =	273.15	p_{TOTAL} = 118.915 kPa(abs)	118.916	120.767	
t[°C] =	10	T[K] =	283.15	p_{TOTAL} = 170.368 kPa(abs)	170.371	173.960	
t[°C] =	20	T[K] =	293.15	p_{TOTAL} = 237.586 kPa(abs)	237.590	244.059	
t[°C] =	30	T[K] =	303.15	p_{TOTAL} = 323.482 kPa(abs)	323.487	334.511	3.3%
t[°C] =	40	T[K] =	313.15	p_{TOTAL} = 431.129 kPa(abs)	431.135	449.097	= ERROR
t[°C] =	50	T[K] =	323.15	p_{TOTAL} = 563.728 kPa(abs)	563.736	591.940	
t[°C] =	60	T[K] =	333.15	p_{TOTAL} = 724.578 kPa(abs)	724.589	767.523	
t[°C] =	70	T[K] =	343.15	p_{TOTAL} = 917.055 kPa(abs)	917.069	980.723	
t[°C] =	80	T[K] =	353.15	p_{TOTAL} = 1144.583 kPa(abs)	1144.599	1236.857	7.5%
t[°C] =	90	T[K] =	363.15	p_{TOTAL} = 1410.618 kPa(abs)	1410.639	1541.762	= ERROR
t[°C] =	100	T[K] =	373.15	p_{TOTAL} = 1718.635 kPa(abs)	1718.660	1901.913	
t[°C] =	110	T[K] =	383.15	p_{TOTAL} = 2072.110 kPa(abs)	2072.141	2324.628	
t[°C] =	120	T[K] =	393.15	p_{TOTAL} = 2474.514 kPa(abs)	2474.551	2818.469	
t[°C] =	130	T[K] =	403.15	p_{TOTAL} = 2929.300 kPa(abs)	2929.344	3394.358	13.7%
t[°C] =	140	T[K] =	413.15	p_{TOTAL} = 3439.900 kPa(abs)	3439.950	#NUM!	= ERROR
t[°C] =	150	T[K] =	423.15	p_{TOTAL} = 4009.711 kPa(abs)	4009.770	#NUM!	
t[°C] =	160	T[K] =	433.15	p_{TOTAL} = 4642.099 kPa(abs)	4642.167	(pure HCHO is super-critical here)	
t[°C] =	170	T[K] =	443.15	p_{TOTAL} = 5340.384 kPa(abs)	5340.4		
t[°C] =	180	T[K] =	453.15	p_{TOTAL} = 6107.839 kPa(abs)	6107.9		
t[°C] =	190	T[K] =	463.15	p_{TOTAL} = 6947.685 kPa(abs)	6947.7		
t[°C] =	200	T[K] =	473.15	p_{TOTAL} = 7863.082 kPa(abs)	7863.1		
t[°C] =	210	T[K] =	483.15	p_{TOTAL} = 8857.126 kPa(abs)	8857.2		
t[°C] =	220	T[K] =	493.15	p_{TOTAL} = 9932.840 kPa(abs)	9932.9		
t[°C] =	230	T[K] =	503.15	p_{TOTAL} = 11093.173 kPa(abs)	11093.3		
t[°C] =	240	T[K] =	513.15	p_{TOTAL} = 12340.990 kPa(abs)	12341.1		
t[°C] =	250	T[K] =	523.15	p_{TOTAL} = 13679.065 kPa(abs)	13679.2		
t[°C] =	260	T[K] =	533.15	p_{TOTAL} = 15110.081 kPa(abs)	15110.3		
t[°C] =	270	T[K] =	543.15	p_{TOTAL} = 16636.619 kPa(abs)	16636.8		
t[°C] =	280	T[K] =	553.15	p_{TOTAL} = 18261.156 kPa(abs)	18261.4		
t[°C] =	290	T[K] =	563.15	p_{TOTAL} = 19986.060 kPa(abs)	19986.3		
t[°C] =	300	T[K] =	573.15	p_{TOTAL} = 21813.584 kPa(abs)	21813.9		

t[°C] =	0.01	T[K] =	273.16	Error:
J.AIChE		p° [kPa]	0.5935	-2.9%
Sinnott			0.5935	-2.9%
R, P & P			0.6120	0.12%
ACTUAL			0.6112	

t[°C] =	100	T[K] =	373.15	Error:
J.AIChE		p° [kPa]	101.316	-0.0090%
Sinnott			101.317	-0.0075%
R, P & P			101.378	0.053%
ACTUAL			101.325	

t[°C] =	373.7	T[K] =	646.85	Error:
J.AIChE		p° [kPa]	20650	-6.1%
Sinnott			20651	-6.1%
R, P & P			22001	0.0065%
ACTUAL			22000	




Raoult-Antoine:
54F:1M:45W
100000.000
10000.000
1000.000
100.000
10.000
Total saturation pressure [kPa(abs)]
-50
0
50
100
150
200
250
300
Temperature [°C]
J.AIChE, 42(6)
Sinnott
(R, P & P(4))

MONASH UNIVERSITY

DEPARTMENT OF CHEMICAL ENGINEERING

APPENDIX TO CHAPTER 7

PART 2: DETAILED PROCESS DESIGN

Property calculation: VLE

Experimental data from M. Albert, L. Hahnenstein, H. Hasse & G. Maurer, AIChE.J, p. 1743 (Table 1)
&, also, hence recalculated van Laar data

Note: Evaluated at t[°C] = 70 , **as T[K] = 343.15** (approx.)

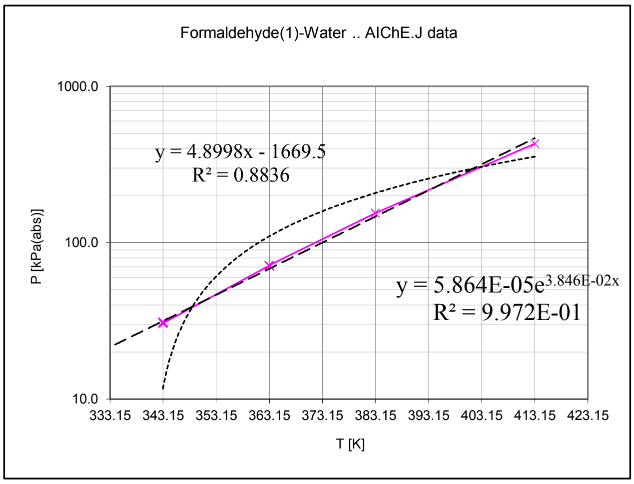
x_1	p [kPa(a)]	y_1
0.030	31	0.029
0.064	30.9	0.054
0.068	31.2	0.056
0.091	30.9	0.071
0.110	30.9	0.083
0.129	30.7	0.093
0.137	30.5	0.098

Substance	Constant (Reid, Prausnitz & Poling[(4)]) A	B	C	D	eq'n	T_c [K]	p_c [bar]
Formaldehyde	-7.29343	1.08395	-1.63882	-2.30677	1	408	65.9
Water	-7.76451	1.45838	-2.7758	-1.23303	1	647.3	221.2
Methanol	-8.54796	0.76982	-3.1085	1.54481	1	512.6	80.9

(1) $\ln(p_{vap}/p_c) = \{A(1 - T/T_c) + B(1 - T/T_c)^{1.5} + C(1 - T/T_c)^3 + D(1 - T/T_c)^6\}.(T_c/T)$

Their data:
Note: In all cases HCHO concentration increases down a column.

	T [K]	t [°C]	P [kPa(abs)]
	343.1	69.95	31.0
	343.1	69.95	30.9
	343.1	69.95	31.2
	343.1	69.95	30.9
	343.2	70.05	30.9
	343.3	70.15	30.7
	343.1	69.95	30.5
MEAN:	343.1428571	69.99286	30.87143
σ:	0.078679579	0.07868	0.221467
	363.1	89.95	71.4
	363.1	89.95	71.4
	363.2	90.05	70.6
	363.1	89.95	71.6
MEAN:	363.125	89.975	71.25
σ:	0.05	0.05	0.443471
	383.1	109.95	153.1
	383.3	110.15	155.0
	383.1	109.95	155.1
	383.0	109.85	155.1
MEAN:	383.125	109.975	154.575
σ:	0.125830574	0.125831	0.984463
	413.2	140.05	405.3
	413.2	140.05	414.4
	413.1	139.95	423.1
	413.2	140.05	423.7
	413.2	140.05	432.9
	413.1	139.95	443.1
	413.1	139.95	442.7
	413.1	139.95	449.1
MEAN:	413.15	140	429.2875
σ:	0.053452249	0.053452	**15.3195**



Hence with:

Henry's law: y = **0.7514** x **or y = x ???**

& Total pressure: P_{BINARY} = 5.86E-05 exp (3.85E-02 T[K])

Note(1): all pressures in kPa(abs).
Note(2): "with inerts" signifies inert gases present to a TOTAL, COMBINED pressure of "P"
Note(3): obviously the "BINARY" refers to the situation with no inerts, although hydrolysis & polymerisation still occur.

	Data for:	x_1	T [K]	P_{BIN} [kPa]	$y_{1\ BINARY}$	p_1	*e.g.* $y_{1\ WITH\ INERTS}$		*Ullmann's*[(5)]			Ratio of
							P = ?		$x_{Mass\ 1}$[#]	p_1	$y_{1\ w\ INERTS}$	$y_{1\ w\ INERTS}$
	(bottom)								[#] Assuming a binary solution.			
TOP	**Abs. Stage 1**	0.402006	335.15	23.23769	0.302067	7.019346	128	0.054839	0.528406	3.487933	0.027249	50%
BOTTOM		*0.42*	*348.15*	*38.3117064*	*0.312309799*	*11.96512131*	*130*	*0.092039395*	*0.542435098*	*7.762824198*	*0.059714032*	65%
TOP	**Abs. Stage 2**	0.195415	323.15	14.64729	0.146835	2.150735	126	0.017069	0.288159	0.943184	0.007486	44%
BOTTOM		*0.196488451*	*336.15*	*24.14881957*	*0.147641422*	*3.565366059*	*128*	*0.027854422*	*0.289558558*	*2.101505518*	*0.016418012*	59%
TOP	**Abs. Stage 3**	0.129216	315.15	10.76796	0.097093	1.045492	124	0.008431	0.198284	0.407343	0.003285	39%
BOTTOM		*0.13020155*	*324.15*	*15.22160042*	*0.097833445*	*1.489181608*	*126*	*0.011818902*	*0.199676262*	*0.726852471*	*0.00576867*	49%
TOP	**Abs. Stage 4**	0	313.15	9.970747	0	0	110	0	0	0	0	#DIV/0!
BOTTOM	**(top)**	*0.096071711*	*316.15*	*11.1901676*	*0.072188284*	*0.807798993*	124	*0.006514508*	*0.150485765*	*0.344611498*	*0.002779125*	43%
NEAR TOP		0.000001	313.15	9.970746937	7.514E-07	7.49202E-06	110	6.81093E-08	1.66672E-06	1.08208E-05	9.83706E-08	144%

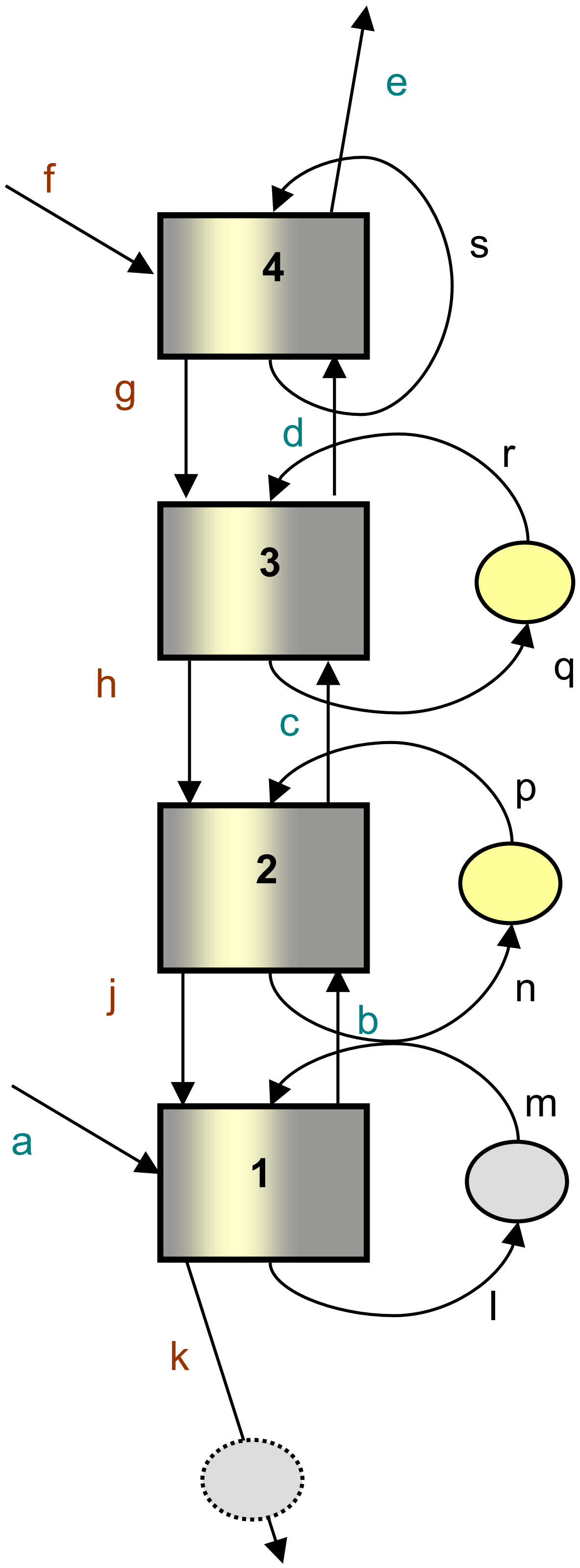
Note(4): Order-of-magnitude concordancy(?) with *Ullmann's*[(5)] - which has **lower** p_{vap}'s.(!)

(Assuming binary liquid)

$p_F[kPa]=0.1333F.\exp\{-F^{\alpha}.(a_0+a_1/T+a_2/T^2)\}$

α = 0.08760 ± 0.00950
a_0 = -12.0127 ± 0.0550
a_1 = 3451.72 ± 17.14
a_2 = 248257.3 ± 5296.8

TOP	**Abs. Stage 4**			5.86E-05	0	0		#DIV/0!	0	#DIV/0!	#DIV/0!	#DIV/0!
BOTTOM	**(top)**											#DIV/0!


e
f
s
4
g
d
r
3
h
q
c
p
2
j
n
b
m
a
1
l
k

(Mass &) Energy Balance over Absorber

NOTE: Heats of solution of methanol [implicitly] considered.
Formic acid is treated as water for VLE.

Total pump-around flow: **84.639** kg.s^{-1} (excluding product)
Total HEAT-EXCHANGED pump-around flow: **84.639** kg.s^{-1} (excluding product)

STAGE 1 (BASE OF COLUMN)

Pump-around flow: **29.737** kg.s^{-1}
Mass fraction of HCHO in liquid from stage above: **0.288897** GOAL SEEK!

STREAMS IN:

No.	Description	HYSIM	Flow [kg.s^{-1}]	t [°C]	T [K]	Species	State	Mass frac. [-]	Mass Flow [kg.s^{-1}]	MR [kg.mol^{-1}]	Mole flow [mol.s^{-1}]	Mole frac. [-]	A / C1	B / C2	C / C3	D / C4	C5	$\bar{\chi}\pi$ [kJ.kg^{-1}.K^{-1}]	ΔH≡ϕ, 298K [kJ.kg^{-1}]	ΔH≡ϕ, T [kJ.kg^{-1}]	ΔH°$_{f, T}$ [kW]	
j	L from stage 2	-	**1.742831**	**63.00**	336.15	HCHO	Aq	**0.2888974**	0.5034995	0.030026	16.76867	0.196488	416.31	-2.6391	0.004984	-		2.70531878	-5555.656	-5452.853	-2745.5091	HCHO
		DEFINE!!!	1.74283148	WATCH T-CROSS	336.15	CH_3OH	Aq	**0.005**	0.0087142	0.032042	0.27196	0.003187	105800	-362.23	0.9379	0	0	2.66429888	-7675.239	-7573.995	-66.000988	CH_3OH
	Combined liquid-IN temperature:		1.74283148		336.15	H_2O	L	**0.7059526**	1.2303564	0.018015	68.29546	0.800258	276370	-2090.1	8.125	-0.01412	9.37E-06	4.1785776	-15866.05	-15707.26	-19325.528	H_2O
	60.20 °C		1.74283148		336.15	HCOOH	Aq	**0.00015**	0.0002614	0.046026	0.00568	6.66E-05						2.192416	-9243.455	-9160.143	-2.3946878	HCOOH
a	Reactor effluent	AbsFeed	**7.920**	90.00	363.15	HCHO	V	0.1804678	1.429305	0.030026	47.60193	0.142986	23.48	0.03157	2.99E-05	-2.3E-08		1.2107	-3862.294	-3783.597	-5407.9144	HCHO
		CHANGED!!!	7.92		363.15	CH_3OH	V	0.003342	0.0264686	0.032042	0.82606	0.002481	21.15	0.07092	2.59E-05	-2.9E-08		1.4480	-6282.379	-6188.261	-163.79466	CH_3OH
	(Should be 7.9159kg.s^{-1})		7.92		363.15	O_2	V	0.000459	0.0036353	0.031999	0.113608	0.000341	28.11	-3.7E-06	1.75E-05	-1.1E-08		0.9261	0	60.1986	0.2188404	O_2
			7.92		363.15	H_2O	V	0.1534721	1.2154989	0.018015	67.47074	0.202668	32.24	0.001924	1.06E-05	-3.6E-09		1.8819	-13433.1	-13310.78	-16179.239	H_2O
			7.92		363.15	H_2	V	0.0098049	0.0776551	0.002016	38.52321	0.115716	27.14	0.009274	-1.4E-05	7.65E-09		14.3718531	0	934.17045	72.5430833	H_2
			7.92		363.15	CO_2	V	0.059157	0.4685232	0.04401	10.64588	0.031978	19.8	0.07344	-5.6E-05	1.72E-08		0.87627156	-8948.007	-8891.049	-4165.6632	CO_2
			7.92		363.15	CO	V	0.0033468	0.0265063	0.02801	0.946301	0.002842	30.87	-0.01285	2.79E-05	-1.3E-08		1.04303748	-3948.533	-3880.736	-102.86381	CO
			7.92		363.15	HCOOH	V	5.976E-05	0.0004733	0.046026	0.010283	3.09E-05	11.71	0.1358	-8.4E-05	2.02E-08		1.04557342	-8231.506	-8163.544	-3.8636254	HCOOH
			7.92		363.15	N_2	V	0.5898907	4.6719343	0.028013	166.775	0.500957	31.15	-0.01357	2.68E-05	-1.2E-08		1.04150997	0	67.698148	316.281298	N_2
m	Pump-around 1	-	29.737	**60.00**	333.15	HCHO	Aq	0.54	16.057959	0.030026	534.7982	0.415637	416.31	-2.6391	0.004984	-		2.6765732	-5555.656	-5461.975	-87708.178	HCHO
			29.736961	NO POLY-MERS!	333.15	CH_3OH	Aq	0.01	0.2973696	0.032042	9.280619	0.007213	105800	-362.23	0.9379	0	0	2.65293796	-7675.239	-7582.386	-2254.7711	CH_3OH
			29.736961		333.15	H_2O	L	0.44982	13.37628	0.018015	742.4997	0.57706	276370	-2090.1	8.125	-0.01412	9.37E-06	4.17834781	-15866.05	-15719.8	-210272.5	H_2O
			29.736961		333.15	HCOOH	Aq	0.00018	0.0053527	0.046026	0.116297	9.04E-05						2.192416	-9243.455	-9166.72	-49.066272	HCOOH

Mass fraction of HCHO in total liquid fed: 52.61% Mole fraction HCHO in total liquid fed: 0.402005981 (average over 298K to T) **SUM = -348058.24**

Check mass balances: 0 Hence equilibrium partial pressure in the vapour: 7.019345926 ~~(From Ulmann's$^{(5)}$)~~ (From AIChE.J & van Laar) *Note: Aqueous c$_p$'s taken as those for the pure liquid.

-7.10543E-15 Hence equilibrium mole fraction in the vapour: 0.05483864 (given a total pressure of: 128 ??? kPa(abs)) ⇒Hence "approach to equilibrium" is: 99.50%

STREAMS OUT:

No.	Description	HYSIM	Flow [kg.s^{-1}]	t [°C]	T [K]	Species	State	Mass frac. [-]	Mass Flow [kg.s^{-1}]	MR [kg.mol^{-1}]	Mole flow [mol.s^{-1}]	Mole frac. [-]	A / C1	B / C2	C / C3	D / C4	C5	$\bar{\chi}\pi$ [kJ.kg^{-1}.K^{-1}]	ΔH≡ϕ, 298K [kJ.kg^{-1}]	ΔH≡ϕ, T [kJ.kg^{-1}]	ΔH°$_{f, T}$ [kW]		
k	Product	-	**2.645503**	75.00	348.15	HCHO	Aq	**0.54**	1.4285716	0.030026	47.5775	0.415637	416.31	-2.6391	0.004984	-		2.83026044	-5555.656	-5414.143	-7734.4904	HCHO	-7734
	(pre-cooling)		2.645503		348.15	CH_3OH	Aq	0.01	0.026455	0.032042	0.825636	0.007213	105800	-362.23	0.9379	0	0	2.71149878	-7675.239	-7539.664	-199.46203	CH_3OH	#REF!
			2.645503		348.15	H_2O	L	0.44982	1.1900002	0.018015	66.05534	0.57706	276370	-2090.1	8.125	-0.01412	9.37E-06	4.18043703	-15866.05	-15657.02	-18631.862	H_2O	
			2.645503		348.15	HCOOH	Aq	0.00018	0.0004762	0.046026	0.010346	9.04E-05						2.192416	-9243.455	-9133.834	-4.3494453	HCOOH	#REF!
b	V from stage 1	-	7.017	**62.00**	335.15	HCHO	V	0.0718554	0.5042329	0.030026	16.7931	0.055279	23.48	0.03157	2.99E-05	-2.3E-08		1.1903	-3862.294	-3818.252	-1925.2885	HCHO	#REF!
			7.01732848		335.15	CH_3OH	V	0.0012437	0.0087277	0.032042	0.272384	0.000897	21.15	0.07092	2.59E-05	-2.9E-08		1.4136	-6282.379	-6230.076	-54.374472	CH_3OH	#REF!
			7.01732848		335.15	O_2	V	0.000518	0.0036353	0.031999	0.113608	0.000374	28.11	-3.7E-06	1.75E-05	-1.1E-08		0.9226	0	34.1363	0.1240961	O_2	#REF!
			7.01732848		335.15	H_2O	V	0.1789649	1.2558551	0.018015	69.71086	0.229474	32.24	0.001924	1.06E-05	-3.6E-09		1.8758	-13433.1	-13363.69	-16782.865	H_2O	#REF!
			7.01732848		335.15	H_2	V	0.0110662	0.0776551	0.002016	38.52321	0.12681	27.14	0.009274	-1.4E-05	7.65E-09		14.3535572	0	531.08162	41.2411865	H_2	41
			7.01732848		335.15	CO_2	V	0.0667666	0.4685232	0.04401	10.64588	0.035044	19.8	0.07344	-5.6E-05	1.72E-08		0.86293916	-8948.007	-8916.078	-4177.3898	CO_2	#REF!
			7.01732848		335.15	CO	V	0.0037773	0.0265063	0.02801	0.946301	0.003115	30.87	-0.01285	2.79E-05	-1.3E-08		1.04230745	-3948.533	-3909.968	-103.63865	CO	87605
			7.01732848		335.15	HCOOH	V	3.684E-05	0.0002585	0.046026	0.005617	1.85E-05	11.71	0.1358	-8.4E-05	2.02E-08		1.01922786	-8231.506	-8193.795	-2.1181955	HCOOH	46.9
			7.01732848		335.15	N_2	V	0.6657711	4.6719343	0.028013	166.775	0.548988	31.15	-0.01357	2.68E-05	-1.2E-08		1.04132941	0	38.529188	180.005835	N_2	348238
l	Pump-around 1	-	29.737	75.00	348.15	HCHO	Aq	0.54	16.057959	0.030026	534.7982	0.415637	416.31	-2.6391	0.004984	-		2.83026044	-5555.656	-5414.143	-86940.078	HCHO	
			29.736961		348.15	CH_3OH	Aq	0.01	0.2973696	0.032042	9.280619	0.007213	105800	-362.23	0.9379	0	0	2.71149878	-7675.239	-7539.664	-2242.0669	CH_3OH	
			29.736961		348.15	H_2O	L	0.44982	13.37628	0.018015	742.4997	0.57706	276370	-2090.1	8.125	-0.01412	9.37E-06	4.18043703	-15866.05	-15657.02	-209432.74	H_2O	
			29.736961		348.15	HCOOH	Aq	0.00018	0.0053527	0.046026	0.116297	9.04E-05						2.192416	-9243.455	-9133.834	-48.890243	HCOOH	

(average over 298K to T) **SUM = -348058.24**

OUT - IN = 4.5286E-08

STAGE 2 (LOWER-MIDDLE SECTION OF COLUMN)

Pump-around flow: **41.158** kg.s^{-1}

Mass fraction of HCHO in liquid from stage above: **0.199489** GOAL SEEK!

STREAMS IN:

No.	Description	HYSIM	Flow	t	T	Species	State	Mass frac.	Mass Flow	MR	Mole flow	Mole frac.	A / C1	B / C2	C / C3	D / C4	C5	$\overline{\chi\pi}$	ΔH≡ϕ, 298K	ΔH≡ϕ, T	ΔH°$_{f,T}$	
			[kg.s^{-1}]	[°C]	[K]			[-]	[kg.s^{-1}]	[kg.mol^{-1}]	[mol.s^{-1}]	[-]						[kJ.kg^{-1}.K^{-1}]	[kJ.kg^{-1}]	[kJ.kg^{-1}]	[kW]	
h	L from stage 3	-	**0.65**	**51.00**	324.15	HCHO	Aq	**0.1994886**	0.1296676	0.030026	4.318481	0.130202	416.31	-2.6391	0.004984	-		2.59631201	-5555.656	-5488.151	-711.6353	HCHO
		DEFINE!!!	0.65	WATCH T-CROSS	324.15	CH_3OH	Aq	**0.002**	0.0013	0.032042	0.040572	0.001223	105800	-362.23	0.9379	0	0	2.61990898	-7675.239	-7607.121	-9.8892575	CH_3OH
	Combined liquid-IN temperature:		0.65		324.15	H_2O	L	**0.7984114**	0.5189674	0.018015	28.8072	0.868533	276370	-2090.1	8.125	-0.01412	9.37E-06	4.17828821	-15866.05	-15757.41	-8177.583	H_2O
	48.05 °C		0.65		324.15	HCOOH	Aq	**0.0001**	0.000065	0.046026	0.001412	4.26E-05						2.192416	-9243.455	-9186.452	-0.5971194	HCOOH
b	V from stage 1	-	7.017	62.000	335.15	HCHO	V	0.0718554	0.5042329	0.030026	16.7931	0.055279	23.48	0.03157	2.99E-05	-2.3E-08		1.1903	-3862.294	-3818.252	-1925.2885	HCHO
			7.01732848		335.15	CH_3OH	V	0.0012437	0.0087277	0.032042	0.272384	0.000897	21.15	0.07092	2.59E-05	-2.9E-08		1.4136	-6282.379	-6230.076	-54.374472	CH_3OH
			7.01732848		335.15	O_2	V	0.000518	0.0036353	0.031999	0.113608	0.000374	28.11	-3.7E-06	1.75E-05	-1.1E-08		0.9226	0	34.1363	0.1240961	O_2
			7.01732848		335.15	H_2O	V	0.1789649	1.2558551	0.018015	69.71086	0.229474	32.24	0.001924	1.06E-05	-3.6E-09		1.8758	-13433.1	-13363.69	-16782.865	H_2O
			7.01732848		335.15	H_2	V	0.0110662	0.0776551	0.002016	38.52321	0.12681	27.14	0.009274	-1.4E-05	7.65E-09		14.3535572	0	531.08162	41.2411865	H_2
			7.01732848		335.15	CO_2	V	0.0667666	0.4685232	0.04401	10.64588	0.035044	19.8	0.07344	-5.6E-05	1.72E-08		0.86293916	-8948.007	-8916.078	-4177.3898	CO_2
			7.01732848		335.15	CO	V	0.0037773	0.0265063	0.02801	0.946301	0.003115	30.87	-0.01285	2.79E-05	-1.3E-08		1.04230745	-3948.533	-3909.968	-103.63865	CO
			7.01732848		335.15	HCOOH	V	3.684E-05	0.0002585	0.046026	0.005617	1.85E-05	11.71	0.1358	-8.4E-05	2.02E-08		1.01922786	-8231.506	-8193.795	-2.1181955	HCOOH
			7.01732848		335.15	N_2	V	0.6657711	4.6719343	0.028013	166.775	0.548988	31.15	-0.01357	2.68E-05	-1.2E-08		1.04132941	0	38.529188	180.005835	N_2
p	Pump-around 2	-	41.158	**48.00**	321.15	HCHO	Aq	0.2888974	11.890551	0.030026	396.0059	0.196488	416.31	-2.6391	0.004984	-		2.57155014	-5555.656	-5496.51	-65356.531	HCHO
			41.1583837		321.15	CH_3OH	Aq	0.005	0.2057919	0.032042	6.422568	0.003187	105800	-362.23	0.9379	0	0	2.60925057	-7675.239	-7615.226	-1567.152	CH_3OH
			41.1583837		321.15	H_2O	L	0.7059526	29.055867	0.018015	1612.853	0.800258	276370	-2090.1	8.125	-0.01412	9.37E-06	4.17849345	-15866.05	-15769.94	-458209.31	H_2O
			41.1583837		321.15	HCOOH	Aq	0.00015	0.0061738	0.046026	0.134137	6.66E-05						2.192416	-9243.455	-9193.029	-56.755533	HCOOH

Mass fraction of HCHO in total liquid fed: 28.75%

Mole fraction HCHO in total liquid fed: 0.19541523

(average over 298K to T)

SUM = -556913.76

Check mass balances: 0
0

Hence equilibrium partial pressure in the vapour: 2.150735239 (~~From Ulmann's~~(5)) (*From AIChE.J & van Laar*)

*Note: Aqueous c_p's taken as those for the pure liquid.

Hence equilibrium mole fraction in the vapour: 0.017069327 (given a total pressure of: 126 kPa(abs))

⇒Hence "approach to equilibrium" is: 99.50%

STREAMS OUT:

No.	Description	HYSIM	Flow	t	T	Species	State	Mass frac.	Mass Flow	MR	Mole flow	Mole frac.	A / C1	B / C2	C / C3	D / C4	C5	$\overline{\chi\pi}$	ΔH≡ϕ, 298K	ΔH≡ϕ, T	ΔH°$_{f,T}$	
			[kg.s^{-1}]	[°C]	[K]			[-]	[kg.s^{-1}]	[kg.mol^{-1}]	[mol.s^{-1}]	[-]						[kJ.kg^{-1}.K^{-1}]	[kJ.kg^{-1}]	[kJ.kg^{-1}]	[kW]	
j	L from stage 2	-	1.742831	63	336.15	HCHO	Aq	0.2888974	0.5034995	0.030026	16.76867	0.196488	416.31	-2.6391	0.004984	-		2.70531878	-5555.656	-5452.853	-2745.5091	HCHO
			1.74283148		336.15	CH_3OH	Aq	0.005	0.0087142	0.032042	0.27196	0.003187	105800	-362.23	0.9379	0	0	2.66429888	-7675.239	-7573.995	-66.000988	CH_3OH
			1.74283148		336.15	H_2O	L	0.7059526	1.2303564	0.018015	68.29546	0.800258	276370	-2090.1	8.125	-0.01412	9.37E-06	4.1785776	-15866.05	-15707.26	-19325.528	H_2O
			1.74283148		336.15	HCOOH	Aq	0.00015	0.0002614	0.046026	0.00568	6.66E-05						2.192416	-9243.455	-9160.143	-2.3946878	HCOOH
c	V from stage 2	-	5.924	**50.00**	323.15	HCHO	V	0.0220105	0.130401	0.030026	4.342906	0.01726	23.48	0.03157	2.99E-05	-2.3E-08		1.1816	-3862.294	-3832.754	-499.79479	HCHO
			5.924497		323.15	CH_3OH	V	0.0002217	0.0013136	0.032042	0.040996	0.000163	21.15	0.07092	2.59E-05	-2.9E-08		1.3989	-6282.379	-6247.407	-8.2064774	CH_3OH
			5.924497		323.15	O_2	V	0.0006136	0.0036353	0.031999	0.113608	0.000452	28.11	-3.7E-06	1.75E-05	-1.1E-08		0.9211	0	23.0281	0.08371444	O_2
			5.924497		323.15	H_2O	V	0.0919008	0.5444662	0.018015	30.2226	0.120116	32.24	0.001924	1.06E-05	-3.6E-09		1.8733	-13433.1	-13386.27	-7288.3702	H_2O
			5.924497		323.15	H_2	V	0.0131075	0.0776551	0.002016	38.52321	0.153106	27.14	0.009274	-1.4E-05	7.65E-09		14.3452205	0	358.63051	27.8494819	H_2
			5.924497		323.15	CO_2	V	0.0790824	0.4685232	0.04401	10.64588	0.042311	19.8	0.07344	-5.6E-05	1.72E-08		0.85708331	-8948.007	-8926.58	-4182.3101	CO_2
			5.924497		323.15	CO	V	0.004474	0.0265063	0.02801	0.946301	0.003761	30.87	-0.01285	2.79E-05	-1.3E-08		1.04208198	-3948.533	-3922.481	-103.97033	CO
			5.924497		323.15	HCOOH	V	1.048E-05	6.209E-05	0.046026	0.001349	5.36E-06	11.71	0.1358	-8.4E-05	2.02E-08		1.00771392	-8231.506	-8206.313	-0.5095089	HCOOH
			5.924497		323.15	N_2	V	0.7885791	4.6719343	0.028013	166.775	0.662826	31.15	-0.01357	2.68E-05	-1.2E-08		1.04133907	0	26.033477	121.626693	N_2
n	Pump-around 2	-	41.158	63.00	336.15	HCHO	Aq	0.2888974	11.890551	0.030026	396.0059	0.196488	416.31	-2.6391	0.004984	-		2.70531878	-5555.656	-5452.853	-64837.432	HCHO
			41.1583837		336.15	CH_3OH	Aq	0.005	0.2057919	0.032042	6.422568	0.003187	105800	-362.23	0.9379	0	0	2.66429888	-7675.239	-7573.995	-1558.667	CH_3OH
			41.1583837		336.15	H_2O	L	0.7059526	29.055867	0.018015	1612.853	0.800258	276370	-2090.1	8.125	-0.01412	9.37E-06	4.1785776	-15866.05	-15707.26	-456388.07	H_2O
			41.1583837		336.15	HCOOH	Aq	0.00015	0.0061738	0.046026	0.134137	6.66E-05						2.192416	-9243.455	-9160.143	-56.552501	HCOOH

(average over 298K to T)

SUM = -556913.76

OUT - IN = 8.2655E-09

STAGE 3 (UPPER-MIDDLE SECTION OF COLUMN)

Pump-around flow: 13.744 kg.s^{-1}

Mass fraction of HCHO in liquid from stage above: 0.150415 GOAL SEEK!

STREAMS IN:

No.	Description	HYSIM	Flow [kg.s^{-1}]	t [°C]	T [K]	Species	State	Mass frac. [-]	Mass Flow [kg.s^{-1}]	MR [kg.mol^{-1}]	Mole flow [mol.s^{-1}]	Mole frac. [-]	A / C1	B / C2	C / C3	D / C4	C5	$\overline{\chi\pi}$ [kJ.kg^{-1}.K^{-1}]	ΔH≡ϕ, 298K [kJ.kg^{-1}]	ΔH≡ϕ, T [kJ.kg^{-1}]	ΔH°$_{f, T}$ [kW]	
g	L from stage 4	-	0.40	43.00	316.15	HCHO	Aq	0.1504147	0.0601659	0.030026	2.00378	0.096072	416.31	-2.6391	0.004984	-		2.53249354	-5555.656	-5510.071	-331.51834	HCHO
		DEFINE!!!	0.4	WATCH T-CROSS	316.15	CH_3OH	Aq	0.001	0.0004	0.032042	0.012484	0.000599	105800	-362.23	0.9379	0	0	2.59187684	-7675.239	-7628.585	-3.051434	CH_3OH
	Combined liquid-IN temperature:		0.4		316.15	H_2O	L	0.8485353	0.3394141	0.018015	18.84043	0.903309	276370	-2090.1	8.125	-0.01412	9.37E-06	4.17910619	-15866.05	-15790.82	-5359.6279	H_2O
	40.09 °C		0.4		316.15	HCOOH	Aq	0.00005	0.00002	0.046026	0.000435	2.08E-05						2.192416	-9243.455	-9203.991	-0.1840798	HCOOH
c	V from stage 2	-	5.924	50.000	323.15	HCHO	V	0.0220105	0.130401	0.030026	4.342906	0.01726	23.48	0.03157	2.99E-05	-2.3E-08		1.1816	-3862.294	-3832.754	-499.79479	HCHO
			5.924497		323.15	CH_3OH	V	0.0002217	0.0013136	0.032042	0.040996	0.000163	21.15	0.07092	2.59E-05	-2.9E-08		1.3989	-6282.379	-6247.407	-8.2064774	CH_3OH
			5.924497		323.15	O_2	V	0.0006136	0.0036353	0.031999	0.113608	0.000452	28.11	-3.7E-06	1.75E-05	-1.1E-08		0.9211	0	23.0281	0.08371444	O_2
			5.924497		323.15	H_2O	V	0.0919008	0.5444662	0.018015	30.2226	0.120116	32.24	0.001924	1.06E-05	-3.6E-09		1.8733	-13433.1	-13386.27	-7288.3702	H_2O
			5.924497		323.15	H_2	V	0.0131075	0.0776551	0.002016	38.52321	0.153106	27.14	0.009274	-1.4E-05	7.65E-09		14.3452205	0	358.63051	27.8494819	H_2
			5.924497		323.15	CO_2	V	0.0790824	0.4685232	0.04401	10.64588	0.042311	19.8	0.07344	-5.6E-05	1.72E-08		0.85708331	-8948.007	-8926.58	-4182.3101	CO_2
			5.924497		323.15	CO	V	0.004474	0.0265063	0.02801	0.946301	0.003761	30.87	-0.01285	2.79E-05	-1.3E-08		1.04208198	-3948.533	-3922.481	-103.97033	CO
			5.924497		323.15	HCOOH	V	1.048E-05	6.209E-05	0.046026	0.001349	5.36E-06	11.71	0.1358	-8.4E-05	2.02E-08		1.00771392	-8231.506	-8206.313	-0.5095089	HCOOH
			5.924497		323.15	N_2	V	0.7885791	4.6719343	0.028013	166.775	0.662826	31.15	-0.01357	2.68E-05	-1.2E-08		1.04133907	0	26.033477	121.626693	N_2
r	Pump-around 3	-	13.744	40.00	313.15	HCHO	Aq	0.1994886	2.7417246	0.030026	91.31107	0.130202	416.31	-2.6391	0.004984	-		2.51038749	-5555.656	-5518	-15128.836	HCHO
			13.7437671	WATCH T-APROACH	313.15	CH_3OH	Aq	0.002	0.0274875	0.032042	0.85786	0.001223	105800	-362.23	0.9379	0	0	2.58168676	-7675.239	-7636.513	-209.90892	CH_3OH
			13.7437671		313.15	H_2O	L	0.7984114	10.973181	0.018015	609.1068	0.868533	276370	-2090.1	8.125	-0.01412	9.37E-06	4.17964476	-15866.05	-15803.35	-173413.03	H_2O
			13.7437671		313.15	HCOOH	Aq	0.0001	0.0013744	0.046026	0.029861	4.26E-05						2.192416	-9243.455	-9210.568	-12.658791	HCOOH

Mass fraction of HCHO in total liquid fed: 19.81% Mole fraction HCHO in total liquid fed: 0.12921583 (average over 298K to T) **SUM = -206392.42**

Check mass balances: 0 Hence equilibrium partial pressure in the vapour: 1.045491577 ~~(From Ulmann's~~[5]~~)~~ *(From AIChE.J & van Laar)* *Note: Aqueous c_p's taken as those for the pure liquid.

0 Hence equilibrium mole fraction in the vapour: 0.008431384 (given a total pressure of: 124 kPa(abs)) ⇒Hence "approach to equilibrium" is: 99.50%

STREAMS OUT:

No.	Description	HYSIM	Flow [kg.s^{-1}]	t [°C]	T [K]	Species	State	Mass frac. [-]	Mass Flow [kg.s^{-1}]	MR [kg.mol^{-1}]	Mole flow [mol.s^{-1}]	Mole frac. [-]	A / C1	B / C2	C / C3	D / C4	C5	$\overline{\chi\pi}$ [kJ.kg^{-1}.K^{-1}]	ΔH≡ϕ, 298K [kJ.kg^{-1}]	ΔH≡ϕ, T [kJ.kg^{-1}]	ΔH°$_{f, T}$ [kW]	
h	L from stage 3	-	0.65	51	324.15	HCHO	Aq	0.1994886	0.1296676	0.030026	4.318481	0.130202	416.31	-2.6391	0.004984	-		2.59631201	-5555.656	-5488.151	-711.6353	HCHO
			0.65		324.15	CH_3OH	Aq	0.002	0.0013	0.032042	0.040572	0.001223	105800	-362.23	0.9379	0	0	2.61990898	-7675.239	-7607.121	-9.8892575	CH_3OH
			0.65		324.15	H_2O	L	0.7984114	0.5189674	0.018015	28.8072	0.868533	276370	-2090.1	8.125	-0.01412	9.37E-06	4.17828821	-15866.05	-15757.41	-8177.583	H_2O
			0.65		324.15	HCOOH	Aq	0.0001	0.000065	0.046026	0.001412	4.26E-05						2.192416	-9243.455	-9186.452	-0.5971194	HCOOH
d	V from stage 3	-	5.674	42.00	315.15	HCHO	V	0.0107321	0.0608993	0.030026	2.028205	0.008476	23.48	0.03157	2.99E-05	-2.3E-08		1.1758	-3862.294	-3842.305	-233.99363	HCHO
			5.674497		315.15	CH_3OH	V	7.288E-05	0.0004136	0.032042	0.012907	5.39E-05	21.15	0.07092	2.59E-05	-2.9E-08		1.3890	-6282.379	-6258.766	-2.5885082	CH_3OH
			5.674497		315.15	O_2	V	0.0006406	0.0036353	0.031999	0.113608	0.000475	28.11	-3.7E-06	1.75E-05	-1.1E-08		0.9202	0	15.6426	0.05686569	O_2
			5.674497		315.15	H_2O	V	0.0643075	0.3649129	0.018015	20.25583	0.084646	32.24	0.001924	1.06E-05	-3.6E-09		1.8717	-13433.1	-13401.28	-4890.3004	H_2O
			5.674497		315.15	H_2	V	0.0136849	0.0776551	0.002016	38.52321	0.160982	27.14	0.009274	-1.4E-05	7.65E-09		14.3394902	0	243.77133	18.930083	H_2
			5.674497		315.15	CO_2	V	0.0825665	0.4685232	0.04401	10.64588	0.044487	19.8	0.07344	-5.6E-05	1.72E-08		0.85313135	-8948.007	-8933.504	-4185.5541	CO_2
			5.674497		315.15	CO	V	0.0046711	0.0265063	0.02801	0.946301	0.003954	30.87	-0.01285	2.79E-05	-1.3E-08		1.04196167	-3948.533	-3930.82	-104.19136	CO
			5.674497		315.15	HCOOH	V	3.011E-06	1.709E-05	0.046026	0.000371	1.55E-06	11.71	0.1358	-8.4E-05	2.02E-08		0.99996278	-8231.506	-8214.507	-0.1403648	HCOOH
			5.674497		315.15	N_2	V	0.8233213	4.6719343	0.028013	166.775	0.696925	31.15	-0.01357	2.68E-05	-1.2E-08		1.04137533	0	17.703381	82.7090306	N_2
q	Pump-around 3	-	13.744	51.00	324.15	HCHO	Aq	0.1994886	2.7417246	0.030026	91.31107	0.130202	416.31	-2.6391	0.004984	-		2.59631201	-5555.656	-5488.151	-15047	HCHO
			13.7437671		324.15	CH_3OH	Aq	0.002	0.0274875	0.032042	0.85786	0.001223	105800	-362.23	0.9379	0	0	2.61990898	-7675.239	-7607.121	-209.101	CH_3OH
			13.7437671		324.15	H_2O	L	0.7984114	10.973181	0.018015	609.1068	0.868533	276370	-2090.1	8.125	-0.01412	9.37E-06	4.17828821	-15866.05	-15757.41	-172908.92	H_2O
			13.7437671		324.15	HCOOH	Aq	0.0001	0.0013744	0.046026	0.029861	4.26E-05						2.192416	-9243.455	-9186.452	-12.625645	HCOOH

(average over 298K to T) **SUM = -206392.42**

OUT - IN = 2.0373E-10

STAGE 4 (TOP OF COLUMN)

Pump-around flow: **0.000** $kg.s^{-1}$

Mass fraction of HCHO in liquid from stage above: **0** GOAL SEEK!

STREAMS IN:

No.	Description	HYSIM	Flow $[kg.s^{-1}]$	t [°C]	T [K]	Species	State	Mass frac. [-]	Mass Flow $[kg.s^{-1}]$	MR $[kg.mol^{-1}]$	Mole flow $[mol.s^{-1}]$	Mole frac. [-]	A / C1	B / C2	C / C3	D / C4	C5	$\bar{\chi}\pi$ $[kJ.kg^{-1}.K^{-1}]$	$\Delta H \equiv \phi$, 298K $[kJ.kg^{-1}]$	$\Delta H \equiv \phi$, T $[kJ.kg^{-1}]$	$\Delta H^o_{f,T}$ [kW]	
f	Fresh DM Water	AbsWater	**0.3275**	**37.00**	310.15	HCHO	Aq	0	0	0.030026	0	0	416.31	-2.6391	0.004984	-		2.48927736	-5555.656	-5525.784	0	HCHO
	NOTE:	DEFINE!!!	0.3275	MAX'M SUMMER	310.15	CH_3OH	Aq	0	0	0.032042	0	0	105800	-362.23	0.9379	0	0	2.57167231	-7675.239	-7644.379	0	CH_3OH
	Hence combined temperature:		0.3275		310.15	H_2O	L	1	0.3275	0.018015	18.17909	1	276370	-2090.1	8.125	-0.01412	9.37E-06	4.1803182	-15866.05	-15815.88	-5179.7016	H_2O
	37.00 °C		0.3275		310.15	HCOOH	Aq	0	0	0.046026	0	0						2.192416	-9243.455	-9217.146	0	HCOOH
d	V from stage 3	-	5.674	42.00	315.15	HCHO	V	0.0107321	0.0608993	0.030026	2.028205	0.008476	23.48	0.03157	2.99E-05	-2.3E-08		1.1758	-3862.294	-3842.305	-233.99363	HCHO
			5.674497		315.15	CH_3OH	V	7.288E-05	0.0004136	0.032042	0.012907	5.39E-05	21.15	0.07092	2.59E-05	-2.9E-08		1.3890	-6282.379	-6258.766	-2.5885082	CH_3OH
			5.674497		315.15	O_2	V	0.0006406	0.0036353	0.031999	0.113608	0.000475	28.11	-3.7E-06	1.75E-05	-1.1E-08		0.9202	0	15.6426	0.05686569	O_2
			5.674497		315.15	H_2O	V	0.0643075	0.3649129	0.018015	20.25583	0.084646	32.24	0.001924	1.06E-05	-3.6E-09		1.8717	-13433.1	-13401.28	-4890.3004	H_2O
			5.674497		315.15	H_2	V	0.0136849	0.0776551	0.002016	38.52321	0.160982	27.14	0.009274	-1.4E-05	7.65E-09		14.3394902	0	243.77133	18.930083	H_2
			5.674497		315.15	CO_2	V	0.0825665	0.4685232	0.04401	10.64588	0.044487	19.8	0.07344	-5.6E-05	1.72E-08		0.85313135	-8948.007	-8933.504	-4185.5541	CO_2
			5.674497		315.15	CO	V	0.0046711	0.0265063	0.02801	0.946301	0.003954	30.87	-0.01285	2.79E-05	-1.3E-08		1.04196167	-3948.533	-3930.82	-104.19136	CO
			5.674497		315.15	HCOOH	V	3.011E-06	1.709E-05	0.046026	0.000371	1.55E-06	11.71	0.1358	-8.4E-05	2.02E-08		0.99996278	-8231.506	-8214.507	-0.1403648	HCOOH
			5.674497		315.15	N_2	V	0.8233213	4.6719343	0.028013	166.775	0.696925	31.15	-0.01357	2.68E-05	-1.2E-08		1.04137533	0	17.703381	82.7090306	N_2
s	Pump-around 4	-	0.000	**40.00**	313.15	HCHO	Aq	0.1504147	0	0.030026	0	#DIV/0!	416.31	-2.6391	0.004984	-		2.51038749	-5555.656	-5518	0	HCHO
	(Note: no change from below)		0		313.15	CH_3OH	Aq	0.001	0	0.032042	0	#DIV/0!	105800	-362.23	0.9379	0	0	2.58168676	-7675.239	-7636.513	0	CH_3OH
			0		313.15	H_2O	L	0.8485353	0	0.018015	0	#DIV/0!	276370	-2090.1	8.125	-0.01412	9.37E-06	4.17964476	-15866.05	-15803.35	0	H_2O
			0		313.15	HCOOH	Aq	0.00005	0	0.046026	0	#DIV/0!						2.192416	-9243.455	-9210.568	0	HCOOH

Mass fraction of HCHO in total liquid fed: 0.00% Mole fraction HCHO in total liquid fed: 0 (average over 298K to T) **SUM = -14494.774**

Check mass balances: 0 Hence equilibrium partial pressure in the vapour: 0 ~~(From Ulmann's (5))~~ (*From AIChE.J & van Laar*) *Note: Aqueous c_p's taken as those for the pure liquid.

8.88178E-16 Hence equilibrium mole fraction in the vapour: 0 (given a total pressure of: 110 kPa(abs)) ⇒Hence "approach to equilibrium" is: **98.78%**

STREAMS OUT:

No.	Description	HYSIM	Flow $[kg.s^{-1}]$	t [°C]	T [K]	Species	State	Mass frac. [-]	Mass Flow $[kg.s^{-1}]$	MR $[kg.mol^{-1}]$	Mole flow $[mol.s^{-1}]$	Mole frac. [-]	A / C1	B / C2	C / C3	D / C4	C5	$\bar{\chi}\pi$ $[kJ.kg^{-1}.K^{-1}]$	$\Delta H \equiv \phi$, 298K $[kJ.kg^{-1}]$	$\Delta H \equiv \phi$, T $[kJ.kg^{-1}]$	$\Delta H^o_{f,T}$ [kW]	
g	L from stage 4	-	0.4	43	316.15	HCHO	Aq	0.1504147	0.0601659	0.030026	2.00378	0.096072	416.31	-2.6391	0.004984	-		2.53249354	-5555.656	-5510.071	-331.51834	HCHO
			0.4		316.15	CH_3OH	Aq	0.001	0.0004	0.032042	0.012484	0.000599	105800	-362.23	0.9379	0	0	2.59187684	-7675.239	-7628.585	-3.051434	CH_3OH
			0.4		316.15	H_2O	L	0.8485353	0.3394141	0.018015	18.84043	0.903309	276370	-2090.1	8.125	-0.01412	9.37E-06	4.17910619	-15866.05	-15790.82	-5359.6279	H_2O
			0.4		316.15	HCOOH	Aq	0.00005	0.00002	0.046026	0.000435	2.08E-05						2.192416	-9243.455	-9203.991	-0.1840798	HCOOH
e	V from stage 4	Ohead_Total	5.602	**37.50**	310.65	HCHO	V	0.0001309	0.0007334	0.030026	0.024425	0.000103	23.48	0.03157	2.99E-05	-2.3E-08		1.1725	-3862.294	-3847.637	-2.8218137	HCHO
			5.601997		310.65	CH_3OH	V	2.424E-06	1.358E-05	0.032042	0.000424	1.79E-06	21.15	0.07092	2.59E-05	-2.9E-08		1.3835	-6282.379	-6265.085	-0.0850878	CH_3OH
			5.601997		310.65	O_2	V	0.0006489	0.0036353	0.031999	0.113608	0.00048	28.11	-3.7E-06	1.75E-05	-1.1E-08		0.9196	0	11.4951	0.04178834	O_2
			5.601997		310.65	H_2O	V	0.063013	0.3529988	0.018015	19.5945	0.082809	32.24	0.001924	1.06E-05	-3.6E-09		1.8707	-13433.1	-13409.72	-4733.6134	H_2O
			5.601997		310.65	H_2	V	0.013862	0.0776551	0.002016	38.52321	0.162804	27.14	0.009274	-1.4E-05	7.65E-09		14.336205	0	179.20256	13.9159897	H_2
			5.601997		310.65	CO_2	V	0.083635	0.4685232	0.04401	10.64588	0.044991	19.8	0.07344	-5.6E-05	1.72E-08		0.85089134	-8948.007	-8937.371	-4187.3659	CO_2
			5.601997		310.65	CO	V	0.0047316	0.0265063	0.02801	0.946301	0.003999	30.87	-0.01285	2.79E-05	-1.3E-08		1.0419047	-3948.533	-3935.51	-104.31566	CO
			5.601997		310.65	HCOOH	V	-5.2E-07	-2.91E-06	0.046026	-6.33E-05	-2.67E-07	11.71	0.1358	-8.4E-05	2.02E-08		0.99557618	-8231.506	-8219.061	0.02393859	HCOOH
			5.601997		310.65	N_2	V	0.8339766	4.6719343	0.028013	166.775	0.704812	31.15	-0.01357	2.68E-05	-1.2E-08		1.04140635	0	13.017579	60.8172753	N_2
s	Pump-around 4	-	0.000	43.00	316.15	HCHO	Aq	0.1504147	0	0.030026	0	#DIV/0!	416.31	-2.6391	0.004984	-		2.53249354	-5555.656	-5510.071	0	HCHO
	(Note: no change from above)		0		316.15	CH_3OH	Aq	0.001	0	0.032042	0	#DIV/0!	105800	-362.23	0.9379	0	0	2.59187684	-7675.239	-7628.585	0	CH_3OH
			0		316.15	H_2O	L	0.8485353	0	0.018015	0	#DIV/0!	276370	-2090.1	8.125	-0.01412	9.37E-06	4.17910619	-15866.05	-15790.82	0	H_2O
			0		316.15	HCOOH	Aq	0.00005	0	0.046026	0	#DIV/0!						2.192416	-9243.455	-9203.991	0	HCOOH

(average over 298K to T) **SUM = -14647.785**

Serpentine inter-cooling req'd b/n TRAYS?

OUT - IN = -153.01063

ABSORBER DETAILED DESIGN

Model of a simplified case:

Stage 1

Reference(s):

Perry[(6)], p. 14-20, 14-10.
"van Laar VLE" worksheet [by D.I.V.], & the relevant references therein.
"Diam.", "Visc.", "Gdiff" & "Ldiff" worksheets [D.I.V.], & references therein.
HYSIM material
I. Hahnenstein, H. Hasse, Y.-Q. Liu and G. Maurer; AIChE Symposium series
Onda *et alii* - original reference.

Assumptions:

Assume:	Comment:
1. Straight operating line (*i.e.* dilute solutions - small mass transfer)	This implies constant flowrates.
2. Straight equilibrium line (*i.e.* Henry's law is valid: $y_i = H_i.x_i$)	This may be reasonable, based on data presented in worksheet "van Laar VLE".
3. Absorption heat effects are negligible	This may or may not be valid: - Hysim's simulation says a large amount of heat [in kW] is evolved - however the absorber also has pump-around cooling, with large(?) liquid flow and so the actual temperature PROFILES in the absorber will not be great

Note: Perry's definition of the assumption is ambiguous, if not confusing.

Additionally, reaction is ignored.

Data:

Temperature at bottom of stage:	LIQUID:	75.00 °C	GAS:	90.00 °C	
Temperature at top of stage:	LIQUID:	60.20 °C	GAS:	62.00 °C	It is assumed that thermal equilibrium is (almost) reached.
	Thus a nominal column temperature of	67.60214	°C will be used here		± 10°C, say.

Pressures:	TOP:	125	kPa(abs)	Estimate.
	BOTTOM:	130	kPa(abs)	
	AVERAGE:	127.5	kPa(abs)	
Henry's constant: ("m")	By linear regression of AIChE.J data in worksheet "van Laar VLE":	0.7514	(70°C)	This was only based on x_{HCHO} under 0.20
	By weighted least squares regression of the above: (approx.)	1	(70°C)	
	Data from Ullmann's[(5)] & Walker[(3)]:	<< 1		This assumes equilibrium of reaction.
	All other estimates, including Raoult's law:	>> 1	(60°C)	This doesn't consider liquid-phase formation of nonvolatiles.
	Hence use the value:	0.7514		On the conservative side. THESE DO NOT CONSIDER INERTS PRESENT
Flows:	TOTAL liquid inflow:	1372.037	$mol.s^{-1}$	
	TOTAL liquid outflow:	1401.164	$mol.s^{-1}$	
	RATIO of BOTTOM to TOP liquid flows:	1.021229		Thus the flow may be considered constant.
	Average stage TOTAL liquid flow:	1386.6	$mol.s^{-1}$	This average is justified by the high pump-around rate.
	Vapour inflow:	332.913	$mol.s^{-1}$	Note: no vapour recirculation.
	Vapour outflow:	303.7859	$mol.s^{-1}$	
	RATIO of BOTTOM to TOP vapour flows:	1.09588		This is really NOT too large to assume constant flow.
	Average (total) vapour flow:	318.3495	$mol.s^{-1}$	
Mean molar masses:	GAS:	0.0231	$kg.mol^{-1}$	Worksheet "Diam."
	LIQUID:	0.022944	$kg.mol^{-1}$	Worksheet "Diam."
Mole-fractions:	Mole-fraction of formaldehyde in vapour: TOP:	0.055279		
	BOTTOM:	0.1430		
	AVERAGE:	0.099133		NOTE: This average for reference only.
	Mole-fraction of formaldehyde in liquid: TOP:	0.4020		(based on a 99.5% nominal aproach to equilibrium) There will be some formaldehyde in the pump-around liquid(!)…
	BOTTOM:	0.4156		...but too high would cause more formaldehyde to escape more easily.
	AVERAGE:	0.408822		The similarity is due to the large pump-around.
	Mole-fraction IN EQUILIBRIUM WITH liquid: TOP:	0.0548		Note that temperature is the dominant effect here.
	BOTTOM:	0.0920		
	AVERAGE:	0.073439		
Equilibrium:	Hence "**m**": TOP:	0.136412		Defined by $y_{equilibrium} \equiv m.x$
	BOTTOM:	0.221442		
	AVERAGE:	0.179636		Actual mean: 0.178927
Diameter:		**1.8**	m	Calculated in worksheet "Diam."
Flooding:	DESIGN:	73%		Worksheet "Diam."
	TURNDOWN:	44%		Worksheet "Diam."
Internals:	Type:	Pall rings		
	Material:	S.S.		
	σ_c:	75	$mN.m^{-1}$	Sinnott[(2)]
	Nominal size:	0.051	m	*I.e.* 2 inches.
	a_t:	102	$m^2.m^{-3}$	
Fluid properties:	μ_G:	1.66E-05	Pa.s	See worksheet "Visc.".

μ_L:		1.89E-03	Pa.s	Worksheet "Diam."
D_G:		**0.174**	$cm^2.s^{-1}$	See worksheet "GDiff".
D_L:		**3.5E-05**	$cm^2.s^{-1}$	See worksheet "LDiff".
ρ_G:		1.04	$kg.m^{-3}$	Worksheet "Diam."
ρ_L:		1132	$kg.m^{-3}$	Worksheet "Diam."
σ:	WATER, 303.15K:	71.40	$dyn.cm^{-1}$	Perry(6)
	WATER, 293.15K:	70	$mN.m^{-1}$	Sinnott(2)
	WATER, 293K:	72.8	$dyn.cm^{-1}$	R, P & P(4)
	WATER, 303K:	71.18	$dyn.cm^{-1}$	R, P & P(4)
	METHANOL, 333K:	19.41	$dyn.cm^{-1}$	R, P & P(4)
	ACETONE, 318K:	21.22	$dyn.cm^{-1}$	R, P & P(4)
	FORMAMIDE, 338K:	53.66	$dyn.cm^{-1}$	R, P & P(4)
	METHYL FORMATE, 298K:	24.62	$dyn.cm^{-1}$	R, P & P(4)
	METHYL FORMATE, 323K:	20.05	$dyn.cm^{-1}$	R, P & P(4)
	METHYL FORMATE, 373K:	12.90	$dyn.cm^{-1}$	R, P & P(4)
	ASSUME:	**60**	$dyn.cm^{-1}$	Surface tension reduces with T rising.

Mass-transfer coefficients:

Liquid "film": Calculated; see below.

Vapour "film": Calculated; see below.

Overall: Calculated; see below.

Equations:

Height: $h_{bed} = H_{Oy}.N_{Oy}$

H_{Oy}: $H_{Oy} = G_M/[(K_y.a).y^*_{BM}]$

where:

$y^*_{BM} = \{(1 - y) - (1 - y^*)\} / \ln\{(1 - y)/(1 - y^*)\}$

with y^* the equilibrium gas-phase mole fraction, such that $y^* = m.x$

and the rate of mass transfer, $N_i = K_y.(y_i - y^*_i)$, defines the overall gas-phase mass transfer coefficient

This K_y can also be expressed in terms of the "film" coefficients, *viz.* :

$1/K_y = 1/k_y + m/k_x$

NOTE: Poxy W. M. Edwards (& predecessors) use a different notation - care!!

From Onda *et alii* :

$k_L.(\rho_L/\mu_L.g)^{1/3} / \{(\mu_L/\rho_L.D_L)^{-1/2}.(a_t.D_p)^{0.4}\}$ is correlated against $(Re)_L = L/(a_w.\mu_L)$

$\{(k_G.R.T)/(a_t.D_G)\} / \{(\mu_G/\rho_G.D_G)^{-1/3}.(a_t.D_p)^{-2.0}\}$ is correlated against $(Re)_G = G/(a_t.\mu_G)$

$a_w/a_t = 1 - \exp\{-1.45(\sigma_c/\sigma)^{0.75}.(L/a_t.\mu_L)^{0.1} \times (L^2.a_t/(\rho_L{}^2.g))^{-0.05}.(L^2/(\rho_L.\sigma.a_t))^{0.2}\}$

Where $[G] = [L] = kg.m^{-2}.s^{-1}$ a_w is the "effective" - wetted - area per volume

Where: $K_G = K_y / P$ Where: $k_G = k_y / P$ Where: $k_L = k_x / \rho_L$ From Uhlherr, CHE3102 notes.

Alternatively, an estimate may be obtained from Cornell's method (*Sinnott* (2) *, updated by Bolles/Fair*)

$H_y[m] = 0.0190283.\psi_h[m].(Sc)_v{}^{0.5}.(D_c/0.3048)^{1.24}.(Z/3.048)^{(1/3)} / \{L.(\mu_L/\mu_w)^{0.16}.(\rho_w/\rho_L)^{1.25}.(\sigma_w/\sigma_L)^{0.8}\}^{0.6}$

$H_x[m] = \phi_h[m].(Sc)_L{}^{0.5}.K_3.(Z/3.048)^{0.15}$

Where D_c is a "corrected" diameter: the lesser of {diameter} or {2 × 0.3048}.

Where μ_w = 1.002 mPa.s ρ_w = 998.2032 $kg.m^{-3}$ σ_w = 70 $mN.m^{-1}$ (All at 20°C)

And $H_{Oy} = H_y + (m.G_M/L_M).H_x$ *NOTE: use of the coefficient $(m.G_M/L_M)$ implied the subscripts "Oy", "y" and "x" by CHE3102/Uhlherr.*

N_{Oy}: Colburn's equation of 1939 is:

$N_{Oy} = 1/\{1 - (m.G_M/L_M)\} \times \ln[\{1 - (m.G_M/L_M)\} \times \{(y_1 - m.x_2)/(y_2 - m.x_2)\} + m.G_M/L_M]$ "m" is a Henry's law-type constant here: $y_{equilibrium\ 1} \equiv m.x_1$

Note: the G_M and L_M are (moles per time) per unit area (of the column).

Feintuch/Treybal(1978) present an "Edmister-type approach":

$N_{Oy} = \ln[\{(y_1 - y_2^*)/(y_2-y_2^*)\}.(1-1/A_E) + 1/A_E] / (1 - 1/A_E)$

where $A_E = [A_{BOTTOM}.(A_{TOP} + 1) + 0.25]^{0.5} - 0.5$

and $(1/A_i) = (m_i.G_i/L_i)$

Calculations:

N_{Oy}: **According to Colburn:**

$(m.G_M/L_M)$ = 0.041243

$\{1 - (m.G_M/L_M)\}$ = 0.958757

∴ N_{Oy} = **5.482**

According to Feintuch & Treybal:

A_{BOTTOM} = 19.00635

A_{TOP} = 33.10883

The big difference here means the more sophisticated average is probably worth calculating!

A_E = 24.96634 (*cf.* arithmetic mean of 26.05759)

∴ N_{Oy} = 5.477

This non-simple short-cut method has resulted in a VERY SIMILAR result to the result from Colburn.

<u>H_{Oy}:</u> y^*_{BM} = TOP: 0.944941

BOTTOM: 0.882242

AVERAGE: 0.913592 "Averages" are just simple, arithmetic.

G_M = TOP: 130.8265 $mol.m^{-2}.s^{-1}$

BOTTOM: 119.3803 $mol.m^{-2}.s^{-1}$

AVERAGE: 125.1034 $mol.m^{-2}.s^{-1}$

From the data of Onda *et alii*:

L = 12.5021 $kg.m^{-2}.s^{-1}$

OKAY $(\sigma_c/\sigma)^{0.75}$ = 1.1822 $(L/a_t.\mu_L)^{0.1}$ = 1.5175 $(L^2.a_t/(\rho_L{}^2.g))^{-0.05}$ = OKAY 1.3958 $(L^2/(\rho_L.\sigma.a_t))^{0.2}$ = OKAY 0.4685

Bolles/Fair: $0.3<(\sigma_c/\sigma)<2$ *Bolles/Fair: $2.5e-9<Fr_L<0.018$* *Bolles/Fair: $1.2e-8<We_L<0.27$*

a_w = 83.4 $m^2.m^{-3}$

$(Re)_L$ = 7.92E+01 OKAY $(\mu_L/\rho_L.D_L)^{-1/2}$ = 0.046027 $(a_t.D_p)^{0.4}$ = 1.934052

Bolles/Fair: $0.04<Re_L<500$

Hence: $k_L.(\rho_L/\mu_L.g)^{1/3}$ = 0.00985 where 0.0060 (*cf.* 0.0051) is the constant for this large, modern packing

Thus, k_L = 0.00025 $m.s^{-1}$

ρ_B = 49341 $mol.m^{-3}$

∴ k_x = 12.35 $mol.m^{-2}.s^{-1}$

G = 2.8898 $kg.m^{-2}.s^{-1}$

$(Re)_G$ = 1.71E+03 OFF SCALE! $(\mu_G/\rho_G.D_G)^{-1/3}$ = 1.027408 $(a_t.D_p)^{-2.0}$ = 0.036954

Hence: $(k_G.R.T)/(a_t.D_G)$ = 41.708 where 6.00 (*cf.* 5.23) is the constant for this large, modern packing

Thus, k_G = 2.54E-05 $mol.Pa^{-1}.m^{-2}.s^{-1}$ 0.000258 $mol.atm^{-1}.cm^{-2}.s^{-1}$

P = 128 kPa(abs)

∴ k_y = 3.24 $mol.m^{-2}.s^{-1}$

We see that the gas-phase resistance is dominant.... (...also, "m" is small).

Hence: K_y = 3.098 $mol.m^{-2}.s^{-1}$

∴ H_{Oy} = **0.530** m

`cf. The data of the Norton Co. (for specific conditions) in Perry(6), p. 14-34, T14-4:`

`K_y.a.y*_BM =` 114 $kmol.h^{-1}.m^{-3}$

i.e. 31.667 $mol.m^{-3}.s^{-1}$

Whence H_{Oy} = 3.951 m

<u>Height:</u> h_{bed} = **2.91 m**

<u>H_{Oy}:</u> **By Cornell's (updated) method:**

Flooding: 73% K_3 = 0.69

(At design percentage flooding, from charts in Bolles/Fair & Sinnott(2))

Flooding: 73% ψ_h = 140 ft 42.672 m

$L[lb_m.h^{-1}ft^{-2}]$: 9.22E+03 ϕ_h = 0.105 ft 0.032004 m

(At design percentage flooding, from charts in Bolles/Fair: specific to metal Pall rings.)

Estimated height, "Z" = 1.93 m

$(Sc)_v{}^{0.5}$ = 0.960253 D_c = 0.6096 m

$\{L.(\mu_L/\mu_w)^{0.16}.(\rho_w/\rho_L)^{1.25}.(\sigma_w/\sigma_L)^{0.8}\}$ = 13.37842 $kg.m^{-2}.s^{-1}$

H_y = 0.333588 m

$(Sc)_L{}^{0.5}$ = 21.7266

H_x = 0.447998 m

∴ H_{Oy} = **0.352** m

(We note that the extraordinarily low value of $m.G_M/L_M$ means the contribution of H_x is ~negligible.)

<u>Height:</u> h_{bed} = 1.93 m (or **2.25** **m** without height-correction)

ABSORBER DETAILED DESIGN

Model of a simplified case:

Stage 2

Reference(s):

Perry[(6)], p. 14-20, 14-10.
"van Laar VLE" worksheet [by D.I.V.], & the relevant references therein.
"Diam.", "Visc.", "Gdiff" & "Ldiff" worksheets [D.I.V.], & references therein.
HYSIM material
I. Hahnenstein, H. Hasse, Y.-Q. Liu and G. Maurer; AIChE Symposium series
Onda *et alii* - original reference.

Assumptions:

Assume:	Comment:
1. Straight operating line (*i.e.* dilute solutions - small mass transfer)	This implies constant flowrates.
2. Straight equilibrium line (*i.e.* Henry's law is valid: $y_i = H_i.x_i$)	This may be reasonable, based on data presented in worksheet "van Laar VLE".
3. Absorption heat effects are negligible	This may or may not be valid: - Hysim's simulation says a large amount of heat [in kW] is evolved - however the absorber also has pump-around cooling, with large(?) liquid flow and so the actual temperature PROFILES in the absorber will not be great

Note: Perry's definition of the assumption is ambiguous, if not confusing.

Additionally, reaction is ignored.

Data:

Temperature at bottom of stage:	LIQUID:	63.00 °C	GAS:	62.00 °C		
Temperature at top of stage:	LIQUID:	48.05 °C	GAS:	50.00 °C		It is assumed that thermal equilibrium is (almost) reached.
	Thus a nominal column temperature of	55.52624	°C will be used here			± 10°C, say.

Pressures:		TOP:	120	kPa(abs)	Estimate.
		BOTTOM:	125	kPa(abs)	
		AVERAGE:	122.5	kPa(abs)	
Henry's constant: ("m")	~~By linear regression of AIChE.J data in worksheet "van Laar VLE":~~		~~0.7514~~	~~(70°C)~~	This was only based on x_{HCHO} under 0.20
	~~By weighted least squares regression of the above: (approx.)~~		~~1~~	~~(70°C)~~	
	~~Data from Ullmann's[(5)] & Walker[(3)]:~~		~~<< 1~~		This assumes equilibrium of reaction.
	~~All other estimates, including Raoult's law:~~		~~>> 1~~	~~(60°C)~~	This doesn't consider liquid-phase formation of nonvolatiles.
	~~Hence use the value:~~		~~0.7514~~		On the conservative side.
					THESE DO NOT CONSIDER INERTS PRESENT
Flows:	TOTAL liquid inflow:		2048.583	$mol.s^{-1}$	
	TOTAL liquid outflow:		2100.757	$mol.s^{-1}$	
	RATIO of BOTTOM to TOP liquid flows:		1.025468		Thus the flow may be considered constant.
	Average stage TOTAL liquid flow:		2074.67	$mol.s^{-1}$	This average is justified by the high pump-around rate.
	Vapour inflow:		303.7859	$mol.s^{-1}$	Note: no vapour recirculation.
	Vapour outflow:		251.6118	$mol.s^{-1}$	
	RATIO of BOTTOM to TOP vapour flows:		1.20736		This is really NOT too large to assume constant flow.
	Average (total) vapour flow:		277.6989	$mol.s^{-1}$	
Mean molar masses:		GAS:	0.023546	$kg.mol^{-1}$	Worksheet "Diam."
		LIQUID:	0.020408	$kg.mol^{-1}$	Worksheet "Diam."
Mole-fractions:	Mole-fraction of formaldehyde in vapour:	TOP:	0.01726		
		BOTTOM:	0.0553		
		AVERAGE:	0.03627		NOTE: This average for reference only. (based on a 99.5% nominal aproach to equilibrium)
	Mole-fraction of formaldehyde in liquid:	TOP:	0.1954		There will be some formaldehyde in the pump-around liquid(!)…
		BOTTOM:	0.1965		...but too high would cause more formaldehyde to escape more easily.
		AVERAGE:	0.195952		The similarity is due to the large pump-around.
	Mole-fraction IN EQUILIBRIUM WITH liquid:	TOP:	0.0171		Note that temperature is the dominant effect here.
		BOTTOM:	0.0279		
		AVERAGE:	0.022462		
Equilibrium:	Hence "**m**":	TOP:	0.087349		Defined by $y_{equilibrium} \equiv m.x$
		BOTTOM:	0.141761		
		AVERAGE:	0.11463		Actual mean: 0.114555
Diameter:			**1.8**	m	Calculated in worksheet "Diam."
Flooding:		DESIGN:	58%		Worksheet "Diam."
		TURNDOWN:	35%		Worksheet "Diam."
Internals:	Type:		Pall rings		
	Material:		S.S.		
	σ_c:		75	$mN.m^{-1}$	Sinnott[(2)]
	Nominal size:		0.051	m	*I.e.* 2 inches.
	a_t:		102	$m^2.m^{-3}$	
Fluid properties:	μ_G:		1.66E-05	Pa.s	See worksheet "Visc.".

μ_L:		5.44E-04	Pa.s	Worksheet "Diam."
D_G:		0.174	$cm^2.s^{-1}$	See worksheet "GDiff".
D_L:		2.9E-05	$cm^2.s^{-1}$	See worksheet "LDiff".
ρ_G:		1.05	$kg.m^{-3}$	Worksheet "Diam."
ρ_L:		1071	$kg.m^{-3}$	Worksheet "Diam."
σ:	WATER, 303.15K:	71.40	$dyn.cm^{-1}$	Perry[(6)]
	WATER, 293.15K:	70	$mN.m^{-1}$	Sinnott[(2)]
	WATER, 293K:	72.8	$dyn.cm^{-1}$	R, P & P[(4)]
	WATER, 303K:	71.18	$dyn.cm^{-1}$	R, P & P[(4)]
	METHANOL, 333K:	19.41	$dyn.cm^{-1}$	R, P & P[(4)]
	ACETONE, 318K:	21.22	$dyn.cm^{-1}$	R, P & P[(4)]
	FORMAMIDE, 338K:	53.66	$dyn.cm^{-1}$	R, P & P[(4)]
	METHYL FORMATE, 298K:	24.62	$dyn.cm^{-1}$	R, P & P[(4)]
	METHYL FORMATE, 323K:	20.05	$dyn.cm^{-1}$	R, P & P[(4)]
	METHYL FORMATE, 373K:	12.90	$dyn.cm^{-1}$	R, P & P[(4)]
	ASSUME:	60	$dyn.cm^{-1}$	Surface tension reduces with T rising.

Mass-transfer coefficients:

Liquid "film":	Calculated;	see below.
Vapour "film":	Calculated;	see below.
Overall:	Calculated;	see below.

Equations:

Height: $h_{bed} = H_{Oy}.N_{Oy}$

H_{Oy}: $H_{Oy} = G_M/[(K_y.a).y^*_{BM}]$

where:

$y^*_{BM} = \{(1 - y) - (1 - y^*)\} / \ln\{(1 - y)/(1 - y^*)\}$

with y^* the equilibrium gas-phase mole fraction, such that $y^* = m.x$

and the rate of mass transfer, $N_i = K_y.(y_i - y^*_i)$, defines the overall gas-phase mass transfer coefficient

This K_y can also be expressed in terms of the "film" coefficients, *viz.* :

$1/K_y = 1/k_y + m/k_x$

NOTE: Poxy W. M. Edwards (& predecessors) use a different notation - care!!

From Onda *et alii* :

$k_L.(\rho_L/\mu_L.g)^{1/3} / \{(\mu_L/\rho_L.D_L)^{-1/2}.(a_t.D_p)^{0.4}\}$ is correlated against $(Re)_L = L/(a_w.\mu_L)$

$\{(k_G.R.T)/(a_t.D_G)\} / \{(\mu_G/\rho_G.D_G)^{-1/3}.(a_t.D_p)^{-2.0}\}$ is correlated against $(Re)_G = G/(a_t.\mu_G)$

$a_w/a_t = 1 - \exp\{-1.45(\sigma_c/\sigma)^{0.75}.(L/a_t.\mu_L)^{0.1} \times (L^2.a_t/(\rho_L{}^2.g))^{-0.05}.(L^2/(\rho_L.\sigma.a_t))^{0.2}\}$

Where $[G] = [L] = kg.m^{-2}.s^{-1}$ a_w is the "effective" - wetted - area per volume

Where: $K_G = K_y / P$ Where: $k_G = k_y / P$ Where: $k_L = k_x / \rho_L$ From Uhlherr, CHE3102 notes.

Alternatively, an estimate may be obtained from Cornell's method (*Sinnott* [(2)], *updated by Bolles/Fair*)

$H_y[m] = 0.0190283.\psi_h[m].(Sc)_v{}^{0.5}.(D_c/0.3048)^{1.24}.(Z/3.048)^{(1/3)} / \{L.(\mu_L/\mu_w)^{0.16}.(\rho_w/\rho_L)^{1.25}.(\sigma_w/\sigma_L)^{0.8}\}^{0.6}$

$H_x[m] = \phi_h[m].(Sc)_L{}^{0.5}.K_3.(Z/3.048)^{0.15}$

Where D_c is a "corrected" diameter: the lesser of {diameter} or {2 × 0.3048}.

Where μ_w = 1.002 mPa.s ρ_w = 998.2032 $kg.m^{-3}$ σ_w = 70 $mN.m^{-1}$ (All at 20°C)

And $H_{Oy} = H_y + (m.G_M/L_M).H_x$ *NOTE: use of the coefficient* $(m.G_M/L_M)$ *implied the subscripts "Oy", "y" and "x" by CHE3102/Uhlherr.*

N_{Oy}: Colburn's equation of 1939 is:

$N_{Oy} = 1/\{1 - (m.G_M/L_M)\} \times \ln[\{1 - (m.G_M/L_M)\} \times \{(y_1 - m.x_2)/(y_2 - m.x_2)\} + m.G_M/L_M]$

Note: the G_M and L_M are (moles per time) per unit area (of the column).

"m" is a Henry's law-type constant here:

$\mathbf{y_{equilibrium\ 1} \equiv m.x_1}$

Feintuch/Treybal(1978) present an "Edmister-type approach":

$N_{Oy} = \ln[\{(y_1 - y_2^*)/(y_2-y_2^*)\}.(1-1/A_E) + 1/A_E] / (1 - 1/A_E)$

where $A_E = [A_{BOTTOM}.(A_{TOP} + 1) + 0.25]^{0.5} - 0.5$

and $(1/A_i) = (m_i.G_i/L_i)$

Calculations:

N_{Oy}: **According to Colburn:**

$(m.G_M/L_M)$ = 0.015343

$\{1 - (m.G_M/L_M)\}$ = 0.984657

∴ N_{Oy} = **5.365**

According to Feintuch & Treybal:

A_{BOTTOM} = 48.78104

A_{TOP} = 93.21043

The big difference here means the more sophisticated average is probably worth calculating!

A_E = 67.29331 (*cf.* arithmetic mean of 70.99574)

$\therefore N_{Oy} =$ 5.363

This non-simple short-cut method has resulted in a VERY SIMILAR result to the result from Colburn.

H_{Oy}: $y^*_{BM} =$ TOP: 0.982835
BOTTOM: 0.958368
AVERAGE: 0.970601

"Averages" are just simple, arithmetic.

$G_M =$ TOP: 119.3803 $mol.m^{-2}.s^{-1}$
BOTTOM: 98.8772 $mol.m^{-2}.s^{-1}$
AVERAGE: 109.1288 $mol.m^{-2}.s^{-1}$

From the data of Onda *et alii*:

$L =$ 16.6389 $kg.m^{-2}.s^{-1}$

OKAY $(\sigma_c/\sigma)^{0.75} =$ 1.1822 $(L/a_t.\mu_L)^{0.1} =$ 1.7689 $(L^2.a_t/(\rho_L^2.g))^{-0.05} =$ 1.3490 OKAY $(L^2/(\rho_L.\sigma.a_t))^{0.2} =$ 0.5311 OKAY

Bolles/Fair: $0.3<(\sigma_c/\sigma)<2$ *Bolles/Fair: $2.5e-9<Fr_L<0.018$* *Bolles/Fair: $1.2e-8<We_L<0.27$*

$a_w =$ 90.4 $m^2.m^{-3}$

$(Re)_L =$ 3.38E+02 OKAY $(\mu_L/\rho_L.D_L)^{-1/2} =$ 0.075777 $(a_t.D_p)^{0.4} =$ 1.934052

Bolles/Fair: $0.04<Re_L<500$

Hence: $k_L.(\rho_L/\mu_L.g)^{1/3} =$ 0.04270 where 0.0060 (*cf.* 0.0051) is the constant for this large, modern packing

Thus, $k_L =$ 0.000729 $m.s^{-1}$
$\rho_B =$ 52479 $mol.m^{-3}$
$\therefore k_x =$ 38.26 $mol.m^{-2}.s^{-1}$

$G =$ 2.5696 $kg.m^{-2}.s^{-1}$
$(Re)_G =$ 1.52E+03 OFF SCALE! $(\mu_G/\rho_G.D_G)^{-1/3} =$ 1.032485 $(a_t.D_p)^{-2.0} =$ 0.036954
Hence: $(k_G.R.T)/(a_t.D_G) =$ 38.606 where 6.00 (*cf.* 5.23) is the constant for this large, modern packing

Thus, $k_G =$ 2.5E-05 $mol.Pa^{-1}.m^{-2}.s^{-1}$ 0.000253 $mol.atm^{-1}.cm^{-2}.s^{-1}$
$P =$ 123 kPa(abs)
$\therefore k_y =$ 3.06 $mol.m^{-2}.s^{-1}$

We see that the gas-phase resistance is dominant.... (...also, "m" is small).
Hence: $K_y =$ 3.033 $mol.m^{-2}.s^{-1}$

$\therefore H_{Oy} =$ **0.410** m

***cf.* The data of the Norton Co. (for specific conditions) in Perry[(6)], p. 14-34, T14-4:**

$K_y.a.y^*_{BM} =$ 114 $kmol.h^{-1}.m^{-3}$
i.e. 31.667 $mol.m^{-3}.s^{-1}$
Whence $H_{Oy} =$ 3.446 m

Height: $h_{bed} =$ **2.20 m**

H_{Oy}: **By Cornell's (updated) method:**

Flooding: 58% $K_3 =$ 0.90
(At design percentage flooding, from charts in Bolles/Fair & Sinnott[(2)])
Flooding: 58% $\psi_h =$ 140 ft 42.672 m
$L[lb_m.h^{-1}ft^{-2}]$: 1.23E+04 $\phi_h =$ 0.120 ft 0.036576 m
(At design percentage flooding, from charts in Bolles/Fair: specific to metal Pall rings.)
Estimated height, "Z" = 1.53 m
$(Sc)_v^{0.5} =$ 0.953179 $D_c =$ 0.6096 m
$\{L.(\mu_L/\mu_w)^{0.16}.(\rho_w/\rho_L)^{1.25}.(\sigma_w/\sigma_L)^{0.8}\} =$ 15.63202 $kg.m^{-2}.s^{-1}$
$H_y =$ 0.279133 m

$(Sc)_L^{0.5} =$ 13.19657
$H_x =$ 0.391743 m

$\therefore H_{Oy} =$ **0.285** m
(We note that the extraordinarily low value of $m.G_M/L_M$ means the contribution of H_x is ~negligible.)

Height: $h_{bed} =$ 1.53 m (or **1.93 m** without height-correction)

ABSORBER DETAILED DESIGN

Model of a simplified case:

Stage 3

Reference(s): Perry[(6)], p. 14-20, 14-10.
"van Laar VLE" worksheet [by D.I.V.], & the relevant references therein.
"Diam.", "Visc.", "Gdiff" & "Ldiff" worksheets [D.I.V.], & references therein.
HYSIM material
I. Hahnenstein, H. Hasse, Y.-Q. Liu and G. Maurer; AIChE Symposium series
Onda *et alii* - original reference.

Assumptions:

Assume:	Comment:
1. Straight operating line (*i.e.* dilute solutions - small mass transfer)	This implies constant flowrates.
2. Straight equilibrium line (*i.e.* Henry's law is valid: $y_i = H_i.x_i$)	This may be reasonable, based on data presented in worksheet "van Laar VLE".
3. Absorption heat effects are negligible	This may or may not be valid: - Hysim's simulation says a large amount of heat [in kW] is evolved - however the absorber also has pump-around cooling, with large(?) liquid flow and so the actual temperature PROFILES in the absorber will not be great

Note: Perry's definition of the assumption is ambiguous, if not confusing.

Additionally, reaction is ignored.

Data:

Temperature at bottom of stage:	LIQUID:	51.00 °C	GAS:	50.00 °C		
Temperature at top of stage:	LIQUID:	40.09 °C	GAS:	42.00 °C		It is assumed that thermal equilibrium is (almost) reached.

Thus a nominal column temperature of 45.54601 °C will be used here ± 10°C, say.

Pressures:		TOP:	115	kPa(abs)	Estimate.
		BOTTOM:	120	kPa(abs)	
		AVERAGE:	117.5	kPa(abs)	
Henry's constant: ("m")	By linear regression of AIChE.J data in worksheet "van Laar VLE":		0.7514	(70°C)	This was only based on x_{HCHO} under 0.20
	By weighted least squares regression of the above:	(approx.)	1	(70°C)	
	Data from Ullmann's[(5)] & Walker[(3)]:		<< 1		This assumes equilibrium of reaction.
	All other estimates, including Raoult's law:		>> 1	(60°C)	This doesn't consider liquid-phase formation of nonvolatiles.
	Hence use the value:		0.7514		On the conservative side. THESE DO NOT CONSIDER INERTS PRESENT
Flows:	TOTAL liquid inflow:		722.1627	$mol.s^{-1}$	
	TOTAL liquid outflow:		734.4732	$mol.s^{-1}$	
	RATIO of BOTTOM to TOP liquid flows:		1.017047		Thus the flow may be considered constant.
	Average stage TOTAL liquid flow:		728.318	$mol.s^{-1}$	This average is justified by the high pump-around rate.
	Vapour inflow:		251.6118	$mol.s^{-1}$	Note: no vapour recirculation.
	Vapour outflow:		239.3013	$mol.s^{-1}$	
	RATIO of BOTTOM to TOP vapour flows:		1.051444		This is really NOT too large to assume constant flow.
	Average (total) vapour flow:		245.4566	$mol.s^{-1}$	
Mean molar masses:		GAS:	0.023713	$kg.mol^{-1}$	Worksheet "Diam."
		LIQUID:	0.019585	$kg.mol^{-1}$	Worksheet "Diam."
Mole-fractions:	Mole-fraction of formaldehyde in vapour:	TOP:	0.008476		
		BOTTOM:	0.0173		
		AVERAGE:	0.012868		NOTE: This average for reference only. (based on a 99.5% nominal aproach to equilibrium)
	Mole-fraction of formaldehyde in liquid:	TOP:	0.1292		There will be some formaldehyde in the pump-around liquid(!)…
		BOTTOM:	0.1302		...but too high would cause more formaldehyde to escape more easily.
		AVERAGE:	0.129709		The similarity is due to the large pump-around.
	Mole-fraction IN EQUILIBRIUM WITH liquid:	TOP:	0.0084		Note that temperature is the dominant effect here.
		BOTTOM:	0.0118		
		AVERAGE:	0.010125		
Equilibrium:	Hence "**m**":	TOP:	0.06525		Defined by $y_{equilibrium} \equiv m.x$
		BOTTOM:	0.090774		
		AVERAGE:	0.078061		Actual mean: 0.078012
Diameter:			**1.8**	m	Calculated in worksheet "Diam."
Flooding:		DESIGN:	53%		Worksheet "Diam."
		TURNDOWN:	32%		Worksheet "Diam."
Internals:	Type:		Pall rings		
	Material:		S.S.		
	σ_c:		75	$mN.m^{-1}$	Sinnott[(2)]
	Nominal size:		0.051	m	*I.e.* 2 inches.
	a_t:		102	$m^2.m^{-3}$	
Fluid properties:	μ_G:		1.66E-05	Pa.s	See worksheet "Visc.".

μ_L:		6.28E-04	Pa.s	Worksheet "Diam."
D_G:		**0.174**	$cm^2.s^{-1}$	See worksheet "GDiff".
D_L:		**2.4E-05**	$cm^2.s^{-1}$	See worksheet "LDiff".
ρ_G:		1.04	$kg.m^{-3}$	Worksheet "Diam."
ρ_L:		1050	$kg.m^{-3}$	Worksheet "Diam."
σ:	WATER, 303.15K:	71.40	$dyn.cm^{-1}$	Perry[(6)]
	WATER, 293.15K:	70	$mN.m^{-1}$	Sinnott[(2)]
	WATER, 293K:	72.8	$dyn.cm^{-1}$	R, P & P[(4)]
	WATER, 303K:	71.18	$dyn.cm^{-1}$	R, P & P[(4)]
	METHANOL, 333K:	19.41	$dyn.cm^{-1}$	R, P & P[(4)]
	ACETONE, 318K:	21.22	$dyn.cm^{-1}$	R, P & P[(4)]
	FORMAMIDE, 338K:	53.66	$dyn.cm^{-1}$	R, P & P[(4)]
	METHYL FORMATE, 298K:	24.62	$dyn.cm^{-1}$	R, P & P[(4)]
	METHYL FORMATE, 323K:	20.05	$dyn.cm^{-1}$	R, P & P[(4)]
	METHYL FORMATE, 373K:	12.90	$dyn.cm^{-1}$	R, P & P[(4)]
	ASSUME:	**60**	$dyn.cm^{-1}$	Surface tension reduces with T rising.

Mass-transfer coefficients:

Liquid "film":	Calculated;	see below.
Vapour "film":	Calculated;	see below.
Overall:	Calculated;	see below.

Equations:

Height: $h_{bed} = H_{Oy}.N_{Oy}$

H_{Oy}: $H_{Oy} = G_M/[(K_y.a).y^*_{BM}]$

where:

$y^*_{BM} = \{(1 - y) - (1 - y^*)\} / \ln\{(1 - y)/(1 - y^*)\}$

with y^* the equilibrium gas-phase mole fraction, such that $y^* = m.x$

and the rate of mass transfer, $N_i = K_y.(y_i - y^*_i)$, defines the overall gas-phase mass transfer coefficient

This K_y can also be expressed in terms of the "film" coefficients, *viz.* :

$1/K_y = 1/k_y + m/k_x$

NOTE: Poxy W. M. Edwards (& predecessors) use a different notation - care!!

From Onda *et alii* :

$k_L.(\rho_L/\mu_L.g)^{1/3} / \{(\mu_L/\rho_L.D_L)^{-1/2}.(a_t.D_p)^{0.4}\}$ is correlated against $(Re)_L = L/(a_w.\mu_L)$

$\{(k_G.R.T)/(a_t.D_G)\} / \{(\mu_G/\rho_G.D_G)^{-1/3}.(a_t.D_p)^{-2.0}\}$ is correlated against $(Re)_G = G/(a_t.\mu_G)$

$a_w/a_t = 1 - \exp\{-1.45(\sigma_c/\sigma)^{0.75}.(L/a_t.\mu_L)^{0.1} \times (L^2.a_t/(\rho_L{}^2.g))^{-0.05}.(L^2/(\rho_L.\sigma.a_t))^{0.2}\}$

Where $[G] = [L] = kg.m^{-2}.s^{-1}$ a_w is the "effective" - wetted - area per volume

Where: $K_G = K_y / P$ Where: $k_G = k_y / P$ Where: $k_L = k_x / \rho_L$ From Uhlherr, CHE3102 notes.

Alternatively, an estimate may be obtained from Cornell's method (*Sinnott* [(2)] *, updated by Bolles/Fair*)

$H_y[m] = 0.0190283.\psi_h[m].(Sc)_v{}^{0.5}.(D_c/0.3048)^{1.24}.(Z/3.048)^{(1/3)} / \{L.(\mu_L/\mu_w)^{0.16}.(\rho_w/\rho_L)^{1.25}.(\sigma_w/\sigma_L)^{0.8}\}^{0.6}$

$H_x[m] = \phi_h[m].(Sc)_L{}^{0.5}.K_3.(Z/3.048)^{0.15}$

Where D_c is a "corrected" diameter: the lesser of {diameter} or {2 × 0.3048}.

Where μ_w = 1.002 mPa.s ρ_w = 998.2032 $kg.m^{-3}$ σ_w = 70 $mN.m^{-1}$ (All at 20°C)

And $H_{Oy} = H_y + (m.G_M/L_M).H_x$ *NOTE: use of the coefficient* $(m.G_M/L_M)$ *implied the subscripts "Oy", "y" and "x" by CHE3102/Uhlherr.*

N_{Oy}: Colburn's equation of 1939 is:

$N_{Oy} = 1/\mathbf{\{1 - (m.G_M/L_M)\}} \times \ln[\mathbf{\{1 - (m.G_M/L_M)\}} \times \{(y_1 - m.x_2)/(y_2 - m.x_2)\} + \mathbf{m.G_M/L_M}]$ "m" is a Henry's law-type constant here:

Note: the G_M and L_M are (moles per time) per unit area (of the column). $\mathbf{y_{equilibrium\ 1} \equiv m.x_1}$

Feintuch/Treybal(1978) present an "Edmister-type approach":

$N_{Oy} = \ln[\{(y_1 - y_2{}^*)/(y_2 - y_2{}^*)\}.(1-1/A_E) + 1/A_E] / (1 - 1/A_E)$

where $A_E = [A_{BOTTOM}.(A_{TOP} + 1) + 0.25]^{0.5} - 0.5$

and $(1/A_i) = (m_i.G_i/L_i)$

Calculations:

N_{Oy}: **According to Colburn:**

$(m.G_M/L_M)$ = 0.026308

$\{1 - (m.G_M/L_M)\}$ = 0.973692

$\therefore N_{Oy}$ = **5.414**

According to Feintuch & Treybal:

A_{BOTTOM} = 32.15762

A_{TOP} = 46.24948

The big difference here means the more sophisticated average is probably worth calculating!

A_E = 38.48309 (*cf.* arithmetic mean of 39.20355)

$\therefore N_{Oy} =$ **5.413**

This non-simple short-cut method has resulted in a VERY SIMILAR result to the result from Colburn.

$\underline{H_{Oy}}$: $y^*_{BM} =$ TOP: 0.991547

BOTTOM: 0.985458

AVERAGE: 0.988502

"Averages" are just simple, arithmetic.

$G_M =$ TOP: 98.8772 $mol.m^{-2}.s^{-1}$

BOTTOM: 94.03947 $mol.m^{-2}.s^{-1}$

AVERAGE: 96.45834 $mol.m^{-2}.s^{-1}$

From the data of Onda *et alii*:

L = 5.6055 $kg.m^{-2}.s^{-1}$

OKAY $(\sigma_c/\sigma)^{0.75} =$ 1.1822 $(L/a_t.\mu_L)^{0.1} =$ 1.5638 $(L^2.a_t/(\rho_L{}^2.g))^{-0.05} =$ 1.5011 OKAY $(L^2/(\rho_L.\sigma.a_t))^{0.2} =$ 0.3450 OKAY

Bolles/Fair: $0.3<(\sigma_c/\sigma)<2$ *Bolles/Fair: $2.5e-9<Fr_L<0.018$* *Bolles/Fair: $1.2e-8<We_L<0.27$*

$a_w =$ 76.6 $m^2.m^{-3}$

$(Re)_L =$ 1.17E+02 OKAY $(\mu_L/\rho_L.D_L)^{-1/2} =$ 0.063423 $(a_t.D_p)^{0.4} =$ 1.934052

Bolles/Fair: $0.04<Re_L<500$

Hence: $k_L.(\rho_L/\mu_L.g)^{1/3} =$ 0.01756 where 0.0060 (*cf.* 0.0051) is the constant for this large, modern packing

Thus, $k_L =$ 0.000317 $m.s^{-1}$

$\rho_B =$ 53626 $mol.m^{-3}$

$\therefore k_x =$ 16.98 $mol.m^{-2}.s^{-1}$

G = 2.2873 $kg.m^{-2}.s^{-1}$

$(Re)_G =$ 1.35E+03 OFF SCALE! $(\mu_G/\rho_G.D_G)^{-1/3} =$ 1.028897 $(a_t.D_p)^{-2.0} =$ 0.036954

Hence: $(k_G.R.T)/(a_t.D_G) =$ 35.462 where 6.00 (*cf.* 5.23) is the constant for this large, modern packing

Thus, $k_G =$ 2.37E-05 $mol.Pa^{-1}.m^{-2}.s^{-1}$ 0.00024 $mol.atm^{-1}.cm^{-2}.s^{-1}$

P = 118 kPa(abs)

$\therefore k_y =$ 2.78 $mol.m^{-2}.s^{-1}$

We see that the gas-phase resistance is [VERY!] dominant.... (...also, "m" is small).

Hence: $K_y =$ 2.746 $mol.m^{-2}.s^{-1}$

$\therefore H_{Oy} =$ **0.464** m

***cf.* The data of the Norton Co. (for specific conditions) in Perry(6), p. 14-34, T14-4:**

$K_y.a.y^*_{BM} =$ 114 $kmol.h^{-1}.m^{-3}$

i.e. 31.667 $mol.m^{-3}.s^{-1}$

Whence $H_{Oy} =$ 3.046 m

Height: $h_{bed} =$ **2.51 m**

$\underline{H_{Oy}}$: **By Cornell's (updated) method:**

Flooding: 53% $K_3 =$ 0.94

(At design percentage flooding, from charts in Bolles/Fair & Sinnott(2))

Flooding: 53% $\psi_h =$ 140 ft 42.672 m

$L[lb_m.h^{-1}ft^{-2}]$: 4.13E+03 $\phi_h =$ 0.088 ft 0.026822 m

(At design percentage flooding, from charts in Bolles/Fair: specific to metal Pall rings.)

Estimated height, "Z" = 3.95 m

$(Sc)_v{}^{0.5} =$ 0.958168 $D_c =$ 0.6096 m

$\{L.(\mu_L/\mu_w)^{0.16}.(\rho_w/\rho_L)^{1.25}.(\sigma_w/\sigma_L)^{0.8}\} =$ 5.522268 $kg.m^{-2}.s^{-1}$

$H_y =$ 0.718652 m

$(Sc)_L{}^{0.5} =$ 15.76725

$H_x =$ 0.413303 m

$\therefore H_{Oy} =$ **0.730** m

(We note that the extraordinarily low value of $m.G_M/L_M$ means the contribution of H_x is ~negligible.)

Height: $h_{bed} =$ **3.95 m** (or 3.62 m without height-correction)

ABSORBER DETAILED DESIGN

Model of a simplified case:

Stage 4

Reference(s): Perry[(6)], p. 14-20, 14-10.
"van Laar VLE" worksheet [by D.I.V.], & the relevant references therein.
"Diam.", "Visc.", "Gdiff" & "Ldiff" worksheets [D.I.V.], & references therein.
HYSIM material
I. Hahnenstein, H. Hasse, Y.-Q. Liu and G. Maurer; AIChE Symposium series
Onda *et alii* - original reference.

Assumptions:

Assume:	Comment:
1. Straight operating line (*i.e.* dilute solutions - small mass transfer)	This implies constant flowrates.
2. Straight equilibrium line (*i.e.* Henry's law is valid: $y_i = H_i.x_i$)	This may be reasonable, based on data presented in worksheet "van Laar VLE".
3. Absorption heat effects are negligible	This may or may not be valid: - Hysim's simulation says a large amount of heat [in kW] is evolved - however the absorber also has pump-around cooling, with large(?) liquid flow and so the actual temperature PROFILES in the absorber will not be great

Note: Perry's definition of the assumption is ambiguous, if not confusing.

Additionally, reaction is ignored.

Data:

			Value	Unit	Comment
Temperature at bottom of stage:	LIQUID:		43.00	°C	
	GAS:		42.00	°C	
Temperature at top of stage:	LIQUID:		37.00	°C	It is assumed that thermal equilibrium is (almost) reached.
	GAS:		37.50	°C	
	Thus a nominal column temperature of		40	°C will be used here	± 10°C, say.
Pressures:		TOP:	110	kPa(abs)	Estimate.
		BOTTOM:	115	kPa(abs)	
		AVERAGE:	112.5	kPa(abs)	
Henry's constant:	By linear regression of AIChE.J data in worksheet "van Laar VLE":		0.7514	(70°C)	This was only based on x_{HCHO} under 0.20
("m")	By weighted least squares regression of the above:	(approx.)	1	(70°C)	
	Data from Ullmann's[(5)] & Walker[(3)]:		<< 1		This assumes equilibrium of reaction.
	All other estimates, including Raoult's law:		>> 1	(60°C)	This doesn't consider liquid-phase formation of nonvolatiles.
	Hence use the value:		0.7514		On the conservative side. THESE DO NOT CONSIDER INERTS PRESENT
Flows:	TOTAL liquid inflow:		18.17909	$mol.s^{-1}$	
	TOTAL liquid outflow:		20.85713	$mol.s^{-1}$	
	RATIO of BOTTOM to TOP liquid flows:		1.147314		Thus the flow may NOT be considered constant.
	Average stage TOTAL liquid flow:		19.51811	$mol.s^{-1}$	Not justified, due to the absence of any (high) pump-around.
	Vapour inflow:		239.3013	$mol.s^{-1}$	Note: no vapour recirculation.
	Vapour outflow:		236.6233	$mol.s^{-1}$	
	RATIO of BOTTOM to TOP vapour flows:		1.011318		This is really NOT too large to assume constant flow.
	Average (total) vapour flow:		237.9623	$mol.s^{-1}$	
Mean molar masses:		GAS:	0.023675	$kg.mol^{-1}$	Worksheet "Diam."
		LIQUID:	0.018015	$kg.mol^{-1}$	Worksheet "Diam."
Mole-fractions:	Mole-fraction of formaldehyde in vapour:	TOP:	0.000103		Entering zero here would give infinite height.
		BOTTOM:	0.0085		
		AVERAGE:	0.004289		NOTE: This average for reference only.
	Mole-fraction of formaldehyde in liquid:	TOP:	0.0000		(based on a 99.5% nominal aproach to equilibrium) There will be some formaldehyde in the pump-around liquid(!)…
		BOTTOM:	0.0961		...but too high would cause more formaldehyde to escape more easily.
		AVERAGE:	0.048036		The disimilarity is due to the absence of a (large) pump-around.
	Mole-fraction IN EQUILIBRIUM WITH liquid:	TOP:	0.0000		Note that temperature is the dominant effect here.
		BOTTOM:	0.0065		
		AVERAGE:	0.003257		
Equilibrium:	Hence "**m**":	TOP:	0.068109		Defined by $y_{equilibrium} \equiv m.x$
		BOTTOM:	0.067809		We see that for this reducing concentration which varies little absolutely,
		AVERAGE:	0.067809		"m" is quite constant. Thus bottom value can be taken as value everywhere at top. Actual mean: 0.067959
Diameter:			**1.8**	m	Calculated in worksheet "Diam."
Flooding:		DESIGN:	179%	Minute liquid flow!	Worksheet "Diam."
		TURNDOWN:	107%	Minute liquid flow!	Worksheet "Diam."
Internals:	Type:		Pall rings	???	
	Material:		S.S.	?	
	σ_c:		75	$mN.m^{-1}$?	Sinnott[(2)]
	Nominal size:		0.051	m ???	*I.e.* 2 inches.
	a_t:		102	$m^2.m^{-3}$???	
Fluid properties:	μ_G:		1.66E-05	Pa.s	See worksheet "Visc.".

μ_L:		7.58E-04	Pa.s	Worksheet "Diam."
D_G:		0.174	$cm^2.s^{-1}$	See worksheet "GDiff".
D_L:		2.2E-05	$cm^2.s^{-1}$	See worksheet "LDiff".
ρ_G:		1.01	$kg.m^{-3}$	Worksheet "Diam."
ρ_L:		995	$kg.m^{-3}$	Worksheet "Diam."
σ:	WATER, 303.15K:	71.40	$dyn.cm^{-1}$	Perry[(6)]
	WATER, 293.15K:	70	$mN.m^{-1}$	Sinnott[(2)]
	WATER, 293K:	72.8	$dyn.cm^{-1}$	R, P & P[(4)]
	WATER, 303K:	71.18	$dyn.cm^{-1}$	R, P & P[(4)]
	METHANOL, 333K:	19.41	$dyn.cm^{-1}$	R, P & P[(4)]
	ACETONE, 318K:	21.22	$dyn.cm^{-1}$	R, P & P[(4)]
	FORMAMIDE, 338K:	53.66	$dyn.cm^{-1}$	R, P & P[(4)]
	METHYL FORMATE, 298K:	24.62	$dyn.cm^{-1}$	R, P & P[(4)]
	METHYL FORMATE, 323K:	20.05	$dyn.cm^{-1}$	R, P & P[(4)]
	METHYL FORMATE, 373K:	12.90	$dyn.cm^{-1}$	R, P & P[(4)]
	ASSUME:	60	$dyn.cm^{-1}$	Surface tension reduces with T rising.

Mass-transfer coefficients:

Liquid "film":	Calculated;	see below.
Vapour "film":	Calculated;	see below.
Overall:	Calculated;	see below.

Equations:

Height: $h_{bed} = H_{Oy}.N_{Oy}$

H_{Oy}: $H_{Oy} = G_M/[(K_y.a).y^*_{BM}]$

where:

$y^*_{BM} = \{(1 - y) - (1 - y^*)\} / \ln\{(1 - y)/(1 - y^*)\}$

with y^* the equilibrium gas-phase mole fraction, such that $y^* = m.x$

and the rate of mass transfer, $N_i = K_y.(y_i - y^*_i)$, defines the overall gas-phase mass transfer coefficient

This K_y can also be expressed in terms of the "film" coefficients, *viz.* :

$1/K_y = 1/k_y + m/k_x$

NOTE: Poxy W. M. Edwards (& predecessors) use a different notation - care!!

From Onda *et alii* :

$k_L.(\rho_L/\mu_L.g)^{1/3} / \{(\mu_L/\rho_L.D_L)^{-1/2}.(a_t.D_p)^{0.4}\}$ is correlated against $(Re)_L = L/(a_w.\mu_L)$

$\{(k_G.R.T)/(a_t.D_G)\} / \{(\mu_G/\rho_G.D_G)^{-1/3}.(a_t.D_p)^{-2.0}\}$ is correlated against $(Re)_G = G/(a_t.\mu_G)$

$a_w/a_t = 1 - \exp\{-1.45(\sigma_c/\sigma)^{0.75}.(L/a_t.\mu_L)^{0.1} \times (L^2.a_t/(\rho_L{}^2.g))^{-0.05}.(L^2/(\rho_L.\sigma.a_t))^{0.2}\}$

Where $[G] = [L] = kg.m^{-2}.s^{-1}$ a_w is the "effective" - wetted - area per volume

Where: $K_G = K_y / P$ Where: $k_G = k_y / P$ Where: $k_L = k_x / \rho_L$ From Uhlherr, CHE3102 notes.

Alternatively, an estimate may be obtained from Cornell's method (*Sinnott* [(2)] *, updated by Bolles/Fair*)

$H_y[m] = 0.0190283.\psi_h[m].(Sc)_v{}^{0.5}.(D_c/0.3048)^{1.24}.(Z/3.048)^{(1/3)} / \{L.(\mu_L/\mu_w)^{0.16}.(\rho_w/\rho_L)^{1.25}.(\sigma_w/\sigma_L)^{0.8}\}^{0.6}$

$H_x[m] = \phi_h[m].(Sc)_L{}^{0.5}.K_3.(Z/3.048)^{0.15}$

Where D_c is a "corrected" diameter: the lesser of {diameter} or {2 × 0.3048}.

Where μ_w = 1.002 mPa.s ρ_w = 998.2032 $kg.m^{-3}$ σ_w = 70 $mN.m^{-1}$ (All at 20°C)

And $H_{Oy} = H_y + (m.G_M/L_M).H_x$ *NOTE: use of the coefficient* $(m.G_M/L_M)$ *implied the subscripts "Oy", "y" and "x" by CHE3102/Uhlherr.*

N_{Oy}: Colburn's equation of 1939 is:

$N_{Oy} = 1/\{1 - (m.G_M/L_M)\} \times \ln[\{1 - (m.G_M/L_M)\} \times \{(y_1 - m.x_2)/(y_2 - m.x_2)\} + m.G_M/L_M]$ "m" is a Henry's law-type constant here:

Note: the G_M and L_M are (moles per time) per unit area (of the column). $y_{equilibrium\ 1} \equiv m.x_1$

Feintuch/Treybal(1978) present an "Edmister-type approach":

$N_{Oy} = \ln[\{(y_1 - y_2^*)/(y_2-y_2^*)\}.(1-1/A_E) + 1/A_E] / (1 - 1/A_E)$

where $A_E = [A_{BOTTOM}.(A_{TOP} + 1) + 0.25]^{0.5} - 0.5$

and $(1/A_i) = (m_i.G_i/L_i)$

Calculations:

N_{Oy}: **According to Colburn:**

$(m.G_M/L_M)$ = 0.826716

$\{1 - (m.G_M/L_M)\}$ = 0.173284

∴ N_{Oy} = **14.978**

According to Feintuch & Treybal:

A_{BOTTOM} = 1.285356

A_{TOP} = 1.127999

The big difference here means the more sophisticated average is probably worth calculating!

A_E = 1.227783 (*cf.* arithmetic mean of 1.206677)

$\therefore N_{Oy}$ = 14.961 (Note: using A_{BOTTOM} only yields: 13.264)

This non-simple short-cut method has resulted in a VERY CLOSE result to the result from Colburn.

However previous results so close to Colburn, that we will assume that result is good here too.

$\underline{H_{Oy}}$: y^*_{BM} = TOP: 0.999948

BOTTOM: 0.992505

AVERAGE: 0.996227 "Averages" are just simple, arithmetic.

G_M = TOP: 94.03947 $mol.m^{-2}.s^{-1}$

BOTTOM: 92.98707 $mol.m^{-2}.s^{-1}$

AVERAGE: 93.51327 $mol.m^{-2}.s^{-1}$

From the data of Onda *et alii*:

L = 0.1382 $kg.m^{-2}.s^{-1}$ OKAY OKAY

OKAY $(\sigma_c/\sigma)^{0.75}$ = 1.1822 $(L/a_t.\mu_L)^{0.1}$ = 1.0599 $(L^2.a_t/(\rho_L^2.g))^{-0.05}$ = 2.1622 $(L^2/(\rho_L.\sigma.a_t))^{0.2}$ = 0.0793

Bolles/Fair: 0.3<(σ_c / σ)<2 *Bolles/Fair: 2.5e-9<Fr_L<0.018* *Bolles/Fair: 1.2e-8<We_L<0.27*

a_w = 27.3 $m^2.m^{-3}$

$(Re)_L$ = 6.68E+00 *OKAY* $(\mu_L/\rho_L.D_L)^{-1/2}$ = 0.053323 $(a_t.D_p)^{0.4}$ = 1.934052

Bolles/Fair: 0.04<Re_L<500

Hence: $k_L.(\rho_L/\mu_L.g)^{1/3}$ = 0.00220 where 0.0060 (*cf.* 0.0051) is the constant for this large, modern packing

Thus, k_L = 4.29E-05 $m.s^{-1}$

ρ_B = 55255 $mol.m^{-3}$

$\therefore k_x$ = 2.37 $mol.m^{-2}.s^{-1}$

G = 2.2139 $kg.m^{-2}.s^{-1}$

$(Re)_G$ = 1.31E+03 OFF SCALE! $(\mu_G/\rho_G.D_G)^{-1/3}$ = 1.018091 $(a_t.D_p)^{-2.0}$ = 0.036954

Hence: $(k_G.R.T)/(a_t.D_G)$ = 34.298 where 6.00 (*cf.* 5.23) is the constant for this large, modern packing

Thus, k_G = 2.34E-05 $mol.Pa^{-1}.m^{-2}.s^{-1}$ 0.000237 $mol.atm^{-1}.cm^{-2}.s^{-1}$

P = 113 kPa(abs)

$\therefore k_y$ = 2.63 $mol.m^{-2}.s^{-1}$

We see that the gas-phase resistance is dominant.... (...also, "m" is small).

Hence: K_y = 2.443 $mol.m^{-2}.s^{-1}$

$\therefore H_{Oy}$ = **1.407** m

***cf.* The data of the Norton Co. (for specific conditions) in Perry[(6)], p. 14-34, T14-4:**

$K_y.a.y^*_{BM}$ = 114 $kmol.h^{-1}.m^{-3}$

i.e. 31.667 $mol.m^{-3}.s^{-1}$

Whence H_{Oy} = 2.953 m

Height: h_{bed} = **21.08 m**

$\underline{H_{Oy}}$: **By Cornell's (updated) method:**

Flooding: **179%** K_3 = 1 **??? - Off chart!**

(At design percentage flooding, from charts in Bolles/Fair & Sinnott(2))

Flooding: **179%** ψ_h = 150 ft 45.72 m **??? - Off chart!**

$L[lb_m.h^{-1}ft^{-2}]$: **1.02E+02** ϕ_h = 0.051 ft 0.015545 m **??? - [Just] Off chart!**

(At design percentage flooding, from charts in Bolles/Fair: specific to metal Pall rings.)

Estimated height, "Z" = 529.71 m

$(Sc)_v^{0.5}$ = 0.973464 D_c = 0.6096 m

$\{L.(\mu_L/\mu_w)^{0.16}.(\rho_w/\rho_L)^{1.25}.(\sigma_w/\sigma_L)^{0.8}\}$ = **0.149992** $kg.m^{-2}.s^{-1}$

H_y = 34.84471 m

$(Sc)_L^{0.5}$ = 18.75357

H_x = 0.631935 m

$\therefore H_{Oy}$ = **35.367** m

(We note that the extraordinarily low value of $m.G_M/L_M$ means the contribution of H_x is ~negligible.)

Height: h_{bed} = **529.71 m** (or 94.92 m without height-correction)

Diameter computation

Design for a pressure drop of 42 mm(H_2O).m^{-1} at the design condition.
==> approx. 412 Pa.m^{-1}
i.e. 20.58 kPa for a 50 m column.

Note: Assuming a CONSTANT DIAMETER for the entire column, this would have to be evaluated for all stages,
for the full range of possible operating conditions.
Each evaluated at the top of the stage (the lower values).

	STAGE 1 Design	0.6×Design	**STAGE 2** Design	0.6×Design	**STAGE 3** Design	0.6×Design	**STAGE 4: Option a** Design	0.6×Design	**STAGE 4: Option b** Design	0.6×Design	
Lower gas flow rate [mol.s^{-1}]	303.79	182.27	251.61	150.97	239.30	143.58	236.62	141.97	236.62	141.97	
Lower gas flow rate [kg.s^{-1}]	7.0173	4.2104	5.9245	3.5547	5.6745	3.4047	5.6020	3.3612	5.6020	3.3612	
Mean M_R [kg.mol^{-1}]	0.02310	0.02310	0.02355	0.02355	0.02371	0.02371	0.02367	0.02367	0.02367	0.02367	
Lower liquid flow rate [mol.s^{-1}]	1372.04	823.22	2048.58	1229.15	722.16	433.30	18.18	10.91	18.18	10.91	
Lower liquid flow rate [kg.s^{-1}]	31.4798	18.8879	41.8084	25.0850	14.1438	8.4863	0.3275	0.1965	0.3275	0.1965	
Mean M_R [kg.mol^{-1}]	0.02294	0.02294	0.02041	0.02041	0.01959	0.01959	0.01802	0.01802	0.01802	0.01802	
p [kPa(abs)]	125	125	120	120	115	115	110	110	110	110	
Temperature [K]	335.15	335.15	323.15	323.15	315.15	315.15	310.65	310.65	310.65	310.65	
	62.00	62	50.00	50	42.00	42	37.50	37.5	37.50	37.5	
Ideal gas density [mol.m^{-3}]	44.857	44.857	44.662	44.662	43.888	43.888	42.588	42.588	42.588	42.588	
Ideal gas density [kg.m^{-3}]	1.036	1.036	1.052	1.052	1.041	1.041	1.008	1.008	1.008	1.008	
Liquid mass fraction HCHO [-]	0.526098	0.526098083	0.287507	0.287507374	0.198101	0.198100722	0	0	0	0	
Liquid mass fraction CH_3OH [-]	0.009723	0.009723183	0.004953	0.004953359	0.001972	0.001971719	0	0	0	0	
a	1.151	1.151	1.092	1.092	1.092	1.092	1.092	1.092	1.092	1.092	
b	0.5015	0.5015	0.30	0.30	0.30	0.30	0.30	0.30	0.30	0.30	
c	0.0161	0.0161	0	0	0	0	0	0	0	0	
Liquid density [kg.m^{-3}]	1132.1	1132.1	1071.0	1071.0	1050.3	1050.3	995.4	995.4	995.4	995.4	
$\rho/1000 = a + 0.30(X_F-b) - 0.25(X_M-c) - \mathbf{10^{-4}}.\{5.5(X_F-0.30) + 5.4\}.(t[°C]-20)$					(*Ullmann's* (5))						
And note the misprinted exponent in the original.											
Compare with *Walker* (3): Values greater than 1000 okay.											
Compare with *K-O* (4):	1134.8	1134.8	1071.9	1071.9	1050.4	1050.4	993.5	993.5	993.5	993.5	
$\rho/1000 = \{1.119 + 0.30(X_F-0.45) - 0.27(X_M)\}.\{1.0 + 0.00055.(55-t[°C])\}$											
$\therefore (L / G).(\rho_V / \rho_L)^{0.5}$	1.36E-01	1.36E-01	2.21E-01	2.21E-01	7.85E-02	7.85E-02	1.86E-03	1.86E-03	1.86E-03	1.86E-03	
From Fig. 11.44: K_4	1.2	1.2	1.2	1.2	1.3	1.3	0.13	0.13	???	???	
							(extrapol'n of Treybal)		(very large)		
cf. K_4 at flooding	2.8	2.8	3.2	3.2	3.5	3.5	0.32	0.32	???	???	
							(extrapol'n of Treybal)		(very large)		
Percentage of flooding	65%	65%	61%	61%	61%	61%	64%	64%	#VALUE!	#VALUE!	
Sinnott (2) calls 66% "satisfactory"							**(out of range)**		**(out of range)**		
Liquid viscosity [mPa.s]	1.892	1.892	1.226	1.226	1.054	1.054	0.380	0.380	0.380	0.380	
From *Ullmann's* (5) = *K-O* (4): $\eta = 1.28 + 3.9XF + 5X_M - 0.024t[°C]$					Out of range ==> compare with values for water						
	0.450	0.450	0.544	0.544	0.628	0.628	0.758	0.758	0.758	0.758	
Hence:	1.892	1.892	1.226	1.226	0.841	0.841	0.758	0.758	0.758	0.758	
Packing	Pall rings	Pall rings	Pall rings	Pall rings	Pall rings	Pall rings	Pall rings	Pall rings	Plastic gauze		*or trays???*
Size [mm]	50	50	50	50	50	50	50	50	(*e.g.* Sulzer, Type BX)		
F_p [m^{-1}] *Table 11.3, Sinnott* (2)	66	66	66	66	66	66	66	66			$c_{G,MAX}$...···
a [m^2.m^{-3}] *Table 11.3, Sinnott* (2)	102	102	102	102	102	102	102	102			
$\therefore G^2 = \{K_4.\rho_V.(\rho_L-\rho_V)\}/\{13.1F_P.(\mu_L/\rho_L)^{0.1}\}$ [kg.m^{-2}.s^{-1}]^2									Largest A	Smallest A	
	6.151	6.151	6.134	6.134	6.683	6.683	**0.617**	**0.617**	0.6	5	G.$\rho_V^{0.5}$ [(m^3.m^{-2}.s^{-1}).(kg.m^{-3})$^{0.5}$]
G [kg.m^{-2}.s^{-1}]	2.480	2.480	2.477	2.477	2.585	2.585	0.785	0.785	0.5975	4.9795	G [m^3.m^{-2}.s^{-1}] = "F"
									F[m^3.m^{-2}.s^{-1}]=	1.5	is typical
Whence A [m^2]	2.829	1.698	2.392	1.435	2.195	1.317	7.133	4.280	0.6025	5.0206	G [kg.m^{-2}.s^{-1}]
$\therefore$ L [kg.m^{-2}.s^{-1}]	11.126	11.126	17.477	17.477	6.443	6.443	0.046	0.046	9.29837	0.669482656	$\therefore$ A [m^2]
G_M [mol.m^{-2}.s^{-1}]	107.369	107.369	105.182	105.182	109.019	109.019	33.173	33.173	Fortunately the	**2.5447**	m^2
L_M [mol.m^{-2}.s^{-1}]	484.927	484.927	856.378	856.378	328.996	328.996	2.549	2.549	chosen for the bottom three stages		
Thus diameter [m]	1.898	1.470	1.745	1.352	1.672	1.295	3.014	2.334	is right within this range!		
									...so use that value for the top stage too.		
Say diameter of column (bottom 3 stages) is				**1.8** m					2.5447	2.5447	A [m^2]
Column area [m^2]				2.5447					2.2014	1.3209	G [kg.m^{-2}.s^{-1}]
Packing size to column diameter ratio:				36.0					**2.1834**	**1.3101**	G [m^3.m^{-2}.s^{-1}] = "F"
Sinnott (2): "a larger packing size could be considered"									0.128699	0.0772	L [kg.m^{-2}.s^{-1}]
Percentage flooding at selected diameter:									**0.465441**	**0.2793**	L [m^3.m^{-2}.h^{-1}]
	72.8%	43.7%	57.6%	34.5%	52.6%	**31.5%**	**178.7%**	**107.2%**	Fortunately this is within the range:		
This should be okay.							CLEARLY PALL		Minimum:	**0.05**	m^3.m^{-2}.h^{-1}
							RINGS DON'T APPLY		Maximum:	**60**	m^3.m^{-2}.h^{-1}
G [kg.m^{-2}.s^{-1}]	2.7576	1.6546	2.3282	1.3969	2.2299	1.3380	2.2014	1.3209	Typical:	**4**	m^3.m^{-2}.h^{-1}
L [kg.m^{-2}.s^{-1}]	12.371	7.422	16.430	9.858	5.558	3.335	0.129	0.077	13.2	5.3	Pressure drop [kPa.m^{-1}]
G_M [mol.m^{-2}.s^{-1}]	119.380	71.628	98.877	59.326	94.039	56.424	92.987	55.792			(*from Sulzer-Chemtech chart*)
L_M [mol.m^{-2}.s^{-1}]	539.176	323.506	805.042	483.025	283.792	170.275	7.144	4.286			
									6.4	8.8	Typical NTU.m^{-1}
											Is this H_{OG}^{-1} xor H_{OL}^{-1}???
									Note: This is NOT for the (reacting) HCHO–H_2O system		

Gas viscosity computation

Using the method of Wilke, given by R, P & P[(4)]

Molar mass:			
	Water (1)	18.0152	$g.mol^{-1}$
	Formaldehyde (2)	30.0262	$g.mol^{-1}$
	Hydrogen (3)	2.0158	$g.mol^{-1}$
	Nitrogen (4)	28.0134	$g.mol^{-1}$

	STAGE 1	STAGE 2	STAGE 3	STAGE 4	
Temperature:					
t [°C]	76	56	46	39.75	Average for gas.
T [K]	349.15	329.15	319.15	312.9	
Composition: mole fraction					
Water (1)	0.202668	0.229474	0.120116	0.084646	
Formaldehyde (2)	0.142986	0.055279	0.01726	0.008476	
Hydrogen (3)	0.115716	0.12681	0.153106	0.160982	
Nitrogen (4)	0.538631	0.588437	0.709518	0.745897	

This is entering, so not at equilibrium.

Nitrogen mole fraction decreased by taking value at bottom of stage, but increased by assuming all other components as nitrogen.

Approx. pure component viscosity [Pa.s]:					
Water (1)	1.11E-05	1.04E-05	1.00E-05	9.87E-06	From Y&R[(5)], rounded to nearest 5°C
Formaldehyde (2)	1.12E-05	1.05E-05	1.02E-05	1.00E-05	Assume as for methanol: Perry[(6)], to nearest 10°C
Hydrogen (3)	1.00E-05	9.50E-06	9.50E-06	9.00E-06	Perry[(6)], to nearest ~25K
Nitrogen (4)	2.00E-05	1.90E-05	1.90E-05	1.80E-05	Perry[(6)], to nearest ~25K

Wilke's parameter's: $\phi_{ij} = \{1 + (\eta_i/\eta_j)^{1/2}.(M_j/M_i)^{1/4}\}^2 / \{8(1 + Mi/Mj)\}^{1/2}$

	STAGE 1	STAGE 2	STAGE 3	STAGE 4
i = 1				
ϕ_{i1}	1	1	1	1
ϕ_{i2}	1.269471	1.269066	1.262202	1.266702
ϕ_{i3}	0.290487	0.288971	0.284755	0.289163
ϕ_{i4}	0.925623	0.919832	0.90374	0.920565
i = 2				
ϕ_{i1}	0.768523	0.768739	0.772445	0.770009
ϕ_{i2}	1	1	1	1
ϕ_{i3}	0.209955	0.208986	0.206894	0.209371
ϕ_{i4}	0.739786	0.735653	0.726742	0.737295
i = 3				
ϕ_{i1}	2.338808	2.359044	2.417614	2.356457
ϕ_{i2}	2.792292	2.816461	2.870285	2.8068
ϕ_{i3}	1	1	1	1
ϕ_{i4}	1.910394	1.910394	1.910394	1.910394
i = 4				
ϕ_{i1}	1.072542	1.080692	1.104258	1.07965
ϕ_{i2}	1.415965	1.426829	1.451003	1.422487
ϕ_{i3}	0.274938	0.274938	0.274938	0.274938
ϕ_{i4}	1	1	1	1

Terms in series:				
i = 1	2.45E-06	2.72E-06	1.45E-06	1.01E-06
i = 2	2.22E-06	8.4E-07	2.68E-07	1.29E-07
i = 3	5.73E-07	6.18E-07	7.87E-07	8.01E-07
i = 4	1.09E-05	1.18E-05	1.48E-05	1.5E-05
∴ SUM = viscosity of mixture [Pa.s]:				
	1.61E-05	1.59E-05	1.73E-05	1.7E-05

It turns out that the decrease in temperature (==> decreasing viscosity) almost exactly compensates for the increase in mole fraction of nitrogen (which has double the viscosity of the others)!

Thus, in ALL cases in the absorber, take the gas viscosity as: 1.66E-05 Pa.s

Comparison with mole-fraction weighted means:

	1.58E-05	1.54E-05	1.63E-05	1.58E-05
"ERROR"	-2.1%	-3.7%	-5.9%	-6.9%

Hence the viscosity would have been underestimated by an average factor of 4.7%

However we see that, although in some cases Wilke's method gives identical values as experiment (methane–propane at 498K), in other cases errors may be +12% (nitrogen–hydrogen at 373K, $y_N = 0.2$) or -12% (ammonia–hydrogen at 306K, $y_A = 0.399$).

Only Reichenberg's method is consistently accurate to **no more than** ±4.8% w.r.t. experiment (these extremes occur for the same conditions as for Wilke's method, above).
As may be guessed, Reichenberg's method is more involved.

Gas-phase diffusivity computation

Assuming binary diffusion:
Formaldehyde in nitrogen (main constituent)

Use the method of Fuller *et alii* (1965–1969), recommended by R, P & P(4)

(Average abs. error = 5.4%)

$$\mathbf{D_{AB}}[\mathrm{cm}^2.\mathrm{s}^{-1}] = \mathbf{0.00143\ T}[\mathrm{K}]^{1.75} \mathbf{/\ \{P}[\mathrm{bar}]\mathbf{.M_{AB}}[\mathrm{g.mol}^{-1}]\}^{1/2}\mathbf{.[\ (\Sigma_v)_A{}^{1/3} + (\Sigma_v)_B{}^{1/3}\ ]\}^2}$$

where $\mathbf{M_{AB} = 2 / (1/M_A + 1/M_B)}$
and Σ_v is the "diffusion volume" sum - atoms (xor =molecule):

Σ_v

Atomic and Structural Diffusion Volume Increments

C	15.9
H	2.31
O	6.11
N	4.54
Aromatic ring	-18.3
Heterocyclic ring	-18.3
F	14.7
Cl	21.0
Br	21.9
I	29.8
S	22.9

Diffusion Volumes of Simple Molecules

He	2.67
Ne	5.98
Ar	16.2
Kr	24.5
Xe	32.7
H_2	6.12
D_2	6.84
N_2	18.5
O_2	16.3
Air	19.7
CO	18.0
CO_2	26.9
N_2O	35.9
NH_3	20.7
H_2O	13.1
SF_6	71.3
Cl_2	38.4
Br_2	69.0
SO_2	41.8

Thus, for formaldehyde:

(Sv)A	26.63	
M_A	30.0262	g.mol^{-1}

For nitrogen:

(Sv)B	18.5	(*cf.* 9.08 for individual contributions)
M_B	28.0134	g.mol^{-1}

Hence: $\mathbf{[\ (\Sigma_v)_A{}^{1/3} + (\Sigma_v)_B{}^{1/3}\ ]}$ = 5.631019

	STAGE 1	**STAGE 2**	**STAGE 3**	**STAGE 4**
p [kPa(abs)]	125	120	115	110
Temperature [K]	335.15	323.15	315.15	310.65
Temperature [°C]	62.00	50.00	42.00	37.50
M_{AB}	28.98	28.98	28.98	28.98
Hence DAB[cm2.s-1] =	0.176	0.172	0.172	0.175

Again this is so invariant that it may be taken as constant across the entire column: **0.174 cm2.s-1**

(We note that the decreasing temperature is compensated for by [commensurately?] decreasing pressure.)

Use the method of Gilliland (1934), recommended by Holman(7)

$$D_{AB}[cm^2.s^{-1}] = 435.7\ T[K]^{1.5} / \{P[Pa].M_{AB}[g.mol^{-1}]^{1/2}.[\ (\Sigma_v)_A^{1/3} + (\Sigma_v)_B^{1/3}\ ]\}^2$$

where $M_{AB} = 2 / (1/M_A + 1/M_B)$

and Σ_v is the molecular volume - summation of atomic contributions:

Σ_v

Atomic and Structural Diffusion Volume Increments

C	14.8
H	3.7
O	
in aldehydes/ketones	7.4
in methyl esters	9.1
in ethyl esters	9.9
in higher esters/ethers	11
in acids	12
in union with S/P/N	8.3
N	
in primary amines	10.5
in secondary amines	1.20
F	8.7
Cl	
terminal	21.6
medial	24.6
Br	27.0
I	37.0
S	25.6
P	27.0

Diffusion Volumes of Simple Molecules

H_2	14.3
N_2	15.6
O_2	7.4
Air	29.9
CO_2	34.0
H_2O	18.8

Thus, for formaldehyde:

(Sv)A 29.6

M_A 30.0262 $g.mol^{-1}$

For nitrogen:

(Sv)B 15.6

M_B 28.0134 $g.mol^{-1}$

Hence: $[\ (\Sigma_v)_A^{1/3} + (\Sigma_v)_B^{1/3}\ ] =$ 5.592027

	STAGE 1	**STAGE 2**	**STAGE 3**	**STAGE 4**
p [kPa(abs)]	125	120	115	110
Temperature [K]	335.15	323.15	315.15	310.65
Temperature [°C]	62.00	50.00	42.00	37.50
M_{AB}	28.98	28.98	28.98	28.98
Hence DAB[cm2.s-1] =	0.127	0.125	0.126	0.129

Again this is so invariant that it may be taken as constant across the entire column: **0.127 cm2.s-1**

(We note that the decreasing temperature is compensated for by [commensurately?] decreasing pressure.)

NOTE: DUE TO THE OBVIOUS ERRORS IN ESTIMATING BINARY GAS DIFFUSION COEFFICIENTS, COMPUTATION OF DIFFUSIVITIES FOR THE MIXTURE WOULD CLEARLY **NOT** BE JUSTIFIED.

Liquid-phase diffusivity computation

Assuming binary diffusion:
Formaldehyde in water (main constituent)
NOTE: While the correlations are for **dilute** solute diffusion, the hydrolysis of HCHO renders this **valid** here.

Use the correlation of Hayduk and Minhas (1982), recommended by R, P & P(4)

In aqueous solutions: (Average abs. error = ~10%)

$\mathbf{D^{o}_{AB}}[cm^2.s^{-1}]$ **=** $\mathbf{1.25 \times 10^{-8}.(V_A^{-0.19} - 0.292).T[K]^{1.52}.\eta_w^{\varepsilon^*}}$

where ε^* **=** $\mathbf{(9.58/V_A) - 1.12}$

η_w is the viscosity of water [mPa.s]

and $\mathbf{V_A}$ is the molar volume of the solute at its normal b.p. [$cm^3.mol^{-1}$]

From Ullmann's(5):

"Formaldehyde liquefies at -19.2°C, the density of the liquid being 0.8153 $g.cm^{-3}$ at 20°C [....]"

Given a molar mass of: 30.026 $g.mol^{-1}$

This yields $\mathbf{V_A}$ = 36.828 $cm^3.mol^{-1}$

whence ε^* **=** -0.85987

	STAGE 1	**STAGE 2**	**STAGE 3**	**STAGE 4**
p [kPa(abs)]	125	120	115	110
Temperature [K]	335.15	323.15	315.15	310.65
Temperature [°C]	62.00	50.00	42.00	37.50
From *Rogers & Mayhew* (5)				
Viscosity of liquid water (to nearest 5°C) = η_w [mPa]:	0.463	0.544	0.651	0.718
Hence D°AB[cm2.s-1] =	**3.5E-05**	**2.9E-05**	**2.4E-05**	**2.2E-05**

This probably should **not** be taken as constant across the whole column: 2.8E-05 cm2.s-1

MONASH UNIVERSITY
DEPARTMENT OF CHEMICAL ENGINEERING

Appendix to Chapter 7

Part 3: Detailed Mechanical Design

CLIENT: CHE4117

PROJECT: FORMALDEHYDE

DESIGN OF: ABSORBER TRAYS

SHEET 1 of 7

DATE 11/09/1999

BY DIV

CHKD.

① NUMBER OF IDEAL STAGES

From the method of <u>Treybal & Feintuch</u> presented in worksheet "Bed 4", it has been shown that

$$N_{oy} = \frac{\ln\left[\left(\frac{y_1 - y_2^*}{y_2 - y_2^*}\right)\cdot\left(1 - \frac{1}{A_E}\right) + \frac{1}{A_E}\right]}{1 - \frac{1}{A_E}} \doteqdot 15$$

<u>Treybal</u>(3) presents the relevant Kremser equation for calculating the number of ideal plates:

$$N_p = \frac{\log_{10}\left[\left(\frac{y_{N_p+1}}{y_1}\right)\cdot\left(1 - \frac{1}{A_E}\right) + \frac{1}{A_E}\right]}{\log_{10}(A_E)}$$

for the absorption section, with pure water "solvent".

As before $A_E \doteqdot 1.2278$

$y_{N_p+1} = 0.0085$ (entering)

$y_1 = 0.0001032$ (exiting)

$\Rightarrow N_p = 13.54$

13.54 ideal trays.

We see that this is of the same order of magnitude as N_{oy}, as expected.

<u>Sinnott</u>(2) gives a correlation <u>specifically</u> for the plate efficiency of absorbers, due to O'Connell (1946).

given $x \equiv 0.062\left(\frac{\rho_s}{\mu_s K M_s}\right)$

$$\Rightarrow x = 0.062\left(\frac{1000\ \text{kg}\cdot\text{m}^{-3}}{0.8\ \text{mPa}\cdot\text{s} * 0.067959 * 18.015\ \text{g}\cdot\text{mol}^{-1}}\right)$$

$x = 6.33 \times 10^1$

From Fig. 11.14 of <u>Sinnott</u>(2)

Efficiency $\simeq 56\%$ (bubble-caps).

~~$E_0 = 56\%$~~

While this may seem quite low, it is higher than it might have been, had K been much larger.

MONASH

CLIENT: CHE4117

PROJECT: FORMALDEHYDE

DESIGN OF: ABSORBER TRAYS

SHEET 2 of 7

DATE 11/09/1999

BY DIV

CHKD.

Hence the actual number of plates required is

$(13.54)(0.56)^{-1} \doteq 24$ actual trays

Perry(6) & VLE data indicate 56% too low : take 21 trays ($E_o = 64.5\%$)

~~24 real trays.~~ $E_o = 64.5\%$
21 real trays.

② PLATE SPACING

Sinnott(2), p. 510 recommends plate spacings of 0.3 to 0.6 m for this diameter column (1.8m), which can be adjusted after detailed design, with larger spacings for manholes/"manways". Typically estimate 0.5m

J.R. Backhurst & J.R. Harker (1973) recommend plate spacings of 0.46m for sieve trays in columns of diameter ≤ 1.2m to avoid mechanical problems of "supporting a tall, slender column," with spacings down to 0.15m possible. Larger columns have sieve tray spacings of 0.6 to 0.9m. [p.166]

For valve trays the sieve tray recommendations may be used, except that 1.22m spacings are preferred for "very large diameter columns". However this may be able to be reduced based on subsequent calculation of hydraulic parameters, subject to acceptable entrainments.

With these recommendations in mind, and also remembering that bubble-cap trays (for the low liquid flow and heat exchange) will be used with "serpentine" cooling coils, a spacing of 0.75m is selected.

Normal spacing
$= 0.75m = l_t$

MONASH

CLIENT: CHE4117

PROJECT: FORMALDEHYDE

DESIGN OF: ABSORBER TRAYS.

SHEET 3 of 7

DATE 11/09/1999

BY DIV

CHKD.

However there shall be manhole spacing every 7 trays (or 5.25m). Manholes may be a significant cost, and so provision is made for access through tray sections. Manholes must accomodate a person and tray sections. Backhurst & Harker list sizes from 0.37 m to 0.61m, inner diameter. As manholes are not installed between each plate, a diameter of 0.61m (24 inches) can be afforded. Say total tray-to-tray manway spacing is $(0.61m + 0.75m) = 1.36m$

manholes every 7 trays.

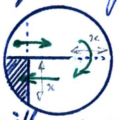
0.61m internal diameter manholes

1.36m tray-to-tray manway spacing.

③ PLATE LAYOUT.

Perry(6), p. 18-8 gives equilateral triangle layouts of bubble-caps as the general arrangement, with spacings between cap centres of {diameter + 25mm} to {diameter + 50mm} as the general arrangement. A typical cap diameter is said to be 100 mm for a 1.8 m diameter column. There is significant periphery waste.

For the low liquid flow Sinnott(3), p. 514 recommends reverse flow:



— see also Figure of p. 523. However this will again reduce the number of available caps. Thus 75mm caps will be used at 125 mm equilateral spacing

Reverse flow baffle.

Cap diameter = 75mm

Cap spacing = 125mm

MONASH

CLIENT: CHE4117

PROJECT: FORMALDEHYDE

DESIGN OF: ABSORBER TRAYS

SHEET 4 of 7

DATE 11/09/1999

BY DIV

CHKD.

④ PLATE PRESSURE DROP.

Perry(6) gives pressure drop correlation equations, from Smith, for bubble-caps [p. 18-9]. However dimensions of the caps are required.

④(a) BUBBLE CAP DIMENSIONS.

Dimensions will be assumed as follows:

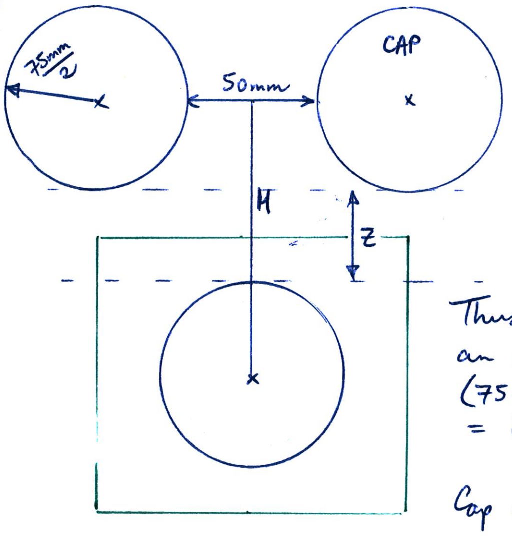
For the 75mm diameter caps selected

circumference = 236 mm

Say 40 slots of width 3mm and height 10mm

$h_{sh} = 10$ mm

40 3mm x 10mm slots



$H = \left(125^2 - \left(\frac{125}{2}\right)^2\right)^{\frac{1}{2}}$

$\therefore H = 108$ mm

$\Rightarrow Z = 33$ mm (cf. 33.25)

Thus each cap fits into an area

$(75 + 33)$ mm $\times$ $(75 + 50)$ mm

$= 13532$ mm^2

Cap area $= 4418$ mm^2

From Table 18-3 of Perry(6), a typical "active area" would be 0.66 * {total cross sectional area}.

Note: Increase in this fraction due to selecting a lower cap size would be compensated for by decrease due to the reverse flow baffle.

Total area $= \frac{\pi}{4} \times (1.8)^2 = 2.545$ m^2

$\Rightarrow$ Active area ≈ 1.679 m^2

Hence we might estimate $\frac{1.679 \times 10^6}{13532} = 124$ caps per tray,

or, rounding down 100 caps per tray.

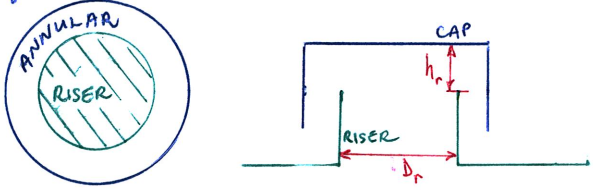
100 caps per tray

MONASH

CLIENT: CHE4117		SHEET	5 of 7
PROJECT: FORMALDEHYDE		DATE	12/09/1999
		BY	DIV
DESIGN OF: ABSORBER TRAYS		CHKD.	

Slot area = $40 \times 3 \times 10$ = 1200 mm^2 per cap

By assumption from Fig. 18-136 of Perry (6), it will be assumed that the ratio of annular area to riser area is 1.0, with the reversal area equal to 1.35 times {average of riser and annular areas} (equal here).



Reversal area is taken as $(\pi D_r) . h_r$.

④(b) PRESSURE DROP

With these specifications the head-loss coefficient for dry bubble-caps, K_2, is approx. 16.6

$K_2 = 16.6$

Given that cap area = riser area + annular area, here riser area = $4418 \div 2 = 2209$ mm^2

$\Rightarrow D_r = 53$ mm

(Reversal area = 2982 mm^2) $\Rightarrow h_r \doteq 18$ mm

Riser diameter = 53 mm

Hence linear gas velocity through risers:

$$U_h = \frac{(238\,mol.s^{-1})(43\,mol.m^{-3})^{-1}}{100 \times (2209 \times 10^{-6})m^2} = 25\ ms^{-1}$$

$U_h = 25\ m.s^{-1}$

Given $\rho_L = 1000\ kg.m^{-3}$ (as for water)

$\rho_G = 1.02\ kg.m^{-3}$

$$\Rightarrow K_2 \frac{\rho_G}{\rho_L} U_h^2 = 10.6\ mm(liquid) \sim 10.6\ mm(H_2O).$$

As linear velocity through the slots, U_s is

$$U_s = \frac{(238)(43)^{-1}}{1200 \times 10^{-4}} = 46\ ms^{-1}$$

$U_s = 46ms^{-1}$

then

$$K_1 = 3.73 \left(\frac{\rho_G}{\rho_L - \rho_G}\right)^{\frac{1}{5}} h_{sh}^{\frac{4}{5}} U_s^{\frac{2}{5}} \doteq 27.4\ mm\ (H_2O)$$

Hence the pressure drop across the disperser is

$$h_d = K_1 + K_2 \frac{\rho_G}{\rho_L} U_h^2 \doteq 27.4 + 10.6 = 38.0mm (H_2O)$$

$h_d \doteq 38.0\ mm\ (H_2O)$

MONASH

CLIENT: CHE4117

PROJECT: FORMALDEHYDE

DESIGN OF: ABSORBER TRAYS

SHEET 6 of 7

DATE 12/09/1999

BY DIV

CHKD.

WEIR DIMENSIONS are needed to find the pressure drop through the aerated liquid.

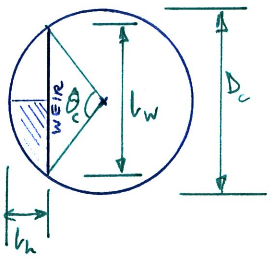
Sinnott[(2)], p. 526, recommends 40 to 50 mm as weir height.

Given the need to cool, we will specify 50mm.

$h_w = 50\,\text{mm}$

Given the low liquid flow, from Sinnott[(2)], p. 527, take

$\frac{l_w}{D_c} \simeq 0.70$, ~~$\frac{l_h}{D_c} \simeq 0.10$~~, $\theta_c \simeq 89°$ (approx.)



$\Rightarrow l_w \simeq 1{\cdot}26\,\text{m}$

~~$l_h \simeq 0{\cdot}18\,\text{m}$~~

Reference to Perry[(6)], p. 1-26 shows that $\frac{l_h}{l_w} \simeq 0{\cdot}205 \Rightarrow l_h \doteqdot 258\,\text{mm}$

(while $\frac{l_h}{D_c} \simeq 0{\cdot}143$).

$l_w = 1{\cdot}26\,\text{m}$

~~$l_h = 0{\cdot}18\,\text{m}$~~

$l_h = 258\,\text{mm}$

DYNAMIC SEAL HEIGHT.

This is the calculated height of clear liquid (equivalent) above dispersers. From Perry[(6)], pp. 18-10ff. :

$$h_{ds} = h_s + h_{ow} + \tfrac{1}{2} h_{hg}$$

$h_s \equiv$ static slot seal $\doteqdot$ {weir height} − {height of top of slot above floor}

If the bottom of the slot is assumed 10mm above the plate floor

$h_s = 50 - (10+10) = 30\,\text{mm}$

$h_s = 30\,\text{mm}$

$h_{aw} \equiv$ height of crest above weir

From the Francis weir equation : $h_{ow} = 664\left(\frac{\dot{V}_L}{l_w}\right)^{\frac{2}{3}}$

$\therefore h_{ow} = 664\left(\frac{0.35\,\text{kg}\cdot\text{s}^{-1}}{1000\,\text{kg}\cdot\text{m}^{-3} * 1{\cdot}26\,\text{m}}\right)^{\frac{2}{3}} = 2{\cdot}83\,\text{mm}\,(H_2O)$

$h_{ow} = 2{\cdot}8\,\text{mm}\,(H_2O)$

$h_{hg} \equiv$ hydraulic gradient across plate.

From Fig. 18-17

$h_{hg}' \doteqdot 0.05$ inches

With $U_a \equiv$ linear gas velocity through active area

$$U_a = \frac{(238)(43)^{-1}}{0.66\,\frac{\pi}{4}(1{\cdot}8)^2} \doteqdot 3{\cdot}3\,\text{ms}^{-1}$$

Say $C_{vf} = 1{\cdot}5 \quad\Rightarrow\quad h_{hg} \doteqdot 1{\cdot}9\,\text{mm}\,(H_2O)$

$h_{hg} = 1{\cdot}9\,\text{mm}\,(H_2O)$

Thus $h_{ds} = 30 + 2{\cdot}8 + 1{\cdot}9 = 34{\cdot}7\,\text{mm}\,(H_2O)$

$h_{ds} = 34{\cdot}7\,\text{mm}\,(H_2O)$

From Fig. 18-15, the aeration factor, $\beta \doteqdot 0{\cdot}58$

$\beta = 0{\cdot}58$

and the relative froth density, $\phi_t \doteqdot 0.18$

MONASH

CLIENT: CHE4117
PROJECT: FORMALDEHYDE
DESIGN OF: ABSORBER TRAYS

SHEET 7 of 7.
DATE 12/09/1999
BY DJV
CHKD.

Hence the pressure drop through the aerated liquid is

$h_l' = \beta . h_{ds} = 20.1 \text{ mm } (H_2O) \simeq 20 \text{ mm } (H_2O)$

$h_l' \doteqdot 20 \text{ mm } (H_2O)$

Hence the actual height of froth on the plates is

$h_f = h_l' \div \phi_t \simeq 112 \text{ mm}$

$h_f \simeq 112 \text{ mm}$

Though this was larger than anticipated, the tray spacing of 0.75m is still valid.

Finally, the total pressure drop across one plate is thus

$h_t = h_d + h_l' = 38. + 20. = 58 \text{ mm}(H_2O) . \text{plate}^{-1}$

$h_t = 58 \text{ mm}(H_2O). \text{plate}^{-1}$

For 21 plates $h_t \doteqdot 12 \text{ kPa}$

This is acceptable.

$(-\Delta p) \doteqdot 12 \text{ kPa}$ for all 21 plates

⑤ DOWNCOMER DESIGN. — Assumed segmental.

From Perry(6), p. 18-7 $h_{dc}' = \frac{1}{\phi_{dc}} \cdot h_{dc} = \frac{1}{\phi_{dc}} \left[h_t + h_w + h_{ow} + h_{da} + h_{hg} \right]$

$\left. \begin{array}{l} h_t = 58 \text{ mm}, \; h_w = 50 \text{ mm}, \; h_{ow} = 2{\cdot}8 \text{ mm} \\ \text{and } h_{hg} = 1{\cdot}9 \text{ mm} \end{array} \right\}$ from ④.

ϕ_{dc} is the average relative froth density in the downcomer, and is taken as 0.5

$h_{da} \equiv$ head loss due to liquid flow under downcomer apron [From p. 18-10]

Taking a liquid-seal depth of 25mm from top of liquid on plate to bottom of downcomer.

Liquid seal = 25mm $= h_{ap}$

Thus the minimum flow area under the apron is

$A_{da} = \left(\tfrac{1}{2} \times 1{\cdot}26 \text{m}\right) \times (50 - 25) \times 10^{-3} \text{ m} = 0.01575 \text{m}^2$

Whence $h_{da} = 165{\cdot}2 \left(\frac{3{\cdot}5 \text{ kg.s}^{-1}}{1000 \text{ kg.m}^{-3} \times 0.01575 \text{m}^2} \right)^2 = 8{\cdot}2 \text{ mm}$

$h_{da} = 8{\cdot}2 \text{ mm } (H_2O)$

Thus $h_{dc} \doteqdot 121 \text{ mm}$ (clear liquid)

$\Rightarrow h_{dc}' = 242 \text{ mm}$ (aerated liquid)

$h_{dc}' = 242 \text{ mm}$ (aerated liquid)

So again the plate spacing of 0.75m is satisfactory [see Sinnott(2), p. 532]

Check downcomer residence time (should be greater than 3 seconds for adequate disengagement — Sinnott(2), p 532)

$t_r = \frac{A_d \cdot h_{dc} \cdot \rho_L}{L} = \frac{(0.127 \text{m}^2)(0.121 \text{m})(1000 \text{kg.m}^{-3})}{(0.35 \text{ kg.s}^{-1})} = 44 \text{ s}$

plenty.

[Also Backhurst & Harker, p. 177]

$t_r = 44 \text{s}.$

CLIENT:	CHE4117	SHEET	1 of 1
PROJECT:	FORMALDEHYDE	DATE	19/09/1999
		BY	DIV
DESIGN OF:	ABSORBER INTERNALS (MECHANICAL)	CHKD.	

MONASH

① THICKNESS OF ABSORBER TRAYS.

Assume that the tray may be modeled as a circular plate freely supported and loaded concentrically, as per Morley[(11)], Art. 151, pp. 460ff.

Supposing the load to be 1000 N (or just over 100 kg), distributed over an area much smaller than that of the tray, then the maximum deflection is given (approximately) by:

$$\delta_{MAX} \simeq \frac{5}{3\pi} \frac{Pr^2}{Et^3}$$

in which P is the load (1000 N)
r the radius of the plate (0.9 m)
E is the Young's modulus of elasticity
t the thickness

[Poisson's ratio is assumed $\nu \equiv \frac{1}{m} = \frac{1}{3}$.]

From AS 1210 (1989), Table 3.3.7, for austenitic stainless steels $E \simeq 0.194 \times 10^6$ MPa at 50°c.

∴ For a deflection of 0.010 m, $t \doteqdot 6$ mm

For comparison, $t = 3$ mm yields a heart-attack-inducing $\delta_{MAX} \simeq 0.082$ m.

Suppose two 25 mm pipes were welded to the underside of the support ring, parallel to the weir. This places it approximately 325 mm off-centre, giving a length of 1650 mm.

length = 1650 mm

If this is subject to a uniformly distributed load, then

$$\delta_{MAX} = \frac{5}{384} \frac{Pl^3}{EI}, \text{ whence } I = \frac{1.51\times10^{-8}\,m^4}{2} \text{ for } \delta_{MAX} = 0.020\,m$$

two bars.

[Morley[(11)], p. 187].

For the hollow pipe $I = \frac{\pi}{64}(d_o^4 - d_i^4)$

for $d_o = 25$ mm $\Rightarrow d_i = 0.022$ m = 22 mm

$\Rightarrow$ i.e. thickness = 1.5 mm

Hence specify 3 mm thick plate with two supports, 325 mm of centre, parallel to the weir, with $d_o \overset{!!}{=} 25$ mm and thickness at least 1.5 mm → 2 mm.

From Perry[(6)], p. 6-42, $\frac{3}{4}$" schedule 40 is ample.
(nominal)

3 mm thick trays
2 supports
325 mm off-centre
parallel to weir
$d_o = 25$ mm
thickness = 2 mm
$\frac{3}{4}$", schedule 40.

MONASH

CLIENT: CHE4117		SHEET	1 of 6
PROJECT: FORMALDEHYDE		DATE	19/09/1999
		BY	DJV
DESIGN OF: ABSORBER SHELL (MECHANICAL)		CHKD.	

① COLUMN DIMENSIONS

The column has an internal diameter of 1.8m and a height of — $D_i = 1.8m$

$H =$ 2.90 (Bed 1)
+2.20 (Bed 2)
+2.50 (Bed 3)
+ 21 × 0.75 + 2 × 0.61 (Stage 4 including manways)
+ 1.50 (Vapour space above stage 4)
+ 1.50 (Between bed 3 and stage 4)
+ 3 × (0.5 + 1.5) (Below beds 1 to 3, including liquid hold-up)

$\therefore H = 33.57m$, <u>without</u> ends — $H = 33.57m$

② WALL THICKNESS

This will be taken as constant for the cylindrical shell.

②(a) PRELIMINARY ESTIMATE

Taking a corrosion allowance of 2mm, <u>Sinnott</u>[(2)], p. 739, recommends a "minimum practical wall thickness" of 7mm for this diameter vessel. — $t > 7mm$

②(b) DESIGN PRESSURE [CHE4109]

Operating pressure of the absorber may be taken at a maximum of 130 kPa (abs), at the base.

Design pressure will be taken above <u>Sinnott</u>[(2)]'s recommended + 5 to 10% in view of the added explosion risk

$\Rightarrow p_{DESIGN} = 150$ kPa (abs) — $p_{DESIGN} = 150$ kPa(abs)

As Bontang may be prone to hurricanes of wind speed up to ~ 100 km.h⁻¹, wind speed will be set at a fixed $27 ms^{-1}$

Given $C_D \simeq 1.0$ for cylinders [<u>Potter and Wiggert</u>[(1)]], the drag coefficient.

Equivalent wind pressure, $p_{WIND} = \frac{1}{2} \rho_{AIR} V^2$.

As $\rho_{AIR} \simeq 1$ kg.m⁻³ $\rightarrow p_{WIND} \simeq 365$ Pa

This acts on the projected area.

For the column $\frac{A_{PROJ}}{L} = D_o = 1.8$ m².m⁻¹

$\Rightarrow$ Treat the wind as a uniformly distributed load, $F_{WIND} = 656 N.m^{-1}$

Treating the vessel as a cantilever, $M_{bend} = F_{WIND} \cdot \frac{L^2}{2} = 370$ kN.m
(at the base)

CLIENT: CHE4117
PROJECT: FORMALDEHYDE
DESIGN OF: ABSORBER SHELL (MECHANICAL)
SHEET 2 of 6
DATE 19/09/1999
BY DIV
CHKD.

For a cylinder (ignoring end effects) $I_z = \frac{\pi}{64}(D_o^4 - D_i^4)$

For a thickness of 5mm (ie. without corrosion allowance):

$$I_z = \frac{\pi}{64}\left[-(1.8\,m)^4 - (1.8 + 0.010)^4\,m^4\right] = 0.0115\ m^4$$

Thus $$\sigma_{z\,bend} = \frac{\pm M_{bend} \cdot D_o}{2I_z} \doteqdot \begin{cases} +29.3\ MPa, & \text{upwind} \\ -29.3\ MPa, & \text{downwind} \end{cases}$$

where negative signifies compression.

$\sigma_{z\,bend} = \pm 29.3\ MPa$

$$\sigma_{HOOP} = \frac{P_{DESIGN}\,D_i}{2t} = {}^{+}8.8\ MPa$$

$$\sigma_{AXIAL} = \frac{\sigma_{HOOP}}{2} = +4.4\ MPa$$

$\Big\}\ P_{DESIGN} = 49\ kPa(g)$

$\sigma_{HOOP} = {}^{+}8.8\,MPa$

$\sigma_{AXIAL} = +4.4\,MPa$

There must also be some self-weight:

Mass of shell $\simeq (33.57\,m)\,\frac{\pi}{4}(D_o^2 - D_i^2)(\rho)$

and $\rho \simeq 7.7 \times 10^3\ kg \cdot m^{-3}$ [Perry (6)]

$\Rightarrow m_{SHELL} \simeq 7.3t$

Mass of liquid $\simeq (21 \times 0.050\,m + 3 \times 0.50\,m) \times \frac{\pi}{4}(1.8\,m)^2 \rho$

$m_{LIQUID} \doteqdot 6.5\,t$

There is also packing, trays and other internals

Say $m_{INTERNALS} \doteqdot 10\ t$

$\Rightarrow m_{TOTAL} \simeq 23.8\ t$

$$\therefore \sigma_{SELF\text{-}WEIGHT} = \frac{(23.8 \times 10^3\,kg)(9.78\,ms^{-2})}{\frac{\pi}{4}\left[-(1.8\,m)^2 + (1.81\,m)^2\right]} \doteqdot -8.3\ MPa$$

where the value for gravity used is for sea level, at the equator [Giancoli (2)].

$\sigma_{SELF\text{-}WEIGHT} = -8.3\,MPa$

Thus, at the base of the column:

	UPWIND	DOWNWIND	
σ_z [MPa]	+25.4	−33.2	
σ_{HOOP} [MPa]	+8.8	+8.8	
σ_{RADIAL} [MPa]	~0	~0	(thin shell)

Here the danger of assuming internal pressure to be the dominant factor is clear.

In summary, $\sigma_{MAX} \doteqdot -33.2\ MPa$

$\sigma_{MAX} = -33.2\,MPa$.

MONASH

CLIENT: CHE4117		SHEET	3 of 6
PROJECT: FORMALDEHYDE		DATE	19/09/1999
		BY	DJV
DESIGN OF: ABSORBER SHELL (MECHANICAL)		CHKD.	

For type F316 "high alloy" (stainless) steel, we abstract a value of ~100 MPa as the design tensile strength from AS 1210 (1989).

$\sigma_{MAX.\ TENSILE} \doteqdot 100\ MPa$

This is evaluated at a design temperature of 170°C, corresponding to a complete failure of the cooler on the absorber feed line.

$T_{DESIGN} = 170°C$

As $\sigma_{MAX} \ll \sigma_{MAX.\ TENSILE} \Rightarrow$ this analysis shows 5mm to be an adequate thickness.

Okay for normal operation during cyclone

②(c) WATER TESTING

For a completely flooded column,

$$m_{WATER} = \frac{\pi}{4}\cdot(1{\cdot}8m)^2\cdot(33{\cdot}57m)(1000 kg.m^{-3}) \doteqdot 85{\cdot}4\ t$$

So now $m_{total} = 7{\cdot}3 + 85{\cdot}4 + 10 = 102{\cdot}7t$

$\therefore\ \sigma_{SELF\cdot WEIGHT} \doteqdot -35{\cdot}6\ MPa$

$\sigma_{SELF\cdot WEIGHT} = -35.6 MPa$

Obviously hydraulic testing would not take place during a cyclone. Taking $V_{WIND} = 10\ ms^{-1}$

$\Rightarrow p_{WIND} = 50\ Pa$

Analysing as before,

$$\sigma_{z,bend} = (\pm 29.3)\left(\frac{50}{365}\right) = \pm 4.0\ MPa$$

$\sigma_{z,bend} = \pm 4.0 MPa$

At the base of the column the pressure due to the hydrostatic head is $p = \rho g h$

$\Rightarrow p_{WATER} = 328\ kPa\ (g)$

Thus, now $\sigma_{HOOP} = \frac{p_{WATER}\ D_i}{2t} = {}^{+}58{\cdot}8\ MPa$

$\sigma_{AXIAL} = \frac{\sigma_{HOOP}}{2} = {}^{+}29{\cdot}3\ MPa$

$\sigma_{HOOP} = {}^{+}58{\cdot}8\ MPa$

$\sigma_{AXIAL} = +29{\cdot}3\ MPa$

where again t = 5mm has been used.

Hence, at the base of the column:

	UPWIND	DOWNWIND	
σ_z [MPa]	$-2{\cdot}3$	$-10{\cdot}3$	
σ_{HOOP} [MPa]	$+58{\cdot}8$	$+58{\cdot}8$	
σ_{RADIAL} [MPa]	~ 0	~ 0	(thin wall)

Here $\sigma_{MAX} = +58{\cdot}8\ MPa$ is larger than the previous case, but still substantially below the maximum allowable.

$\Rightarrow$ 7mm thickness (total) is adequate.

$\sigma_{MAX} = +58{\cdot}8\ MPa$

Okay for hydrostatic testing.

②(d) EARTHQUAKE LOADING.

Bontang may be subject to earthquakes.

From Brownell & Young (1959), cited in CHE4109 by Olbrich,

$$F_{HORIZ} = C \cdot m_{VESSEL} \cdot g$$

where C will be taken as 0.10 (empirical correlation)

$C = 0.10$

Assuming hydraulic testing does not take place, $m_{VESSEL} \doteq 23.8t$.

$\Rightarrow F_{HORIZ} = 23.3 kN$

$F_{HORIZ} = 23.3 kN$

The average shear stress due to this force:

$$\tau_{ave.} = \frac{23.3 \times 10^3 N}{\frac{\pi}{4}(-1.8^2 + 1.81^2) m^2} = 822 kPa$$

From Morley(11), Art. 71, p. 161, we observe $\tau_{MAX} = 2\tau_{ave}$ due to F_{HORIZ}. $\Rightarrow \tau_{MAX} \simeq 1.65 MPa$.

$\tau_{MAX} \simeq 1.65 MPa$

Even allowing for the fact that the actual maximum shear stress will be increased by the effect of other forces acting, it is evident that this is not a significant factor ↳ the suggested design is satisfactory from an earthquake-loading perspective.

Okay for earthquakes.

②(e) BUCKLING

Neglecting the stiffening effects of the internals, Sinnott(2), p. 760, gives the following equation for buckling:

$$\sigma_c = 2 \times 10^4 \left(\frac{t}{D_o}\right) MPa.$$

This is the maximum allowable compressive stress.

Here $\sigma_c = 55 MPa$, taking $t = 5mm$.

$\sigma_c = 55 MPa$.

From section ②(b), page 2, we found that the maximum compressive stress was $\simeq 33 MPa$, so the buckling criterion is satisfied.

Okay for buckling. (normal operation at high wind speed).

MONASH

CLIENT: CHE4117
PROJECT: FORMALDEHYDE
DESIGN OF: ABSORBER SHELL (MECHANICAL)

SHEET 5 of 6
DATE 19/09/1999
BY DJV
CHKD.

Alternatively, in the absence of high wind load,

$\sigma_{z, bend} = \pm 4\ MPa$, $\sigma_{SELF\text{-}WEIGHT} = -8.3\ MPa$

$\sigma_{z, bend} = \pm 4\ MPa$
$\sigma_{SELF\text{-}WEIGHT} = -8.3\ MPa$

Thus the limit of maximum compressive stress $= \sigma_c = 55\ MPa$ is reached when

$$\sigma_{HOOP} = -55 MPa,$$

for which $\sigma_{AXIAL} = -27.5\ MPa$

Given $\sigma_{HOOP} = \dfrac{p D_i}{2t}$, this implies

$$p = -306\ kPa(g)$$

Thus, this implies the vessel would withstand even an absolute vacuum inside, with atmospheric pressure outside.

Okay for buckling (vacuum). ?

Comparison with AS1210 (1989), § 3.9.3 gives

$$\frac{D_o}{t} \doteqdot 360, \quad \frac{L}{D_o} \simeq 20 \Rightarrow A \simeq 10^{-5}$$

$$\Rightarrow B \simeq 0.94$$

And $P = \dfrac{4B}{3(D_o/t)} \doteqdot 0.003\ MPa$ nett external overpressure

$$= 3 kPa(g)$$

Equation (13.51) of Sinnott$^{(2)}$, $P_c = 2.2E\left(\frac{t}{D_o}\right)^3$, gives

$$P_c \simeq -9 kPa(g)$$

and the recommended safety factor of 3 then yields a maximum (magnitude) overpressure $P_c = -3 kPa(g)$, as before.

Maximum external overpressure $= 3kPa(g)$

→ NOT SUITABLE FOR NON-NEGLIGIBLE VACUUM
(Note: stiffening effects not considered).

Will fail due to buckling at moderate vacuum.

②(f)

INSTALLATION

Consider the installation of the empty vessel, transported horizontally to site.

If it is raised according to

then, taking the empty mass as 8t $\Rightarrow F = \dfrac{78.2 kN}{2}$

Thus $M_{bend} = (2F) \cdot \dfrac{L}{2} = 1313\ kN.m$

Given $I_z = 0.0115\ m^4$ (as before)

$$\Rightarrow \sigma_{z, bend} = \frac{\pm M_{bend} \cdot D_o}{2 I_z} = \pm 103\ MPa$$

$\sigma_{z, bend} = \pm 103 MPa$.

MONASH

CLIENT: CHE4117

PROJECT: FORMALDEHYDE

DESIGN OF: ABSORBER SHELL (MECHANICAL)

SHEET 6 of 6

DATE DJV

BY 19/09/1999

CHKD.

This is right at the suggested allowable maximum for tensile stress.

However:

* the maximum tensile stress was evaluated at 150°c, however installation at 50°c gives a design tensile strength of 129 MPa [AS1210(1989)] ⇒ OKAY.

* when installed, the 2mm corrosion allowance will still be entirely present ⇒ OKAY

* in practice the vessel may not be lifted from a single point, and certainly would not be lifted from its end. ⇒ OKAY.

OKAY for installation.

MONASH	CLIENT: CHE4117	SHEET	1 of 2
	PROJECT: FORMALDEHYDE	DATE	01/10/1999
		BY	DJV.
	DESIGN OF: ABSORBER ENDS (MECHANICAL)	CHKD.	

① CHARACTERISTICS

Diameter is 1.8 m (internal)

Δp_{MAX} = 328 kPa [see design of ABSORBER SHELL]

$D = 1.8\,m$

$\Delta p_{MAX} = 328\,kPa$.

② TYPE

Sinnott(2) recommends standard torispherical heads "dished ends". Formed head (no joints)

Take ratio of knuckle to crown radius $\geq \frac{6}{100}$

Also crown radius $\leq$ Diameter of cylinder

$\longrightarrow$ Physically $R_c > \frac{D}{2}$

Torispherical

Formed (no joints)

$\frac{R_k}{R_c} \geq \frac{6}{100}$

$R_c \leq D$.

$R_c > \frac{D}{2}$

③ DIMENSIONS.

$0.9\,m < R_c \leq 1.8\,m$

Say $R_c = 1.4\,m$

if $\frac{R_k}{R_c} = \frac{7}{100} \Rightarrow R_k = 0.2\,m$

$R_c = 1.4\,m$

$R_k = 0.2\,m$

④(a) THICKNESS

Calculate using the "stress concentration factor", C_s, of Sinnott(2):

$$C_s = \frac{1}{4}\left(3 + \sqrt{\frac{R_c}{R_k}}\right) = 1.41 \quad (\sim\sqrt{2})$$

$$\delta = 1.0 \quad \text{(formed)}$$

$$\therefore \text{Thickness}_{MAX} = \frac{(328\,kPa)(1.4\,m)(1.41)}{2\sigma_{MAX}(1.0) + (328\,kPa)(1.41 - 0.2)}$$

From AS1210(1989) $\Rightarrow \sigma_{\substack{MAX\\TENSILE}} \doteqdot 100\,MPa$

$$\Rightarrow \text{Thickness}_{MAX} = \frac{0.648}{200 + 0.397} = 0.00323\,m$$

Add 2mm corrosion allowance : Thickness $\simeq$ 5.2mm

$C_s = 1.41$

$\delta = 1.0$

$\sigma_{MAX,TENSILE} = 100\,MPa$

$\text{Thickness}_{MAX} = 3.2\,mm$

Thickness $\simeq$ 5.2mm

④(b) CHECK STRESS

Maximum stress is in toroidal section.

From Sinnott(2)

For the maximum stress : hypothetical inner edge of torus:

$$\sigma_2 = \frac{PR_k}{2t}\left[\frac{D - R_k}{\frac{D}{2} - R_k}\right] = 1.58\,\frac{PR_k}{2t} = 1.58\sigma_1 = 16.2\,MPa$$

$\sigma_1 = 10.25\,MPa$

$\sigma_2 = 16.2\,MPa$

CLIENT: CHE4117		SHEET	2 of 2
PROJECT: FORMALDEHYDE		DATE	01/10/1999
		BY	DIV
DESIGN OF: ABSORBER ENDS (MECHANICAL)		CHKD.	

Both values are far below the maximum allowable

OKAY.

⑤ AUSTRALIAN STANDARD.
Check the above with AS1210(1989)

§ 3.12

$$\frac{D}{t} = \frac{1800}{3.2} = 563 > 100 \Rightarrow$$

particular care should be exercised (buckling)

CARE! (buckling)

Suppose $t = 5mm$ (+2mm corrosion allowance)

$$\Rightarrow \frac{D}{t} = \frac{1800}{5} = 360 > 100 \Rightarrow$$ Care still required.

↳ However this would match the existing shell better.

Thickness = 5mm
+ 2mm corrosion allowance

AMENDMENT 1 :
As $\frac{D}{t} > 300$ $\Rightarrow \frac{P_{MAX}}{\sigma_{MAX, TENSILE}} \leqslant \frac{150\left(\frac{R_k}{D}\right)^{0.84}}{\left(\frac{D}{t_k}\right)^{1.53} \cdot \left(\frac{R_c}{D}\right)^{1.1}}$

is recommended.

Current dimensions give

$$\frac{P_{MAX}}{100 MPa} \leqslant \frac{23.69}{6181.}$$

$$\Rightarrow P_{MAX} \leqslant 0.383 MPa$$

i.e. $P_{MAX} \leqslant 383 kPa$

Note that the initial 3.2mm thickness would have been too low.

$P_{MAX} \leqslant 383 kPa$
OKAY

THICKNESS:

$$t = \frac{P R_c C_s}{2\sigma_{MAX\ TENSILE} J - 0.2P} = \frac{0.649}{200 - 0.0656} = 0.003248$$

$$= 3.2mm$$

(as before).

MONASH

CLIENT: CHE4117		SHEET	1 of 2
PROJECT: FORMALDEHYDE		DATE	01/10/1999
		BY	DJV
DESIGN OF: ABSORBER SUPPORT (MECHANICAL)		CHKD.	

① TYPE : Skirt

Skirt.

② REFERENCE : AS1210 (1989)

AS1210 (1989)

③ TEMPERATURE

Check for excessive discontinuity stresses :

$$t.D.(T-T_{ambient})_{MAX} \simeq (5mm)(1800mm)(90-20) = 6.3\times10^5$$

$$6.3\times10^5 < 16\times10^6$$

OKAY FOR TEMPERATURE.

④ (a) AXIAL COMPRESSIVE STRESS — HYDROSTATIC TEST CONDITION

$$S_a = \left(\frac{4M}{\pi D_o^2 t} + \frac{W}{\pi D_o t}\right)\frac{1}{\cos(\alpha)}$$

$$W = (102.7t)(9.78 ms^{-2}) = 1004 kN \doteqdot 10^6 N$$

$$\text{take } M = (50Pa)(1.8m^2.m^{-1})\frac{(34m)^2}{2} = 52020 \ N.m \doteqdot 5.2\times10^7 \ N.mm$$

Suppose a cylindrical cell of the same thickness as the column :

$$D_o \doteqdot 1810mm \ , \ t = 5mm \ , \ \alpha = 0°$$

$$\Rightarrow S_a = (4.04 + 35.2)(1) = 39.2 \ MPa.$$

④(b) YIELD

$2S_a$ < yield strength $\Rightarrow$ OKAY

YIELD OKAY.

④(c) YOUNG'S MODULUS

$$0.125\frac{Et}{D_o} = 0.125\times\left[\frac{(0.191\times10^6 MPa)(5mm)}{1810mm}\right] \doteqdot 66 < S_a$$

$\Rightarrow$ OKAY

MODULUS OKAY.

⑤ CHECK BASE RING [Sinnott(6)]

circumference (cylindrical) $\doteqdot 1800\pi$ mm

8 bolts $\Rightarrow$ pitch = 706.9mm > 600mm

PITCH OKAY.

$$\therefore A_b \doteqdot \frac{1}{(8)(125MPa)}\left[\frac{4\times52020}{1.8} - 10^6\right] \rightarrow \text{none required FOR HYDRO. TEST.}$$

$$A_b \doteqdot \frac{1}{(8)(125)}\left[\frac{4\times370000}{1.8} - (23.8\times10^3)(9.78)\right] = 589mm^2$$

$$\Rightarrow D_b = 27.4mm$$

CYCLONE LOADING.

$D_b = 27.4mm$

CLIENT: CHE4117

PROJECT: FORMALDEHYDE

DESIGN OF: ABSORBER SUPPORT (MECHANICAL)

SHEET 2 of 2

DATE 1/10/1999

BY DIV.

CHKD.

⑥ WIDTH OF BASE RING

From Sinnott$^{(2)}$:

$$F_b = \left[\frac{4M_s}{\pi D_s^2} + \frac{W}{\pi D_s} \right] \doteqdot t S_a$$

$\therefore F_b = 196 \ \mathrm{N\,m^{-1}}$

$\Rightarrow L_b = \frac{196 \times 10^3}{5} \times \frac{1}{10^3} = 39.2 \ \mathrm{mm}$ $\qquad L_b \geq 40\mathrm{mm}$

⑦ THICKNESS

Choose simple anchor (AS1210 (1989)) ... plus gusset [Sinnott$^{(2)}$]

$\Rightarrow L_r \rightarrow L_b = 39.2\mathrm{mm} \doteqdot 40\mathrm{mm}$

$$\therefore t_b = L_r \sqrt{\frac{3f_c'}{f_r}} \doteqdot 40 \sqrt{\frac{3 \cdot (8.75)}{140}}$$

$$\text{As } f_c' \simeq \frac{10^6 \mathrm{N}}{\frac{\pi}{4}\left[1840^2 - 1800^2\right] \mathrm{mm}^2} = 8.74 \ \mathrm{N.mm^{-2}}$$

$\therefore t_b = 17.3 \ \mathrm{mm} \rightarrow 17\mathrm{mm}$ $\qquad t_b = 17\mathrm{mm}.$

L_b must be greater :
- to accomodate bolt head + spanner
- for inside-skirt provision (50mm)

MONASH

CLIENT: CHE4117		SHEET	1 of 1
PROJECT: FORMALDEHYDE		DATE	03/10/1999
		BY	DIV
DESIGN OF: INSULATION ON ABSORBER		CHKD.	

① CONVECTIVE HEAT TRANSFER COEFFICIENT.

From Holmon (7), fiber-glass blankets for wrapping are recommended, with $k \simeq 0.05\ W.m^{-2}.K^{-1}$.

fiber-glass blankets.
$k = 0.05 W.m^{-2}.K^{-1}$

For a vertical cylinder

$$h = \begin{cases} 1.42\left(\frac{\Delta T}{L}\right)^{1/4} & \text{, laminar} \\ 1.31\,(\Delta T)^{\frac{1}{3}} & \text{, turbulent} \end{cases}$$

where L is "vertical or horizontal dimension".

② TEMPERATURES

if $T_a = 20°C$ (minimum of range)

and $T_{ABS-1} = 75°C$

$\rightarrow T_{WALL_{MIN}} \simeq 48°C$ ... OKAY

But, at the top of stage 1

$T_{ABS-1} = 60°C \longrightarrow T_{WALL_{MIN}} \simeq 40°C$ ... TOO LOW

In that case $\Delta T = 40°C$

$\therefore$ take $h \simeq 3\ W.m^{-2}.K^{-1}$

$h = 3\ W.m^{-2}.K^{-1}$

$$h A \,\Delta T_{surface} = \dot{Q} = \frac{k}{\Delta x} A \,\Delta T_{ins}$$

③ THICKNESS

Suppose the outer surface of the insulation were at 40°C

$$\Rightarrow \quad (3)(40-20) = \frac{0.05}{\Delta x}(60-40)$$

$$\therefore \Delta x \doteq 0.0167\,m = 16.7\,mm$$

$\Rightarrow$ Take insulation thickness as 25mm.

$\Delta x = 25mm$

Tube wall temperature is thus $T_{WALL_{MIN}} \rightarrow 60°C$.

$T_{WALL_{MIN}} \rightarrow 60°C$
OKAY.

MONASH UNIVERSITY

DEPARTMENT OF CHEMICAL ENGINEERING

APPENDIX TO CHAPTER 9

RECORD OF HAZOP MEETING

Stream 3

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Flow	• Pipe blockage • Control valve V-1 malfunction • Pipe rupture or leakage	• Possibility of entering the explosive limits • Visible on flow indicator • Reactor feed will be outside design composition ==> product may be out of spec. • Reactor temperature may increase (less thermal ballast)	• Display flow reading of Stream 3 on panel (control room) • Have alarm for low flow • Have temperature indicator and alarm in reactor • Regular maintenance and inspection of control valve and piping
More	Flow	• Control valve V-1 failure (fail-open to avoid previous deviation)	• Deterioration of catalyst • Decrease in yield	• Install alarm for high flow
Less	Flow	• As for “No Flow”	• As for “No Flow”	• As for “No Flow”
	Pressure	• Control valve V-1 failure • Upstream pipe rupture or leakage	• Reverse flow, possibly including methanol ==> flammability hazard	• Install low pressure alarm and indicator • Install non-return valve
What else?	Instrument air failure	• As for “More Flow”	• As for “More Flow”	• Regular inspection

Stream 6

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Flow	• Upstream pump failure or trip • Pipe blockage • Control valve V-2 failure (fail closed to avoid following deviation) • Pipe rupture or leakage	• Visible on flow indicator • Reactor feed will be outside design composition ==> product will be out of spec. • Reactor temperature will decrease (no reaction), catalyst degradation	• Regular maintenance and inspection • Stand-by pump installed
More	Flow	• Control valve V-2 malfunction	• Product out of specification • Visible on flow indicator	• Install alarm for high flow • Have panel-mounted indicator
	Pressure	• Downstream blockage AND pump-trip failure	• Increased likelihood of rupture and leakage ==> flammability risk	• Pressure indicator and high alarm • Regular maintenance and testing of pump motor trip
	Temperature	• Pump dead-heading, as for “More Pressure”	• As for “More Pressure”	• As for “More Pressure”
Less	Flow	• As for “No Flow”	• As for “No Flow”	• As for “No Flow”
	Pressure	• Control valve V-2 failure • Upstream pipe rupture or leakage • Upstream pump failure or trip	• Reverse flow of methanol ==> flammability hazard • Loss of feedstock	• Install low pressure alarm and indicator (panel mounted) • Install non-return valve • Regular inspection and maintenance
What else?	Instrument air failure	• As for “More Flow”	• As for “More Flow”	• Regular inspection

Stream 7

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Flow	• Upstream pump failure or trip • Pipe blockage • Malfunction of V-1 AND V-2 • Pipe rupture or leakage	• No product • Reactor temperature will decrease (no reaction)	• Provision for indicator on flow controller • Regular maintenance and inspection • Stand-by pump installed
More	Flow	• Malfunction of V-1 AND V-2	• Product out of specification (contact time in reactor affected) • Visible on flow indicators • Possible level increase in vaporiser	• Install alarms for high flow on Streams 3 AND 6 • Have panel-mounted indicators
	Pressure	• Downstream blockage AND pump-trip failure	• Increased likelihood of rupture and leakage ==> flammability risk	• Pressure indicator and high alarm on stream 6 • Regular maintenance and testing of pump motor trip
	Temperature	• Pump dead-heading, as for “More Pressure”	• As for “More Pressure”	• As for “More Pressure”
Less	Flow	• As for “No Flow”	• Less product • Reactor temperature will decrease (less reaction)	• As for “No Flow”
	Pressure	• Control valve V-1 OR V-2 malfunction • Upstream pipe rupture or leakage • Upstream pump failure or trip	• Reverse flow of methanol ==> flammability hazard	• Install low pressure alarm and indicator (panel mounted) • Install non-return valve • Regular inspection and maintenance

Stream 9

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Flow	• Upstream blower (CP-1) failure or trip of steam turbine (TRB-1) • Duct blockage • Duct rupture or leakage • Failure of control valve V-3 (fails closed to avoid feeding a fire)	• Reactor feed will be outside design composition ==> product will be out of spec. • Reactor temperature will decrease (no reaction)	• Provision for indicator on flow controller • Regular maintenance and inspection • (Stand-by compressor and turbine too expensive and impractical)
More	Flow	• Malfunction of V-3 • Steam turbine (TRB-1) goes haywire • Too much off-gas recycle	• Product out of specification (contact time in reactor affected) • Visible on flow indicators • Possibly enter flammability limits	• Install alarm for high flow • Have panel-mounted indicators • Remove all ignition sources • Adjust off-gas recycle
	Pressure	• Downstream blockage (*e.g.* V-3 failure) AND turbine-trip malfunction	• Increased likelihood of rupture and leakage ==> flammability risk (contains hydrogen)	• Pressure indicator and high alarm • Regular maintenance and testing of turbine trip system
	Temperature	• Compressor dead-heading, as for “More Pressure”	• As for “More Pressure”	• As for “More Pressure”
Less	Flow	• As for “No Flow”	• Less product • Reactor temperature will decrease (less reaction) • Product out of spec.	• As for “No Flow”
	Pressure	• Control valve V-3 failure • Upstream pipe rupture or leakage • Upstream blower/turbine failure or trip	• Reverse flow of vapour, possibly including methanol ==> flammability hazard • Product out of spec.	• Install low pressure alarm and indicator (panel mounted) • Regular inspection and maintenance • (Non-return valve impractical)

Stream 10

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Flow	• Downstream pump (P-2A / P-2B) failure • Pipe blockage • Pipe rupture or leakage • Upstream feed system failure • Accidental closure of isolation valves	• No vaporisation due to zero heat transfer ==> Level in vaporiser rises ==> increased rupture risk of vaporiser ==> flammability hazard • Visible on vaporiser level indicator • composition ==> product will be out of spec. • Reactor temperature will decrease (no reaction) • More cooling required in absorber (control system will detect this)	• Provision for panel display of level • Regular maintenance and inspection • Training of operators not to close isolation valves during operation AND interlocks
More	Flow	• Increase in upstream flow • Lower temperature on exit of HX-10 (Stream 13)	• No increase in vaporisation due to limited utility capacity ==> Level in vaporiser rises ==> increased rupture risk of vaporiser ==> flammability hazard • Visible on vaporiser level indicator • Product out of spec.	• Install alarm for high flow • Have panel-mounted indicators
	Pressure	• Downstream blockage of pipe • Accidental closure of isolation valves	• Increased likelihood of rupture and leakage ==> flammability risk (contains methanol)	• High pressure alarm on pump discharges (to existing indicators)
	Temperature	• High temperature of Stream 9 OR 13	• Vapour in pump suction ==> damage to pump	• Install low level alarm to trip pump
Less	Flow	• As for “No Flow”	• Less product • Reactor temperature will decrease (less reaction) • Product out of spec. • More cooling required in absorber (control system will detect this)	• As for “No Flow”
	Pressure	• Low level in vaporiser (HX-1) • Upstream rupture or leakage • Upstream blower/pump failure or trip	• As for “More Temperature”	• As for “More Temperature”
	Temperature	• Inadequate heat transfer in heat exchangers (HX-5 OR HX-10) • Steam utility failure	• Level in vaporiser rises ==> increased rupture risk of vaporiser ==> flammability hazard	• Install panel-mounted temperature indicators and alarms on exits of heat exchangers HX-5 AND HX-10

		• On start-up temperatures of Streams 20 and 21 will be low	• Visible on vaporiser level indicator • Product out of spec.	• Attempt to make up additional duty in OTHER exchanger, ELSE reduce flow of vaporiser feed • Recycle until operating temperature reached

Stream 11

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Flow	• Upstream pump (P-2A / P-2B) failure • Pipe blockage • Pipe rupture or leakage • Upstream feed system failure • Accidental closure of isolation valves	• As for “No Flow” of Stream 10	• As for “No Flow” of Stream 10
More	Flow	• As for “More Flow” of Stream 10	• As for “More Flow” of Stream 10	• As for “More Flow” of Stream 10
	Pressure	• Downstream blockage of pipe (including fouling of heat exchangers, HX-5 OR HX-10) • Accidental closure of isolation valves	• Increased likelihood of rupture and leakage ==> flammability risk (contains methanol)	• High pressure alarm on pump discharges (to existing indicators)
	Temperature	• High temperature of Stream 9 OR 13	• Vapour in pump suction ==> damage to pump	• Install low level alarm to trip pump
Less	Flow	• As for “No Flow”	• As for “Less Flow” of Stream 10	• As for “No Flow”
	Pressure	• Low level in vaporiser (HX-1) • Upstream rupture or leakage • Upstream blower/pump failure or trip	• As for “More Temperature”	• As for “More Temperature”
	Temperature	• As for “Less Temperature” of Stream 10	• As for “Less Temperature” of Stream 10	• As for “Less Temperature” of Stream 10

Stream 12

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Flow	• As for “No Flow” of Stream 11	• As for “No Flow” of Stream 10	• As for “No Flow” of Stream 10
More	Flow	• As for “More Flow” of Stream 10	• As for “More Flow” of Stream 10	• As for “More Flow” of Stream 10
	Pressure	• Downstream blockage of pipe (including fouling of heat exchangers, HX-5 OR HX-10) • Accidental closure of isolation valves	• Increased likelihood of rupture and leakage ==> flammability risk (contains methanol)	• High pressure alarm on pump discharges (to existing indicators)
	Temperature	• High temperature of Stream 9 OR 13	• Vapour in pump suction ==> damage to pump	• Install low level alarm to trip pump
Less	Flow	• As for “No Flow”	• As for “Less Flow” of Stream 10	• As for “No Flow”
	Pressure	• Low level in vaporiser (HX-1) • Upstream rupture or leakage • Upstream blower/pump failure or trip	• As for “More Temperature”	• As for “More Temperature”
	Temperature	• As for “Less Temperature” of Stream 10	• As for “Less Temperature” of Stream 10	• As for “Less Temperature” of Stream 10

Stream 13

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Flow	• As for “No Flow” of Stream 11	• As for “No Flow” of Stream 10	• As for “No Flow” of Stream 10
More	Flow	• As for “More Flow” of Stream 10	• As for “More Flow” of Stream 10	• As for “More Flow” of Stream 10
	Pressure	• Downstream blockage of pipe (including fouling of heat exchangers, HX-5 OR HX-10) • Accidental closure of isolation valves	• Increased likelihood of rupture and leakage ==> flammability risk (contains methanol)	• High pressure alarm on pump discharges (to existing indicators)
	Temperature	• High temperature of Stream 9 OR 13	• Vapour in pump suction ==> damage to pump	• Install low level alarm to trip pump
Less	Flow	• As for “No Flow”	• As for “Less Flow” of Stream 10	• As for “No Flow”
	Pressure	• Low level in vaporiser (HX-1) • Upstream rupture or leakage • Upstream blower/pump failure or trip	• As for “More Temperature”	• As for “More Temperature”
	Temperature	• As for “Less Temperature” of Stream 10	• As for “Less Temperature” of Stream 10	• As for “Less Temperature” of Stream 10

Stream 14

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Flow	• Upstream blockage (including accidental closure of isolation valves) • Upstream leakage or rupture	• No reaction ==> reactor temperature decrease ==> visible on reactor temperature indicator (with alarm) • No product	• Display flow reading of Stream 14 on panel • Have alarm for low flow • Regular maintenance and inspection of ductwork
More	Flow	• More flow of feed streams into vaporiser (HX-1) – see Streams 3, 6, 7 and 9	• Product out of spec. (altered contact time in reactor) • Temperature at inlet to reactor will decrease due to limited heat transfer in Superheater (HX-2) ==> possible degradation of catalyst; product out of spec.	• Install a flow indicator, to be displayed in the control room with integral high flow alarm • Size vaporiser unit and steam system to handle some contingency (say 20% above design) • Temperature indicator AND controller will exist on exit of superheater (HX-2)
	Pressure	• Downstream blockage of duct • Accidental closure of isolation valves downstream	• Increased likelihood of rupture and leakage ==> flammability risk (contains methanol) • Discharge through safety valve at top of vaporiser (HX-1)	• Install high pressure alarm
	Temperature	• High temperature of Stream 9 OR 13	• Vapour in pump suction ==> damage to pump (P-2) • Less heating required in superheater (HX-2) • Composition may be different ==> product out of spec.	• Install low level alarm to trip pump • Temperature indicator AND controller on HX-2
Less	Flow	• As for “No Flow”	• Less reaction ==> reactor temperature decrease ==> visible on reactor temperature indicator (with alarm) • Less product	• As for “No Flow”
	Pressure	• Upstream rupture or leakage • Upstream blower (CP-1) failure OR trip	• Reaction may be affected via a shift in equilibrium (principally of the dehydrogenation reaction) • Saturation mole fractions of condensables in absorber (ABS-1) will increase ==> less effective	• Install low flow alarm • Make the ducts strong

			absorption ==> lower plant yield; product out of spec. • Identifiable by blower trip alarm	
	Temperature	• As for "Less Temperature" of Stream 13	• As for "Less Temperature" of Stream 13	• As for "Less Temperature" of Stream 13
	Percentage of methanol	• Inadequate vaporisation (*e.g.* insufficient steam OR temperature of Stream 20 too low, as on start-up) • Malfunction of ratio controller	• Less reaction • Enter the flammability limits (no longer above the upper limit)	• Have alarm on ratio controller – increase the ratio of methanol supplied, if possible, ELSE feed less feed to process and recycle more off-gas

Stream 118

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Flow	• Blockage in steam lines (including accidental closure of isolation valves; including build-up of deposits [“fouling”] in HX-10) • Upstream leakage or rupture • Failure to add additional fuel (natural gas) to the off-gas burner (RXN-3) on start-up	• No heating in HX-10 ==> less vaporisation occurring ==> less product / out of spec. • Likely to be registered by the pressure indicator on Stream 118	• Display flow reading of Stream 119 on panel • Have alarm for low flow on Stream 119 • Indicate pressure on panel • Regular maintenance and inspection of ductwork
More	Flow	• Malfunction in steam system control valves (including V-4 – which should be fail-open to vaporise methanol out of vaporiser)	• Over heating of vaporiser recycle stream (in HX-10) ==> gas phase in Stream 13 ==> liquid hold-up in base of vaporiser drops ==> cavitation in pump (P-2)	• Install a flow indicator, to be displayed in the control room with integral high flow alarm on Stream 119 • Temperature indicator AND controller will exist on exit of superheater (HX-2), and duty in this exchanger will decrease as required • Low pressure/Level alarms will trip pump (P-2)
	Pressure	• Downstream blockage of line • Accidental closure of isolation valves downstream • Malfunction in steam system control valves (including V-4)	• Increased likelihood of rupture and leakage ==> risk to personnel • Discharge through safety valve on shell-side of HX-10	• Install high pressure alarm at boiler (RXN-3)
	Temperature	• As for “More Pressure” • Very low boiler feed water flow leading to super-heating of the 1200kPa(abs) steam	• Increased risk of materials failures ==> risk to personnel	• Construct steam lines of rugged material
Less	Flow	• As for “No Flow”	• Less heating in HX-10 ==> less vaporisation occurring ==> less product / out of spec. • Likely to be registered by the pressure indicator on Stream 118	• As for “No Flow”
	Pressure	• Upstream rupture or leakage • Upstream pump (on boiler feed water to off-gas burner) failure OR trip	• Control system would attempt to increase the flow (IF necessary), however there is a limit to the flow that can be handled by HX-10	• Detect with low temperature alarm on Stream 13 AND low flow alarm Stream 119 • Ease off on the flow of feedstock to

			• Temperature of Stream 13 would decrease ==> less vaporisation ==> less feed to reactor ==> less product / out of spec.	the vaporiser (HX-1)
	Temperature	• Inadequate heating in boiler (RXN-3) • Heat loss through steam lines	• Control system would attempt to increase the flow (IF necessary), however there is a limit to the flow that can be handled by HX-10 • Temperature of Stream 13 would decrease ==> less vaporisation ==> less feed to reactor ==> less product / out of spec.	• Cover steam lines with adequate insulation and ensure its upkeep • Control temperature of steam at point of generation (RXN-3) • Detect with low temperature alarm on Stream 13 AND low flow alarm Stream 119 • Ease off on the flow of feedstock to the vaporiser (HX-1)
What else?	Personnel performing maintenance on OR near steam lines	• Regular maintenance • Equipment break-down	• Employees suffer burns to their persons	• Cover steam lines with adequate insulation ("Personnel Protection") and ensure its upkeep

Stream 119

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Flow	• As for “No Flow” of Stream 118	• As for “No Flow” of Stream 118	• As for “No Flow” of Stream 118
More	Flow	• As for “More Flow” of Stream 118	• As for “More Flow” of Stream 118	• As for “More Flow” of Stream 118
	Pressure	• As for “More Pressure” of Stream 118	• As for “More Pressure” of Stream 118	• As for “More Pressure” of Stream 118
	Temperature	• Low flow of Stream 12 (*q.v.*) • As for “More Pressure” • Very low boiler feed water flow leading to super-heating of the 1200kPa(abs) steam	• Increased risk of materials failures ==> risk to personnel	• Construct condensate lines of rugged material
Less	Flow	• As for “Less Flow” of Stream 118	• As for “Less Flow” of Stream 118	• As for “Less Flow” of Stream 118
	Pressure	• As for “Less Pressure” of Stream 118	• As for “Less Pressure” of Stream 118	• As for “Less Pressure” of Stream 118
	Temperature	• As for “Less Temperature” of Stream 118	• As for “Less Temperature” of Stream 118	• As for “Less Temperature” of Stream 118
What else?	Personnel performing maintenance on OR near condensate lines	• As for “What else?” of Stream 118	• As for “What else?” of Stream 118	• As for “What else?” of Stream 118

Vaporiser (HX-1)

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Level	• No inlet flows (blockage of inlet lines/closed control valves) • Inlet flows are too hot (vapour)	• Vapour to suction port of pump (P-2) ==> Damage to pumps • Product out of spec.	• Automatic trip on pumps
More	Level	• Inadequate heating in recirculation loop (including due to blockage in pipes)	• Flooding of vaporiser • Blower may have to work harder to blow gas stream (Stream 9) through the increased head of liquid	• Install high level alarm on existing liquid level controller
	Pressure	• Downstream blockage	• Pressure will be relieved through existing safety valve on top of HX-1	• Ensure regular maintenance, testing AND inspection of safety valve
	Temperature	• Upstream blockage or disturbance • High inlet temperatures on streams 9 OR 13 (*q.v.*)	• Increased risk of materials failures ==> risk to personnel; flammability risk	• Construct vaporiser shell of heavy duty materials
Less	Level	• Less inlet flows (blockage of inlet lines/closed control valves) • Inlet flows are too hot (*e.g.* two-phase)	• As for “No Level”	• As for “No Level”
	Pressure	• Blower (CP-1) or pump (P-1) failure • Blockage in lines 7 OR 9 (upstream)	• Reaction may be affected via a shift in equilibrium (principally of the dehydrogenation reaction) • Saturation mole fractions of condensables in absorber (ABS-1) will increase ==> less effective absorption ==> lower plant yield; product out of spec. • Identifiable by blower/pump trip alarm	• Install low flow alarm
	Temperature	• Inadequate heating in recirculation loop (including due to blockage in pipes)	• Flooding of vaporiser • Blower may have to work harder to blow gas stream (Stream 9) through the increased head of liquid	• Install high level alarm on existing liquid level controller

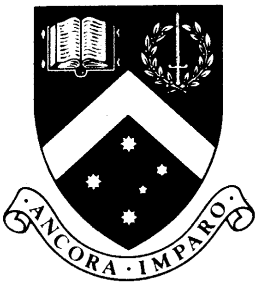
Methanol Heater (HX-10)

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
No	Level (shell-side)	• Blockage in Stream 118 (including Less inlet flows: blockage of inlet lines) • Steam trap failure • Leak in HX-10	• No heat transfer • Loss of containment ==> risk to personnel	• Low flow alarm on Stream 119 • Install liquid level controller with low level alarm
More	Level	• Blockage in Stream 119 (including closed control valves) • Insufficient flow of steam through Stream 118	• Flooding of exchanger shell • Evident due to low flow indicator on stream 119 • Heat transfer [coefficient] would decrease ==> evident due to low temperature indicator on Stream 13	• Install liquid level controller with high level alarm
	Pressure	• As for “More Pressure” of Stream 118	• As for “More Pressure” of Stream 118	• As for “More Pressure” of Stream 118
	Temperature	• As for “More Temperature” of Stream 118	• As for “More Temperature” of Stream 118	• As for “More Temperature” of Stream 118
Less	Level	• As for “No Level”	• As for “No Level”	• As for “No Level”
	Pressure	• If the exchanger were isolated (shell-side) with steam initially present, then the steam would condense ==> decrease in pressure	• This may cause material failure in extreme cases	• Train employees to NOT isolate exchanger while it still contains steam – it must be vented • Install vent if not already present (not marked) ELSE discharge through safety valve
	Temperature	• As for “Less Temperature” of Stream 118	• As for “Less Temperature” of Stream 118	• As for “Less Temperature” of Stream 118

Pumps (P-2A AND P-2B)

GUIDE WORD	DEVIATION	POSSIBLE CAUSES	CONSEQUENCES	ACTION REQUIRED
More	Pressure	• Dead-heading of pump due to downstream obstruction in line	• Possible material failure in extreme cases	• Design pressures rated above operating pressures • Trip pump in case of high pressure alarm (to be installed)
	Temperature	• As for “More Pressure” • High inlet temperatures (see Stream 7)	• Possible material failure in extreme cases (due to reduction in the yield strength of metals at elevated temperatures)	• Design temperatures rated above operating temperatures
Less	Pressure	• Low level in vaporiser (HX-1) ==> Insufficient Net Positive Suction Head (NPSH)	• Cavitation ==> Damage to pump	• Automatic trip on pump, activated by low level alarm on vaporiser (HX-1)
Reverse	Flow	• Check-valve failure	• Damage to pump(s)	• Make sure that those responsible check the check valves to make sure that the check valves will check the flow, as required

MONASH UNIVERSITY
DEPARTMENT OF CHEMICAL ENGINEERING



APPENDIX TO CHAPTER 11

ECONOMIC EVALUATION

1999 currency exchange rates:
Source: The Saturday Age, Business section (from CBA - *not* for currency notes)

One Australian dollar was worth:

DATE	**German DM**			**US $**		
	Buy	**Sell**	AVERAGE	**Buy**	**Sell**	AVERAGE
08 May	1.2290	1.2004	1.215	0.6718	0.6668	0.669
22 May	1.2289	1.2003	1.215	0.6620	0.6570	0.660
10 July	1.2910	1.2610	1.276	0.6692	0.6642	0.667
24 July	1.2209	1.1923	1.207	0.6506	0.6456	0.648
09 October	1.2188	1.1904	1.205	0.6620	0.6570	0.660
Average	1.238	1.209	**1.22**	0.663	0.658	**0.66**

So a German DM is equal to **0.5400** US $.

PURCHASED EQUIPMENT COSTS

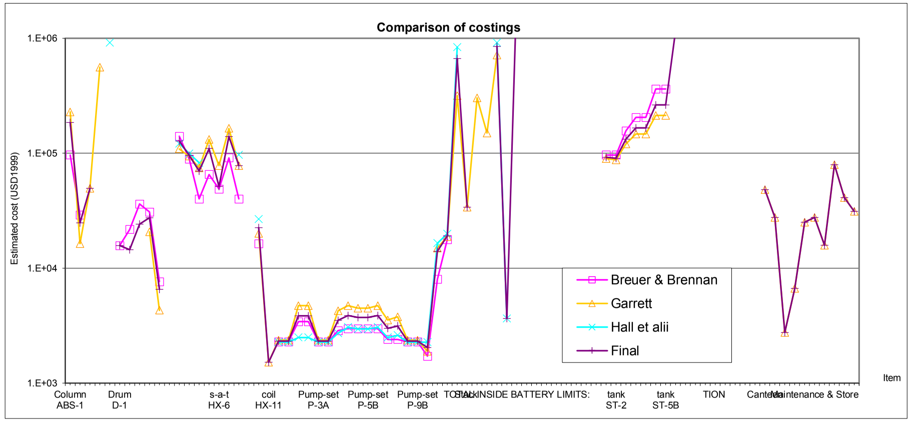
Indonesian, USD$_{1999}$ basis.

ABBREVIATIONS: n.a. = not available, N/A = not applicable, s-a-t = shell-and-tube (heat exchanger)

REFERENCE:	BREUER & BRENNAN	GARRETT	HALL, MATLEY & MCNAUGHTON
Current location factor [B & B; BRENNAN]:	0.769	0.97	0.97
Historical currency conversion factor [B & B]:	0.769	1	1
CE Index for original date [BRENNAN; CE]:	363.0	320	300
CE Index for 1999 [CE]:	390	390	390
Inflation factor:	1.074	1.219	1.3

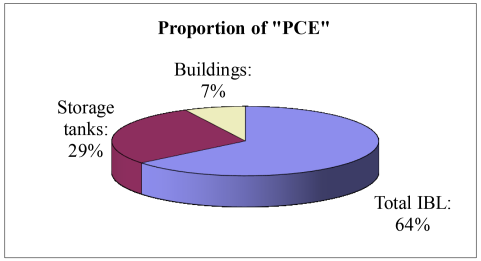
ITEM	**DESCRIP-TION**	**DIMENSION & TYPE**	**B&B Original cost** [AUD$_{1/7/91}$]	**B&B Updated cost** [USD$_{1999}$]	**B&B Type** [–]	**B&B Materials** [–]	**B&B Pressure** [–]	**B&B Final cost** [USD$_{1999}$]	**Garrett Original cost** [USD$_{1987}$]	**Garrett Updated cost** [USD$_{1999}$]	**Garrett Type** [–]	**Garrett Materials** [–]	**Garrett Pressure** [–]	**Garrett Final cost** [USD$_{1999}$]	**HM&M Original cost** [USD$_{Jan82}$]	**HM&M Updated cost** [USD$_{1999}$]	**HM&M Type** [–]	**HM&M Materials** [–]	**HM&M Pressure** [–]	**HM&M Final cost** [USD$_{1999}$]	**FINAL VALUE**	**COMMENTS**
INSIDE BATTERY LIMITS																						
ABS-1	Column	1.8m diameter, 33m height	80.0E+3	50.9E+3	1	1.9	1	96.6E+3	92.0E+3	108.8E+3	1	2.1	1	228.5E+3	no good data available						185E+3	
	Packing	19.3 m^3, 50mm Pall	13.1E+3	8.3E+3	1	3.5	1	29.0E+3	13.1E+3	15.5E+3	1	1.05	1	16.3E+3	no good data available						25E+3	Garrett's data for SS.
	Trays	21 × 1.8m dia., b-caps	n.a.						22.1E+3	26.1E+3	1	1.9	1	49.5E+3	no good data available						50E+3	
CP-1	Blower	Centrifugal 6 m^3.s^{-1} 85kPa	n.a.						190.0E+3	224.6E+3	1	2.5	1	561.5E+3	see below						see below	Garrett with MOTOR
Blower WITH tubine		539kW	N/A						N/A						250.0E+3	315.3E+3	1	2.9	1	914.2E+3	see below	"Gas" turbine specified
D-1	Drum	1.4 cubic metres	13.0E+3	8.3E+3	1	1.9	1	15.7E+3	n.a.						no good data available						16E+3	
D-2	Drum	2.2 cubic metres	18.0E+3	11.4E+3	1	1.9	1	21.7E+3	n.a.					000.0E+0	no good data available						14E+3	
D-3	Drum	12 cubic metres	30.0E+3	19.1E+3	1	1.9	1	36.2E+3	n.a.					000.0E+0	no good data available						24E+3	
HX-1	Column	1.8m diameter, 3m height	25.0E+3	15.9E+3	1	1.9	1.02	30.7E+3	8.4E+3	9.9E+3	1	2.1	1	20.8E+3	no good data available						27E+3	
	Packing	5.1 m^3, 50mm Pall	3.4E+3	2.2E+3	1	3.5	1	7.6E+3	3.5E+3	4.1E+3	1	1.05	1	4.3E+3	no good data available						7E+3	Garrett's data for SS.
									Type factor corrected by subtracting unity according to B & B													
HX-2	s-a-t	Fixed-tube, 148 m^2	60.0E+3	38.1E+3	1	3.5	1.05	140.2E+3	32.0E+3	37.8E+3	0.79	3.48	1.05	109.1E+3	25.0E+3	31.5E+3	1	3.85	1	121.4E+3	128E+3	Hall extrapolated
HX-3	s-a-t	Fixed-tube, 131 m^2	40.0E+3	25.4E+3	1	3.5	1	89.0E+3	29.0E+3	34.3E+3	0.79	3.48	1	94.2E+3	20.5E+3	25.9E+3	1	3.85	1	99.5E+3	96E+3	see RXN-2
HX-4	s-a-t	Fixed-tube, 87.2 m^2	18.0E+3	11.4E+3	1	3.5	1	40.1E+3	23.0E+3	27.2E+3	0.79	3.48	1	74.7E+3	17.0E+3	21.4E+3	1	3.85	1	82.5E+3	70E+3	see RXN-1
HX-5	s-a-t	U-tube 180 m^2	28.0E+3	17.8E+3	1	3.5	1.05	65.4E+3	36.0E+3	42.6E+3	0.85	3.48	1.05	132.1E+3	out of range						110E+3	
HX-6	s-a-t	Floating 75 m^2	22.0E+3	14.0E+3	1	3.5	1	49.0E+3	19.0E+3	22.5E+3	1	3.48	1	78.1E+3	17.5E+0	22.1E+0	1	3.85	1	85.0E+0	51E+3	
HX-7	s-a-t	Floating 210 m^2	41.0E+3	26.1E+3	1	3.5	1	91.2E+3	40.0E+3	47.3E+3	1	3.48	1	164.4E+3	out of range						140E+3	
HX-8	s-a-t	Floating 100 m^2	18.0E+3	11.4E+3	1	3.5	1	40.1E+3	19.0E+3	22.5E+3	1	3.48	1	78.1E+3	20.0E+3	25.2E+3	1	3.85	1	97.1E+3	78E+3	
HX-9	fired boiler	see RXN-3 (1478kW)	see RXN-3						see RXN-3						see RXN-3						see below	see RXN-3
HX-10	s-a-t	Fixed-tube, 13 m^2	7.0E+3	4.5E+3	1	3.5	1.05	16.4E+3	5.9E+3	7.0E+3	0.79	3.48	1.05	20.1E+3	5.5E+3	6.9E+3	1	3.85	1	26.7E+3	22E+3	
HX-11	coil	25mm 273 m	n.a.						627.0E+0	741.2E+0	1	2.05	1	1.5E+3	n.a.						2E+3	Garrett extrapolated
P-1A	Pump-set	0.32kW 7.9 m^3.h^{-1} 9.7m	2.0E+3	1.3E+3	1	1.8	1	2.3E+3	1.0E+3	1.2E+3	1	2.0	1	2.4E+3	1.0E+3	1.3E+3	1	1.8	1	2.3E+3	2E+3	Garrett extrapolated
P-1B	Pump-set	0.32kW 7.9 m^3.h^{-1} 9.7m	2.0E+3	1.3E+3	1	1.8	1	2.3E+3	1.0E+3	1.2E+3	1	2.0	1	2.4E+3	1.0E+3	1.3E+3	1	1.8	1	2.3E+3	2E+3	All conventional, AVS
P-2A	Pump-set	2.55kW 96 m^3.h^{-1} 7.1m	3.0E+3	1.9E+3	1	1.8	1	3.4E+3	2.0E+3	2.4E+3	1	2.0	1	4.7E+3	1.1E+3	1.4E+3	1	1.8	1	2.5E+3	4E+3	
P-2B	Pump-set	2.55kW 96 m^3.h^{-1} 7.1m	3.0E+3	1.9E+3	1	1.8	1	3.4E+3	2.0E+3	2.4E+3	1	2.0	1	4.7E+3	1.1E+3	1.4E+3	1	1.8	1	2.5E+3	4E+3	
P-3A	Pump-set	0.22kW 3.9 m^3.h^{-1} 10.2m	2.0E+3	1.3E+3	1	1.8	1	2.3E+3	1.0E+3	1.2E+3	1	2.0	1	2.4E+3	1.0E+3	1.3E+3	1	1.8	1	2.3E+3	2E+3	All except Hall extrap'd
P-3B	Pump-set	0.22kW 3.9 m^3.h^{-1} 10.2m	2.0E+3	1.3E+3	1	1.8	1	2.3E+3	1.0E+3	1.2E+3	1	2.0	1	2.4E+3	1.0E+3	1.3E+3	1	1.8	1	2.3E+3	2E+3	
P-4A	Pump-set	2.1kW 93 m^3.h^{-1} 3.6m	2.5E+3	1.6E+3	1	1.8	1	2.9E+3	1.8E+3	2.1E+3	1	2.0	1	4.3E+3	1.2E+3	1.5E+3	1	1.8	1	2.7E+3	4E+3	
P-4B	Pump-set	3.0kW 135 m^3.h^{-1} 3.7m	2.6E+3	1.7E+3	1	1.8	1	3.0E+3	2.0E+3	2.4E+3	1	2.0	1	4.7E+3	1.4E+3	1.7E+3	1	1.8	1	3.1E+3	4E+3	
P-5A	Pump-set	2.76kW 6.2 m^3.h^{-1} 82m	2.6E+3	1.7E+3	1	1.8	1	3.0E+3	1.9E+3	2.2E+3	1	2.0	1	4.5E+3	1.3E+3	1.6E+3	1	1.8	1	3.0E+3	4E+3	
P-5B	Pump-set	2.76kW 6.2 m^3.h^{-1} 82m	2.6E+3	1.7E+3	1	1.8	1	3.0E+3	1.9E+3	2.2E+3	1	2.0	1	4.5E+3	1.3E+3	1.6E+3	1	1.8	1	3.0E+3	4E+3	
P-6	Pump-set	3.0kW 135 m^3.h^{-1} 3.7m	2.6E+3	1.7E+3	1	1.8	1	3.0E+3	2.0E+3	2.4E+3	1	2.0	1	4.7E+3	1.4E+3	1.7E+3	1	1.8	1	3.1E+3	4E+3	See P-4B
P-7	Pump-set	1.0kW 47 m^3.h^{-1} 3.9m	2.1E+3	1.3E+3	1	1.8	1	2.4E+3	1.5E+3	1.8E+3	1	2.0	1	3.5E+3	1.1E+3	1.4E+3	1	1.8	1	2.5E+3	3E+3	
P-8	Pump-set	1.3kW 26 m^3.h^{-1} 13m	2.1E+3	1.3E+3	1	1.8	1	2.4E+3	1.6E+3	1.9E+3	1	2.0	1	3.8E+3	1.2E+3	1.5E+3	1	1.8	1	2.6E+3	3E+3	
P-9A	Pump-set	0.32kW 5.9 m^3.h^{-1} 10.2m	2.0E+3	1.3E+3	1	1.8	1	2.3E+3	1.0E+3	1.2E+3	1	2.0	1	2.4E+3	1.0E+3	1.3E+3	1	1.8	1	2.3E+3	2E+3	All except Hall extrap'd
P-9B	Pump-set	0.32kW 5.9 m^3.h^{-1} 10.2m	2.0E+3	1.3E+3	1	1.8	1	2.3E+3	1.0E+3	1.2E+3	1	2.0	1	2.4E+3	1.0E+3	1.3E+3	1	1.8	1	2.3E+3	2E+3	
P-10	Pump-set	0.05kW 1.2 m^3.h^{-1} 9.7m	1.5E+3	953.6E+0	1	1.8	1	1.7E+3	800.0E+0	945.8E+0	1	2.0	1	1.9E+3	1.0E+3	1.3E+3	1	1.8	1	2.3E+3	2E+3	All extrapolated
RXN-1	Cat. Bed	Take as 20% of HX-4						8.0E+3						14.9E+3						16.5E+3	14E+3	Take as 20% of HX-4
RXN-2	Cat. Bed	Take as 20% of HX-3						17.8E+3						18.8E+3						19.9E+3	19E+3	Take as 20% of HX-3
RXN-3	Burner	Fired, box 3.595MW 12.3 ×10^6 btu/h	N/A						200.0E+3	236.4E+3	1	1.34	1	316.8E+3	370.0E+3	466.6E+3	1	1.8	1	839.8E+3	665E+3	Includes HX-9. Box must be extrapolated (circular wouldn't req.)
	Stack	15m	n.a.						12.5E+3	14.8E+3	2.3	1	1	34.0E+3	n.a.						34E+3	
TRB-1	Steam turb	539kW centrifugal 3600rpm	n.a.						85.0E+3	100.5E+3	1.04	2.9	1	303.1E+3	See CP-1						see below	See also under CP-1
	Corresponding motor		N/A						42.0E+3	49.7E+3	1.04	2.9	1	149.8E+3	N/A						see below	
	∴ Blower + Turbine:													714.9E+3						914.2E+3	848E+3	

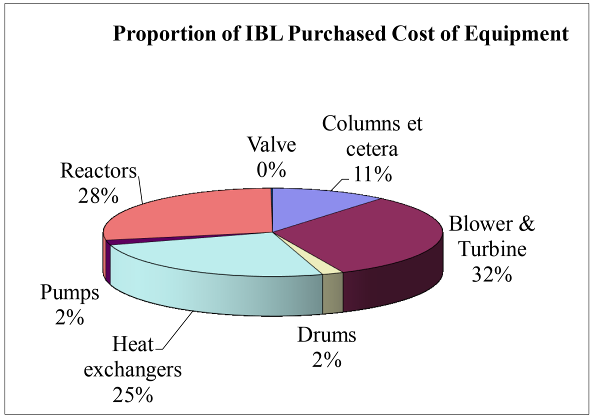
ITEM	DESCRIPTION	DIMENSION & TYPE	Original cost [AUD$_{1/7/91}$]	Updated cost [USD$_{1999}$]	Type [–]	Materials [–]	Pressure [–]	Final cost [USD$_{1999}$]	Original cost [USD$_{1987}$]	Updated cost [USD$_{1999}$]	Type [–]	Materials [–]	Pressure [–]	Final cost [USD$_{1999}$]	Original cost [USD$_{Jan82}$]	Updated cost [USD$_{1999}$]	Type [–]	Materials [–]	Pressure [–]	Final cost [USD$_{1999}$]	FINAL VALUE	COMMENTS
V-1	Exp.Valve	under 1 inch	n.a.						n.a.						1.0E+3	1.3E+3	1	2.9	1	3.7E+3	4E+3	IF h.p. butterfly (negl.)
TOTAL INSIDE BATTERY LIMITS:																					2.7E+6	
STORAGE TANKS																						
ST-1	tank	closed 190 m^3	80.0E+3	50.9E+3	1	1.9	1	96.6E+3	38.0E+3	44.9E+3	1	2.0	1	89.8E+3	Out of range						92E+3	B&B:"pressure vessels"
ST-2	tank	closed 183 m^3	80.0E+3	50.9E+3	1	1.9	1	96.6E+3	37.0E+3	43.7E+3	1	2.0	1	87.5E+3	Out of range						91E+3	Garrett: cone roof
ST-3	tank	closed 330 m^3	130.0E+3	82.6E+3	1	1.9	1	157.0E+3	51.0E+3	60.3E+3	1	2.0	1	120.6E+3	Out of range						133E+3	(*cf.* ellipsoidal)
ST-4A	tank	closed 507 m^3	170.0E+3	108.1E+3	1	1.9	1	205.3E+3	62.0E+3	73.3E+3	1	2.0	1	146.6E+3	Out of range						166E+3	
ST-4B	tank	closed 507 m^3	170.0E+3	108.1E+3	1	1.9	1	205.3E+3	62.0E+3	73.3E+3	1	2.0	1	146.6E+3	Out of range						166E+3	
ST-5A	tank	closed 1120 m^3	300.0E+3	190.7E+3	1	1.9	1	362.4E+3	90.0E+3	106.4E+3	1	2.0	1	212.8E+3	Out of range						263E+3	B&B extrapolated
ST-5B	tank	closed 1120 m^3	300.0E+3	190.7E+3	1	1.9	1	362.4E+3	90.0E+3	106.4E+3	1	2.0	1	212.8E+3	Out of range						263E+3	B&B extrapolated
TOTAL STORAGES:																					1.2E+6	
ITEM	DESCRIPTION	DIMENSION & TYPE	Original cost [AUD$_{1/7/91}$]	Updated cost [USD$_{1999}$]	Type [–]	Materials [–]	Pressure [–]	Final cost [USD$_{1999}$]	Original cost [USD$_{1987}$]	Updated cost [USD$_{1999}$]	Type [–]	Materials [–]	Pressure [–]	Final cost [USD$_{1999}$]	Original cost [USD$_{Jan82}$]	Updated cost [USD$_{1999}$]	Type [–]	Materials [–]	Pressure [–]	Final cost [USD$_{1999}$]	FINAL VALUE	COMMENTS
BUILDINGS																						
Canteen		60 m^2 : ft^2 646	n.a.						40.8E+3	48.2E+3	1	1	1	48.2E+3	n.a.						48E+3	All assumed to be
Control Room		30 m^2 : ft^2 323	n.a.						23.4E+3	27.7E+3	1	1	1	27.7E+3	n.a.						28E+3	equivalent (in cost) to:
Fire Shed		4 m^2 : ft^2 43	n.a.					(Extrapolated) --->	4.7E+3	5.5E+3	0.5	1	1	2.8E+3	n.a.						3E+3	"Office type with
Gate House		12 m^2 : ft^2 129	n.a.						11.3E+3	13.3E+3	0.5	1	1	6.7E+3	n.a.						7E+3	air conditioning,
Laboratory		16 m^2 : ft^2 172	n.a.						14.2E+3	16.7E+3	1.5	1	1	25.1E+3	n.a.						25E+3	restrooms, plaster or
Maintenance & Store		30 m^2 : ft^2 323	n.a.						23.4E+3	27.7E+3	1	1	1	27.7E+3	n.a.						28E+3	equivalent walls,
Medical Centre		9 m^2 : ft^2 97	n.a.						8.9E+3	10.6E+3	1.5	1	1	15.9E+3	n.a.						16E+3	insulation, modest
Offices & Admin.		112 m^2 : ft^2 1206	n.a.						67.2E+3	79.4E+3	1	1	1	79.4E+3	n.a.						79E+3	architectural features."
Religious Centre		49 m^2 : ft^2 527	n.a.						34.7E+3	41.0E+3	1	1	1	41.0E+3	n.a.						41E+3	EXCEPT where type
Toilets & Showers		21 m^2 : ft^2 226	n.a.						17.6E+3	20.8E+3	1.5	1	1	31.2E+3	n.a.						31E+3	factors are used
TOTAL BUILDINGS:																					305.6E+3	

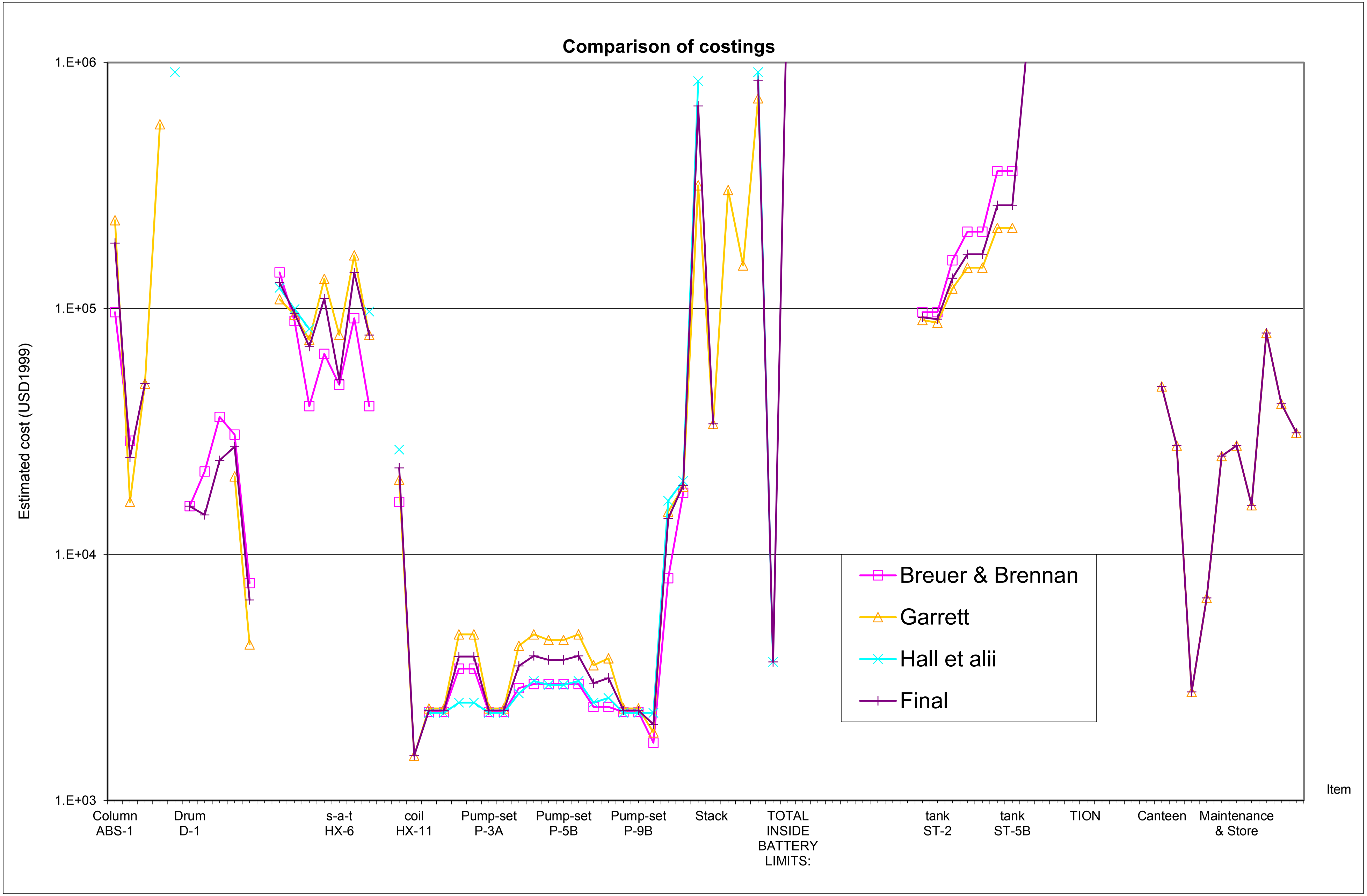


SUMMARY:

Columns *et cetera*	292.8E+3	
Blower & Turbine	847.8E+3	
Drums	54.4E+3	
Heat exchangers	662.5E+3	
Pumps	48.5E+3	
Reactors	732.6E+3	
Valve	3.7E+3	
Total IBL:	***2.6E+6***	Fraction of:
Storage tanks:	***1.2E+6***	0.44
Buildings:	***305.6E+3***	0.12
SUM:	4.1E+6	







Comparison of costings

OPERATING & PRODUCTION COSTS: 100% capacity utilisation

PRODUCT	**Formaldehyde**
PROCESS ROUTE	**Production from methanol via a silver catalyst-type process, with off-gas recycle**

GENERAL DATA	*VALUE*	*UNITS*	*COMMENTS*
PLANT CAPACITY	**80000**	$t.y^{-1}$	
CAPACITY UTILISATION	**1.00**	$(t.y^{-1}).(t.y^{-1})^{-1}$	
FIXED CAPITAL: **I**nside **B**attery **L**imits	2.64	$\times 10^6$ \$	All "\$" symbols denote USD_{1999}. $1AUD_{1999} = 0.66USD_{1999}$.
FIXED CAPITAL: **O**utside **B**attery **L**imits	6.50	$\times 10^6$ \$	
TOTAL FIXED CAPITAL	**13.37**	$\times 10^6$ \$	
PRODUCT SELLING PRICE	**300**	$\$.t_{product}^{-1}$	"Expected" price, Freight On Board. 54%$(kg.kg^{-1})$ basis.
EXPECTED ECONOMIC PLANT LIFE	**10**	y	Minimum value (conservative).

PRODUCTION COST	*UNITS*	*UNIT COST* $[\$.unit^{-1}]$	*UNIT USAGE* $[unit.t_{product}^{-1}]$	**ANNUAL COST** $[\times 10^6\ \$.y^{-1}]$	**COST PER TONNE OF PRODUCT (54% basis)** $[\$.t_{product}^{-1}]$	*COMMENTS*
RAW MATERIALS						From a neighbouring plant in Bontang, by pipeline.
Methanol	t	100	0.6648	5.32	66.48	**The unit cost is adjusted so that the minimum viable**
TOTAL RAW MATERIALS COSTS				**5.32**	**66.48**	**selling price equals the expected selling price.**
						There are two inlets streams!
	UNITS	*UNIT COST* $[\$.unit^{-1}]$	*UNIT USAGE* $[unit.t_{product}^{-1}]$			*COMMENTS*
UTILITIES						
Steam	t	7.92	-0.252	-0.16	-2.00	Surplus steam is exported for profit.
Nitrogen	Nm^3	0.198	0.000	0.00	0.00	Not required during normal operation.
Demineralised water	t	1.65	1.912	0.25	3.15	20% of BFW (Streams 100, 105 and 112) + Streams 2, 33 and 41.
Recirculated cooling wate	$m^3 \approx t$	0.0396	31.57	0.10	1.25	Streams 122, 124, 126 and 128.
Towns water	t	0.396	6.314	0.20	2.50	Taken as 20% of the RCW flow.
Electric power	MWh	29.7	0.0271	0.06	0.81	From actual pump motor requirements (only): 19.95 kW.
Natural gas	GJ	2.64	0.000	0.00	0.00	Only required on start-up.
TOTAL UTILITIES COSTS				**0.46**	**5.71**	*This is only 9% of the Raw Materials cost.*
	NUMBER	*COST PER "UNIT"* $[\$.y^{-1}]$				*COMMENTS*
PROCESS LABOUR						
Operators per shift	2					
(Hours required per day)	(24)					
(Days required per week)	(7)					
(Hours per shift)	(8)					(Ignoring time required during shift change-over)
Shift teams	4					
TOTAL *shift* operators	8	33000		0.26	3.30	
TOTAL *day* operators	0	26400		0.00	0.00	It is assumed that all operators are on a rotating shift,
TOTAL PROCESS LABOUR WAGES				0.26	3.30	such that none are classed as "day" operators

		FRACTION OF TOTAL PROCESS LABOUR WAGES						
PAYROLL OVERHEADS		0.3	0.08	0.99	Plant is not in a highly "developed" country	0.30 ≤	**0.30**	≤ 0.50
	FRACTION OF TOTAL FIXED CAPITAL							
MAINTENANCE LABOUR	0.05		0.67	8.36	See, *e.g.*, Brennan[1], p. 126, and *cf.* p. 118.			
					Assuming "equal division between materials and labour." See also below			
NETT "OPERATING" LABOUR COSTS			**1.01**	**12.65**	*This is 19% of the Raw Materials cost.*			
	FRACTION OF TOTAL FIXED CAPITAL	***FRACTION OF NETT "OPERATING" LABOUR COSTS***						
MAINTENANCE MATERIALS	0.05		**0.67**	**8.36**	See Brennan[1], p. 118: here the *two* fractions sum to	0.02 ≤	**0.10**	≤ 0.12
					The fraction is increased due to high capacity utilisation:		**100%**	,
					and due to the corrosive process fluid (though 316SS is used) which precipitates.			
OPERATING SUPPLIES ≈ CONSUMABLE STORES		0.125	**0.03**	**0.41**	Moderately "dirty" and "complicated" process	0.05 ≤	**0.13**	≤ 0.20
cf.	0.0075		0.10028	1.25344	Alternative to the above	0.005 ≤	**0.008**	≤ 0.01
PLANT OVERHEADS		0.4	**0.11**	**1.32**	Plant is part of a larger petrochemical complex	0.3 ≤	**0.4**	≤ 1.0
INSURANCE	0.015		**0.20**	**2.51**	Moderate risk	0.001 ≤	**0.015**	≤ 0.03
PROPERTY TAXES	0.01		**0.13**	**1.67**	Relatively undeveloped industrial area; incentive	0.01 ≤	**0.01**	≤ 0.04
"BOOK" DEPRECIATION (*not* a cash cost)	0.10		**1.34**	**16.71**	Calculated based on a 10 y plant life	0.05 ≤	**0.10**	≤ 0.2
TOTAL FIXED COSTS			**3.49**	**43.63**				
TOTAL PRODUCTION COST		**FIXED**	**3.49**	**43.63**				
		VARIABLE	5.78	**72.19**	Raw materials & Utilities			
		TOTAL	9.27	**115.82**	*Check: Methanol makes up 57% of the total "production cost."* ✓			
NON-MANUFACTURING COSTS								
	FRACTION OF TOTAL PRODUCTION COST (above)							
Corporate administration	0.025		0.23	2.90	Relatively simple division; mostly central admin.	0.02 ≤	**0.03**	≤ 0.06
cf. Fraction of total fixed capital		0.01375		2.30	Alternative to the above	0.01 ≤	**0.014**	≤ 0.04
Research & Development	0.005		0.05	0.58	An established technology, largely bought into	0.00 ≤	**0.01**	≤ 0.05
cf. Fraction of sales revenue		0.006		1.80	Expected sales revenue = 24 $\times 10^6$ \$(gr).y$^-$	0.00 ≤	**0.006**	≤ 0.06
Selling expenses	0.05		0.46	5.79	Relatively one major customer (contract)	0.05 ≤	**0.05**	≤ 0.025
cf. Fraction of sales revenue		0.020		6.00	Alternative to the above	0.02 ≤	**0.020**	≤ 0.2
TOTAL NON-MANUFACTURING COSTS			0.74	**9.27**				
TOTAL OPERATING COST			10.01	**125.08**	*Check: Methanol makes up 53% of the total "operating cost."* ✓			
MINIMUM PROFIT	Fraction of total fixed capital =	0.20	**2.67**	**33.43** $\$.t_{product}^{-1}$	This is a (pseudo)-commodity ==> Profit margin not so high			
MINIMUM VIABLE SELLING PRICE			12.68	**158.51** $\$.t_{product}^{-1}$	NOTE: The *expected* selling price i **300** $\$.t_{product}^{-1}$			
Recall:								
TOTAL RAW MATERIALS COSTS			5.32	66.48 $\$.t_{product}^{-1}$	Which is only methanol.			
Hence:								
"CONVERSION COST"			4.69	**58.61** $\$.t_{product}^{-1}$				

OPERATING & PRODUCTION COSTS TO "BREAK EVEN": 100% capacity utilisation

PRODUCT	**Formaldehyde**
PROCESS ROUTE	**Production from methanol via a silver catalyst-type process, with off-gas recycle**

GENERAL DATA

	VALUE	*UNITS*	*COMMENTS*
PLANT CAPACITY	**80000**	$t.y^{-1}$	
CAPACITY UTILISATION	**1.00**	$(t.y^{-1}).(t.y^{-1})^{-1}$	
FIXED CAPITAL: **I**nside **B**attery **L**imits	2.64	$\times 10^6$ \$	All "\$" symbols denote USD_{1999}. $1AUD_{1999} = 0.66USD_{1999}$.
FIXED CAPITAL: **O**utside **B**attery **L**imits	6.50	$\times 10^6$ \$	
TOTAL FIXED CAPITAL	**13.37**	$\times 10^6$ \$	
PRODUCT SELLING PRICE	**300**	$\$.t_{product}^{-1}$	"Expected" price, Freight On Board. 54%$(kg.kg^{-1})$ basis.
EXPECTED ECONOMIC PLANT LIFE	**10**	y	Minimum value (conservative).

PRODUCTION COST

	UNITS	*UNIT COST* $[\$.unit^{-1}]$	*UNIT USAGE* $[unit.t_{product}^{-1}]$	ANNUAL COST $[\times 10^6\ \$.y^{-1}]$	COST PER TONNE OF PRODUCT (54% basis) $[\$.t_{product}^{-1}]$	*COMMENTS*
RAW MATERIALS						From a neighbouring plant in Bontang, by pipeline.
Methanol	t	**297.09**	0.6648	15.80	197.49	**The unit cost is adjusted so that the minimum viable**
TOTAL RAW MATERIALS COSTS				**15.80**	**197.49**	**selling price equals the expected selling price.**
						There are two inlets streams!

	UNITS	*UNIT COST* $[\$.unit^{-1}]$	*UNIT USAGE* $[unit.t_{product}^{-1}]$	ANNUAL COST $[\times 10^6\ \$.y^{-1}]$	COST PER TONNE OF PRODUCT (54% basis) $[\$.t_{product}^{-1}]$	*COMMENTS*
UTILITIES						
Steam	t	7.92	-0.252	-0.16	-2.00	Surplus steam is exported for profit.
Nitrogen	Nm^3	0.198	0.000	0.00	0.00	Not required during normal operation.
Demineralised water	t	1.65	1.912	0.25	3.15	20% of BFW (Streams 100, 105 and 112) + Streams 2, 33 and 41.
Recirculated cooling wate	$m^3 \approx t$	0.0396	31.57	0.10	1.25	Streams 122, 124, 126 and 128.
Towns water	t	0.396	6.314	0.20	2.50	Taken as 20% of the RCW flow.
Electric power	MWh	29.7	0.0271	0.06	0.81	From actual pump motor requirements (only): 19.95 kW.
Natural gas	GJ	2.64	0.000	0.00	0.00	Only required on start-up.
TOTAL UTILITIES COSTS				**0.46**	**5.71**	*This is only 3% of the Raw Materials cost.*

	NUMBER	*COST PER "UNIT"* $[\$.y^{-1}]$	ANNUAL COST $[\times 10^6\ \$.y^{-1}]$	COST PER TONNE OF PRODUCT (54% basis) $[\$.t_{product}^{-1}]$	*COMMENTS*
PROCESS LABOUR					
Operators per shift	2				
(Hours required per day)	(24)				
(Days required per week)	(7)				
(Hours per shift)	(8)				(Ignoring time required during shift change-over)
Shift teams	4				
TOTAL *shift* operators	8	33000	0.26	3.30	
TOTAL *day* operators	0	26400	0.00	0.00	It is assumed that all operators are on a rotating shift,
TOTAL PROCESS LABOUR WAGES			0.26	3.30	such that none are classed as "day" operators

	FRACTION OF TOTAL PROCESS LABOUR WAGES								
PAYROLL OVERHEADS		0.3	0.08	0.99		Plant is not in a highly "developed" country	0.30 ≤	**0.30**	≤ 0.50
	FRACTION OF TOTAL FIXED CAPITAL								
MAINTENANCE LABOUR	0.05		0.67	8.36		See, *e.g.*, Brennan[1], p. 126, and *cf.* p. 118.			
						Assuming "equal division between materials and labour." See also below			
NETT "OPERATING" LABOUR COSTS			**1.01**	**12.65**		*This is 6% of the Raw Materials cost.*			
	FRACTION OF TOTAL FIXED CAPITAL	***FRACTION OF NETT "OPERATING" LABOUR COSTS***							
MAINTENANCE MATERIALS	0.05		**0.67**	**8.36**		See Brennan[1], p. 118: here the *two* fractions sum to 0.02 ≤		**0.10**	≤ 0.12
						The fraction is increased due to high capacity utilisation:		**100%**	,
						and due to the corrosive process fluid (though 316SS is used) which precipitates.			
OPERATING SUPPLIES ≈ CONSUMABLE STORES		0.125	**0.03**	**0.41**		Moderately "dirty" and "complicated" process	0.05 ≤	**0.13**	≤ 0.20
cf.	0.0075		0.10028	1.25344		Alternative to the above	0.005 ≤	**0.008**	≤ 0.01
PLANT OVERHEADS		0.4	**0.11**	**1.32**		Plant is part of a larger petrochemical complex	0.3 ≤	**0.4**	≤ 1.0
INSURANCE	0.015		**0.20**	**2.51**		Moderate risk	0.001 ≤	**0.015**	≤ 0.03
PROPERTY TAXES	0.01		**0.13**	**1.67**		Relatively undeveloped industrial area; incentive	0.01 ≤	**0.01**	≤ 0.04
"BOOK" DEPRECIATION (*not* a cash cost)	0.10		**1.34**	**16.71**		Calculated based on a 10 y plant life	0.05 ≤	**0.10**	≤ 0.2
TOTAL FIXED COSTS			**3.49**	**43.63**					
TOTAL PRODUCTION COST		**FIXED**	**3.49**	**43.63**					
		VARIABLE	16.26	**203.20**		Raw materials & Utilities			
		TOTAL	19.75	**246.83**		*Check: Methanol makes up 80% of the total "production cost."* ✓			
NON-MANUFACTURING COSTS									
	FRACTION OF TOTAL PRODUCTION COST (above)								
Corporate administration	0.025		0.49	6.17		Relatively simple division; mostly central admin.	0.02 ≤	**0.03**	≤ 0.06
cf. Fraction of total fixed capital		0.01375		2.30		Alternative to the above	0.01 ≤	**0.014**	≤ 0.04
Research & Development	0.005		0.10	1.23		An established technology, largely bought into	0.00 ≤	**0.01**	≤ 0.05
cf. Fraction of sales revenue		0.006		1.80		Expected sales revenue = $24 \times 10^{6}\ \$(\mathrm{gr}).\mathrm{y}^{-}$	0.00 ≤	**0.006**	≤ 0.06
Selling expenses	0.05		0.99	12.34		Relatively one major customer (contract)	0.05 ≤	**0.05**	≤ 0.025
cf. Fraction of sales revenue		0.020		6.00		Alternative to the above	0.02 ≤	**0.020**	≤ 0.2
TOTAL NON-MANUFACTURING COSTS			1.58	**19.75**					
TOTAL OPERATING COST			21.33	**266.58**		*Check: Methanol makes up 74% of the total "operating cost."* ✓			
MINIMUM PROFIT	Fraction of total fixed capital =	0.20	**2.67**	**33.43**	$\$.\mathrm{t}_{\mathrm{product}}^{-1}$	This is a (pseudo)-commodity ==> Profit margin not so high			
MINIMUM VIABLE SELLING PRICE			24.00	**300**	$\$.\mathrm{t}_{\mathrm{product}}^{-1}$	NOTE: The *expected* selling price **300** $\$.\mathrm{t}_{\mathrm{product}}^{-1}$			
Recall:									
TOTAL RAW MATERIALS COSTS			15.80	197.49	$\$.\mathrm{t}_{\mathrm{product}}^{-1}$	Which is only methanol.			
Hence:									
"CONVERSION COST"			5.53	**69.09**	$\$.\mathrm{t}_{\mathrm{product}}^{-1}$				

OPERATING & PRODUCTION COSTS: 60% capacity utilisation

PRODUCT	**Formaldehyde**
PROCESS ROUTE	**Production from methanol via a silver catalyst-type process, with off-gas recycle**

GENERAL DATA	*VALUE*	*UNITS*	*COMMENTS*
PLANT CAPACITY	**80000**	$t.y^{-1}$	
CAPACITY UTILISATION	**0.60**	$(t.y^{-1}).(t.y^{-1})^{-1}$	The possibility of turndown to 60% is a required attribute.
FIXED CAPITAL: **I**nside **B**attery **L**imits	2.64	$\times 10^6$ \$	All "\$" symbols denote USD_{1999}. $1AUD_{1999} = 0.66USD_{1999}$.
FIXED CAPITAL: **O**utside **B**attery **L**imits	6.50	$\times 10^6$ \$	
TOTAL FIXED CAPITAL	**13.37**	$\times 10^6$ \$	
PRODUCT SELLING PRICE	**300**	$\$.t_{product}^{-1}$	"Expected" price, Freight On Board. 54%($kg.kg^{-1}$) basis.
EXPECTED ECONOMIC PLANT LIFE	**10**	y	Minimum value (conservative).

PRODUCTION COST

	UNITS	*UNIT COST* $[\$.unit^{-1}]$	*UNIT USAGE* $[unit.t_{product}^{-1}]$	ANNUAL COST $[\times 10^6\ \$.y^{-1}]$	COST PER TONNE OF PRODUCT (54% basis) $[\$.t_{product}^{-1}]$	*COMMENTS*
RAW MATERIALS						From a neighbouring plant in Bontang, by pipeline.
Methanol	t	100	0.6648	3.19	66.48	**The unit cost is adjusted so that the minimum viable**
TOTAL RAW MATERIALS COSTS				**3.19**	**66.48**	**selling price equals the expected selling price.**
						There are two inlets streams!

	UNITS	*UNIT COST* $[\$.unit^{-1}]$	*UNIT USAGE* $[unit.t_{product}^{-1}]$	ANNUAL COST $[\times 10^6\ \$.y^{-1}]$	COST PER TONNE OF PRODUCT (54% basis) $[\$.t_{product}^{-1}]$	*COMMENTS*
UTILITIES						
Steam	t	7.92	-0.252	-0.10	-2.00	Surplus steam is exported for profit.
Nitrogen	Nm^3	0.198	0.000	0.00	0.00	Not required during normal operation.
Demineralised water	t	1.65	1.912	0.15	3.15	20% of BFW (Streams 100, 105 and 112) + Streams 2, 33 and 41.
Recirculated cooling wate	$m^3 \approx t$	0.0396	31.57	0.06	1.25	Streams 122, 124, 126 and 128.
Towns water	t	0.396	6.314	0.12	2.50	Taken as 20% of the RCW flow.
Electric power	MWh	29.7	0.0271	0.04	0.81	From actual pump motor requirements (only): 19.95 kW.
Natural gas	GJ	2.64	0.000	0.00	0.00	Only required on start-up.
TOTAL UTILITIES COSTS				**0.27**	**5.71**	*This is only 9% of the Raw Materials cost.*

	NUMBER	*COST PER "UNIT"* $[\$.y^{-1}]$	ANNUAL COST $[\times 10^6\ \$.y^{-1}]$	COST PER TONNE OF PRODUCT (54% basis) $[\$.t_{product}^{-1}]$	*COMMENTS*
PROCESS LABOUR					
Operators per shift	2				
(Hours required per day)	(24)				
(Days required per week)	(7)				
(Hours per shift)	(8)				(Ignoring time required during shift change-over)
Shift teams	4				
TOTAL *shift* operators	8	33000	0.26	5.50	
TOTAL *day* operators	0	26400	0.00	0.00	It is assumed that all operators are on a rotating shift,
TOTAL PROCESS LABOUR WAGES			0.26	5.50	such that none are classed as "day" operators

	FRACTION OF TOTAL PROCESS LABOUR WAGES									
PAYROLL OVERHEADS		0.3		0.08	1.65		Plant is not in a highly "developed" country	0.30 ≤	**0.30**	≤ 0.50
	FRACTION OF TOTAL FIXED CAPITAL									
MAINTENANCE LABOUR	0.05			0.67	13.93		See, *e.g.*, Brennan^1, p. 126, and *cf.* p. 118. Assuming "equal division between materials and labour." See also below			
NETT "OPERATING" LABOUR COSTS				**1.01**	**21.08**		*This is 32% of the Raw Materials cost.*			
	FRACTION OF TOTAL FIXED CAPITAL	***FRACTION OF NETT "OPERATING" LABOUR COSTS***								
MAINTENANCE MATERIALS	0.05			**0.67**	**13.93**		See Brennan^1, p. 118: here the *two* fractions sum to	0.02 ≤	**0.10**	≤ 0.12
							The fraction is increased due to high capacity utilisation:		**60%**	,
							and due to the corrosive process fluid (though 316SS is used) which precipitates.			
OPERATING SUPPLIES ≈ CONSUMABLE STORES		0.125		**0.03**	**0.69**		Moderately "dirty" and "complicated" process	0.05 ≤	**0.13**	≤ 0.20
cf.	0.0075			0.10028	2.08906		Alternative to the above	0.005 ≤	**0.008**	≤ 0.01
PLANT OVERHEADS		0.4		**0.11**	**2.2**		Plant is part of a larger petrochemical complex	0.3 ≤	**0.4**	≤ 1.0
INSURANCE	0.015			**0.20**	**4.18**		Moderate risk	0.001 ≤	**0.015**	≤ 0.03
PROPERTY TAXES	0.01			**0.13**	**2.79**		Relatively undeveloped industrial area; incentive	0.01 ≤	**0.01**	≤ 0.04
"BOOK" DEPRECIATION (*not* a cash cost)	0.10			**1.34**	**27.85**		Calculated based on a 10 y plant life	0.05 ≤	**0.10**	≤ 0.2
TOTAL FIXED COSTS				**3.49**	**72.71**					
TOTAL PRODUCTION COST			**FIXED**	**3.49**	**72.71**					
			VARIABLE	3.47	**72.19**		Raw materials & Utilities			
			TOTAL	6.96	**144.90**		*Check: Here methanol makes up 46% of the total "production cost."* ✗			
NON-MANUFACTURING COSTS										
	FRACTION OF TOTAL PRODUCTION COST (above)									
Corporate administration	0.025			0.17	3.62		Relatively simple division; mostly central admin.	0.02 ≤	**0.03**	≤ 0.06
cf. Fraction of total fixed capital		0.01375			3.83		Alternative to the above	0.01 ≤	**0.014**	≤ 0.04
Research & Development	0.005			0.03	0.72		An established technology, largely bought into	0.00 ≤	**0.01**	≤ 0.05
cf. Fraction of sales revenue		0.006			1.80		Expected sales revenue = 14.4 ×10^6 \$(gr).y$^-$	0.00 ≤	**0.006**	≤ 0.06
Selling expenses	0.05			0.35	7.24		Relatively one major customer (contract)	0.05 ≤	**0.05**	≤ 0.025
cf. Fraction of sales revenue		0.020			6.00		Alternative to the above	0.02 ≤	**0.020**	≤ 0.2
TOTAL NON-MANUFACTURING COSTS				0.56	**11.59**					
TOTAL OPERATING COST				7.51	**156.49**		*Check: Here methanol makes up 42% of the total "operating cost."* ✗			
MINIMUM PROFIT	Fraction of total fixed capital =	0.20		**2.67**	**55.71**	$\$.t_{product}^{-1}$	This is a (pseudo)-commodity ==> Profit margin not so high			
MINIMUM VIABLE SELLING PRICE				10.19	**212.20**	$\$.t_{product}^{-1}$	NOTE: The *expected* selling price i **300** $\$.t_{product}^{-1}$			
Recall:										
TOTAL RAW MATERIALS COSTS				3.19	66.48	$\$.t_{product}^{-1}$	Which is only methanol.			
Hence:										
"CONVERSION COST"				4.32	**90.02**	$\$.t_{product}^{-1}$				

OPERATING & PRODUCTION COSTS TO "BREAK EVEN": 60% capacity utilisation

PRODUCT	**Formaldehyde**
PROCESS ROUTE	**Production from methanol via a silver catalyst-type process, with off-gas recycle**

GENERAL DATA	*VALUE*	*UNITS*	*COMMENTS*
PLANT CAPACITY	**80000**	$t.y^{-1}$	
CAPACITY UTILISATION	**0.60**	$(t.y^{-1}).(t.y^{-1})^{-1}$	The possibility of turndown to 60% is a required attribute.
FIXED CAPITAL: **I**nside **B**attery **L**imits	2.64	$\times 10^6$ \$	All "\$" symbols denote USD_{1999}. $1AUD_{1999} = 0.66USD_{1999}$.
FIXED CAPITAL: **O**utside **B**attery **L**imits	6.50	$\times 10^6$ \$	
TOTAL FIXED CAPITAL	**13.37**	$\times 10^6$ \$	
PRODUCT SELLING PRICE	**300**	$\$.t_{product}^{-1}$	"Expected" price, Freight On Board. 54%$(kg.kg^{-1})$ basis.
EXPECTED ECONOMIC PLANT LIFE	**10**	y	Minimum value (conservative).

PRODUCTION COST	*UNITS*	*UNIT COST*	*UNIT USAGE*	**ANNUAL COST**	**COST PER TONNE OF PRODUCT (54% basis)**	*COMMENTS*
		$[\$.unit^{-1}]$	$[unit.t_{product}^{-1}]$	$[\times 10^6\ \$.y^{-1}]$	$[\$.t_{product}^{-1}]$	
RAW MATERIALS						From a neighbouring plant in Bontang, by pipeline.
Methanol	t	**222.30**	0.6648	7.09	147.77	**The unit cost is adjusted so that the minimum viable**
TOTAL RAW MATERIALS COSTS				**7.09**	**147.77**	**selling price equals the expected selling price.**
						There are two inlets streams!
	UNITS	*UNIT COST*	*UNIT USAGE*			*COMMENTS*
		$[\$.unit^{-1}]$	$[unit.t_{product}^{-1}]$			
UTILITIES						
Steam	t	7.92	-0.252	-0.10	-2.00	Surplus steam is exported for profit.
Nitrogen	Nm^3	0.198	0.000	0.00	0.00	Not required during normal operation.
Demineralised water	t	1.65	1.912	0.15	3.15	20% of BFW (Streams 100, 105 and 112) + Streams 2, 33 and 41.
Recirculated cooling wate	$m^3 \approx t$	0.0396	31.57	0.06	1.25	Streams 122, 124, 126 and 128.
Towns water	t	0.396	6.314	0.12	2.50	Taken as 20% of the RCW flow.
Electric power	MWh	29.7	0.0271	0.04	0.81	From actual pump motor requirements (only): 19.95 kW.
Natural gas	GJ	2.64	0.000	0.00	0.00	Only required on start-up.
TOTAL UTILITIES COSTS				**0.27**	**5.71**	*This is only 4% of the Raw Materials cost.*
	NUMBER	*COST PER "UNIT"*				*COMMENTS*
		$[\$.y^{-1}]$				
PROCESS LABOUR						
Operators per shift	2					
(Hours required per day)	(24)					
(Days required per week)	(7)					
(Hours per shift)	(8)					(Ignoring time required during shift change-over)
Shift teams	4					
TOTAL *shift* operators	8	33000		0.26	5.50	
TOTAL *day* operators	0	26400		0.00	0.00	It is assumed that all operators are on a rotating shift,
TOTAL PROCESS LABOUR WAGES				0.26	5.50	such that none are classed as "day" operators

	FRACTION OF TOTAL PROCESS LABOUR WAGES								
PAYROLL OVERHEADS		0.3	0.08	1.65		Plant is not in a highly "developed" country	0.30 ≤	**0.30**	≤ 0.50
	FRACTION OF TOTAL FIXED CAPITAL								
MAINTENANCE LABOUR	0.05		0.67	13.93		See, *e.g.* , Brennan[1], p. 126, and *cf.* p. 118. Assuming "equal division between materials and labour." See also below			
NETT "OPERATING" LABOUR COSTS			**1.01**	**21.08**		*This is 14% of the Raw Materials cost.*			
	FRACTION OF TOTAL FIXED CAPITAL	***FRACTION OF NETT "OPERATING" LABOUR COSTS***							
MAINTENANCE MATERIALS	0.05		**0.67**	**13.93**		See Brennan[1], p. 118: here the *two* fractions sum to 0.02 ≤		**0.10**	≤ 0.12
						The fraction is increased due to high capacity utilisation:		**60%**	,
						and due to the corrosive process fluid (though 316SS is used) which precipitates.			
OPERATING SUPPLIES ≈ CONSUMABLE STORES		0.125	**0.03**	**0.69**		Moderately "dirty" and "complicated" process	0.05 ≤	**0.13**	≤ 0.20
cf.	0.0075		0.10028	2.08906		Alternative to the above	0.005 ≤	**0.008**	≤ 0.01
PLANT OVERHEADS		0.4	**0.11**	**2.2**		Plant is part of a larger petrochemical complex	0.3 ≤	**0.4**	≤ 1.0
INSURANCE	0.015		**0.20**	**4.18**		Moderate risk	0.001 ≤	**0.015**	≤ 0.03
PROPERTY TAXES	0.01		**0.13**	**2.79**		Relatively undeveloped industrial area; incentive	0.01 ≤	**0.01**	≤ 0.04
"BOOK" DEPRECIATION (*not* a cash cost)	0.10		**1.34**	**27.85**		Calculated based on a 10 y plant life	0.05 ≤	**0.10**	≤ 0.2
TOTAL FIXED COSTS			**3.49**	**72.71**					
TOTAL PRODUCTION COST		**FIXED**	**3.49**	**72.71**					
		VARIABLE	7.37	**153.49**		Raw materials & Utilities			
		TOTAL	10.86	**226.20**		*Check: Here methanol makes up 65% of the total "production cost."* ✗			
NON-MANUFACTURING COSTS									
	FRACTION OF TOTAL PRODUCTION COST (above)								
Corporate administration	0.025		0.27	5.65		Relatively simple division; mostly central admin.	0.02 ≤	**0.03**	≤ 0.06
cf. Fraction of total fixed capital		0.01375		3.83		Alternative to the above	0.01 ≤	**0.014**	≤ 0.04
Research & Development	0.005		0.05	1.13		An established technology, largely bought into	0.00 ≤	**0.01**	≤ 0.05
cf. Fraction of sales revenue		0.006		1.80		Expected sales revenue = 14.4×10^{6} \$(gr).y^{-}	0.00 ≤	**0.006**	≤ 0.06
Selling expenses	0.05		0.54	11.31		Relatively one major customer (contract)	0.05 ≤	**0.05**	≤ 0.025
cf. Fraction of sales revenue		0.020		6.00		Alternative to the above	0.02 ≤	**0.020**	≤ 0.2
TOTAL NON-MANUFACTURING COSTS			0.87	**18.10**					
TOTAL OPERATING COST			11.73	**244.29**		*Check: Here methanol makes up 60% of the total "operating cost."* ✗			
MINIMUM PROFIT	Fraction of total fixed capital =	0.20	**2.67**	**55.71**	$\$.t_{product}^{-1}$	This is a (pseudo)-commodity ==> Profit margin not so high			
MINIMUM VIABLE SELLING PRICE			14.40	**300**	$\$.t_{product}^{-1}$	NOTE: The *expected* selling price **300** $\$.t_{product}^{-1}$			
Recall:									
TOTAL RAW MATERIALS COSTS			7.09	147.77	$\$.t_{product}^{-1}$	Which is only methanol.			
Hence:									
"CONVERSION COST"			4.63	**96.52**	$\$.t_{product}^{-1}$				

WORKING CAPITAL: 80000t.y^{-1} plant with 100% capacity utilisation

PRODUCT	**Formaldehyde**
PROCESS ROUTE	**Production from methanol via a silver catalyst-type process, with off-gas recycle**

GENERAL DATA			
	VALUE	***UNITS***	***COMMENTS***
PLANT CAPACITY	**80000**	t.y^{-1}	All based on a solution of equivalent conc'n 54% by mass.
CAPACITY UTILISATION	**1.00**	(t.y^{-1}).(t.y^{-1})$^{-1}$	Assumed to be "normal" operation.
FIXED CAPITAL: **I**nside **B**attery **L**imits	2.64	$\times 10^6$ \$	All "\$" symbols denote USD$_{1999}$. 1AUD$_{1999}$ = 0.66USD$_{1999}$.
FIXED CAPITAL: **O**utside **B**attery **L**imits	6.50	$\times 10^6$ \$	
TOTAL FIXED CAPITAL	**13.37**	$\times 10^6$ \$	
PRODUCT SELLING PRICE	**300**	\$.t$_{product}^{-1}$	"Expected" price, Freight On Board. 54%(kg.kg^{-1}) basis.
EXPECTED ECONOMIC PLANT LIFE	**10**	y	Minimum value (conservative).

RAW MATERIAL STOCKS

	INVENTORY [weeks]	UNIT USAGE [t.t$_{product}^{-1}$]	UNIT COST [\$.t^{-1}]	VALUE [$\times 10^6$ \$]	COMMENTS
TOTAL = Methanol	0.43	0.6583	100	**0.043**	From a neighbouring plant in Bontang, by pipeline, with small storage tank.

MATERIALS IN PROGRESS INVENTORY

	INVENTORY [weeks of production]	[t]	UNIT VALUE [\$.t^{-1}]	VALUE [$\times 10^6$ \$]	COMMENTS
TOTAL	1.0	1276	104	**0.133**	This low value may still be conservative for such a "short" process. Take "unit value" as average between product and (mean) raw materials Tonnes composed of average of {contributions from each raw material} and {product}

PRODUCT STOCKS

	INVENTORY [weeks]	PRODUCT CASH COST [\$.t^{-1}]	VALUE [$\times 10^6$ \$]	COMMENTS
TOTAL = 54% formaldehyde solution	0.57	108.37	**0.095**	By pipeline to neighbouring resins plant, with moderate storage.
		*NOTE: valued at "***cash*** *operating cost*" (no depreciation!)		
SUB-TOTAL (process materials)			**0.272**	

DEBTORS

	PERIOD [weeks]	PRODUCT SELLING PRICE [\$.t^{-1}]	VALUE [$\times 10^6$ \$]	COMMENTS
TOTAL = Customers	6	300	**2.769**	Assume monthly payments (every ~ **4** weeks)
		*Using the *expected* price		NOTE: Other debtors exist (e.g. insurance, et cetera), but are not considered here
SUB-TOTAL (debtors)			**2.769**	

CREDITORS

	PERIOD [weeks]	COST PER TONNE OF PROD [\$.t$_{product}^{-1}$]	VALUE [$\times 10^6$ \$]	COMMENTS
RAW MATERIALS	6	66.48	(0.614)	Monthly payments assumed (every ~ **4** weeks)
UTILITIES	6	5.71	(0.053)	Monthly payments assumed (every ~ **4** weeks)
WAGES	1.5	12.65	(0.029)	"Paid, say on average, 1.5 weeks in arrears" - Brennan, p. 90 NOTE: Other creditors exist (e.g. "operating supplies"), but are not considered here
SUB-TOTAL (creditors)			**(0.696)**	

TOTAL WORKING CAPITAL	**2.345**	= {Process materials} + {Debtors} - {Creditors}

Cash flows

Note: Basis is USD $_{1999}$ and 54% formaldehyde solution (by mass).

All cash flows in millions of USD$_{1999}$.

Calendar year		1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011
Year number			0	1	2	3	4	5	6	7	8	9	10	11
Fixed capital			-13.37											
Working capital			-1.88	-0.23	-0.23									2.35
Sales volume [t.y^{-1}]			0	60000	72000	80000	80000	80000	80000	80000	80000	80000	80000	0
Selling price [USD$_{1999}$.t^{-1}]	**300**													
Sales revenue			0	18	21.6	24	24	24	24	24	24	24	24	0
Variable cost [USD$_{1999}$.t^{-1}]*	**72.19**													
Variable costs			0	-4.33	-5.20	-5.78	-5.78	-5.78	-5.78	-5.78	-5.78	-5.78	-5.78	0
Fixed costs‡			0	-2.89	-2.89	-2.89	-2.89	-2.89	-2.89	-2.89	-2.89	-2.89	-2.89	0
CASH FLOW BEFORE TAX♣			0	10.77	13.51	15.33	15.33	15.33	15.33	15.33	15.33	15.33	15.33	0
Investment allowance†	**0**													
Tax depreciation rate	**10%**													
Tax depreciation allowance			0	1.34	1.34	1.34	1.34	1.34	1.34	1.34	1.34	1.34	1.34	0
Taxable income			0	9.44	12.17	13.99	13.99	13.99	13.99	13.99	13.99	13.99	13.99	0
Tax rate	**30%**													
Tax payments¶			0	-2.83	-3.65	-4.20	-4.20	-4.20	-4.20	-4.20	-4.20	-4.20	-4.20	0
CASH FLOW AFTER TAX			-15.25	7.71	9.62	11.13	11.13	11.13	11.13	11.13	11.13	11.13	11.13	2.35
CUMULATIVE CASH FLOW AFTER TAX														
• DISCOUNT RATE =	**0%**	0	-15.25	**-7.54**	**2.08**	13.22	24.35	35.48	46.61	57.75	68.88	80.01	91.14	**93.49**
• DISCOUNT RATE =	**5%**	0	-15.25	**-7.90**	**0.82**	10.44	19.60	28.32	36.63	44.54	52.07	59.25	66.08	**67.46**
• DISCOUNT RATE =	**10%**	0	-15.25	-8.24	**-0.29**	**8.08**	15.68	22.59	28.88	34.59	39.78	44.50	48.80	**49.62**
• DISCOUNT RATE =	**20%**	0	-15.25	-8.82	**-2.14**	**4.30**	9.67	14.14	17.87	20.98	23.57	25.73	27.52	**27.84**
• DISCOUNT RATE =	**62%** **(annual)**	0	-15.25	-10.47	-6.79	-4.15	-2.52	-1.50	-0.88	-0.49	-0.25	-0.10	**-0.01**	**0.00**

---

* All non-manufacturing costs are assumed to be fixed.

‡ This therefore 125.08 – 72.19 – 16.71§ USD$_{1999}$.t^{-1}.

§ This is book depreciation.

† This is assumed to be zero.

¶ No tax is paid on the working capital recovered, after Brennan.

♣ Similarly, this does not include the working (or fixed) capital.

We assume all tax is paid in the same year (no delay)

We assume production is 75% in the first year, 90% in the following year and 100% thereafter.

We assume all fixed capital is disbursed in "year zero", along with 80% of the working capital, with the remainder distributed equally over the following two years, with full recovery.

Tax rate estimated at 30%, slightly lower than the 36% corporate rate in Australia.