DME Absorbing Unit Simulation Using PRO/II with PROVISION

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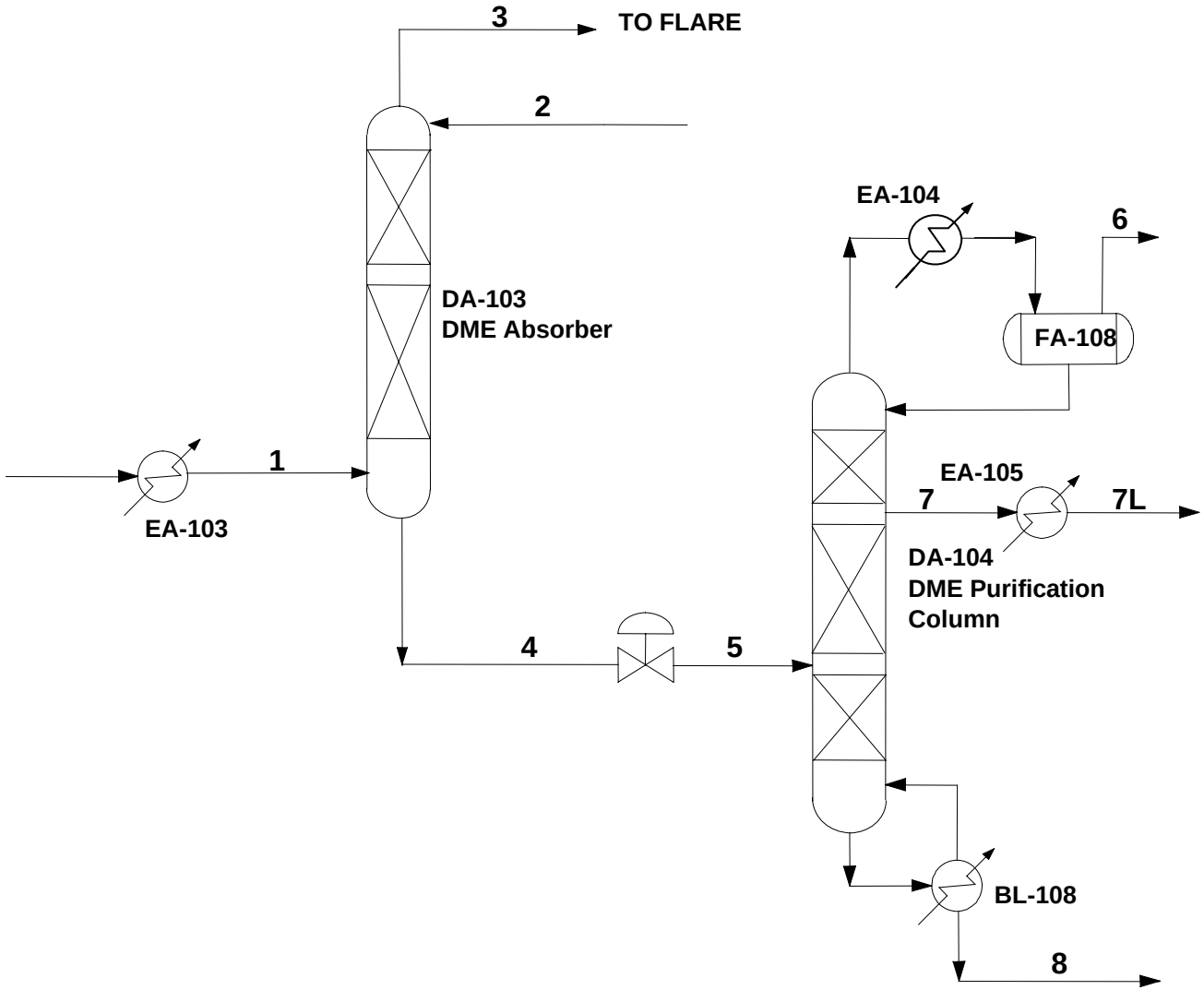
Overall DME Purification Process



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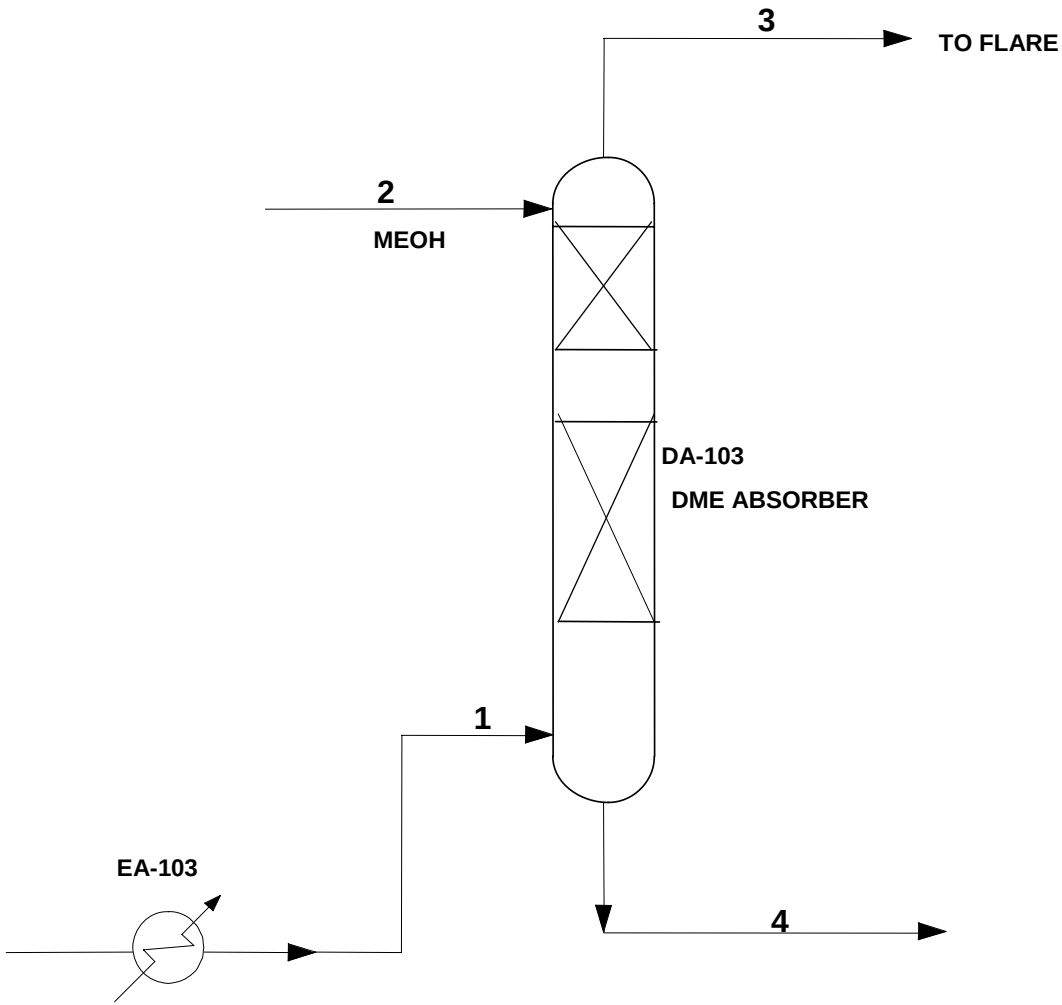
1st Column: DA-103 (DME Absorber)



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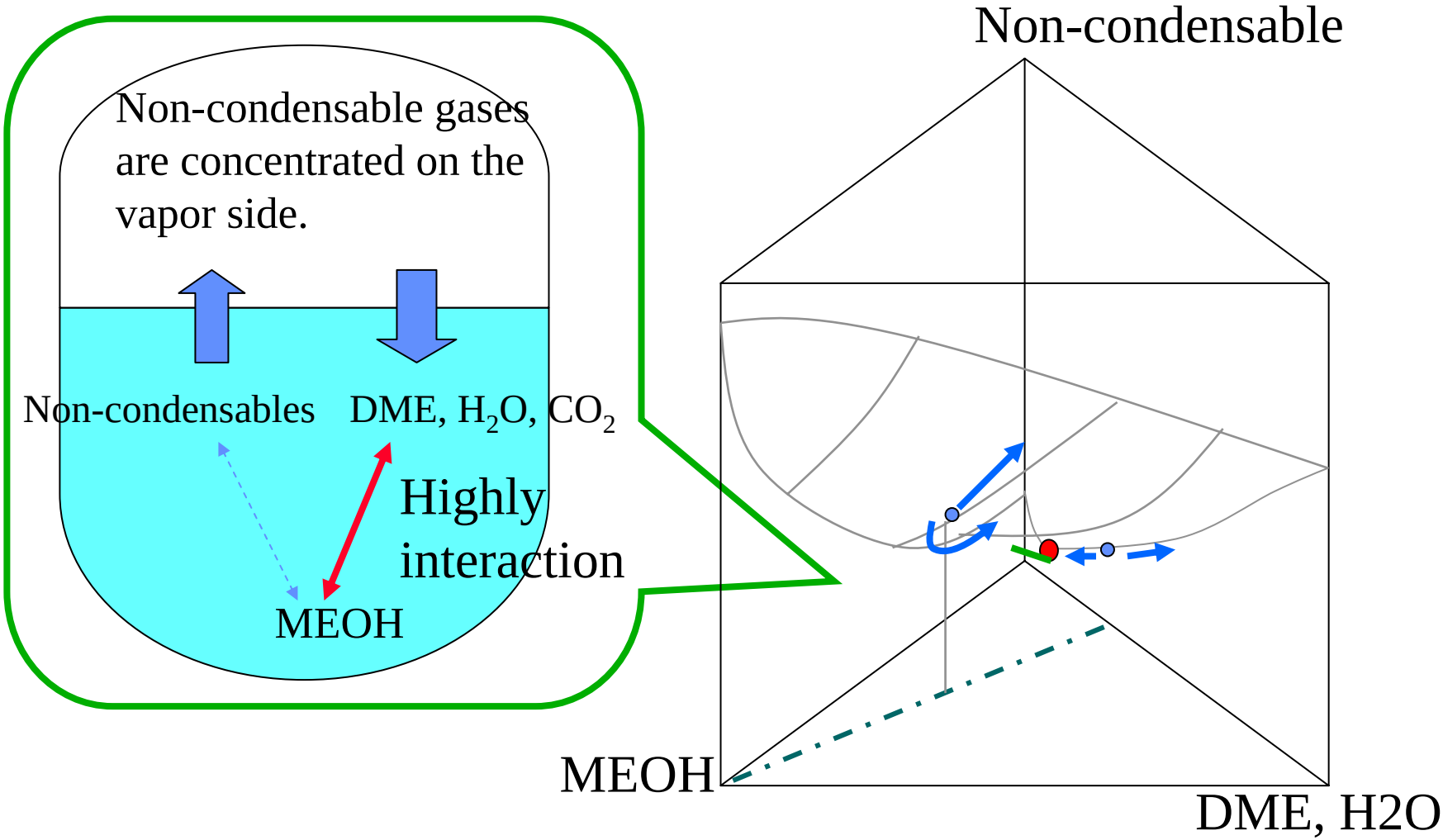
Feedstock Characterization

- Feedstock Compositions for DME Absorber are as:

	1	31
Mole Fraction		
H2	0.137	
CO	0.099	
CO2	0.099	
CH4	0.095	
N2	0.238	
H2O	0.000	5.0 LV%
DME	0.241	
MEOH	0.091	95.0 LV%
Flow rate (K-mole/hr)	1.875	?
Molecular Weight	29.6161	
Flow rate (Kg/hr)	55.5303	
Temperature (^{o}C)	80.0	45.0
Pressure (Kg/cm^{2}G)	50.0	50.0

Theory of Selective Absorption



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Step 1: DME Absorber Simulation

- Primary objective of the absorber is to recovery DME by using methanol as a solvent at a bottom product.

Step 1: DME Absorber Simulation *Continued*

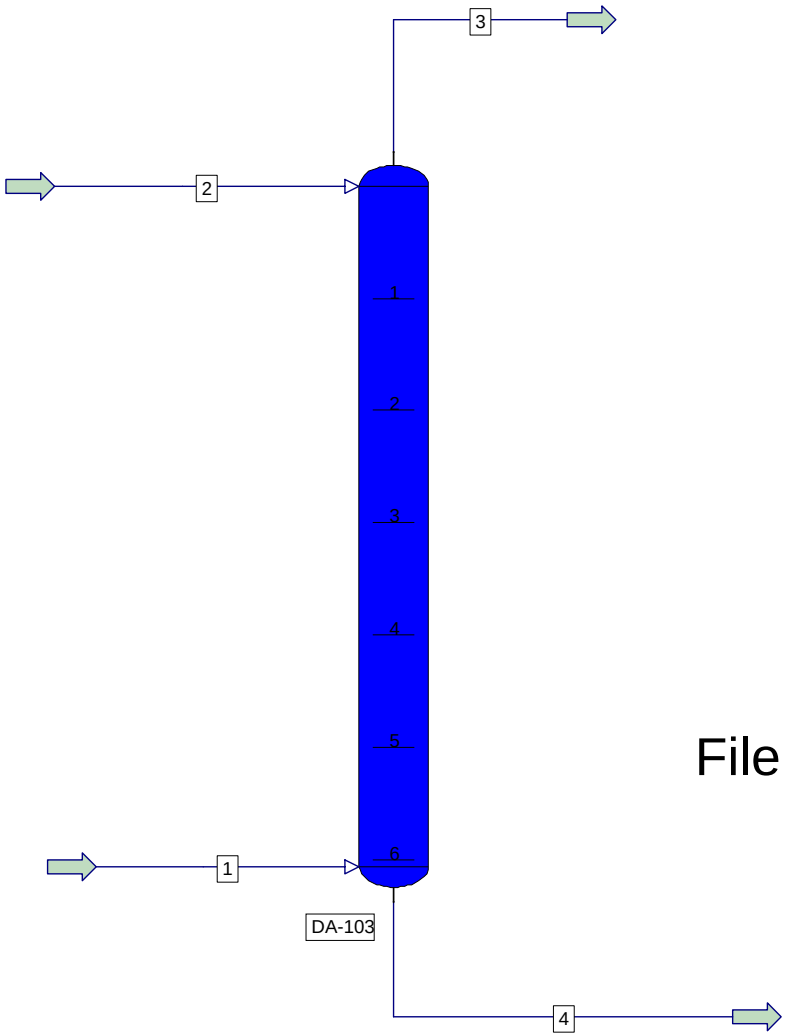
- Consider the following absorber distillation to produce a purified toluene using sulfolane as a solvent.
  - Feed1: Crude Feed (Refer to feedstock characterization)
  - Feed2: Methanol Solvent
    1) Solvent to Feed (MEA) Ratio = Variable
    2) DME Recovery = 90%
    3) Solvent Feed Temperature = 80^{o}C
    4) Solvent Feed Pressure = 50.0 Kg/cm^{2}G
    3) Flow Rate = 1.875 K-mole/hr
  - DME Absorber Column
    1) Number of Theoretical Stages: 6
    3) Overall Tray Efficiencies: ?
    4) Feed Tray Location: 6
    6) Solvent Feed Tray Location: 1

Step 1: DME Absorber Simulation *Continued*

- Selection of appropriate thermodynamic model for the simulation of DME absorber using methanol as a solvent is very important.

  - NRTL (Non Random Two Liquid) activity coefficient model was chosen to explain non-ideal phase behavior of liquid mixture between H_2O, DME and methanol.
  - Henry's law option was also selected for the calculation of non-condensable supercritical gases like H_2, CO, CO_2, CH_4 and N_2 in a liquid mixture.
  - SRK equation of state was used for the vapor phase non-idealities since the system pressure is very high.

Flow Sheet for DME Absorber (DA-103)



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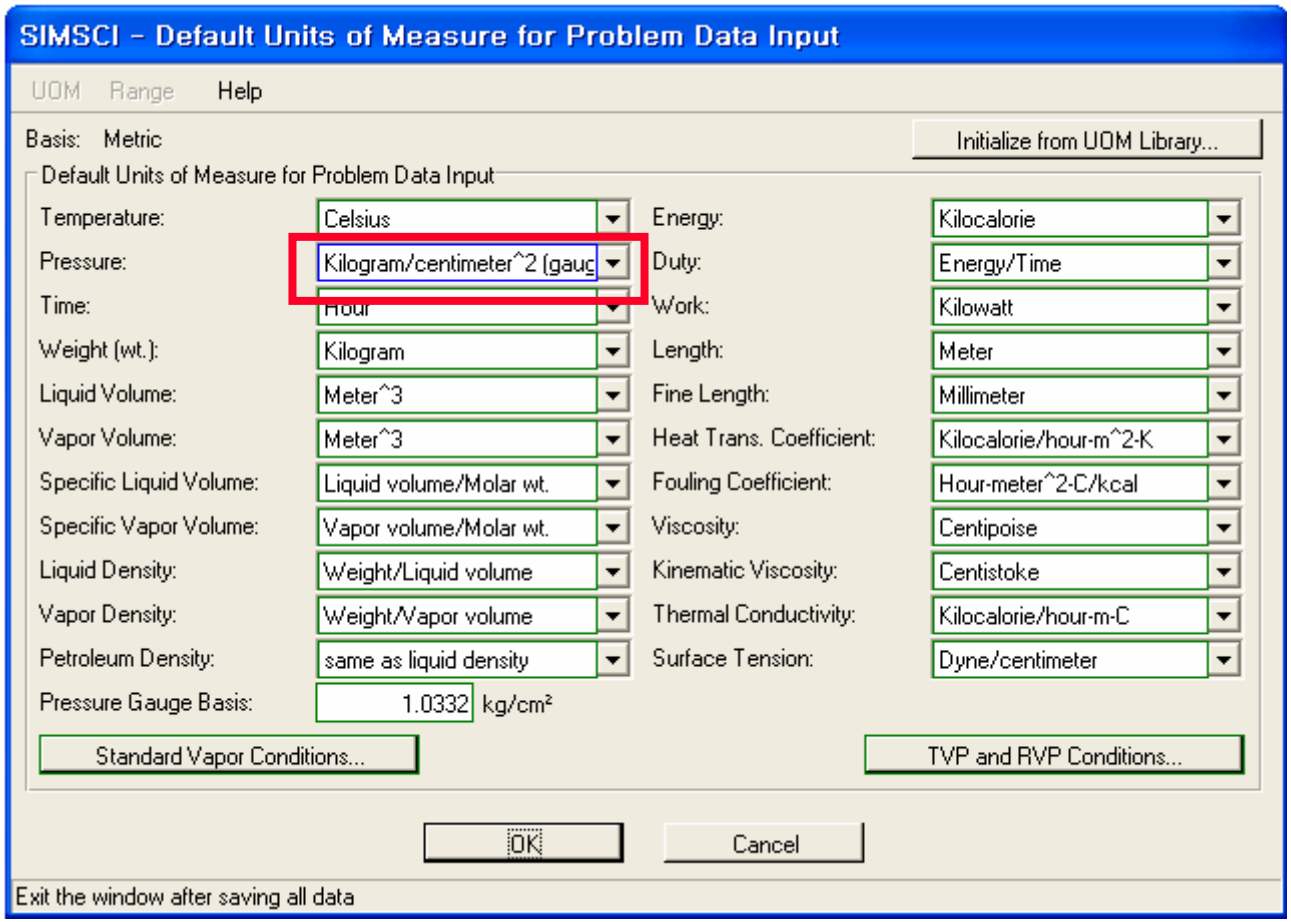
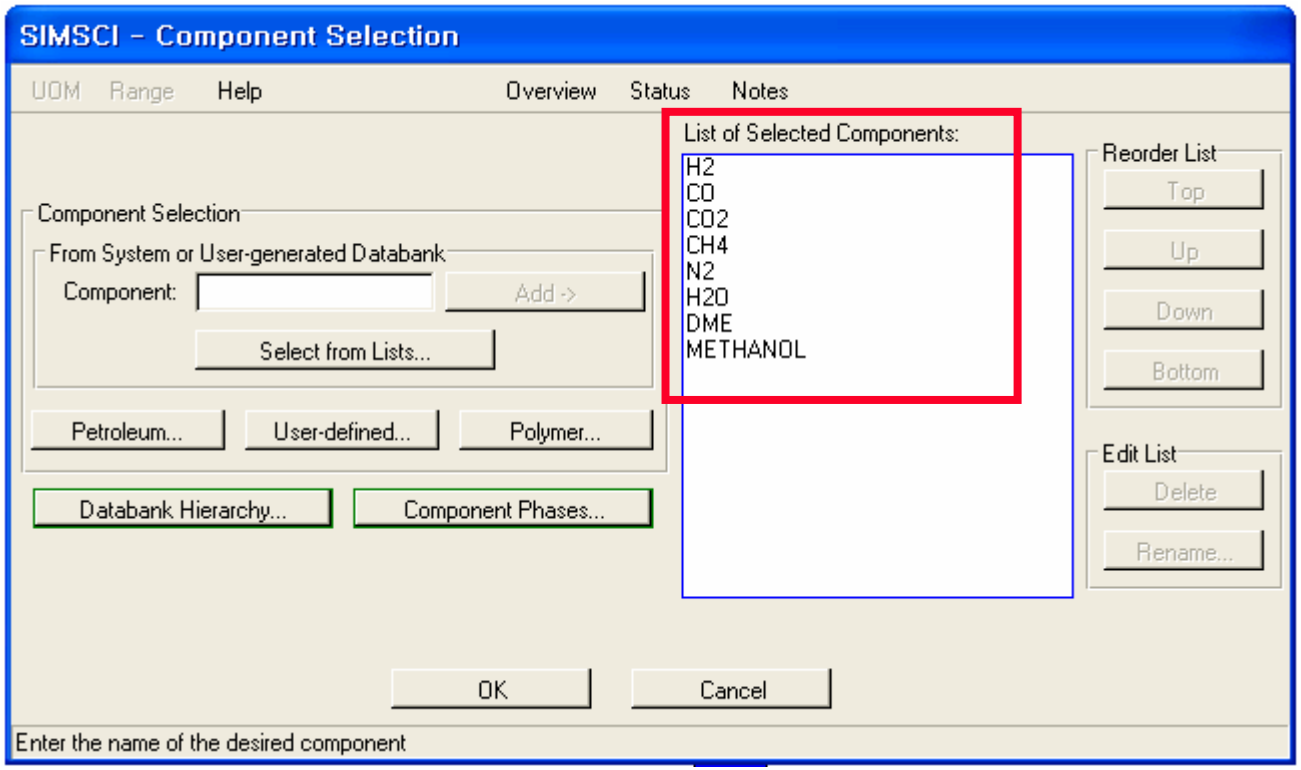
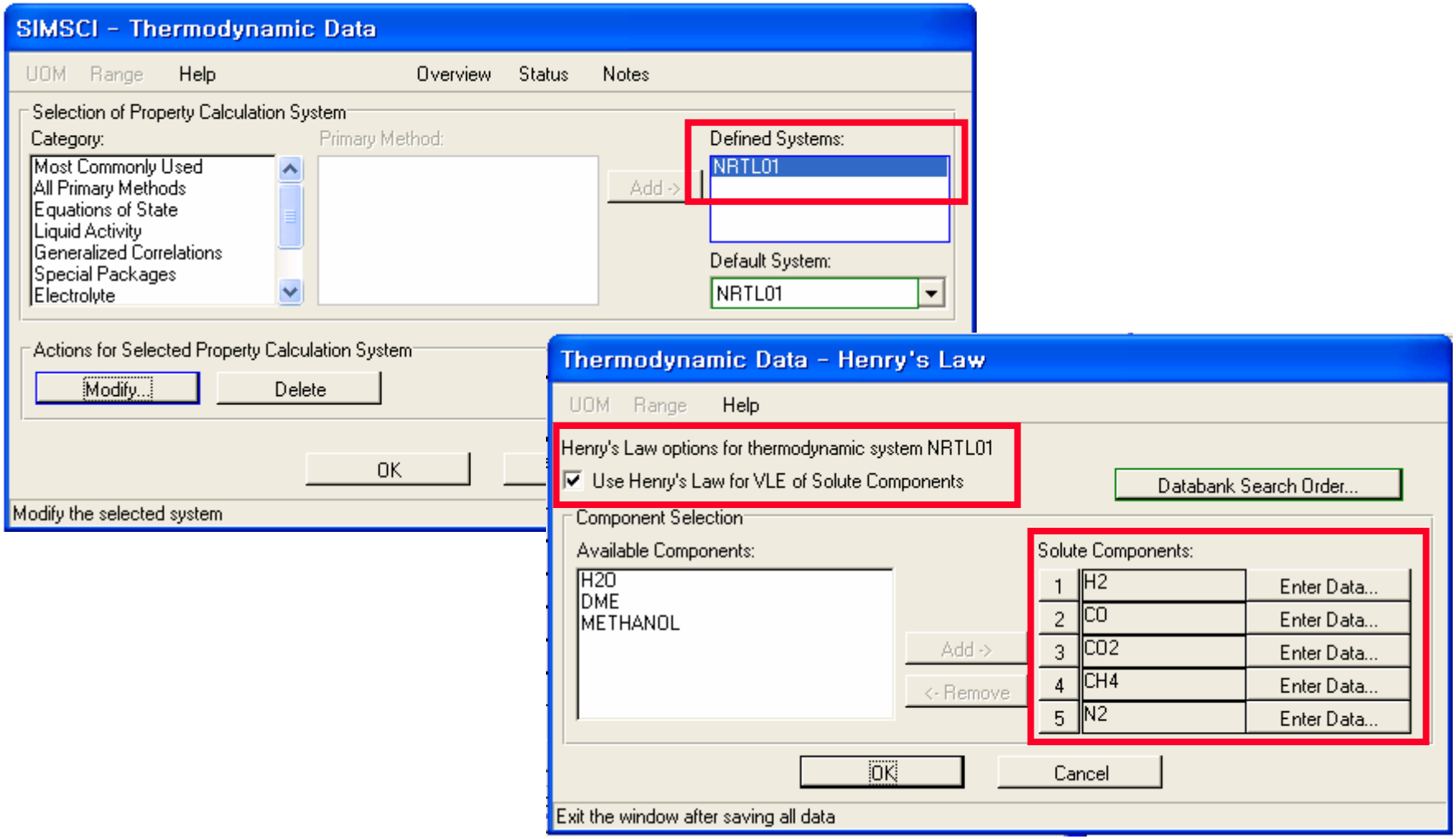
Measure of Unit: Metric Unit



Component Data: Pure Component Selection



Thermodynamic Data: NRTL with Henry's Law Option



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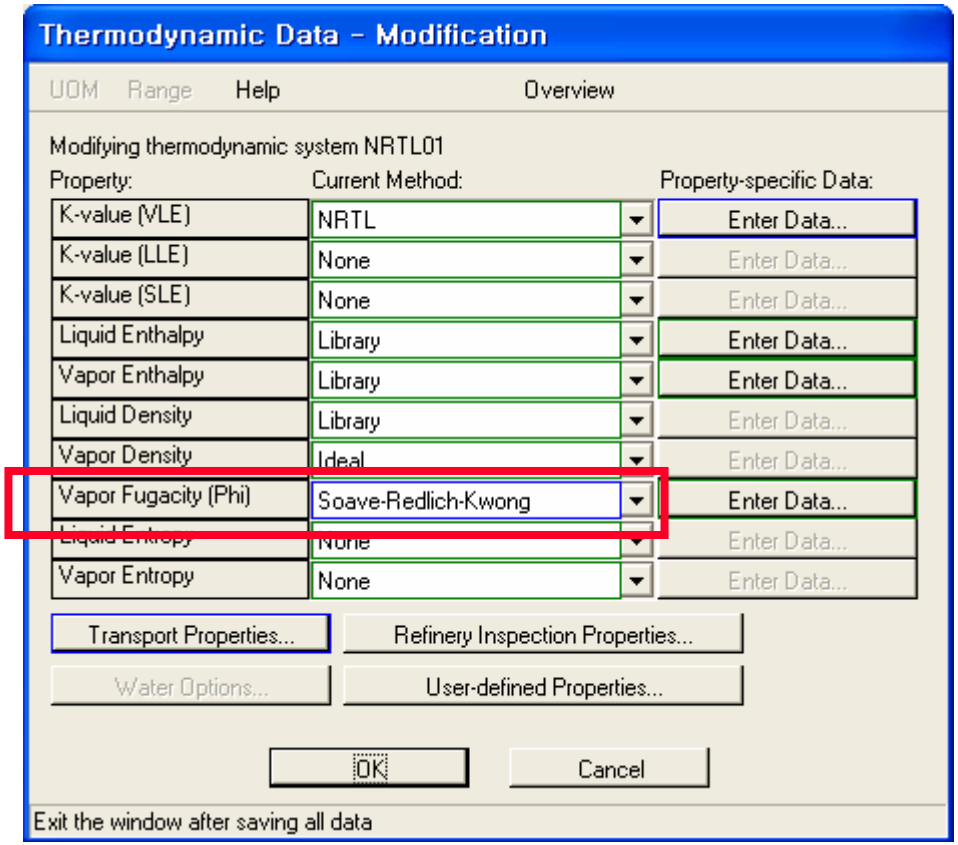
Thermodynamic Data: SRK EOS for Vapor Phase



NRTL BIP's Built in PRO/II Database

VLE LIQUID INTERACTION PARAMETERS FOR SET 'NRTL01'

NRTL BINARY COEFFICIENTS

I	J	A(I,J) / A(J,I)	B(I,J) / B(J,I)	C(I,J) / C(J,I)	ALPHAC / ALPHAT	UNITS FROM
6	7	12.300150	-4019.6919	330053.91	0.2000	DEG K SIMSCI VLEBANK
		-5.168679	2145.8921	74425.09	0.0000	
6	8	0.511068	199.8540	0.00	0.2442	DEG K SIMSCI VLEBANK
		0.736107	-360.6920	0.00	0.0000	
7	8	0.000000	-18.9372	0.00	0.2951	DEG K SIMSCI VLEBANK
		0.000000	653.0060	0.00	0.0000	

6: H2O
7: DME
8: Methanol

Henry's Constants Built in PRO/II Database

HENRY COEFFICIENTS FOR SET 'NRTL01'

LN(H) = C1 + C2/T + C3*LN(T) + C4*P **2: CO, 4: CH4, 7: DME, 8: Methanol**
TEMPERATURE IN K
PRESSURE IN

HENRY COEFFICIENTS

SOLUTE	SOLVENT	C1	C2	C3	C4	FROM
1	6	123.3211	-4881.3198	-14.7884	3.5529E-09	SIMSCI BANK
1	7	230.3261	-8787.0996	-31.9150	0.0000	SIMSCI BANK
1	8	22.4721	271.3300	-0.5485	0.0000	SIMSCI BANK
2	6	173.5801	-7847.1602	-21.8994	9.8692E-10	SIMSCI BANK
2	**7**	**N/A**	**N/A**	**N/A**	**N/A**	**VAPOR PRESSURE**
2	**8**	**N/A**	**N/A**	**N/A**	**N/A**	**VAPOR PRESSURE**
3	6	161.8561	-8498.7197	-20.0841	7.3032E-09	SIMSCI BANK
3	7	141.5061	-6535.3999	-18.2570	0.0000	SIMSCI BANK
3	8	223.9361	-10620.0000	-30.1360	0.0000	SIMSCI BANK
4	6	176.8001	-8132.2300	-22.3559	1.4409E-09	SIMSCI BANK
4	**7**	**N/A**	**N/A**	**N/A**	**N/A**	**VAPOR PRESSURE**
4	8	-56.2439	2617.0000	11.5200	0.0000	SIMSCI BANK
5	6	165.1721	-7260.1401	-20.7005	1.4409E-09	SIMSCI BANK
5	7	232.5161	-9275.2002	-32.1410	0.0000	SIMSCI BANK
5	8	34.6721	-598.8800	-2.2701	0.0000	SIMSCI BANK

Column Profiles Summary

NIT 1, 'DA-103', 'FA-106'

COLUMN SUMMARY

TRAY	TEMP DEG C	PRESSURE KG/CM2G	NET FLOW RATES LIQUID KG-MOL/HR	NET FLOW RATES VAPOR KG-MOL/HR	NET FLOW RATES FEED KG-MOL/HR	NET FLOW RATES PRODUCT KG-MOL/HR	HEATER DUTIES M*KCAL/HR
1	52.5	50.00	3.1		2.9L	1.2V	
2	59.7	50.00	3.2	1.4			
3	66.6	50.00	3.3	1.5			
4	72.7	50.00	3.3	1.5			
5	77.7	50.00	3.4	1.6			
6	80.8	50.00		1.7	1.9M	3.6L	

SPECIFICATIONS

SPECIFICATION NUMBER	PARAMETER TYPE	TRAY NO	COMP NO	SPECIFICATION TYPE	SPECIFIED VALUE	CALCULATED VALUE
1 (ACTIVE)	STRM 4	6	7	MOL RATIO	9.000E-01	9.000E-01

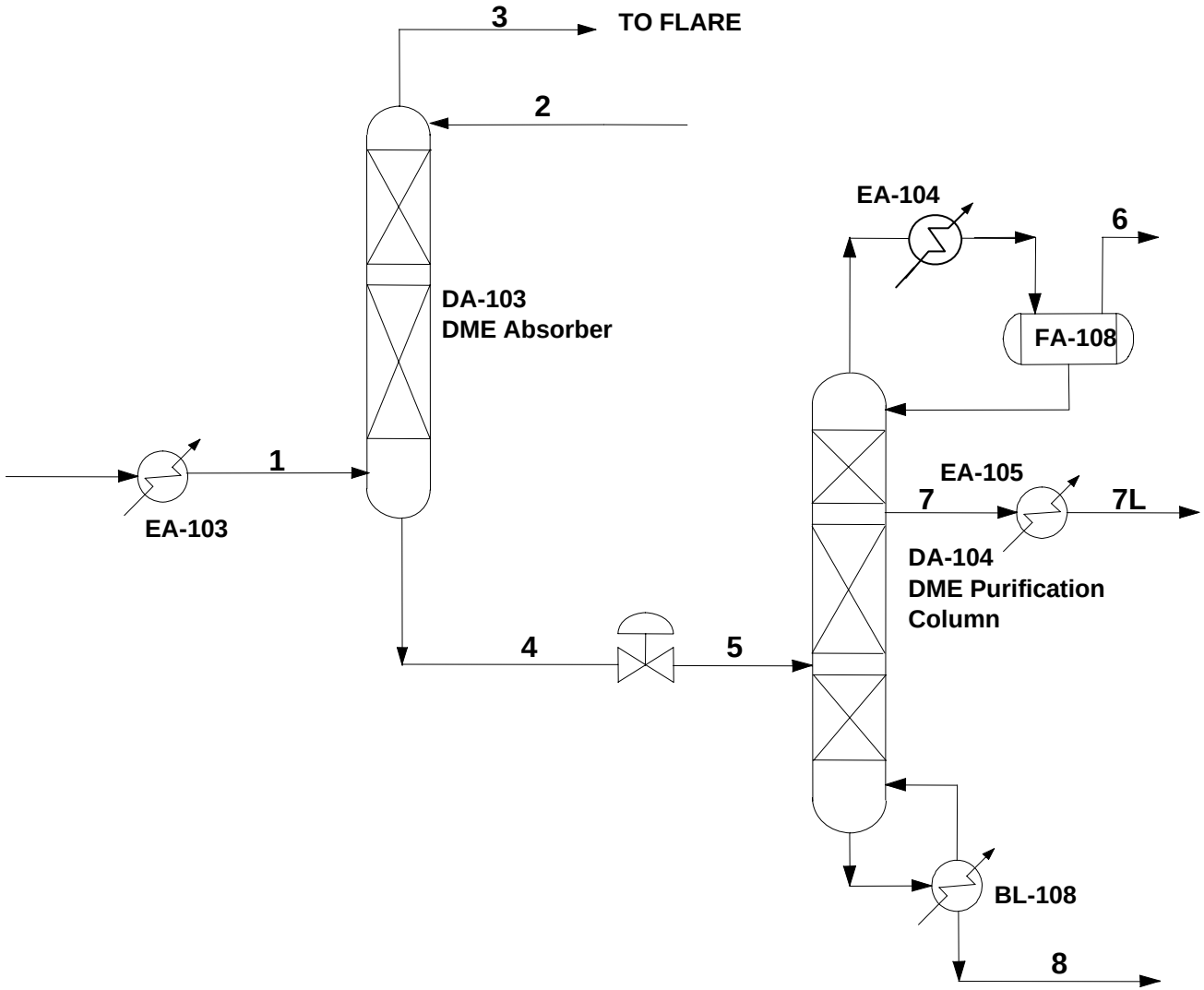
Stream Summary

STREAM ID	1	2	3	4
NAME				
PHASE	MIXED	LIQUID	VAPOR	LIQUID
FLUID RATES, KG-MOL/HR				
1 H2	0.2569	0.0000	0.2515	5.3426E-03
2 CO	0.1856	0.0000	0.1756	0.0100
3 CO2	0.1856	0.0000	0.1187	0.0669
4 CH4	0.1781	0.0000	0.1678	0.0103
5 N2	0.4463	0.0000	0.4336	0.0127
6 H2O	0.0000	0.3077	6.4239E-04	0.3071
7 DME	**0.4519**	0.0000	0.0453	**0.4066**
8 METHANOL	0.1706	2.6192	0.0208	2.7691
TOTAL RATE, KG-MOL/HR	1.8750	2.9269	1.2139	3.5881
TEMPERATURE, C	80.0000	45.0000	52.5122	80.7979
PRESSURE, KG/CM2G	50.0000	49.9998	50.0000	50.0000
ENTHALPY, M*KCAL/HR	4.7385E-03	2.5088E-03	1.1479E-03	6.0993E-03
MOLECULAR WEIGHT	29.6161	30.5672	23.2730	32.5379
MOLE FRAC VAPOR	0.9446	0.0000	1.0000	0.0000
MOLE FRAC LIQUID	0.0554	1.0000	0.0000	1.0000

Stream Summary

TREAM ID	1	2	3	4
NAME				
PHASE	MIXED	LIQUID	VAPOR	LIQUID
FLUID RATES, KG/HR				
1 H2	0.5179	0.0000	0.5071	0.0108
2 CO	5.1995	0.0000	4.9185	0.2811
3 CO2	8.1694	0.0000	5.2260	2.9434
4 CH4	2.8577	0.0000	2.6917	0.1659
5 N2	12.5008	0.0000	12.1459	0.3549
6 H2O	0.0000	5.5439	0.0116	5.5323
7 DME	20.8179	0.0000	2.0848	**18.7331**
8 METHANOL	5.4672	83.9247	0.6653	88.7265
TOTAL RATE, KG/HR	55.5303	89.4686	28.2508	116.7481
TEMPERATURE, C	80.0000	45.0000	52.5122	80.7979
PRESSURE, KG/CM2G	50.0000	49.9998	50.0000	50.0000
ENTHALPY, M*KCAL/HR	4.7385E-03	2.5088E-03	1.1479E-03	6.0993E-03
MOLECULAR WEIGHT	29.6161	30.5672	23.2730	32.5379
WEIGHT FRAC VAPOR	0.9343	0.0000	1.0000	0.0000
WEIGHT FRAC LIQUID	0.0657	1.0000	0.0000	1.0000

Overall DME Purification Process



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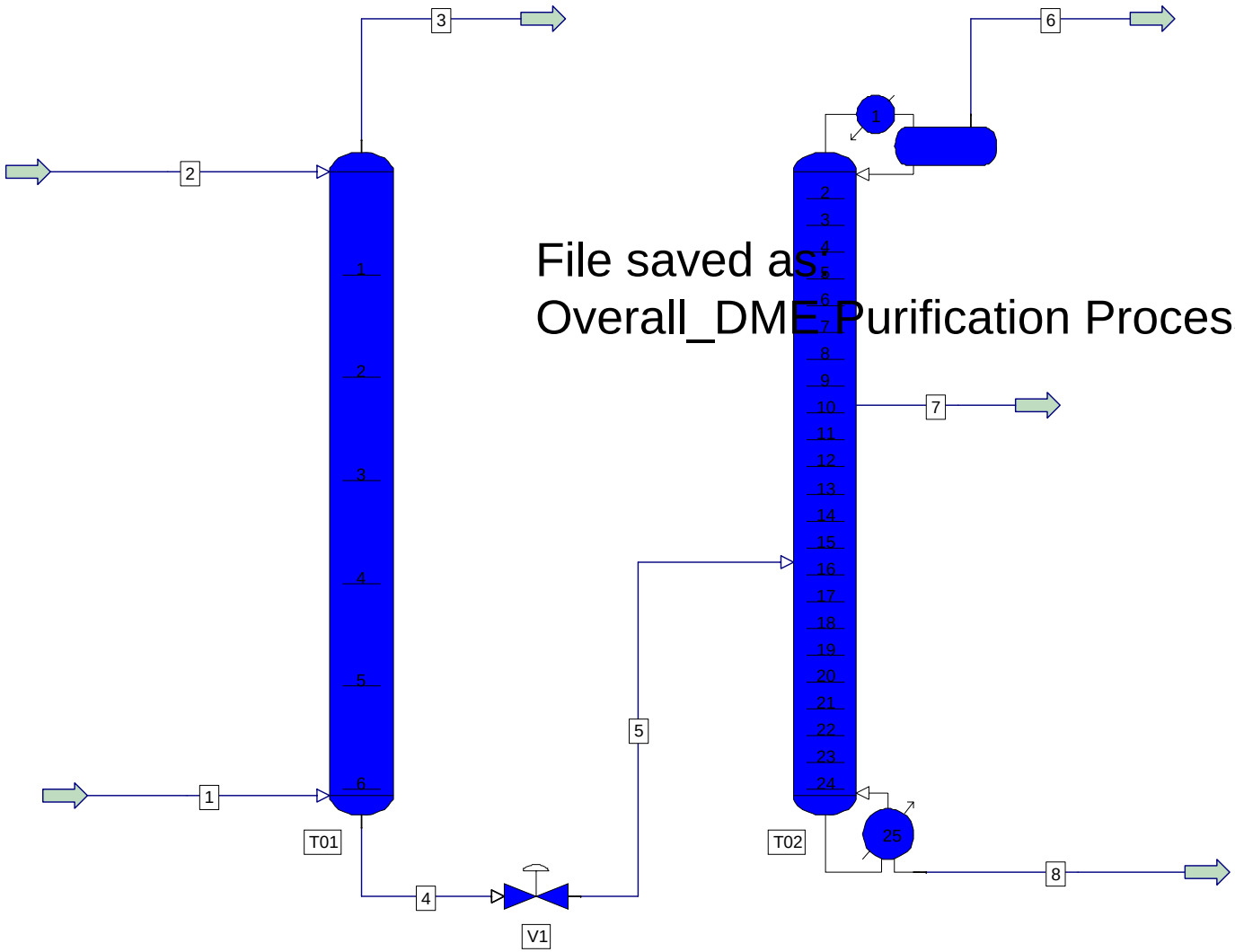
Step 2: DME Purification Column Simulation

- Primary objective of the DME purification column is to obtain a purified DME as a side distillate product.
- Secondary objective of this column is to strip-out CO_2 dissolved in the feed liquid mixture as a top vapor distillate.
- Methanol Solvent is withdrawn as a bottom product.
- Expected DME purity is 98.0 percent by weight.
- Expected methanol purity at column bottom is 95 percent by volume.

Flow Sheet for Overall Process



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Overall_DME Purification Process_New.prz

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Column Summary

COLUMN SUMMARY

TRAY	TEMP DEG C	PRESSURE KG/CM2G	NET FLOW RATES LIQUID KG-MOL/HR	NET FLOW RATES VAPOR KG-MOL/HR	NET FLOW RATES FEED KG-MOL/HR	NET FLOW RATES PRODUCT KG-MOL/HR	HEATER DUTIES M*KCAL/HR
1C	45.0	28.00	1.5			0.2V	-0.0059
2	80.3	28.30	1.9	1.7			
8	89.5	28.38	2.0	2.1			
9	89.6	28.39	2.0	2.1			
10	89.7	28.40	1.6	2.1		0.3L	
15	101.8	28.47	1.2	1.9			
16	114.3	28.48	5.9	1.7	3.6M		
17	117.7	28.50	6.2	2.8			
24	179.2	28.59	5.4	2.1			
25R	183.5	28.60		2.4		3.1L	0.0143

PECIFICATIONS

SPECIFICATION NUMBER	PARAMETER TYPE	TRAY NO	COMP NO	SPECIFICATION TYPE	SPECIFIED VALUE	CALCULATED VALUE
1 (ACTIVE)	TRAY LIQ	1		TEMPERATURE	4.500E+01	4.500E+01
2 (ACTIVE)	STRM 7	10	7	WT PERCENT	9.800E+01	9.800E+01
3 (ACTIVE)	STRM 8	25	8	LV PERCENT	9.500E+01	9.500E+01

Stream Results Around DA-104

STREAM ID	5	6	7	8
NAME				
PHASE	MIXED	VAPOR	LIQUID	LIQUID
FLUID RATES, KG-MOL/HR				
1 H2	5.3460E-03	5.3069E-03	3.8835E-05	5.4934E-12
2 CO	0.0101	0.0100	3.3359E-05	7.7125E-11
3 CO2	0.0670	0.0616	5.3933E-03	1.4158E-06
4 CH4	0.0104	0.0103	6.5979E-05	1.9027E-11
5 N2	0.0127	0.0125	1.5265E-04	1.2924E-11
6 H2O	0.3078	1.2605E-06	8.9925E-04	0.3068
7 DME	**0.4068**	0.0616	**0.3402**	5.0025E-03
8 METHANOL	2.7747	1.0184E-08	1.8700E-03	2.7724
TOTAL RATE, KG-MOL/HR	3.5946	0.1613	0.3486	**3.0842**
TEMPERATURE, C	78.8472	45.0000	89.7423	183.5413
PRESSURE, KG/CM2G	21.9668	28.0000	28.4043	28.6000
ENTHALPY, M*KCAL/HR	6.1067E-03	4.3459E-04	9.2368E-04	0.0132
MOLECULAR WEIGHT	32.5351	39.3927	45.8703	30.6694
MOLE FRAC VAPOR	0.0227	1.0000	0.0000	0.0000
MOLE FRAC LIQUID	0.9773	0.0000	1.0000	1.0000

Stream Results Around DA-104

STREAM ID	5	6	7	8
NAME				
PHASE	MIXED	VAPOR	LIQUID	LIQUID
FLUID RATES, KG/HR				
1 H2	0.0108	0.0107	7.8291E-05	1.1075E-11
2 CO	0.2816	0.2806	9.3441E-04	2.1604E-09
3 CO2	2.9466	2.7090	0.2374	6.2310E-05
4 CH4	0.1663	0.1652	1.0585E-03	3.0525E-10
5 N2	0.3551	0.3508	4.2761E-03	3.6203E-10
6 H2O	5.5441	2.2707E-05	0.0162	5.5270
7 DME	18.7392	2.8368	**15.6714**	0.2305
8 METHANOL	88.9061	3.2632E-07	0.0599	88.8322
TOTAL RATE, KG/HR	116.9498	6.3532	15.9912	94.5897
TEMPERATURE, C	78.8472	45.0000	89.7423	183.5413
PRESSURE, KG/CM2G	21.9668	28.0000	28.4043	28.6000
ENTHALPY, M*KCAL/HR	6.1067E-03	4.3459E-04	9.2368E-04	0.0132
MOLECULAR WEIGHT	32.5351	39.3927	45.8703	30.6694
WEIGHT FRAC VAPOR	0.0249	1.0000	0.0000	0.0000
WEIGHT FRAC LIQUID	0.9751	0.0000	1.0000	1.0000

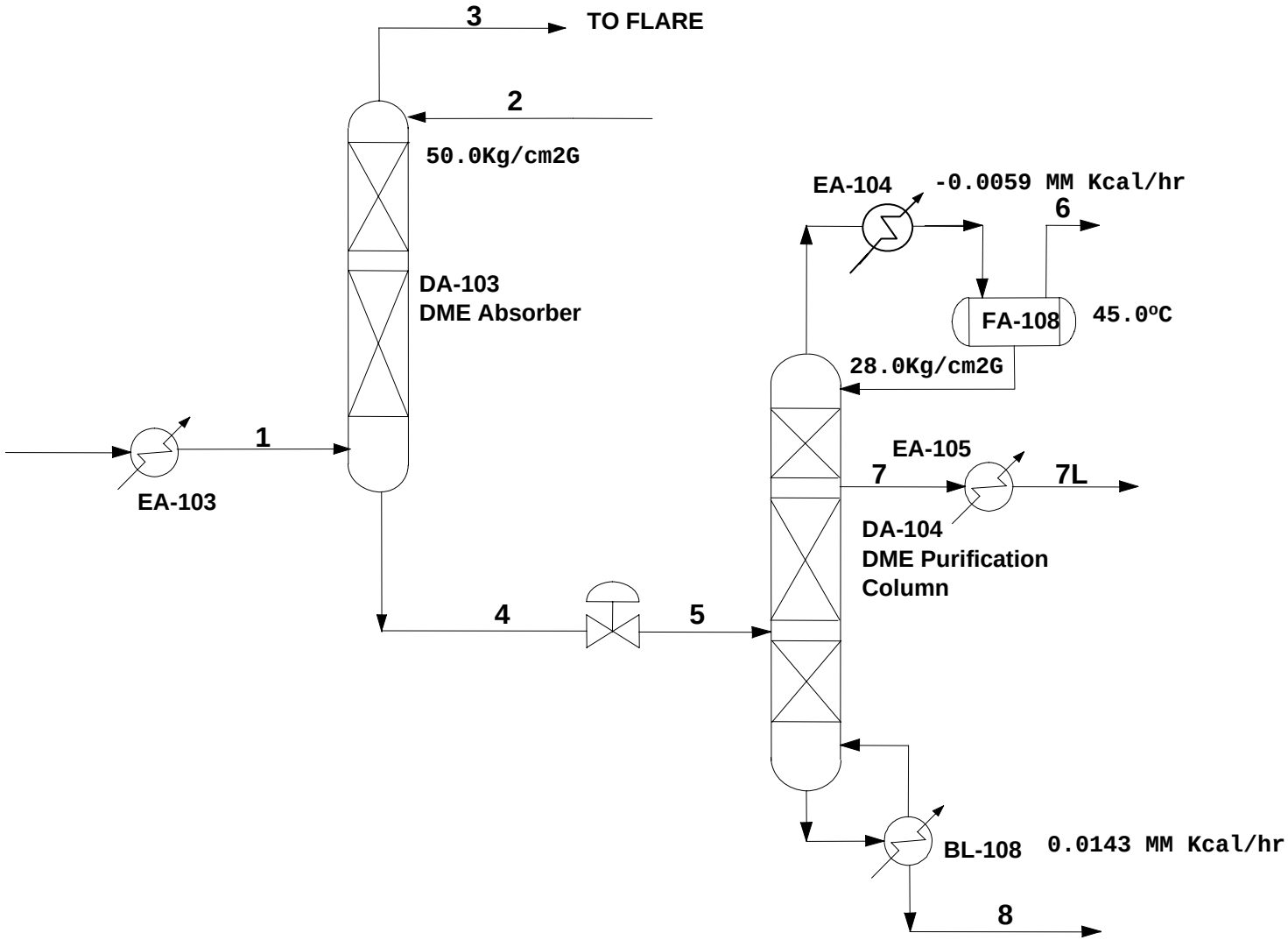
Stream Results Around DA-104

STREAM ID	5	6	7	8
NAME				
PHASE	MIXED	VAPOR	LIQUID	LIQUID
FLUID WEIGHT PERCENTS				
1 H2	9.2155E-03	0.1684	4.8959E-04	1.1708E-11
2 CO	0.2408	4.4175	5.8433E-03	2.2839E-09
3 CO2	2.5196	42.6395	1.4843	6.5874E-05
4 CH4	0.1422	2.6002	6.6192E-03	3.2271E-10
5 N2	0.3037	5.5224	0.0267	3.8274E-10
6 H2O	4.7406	3.5741E-04	0.1013	5.8431
7 DME	16.0232	44.6517	**98.0000**	0.2436
8 METHANOL	76.0207	5.1364E-06	0.3747	93.9132
TOTAL RATE, KG/HR	116.9498	6.3532	15.9912	94.5897
TEMPERATURE, C	78.8472	45.0000	89.7423	183.5413
PRESSURE, KG/CM2G	21.9668	28.0000	28.4043	28.6000
ENTHALPY, M*KCAL/HR	6.1067E-03	4.3459E-04	9.2368E-04	0.0132
MOLECULAR WEIGHT	32.5351	39.3927	45.8703	30.6694
WEIGHT FRAC VAPOR	0.0249	1.0000	0.0000	0.0000
WEIGHT FRAC LIQUID	0.9751	0.0000	1.0000	1.0000

Stream Results Around DA-104

STREAM ID	5	6	7	8
NAME				
PHASE	MIXED	VAPOR	LIQUID	LIQUID
FLUID DRY LV PERCENTS				
1 H2	0.1027	1.7051	4.7411E-03	1.3475E-10
2 CO	0.2345	3.9099	4.9464E-03	2.2977E-09
3 CO2	2.3756	36.5443	1.2167	6.4170E-05
4 CH4	0.3695	6.1432	0.0150	8.6660E-10
5 N2	0.2930	4.8436	0.0224	3.8155E-10
6 H2O	3.6980	2.5344E-04	0.0687	4.7093
7 DME	18.4963	46.8536	98.3486	0.2906
8 METHANOL	74.4304	4.5714E-06	0.3189	**95.0000**
TOTAL RATE, M3/HR	0.1501	8.9723E-03	0.0236	0.1175
TEMPERATURE, C	78.8472	45.0000	89.7423	183.5413
PRESSURE, KG/CM2G	21.9668	28.0000	28.4043	28.6000
ENTHALPY, M*KCAL/HR	6.1067E-03	4.3459E-04	9.2368E-04	0.0132
MOLECULAR WEIGHT	32.5351	39.3927	45.8703	30.6694
MOLE FRAC VAPOR	0.0227	1.0000	0.0000	0.0000
MOLE FRAC LIQUID	0.9773	0.0000	1.0000	1.0000

Simulation Results Summary



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