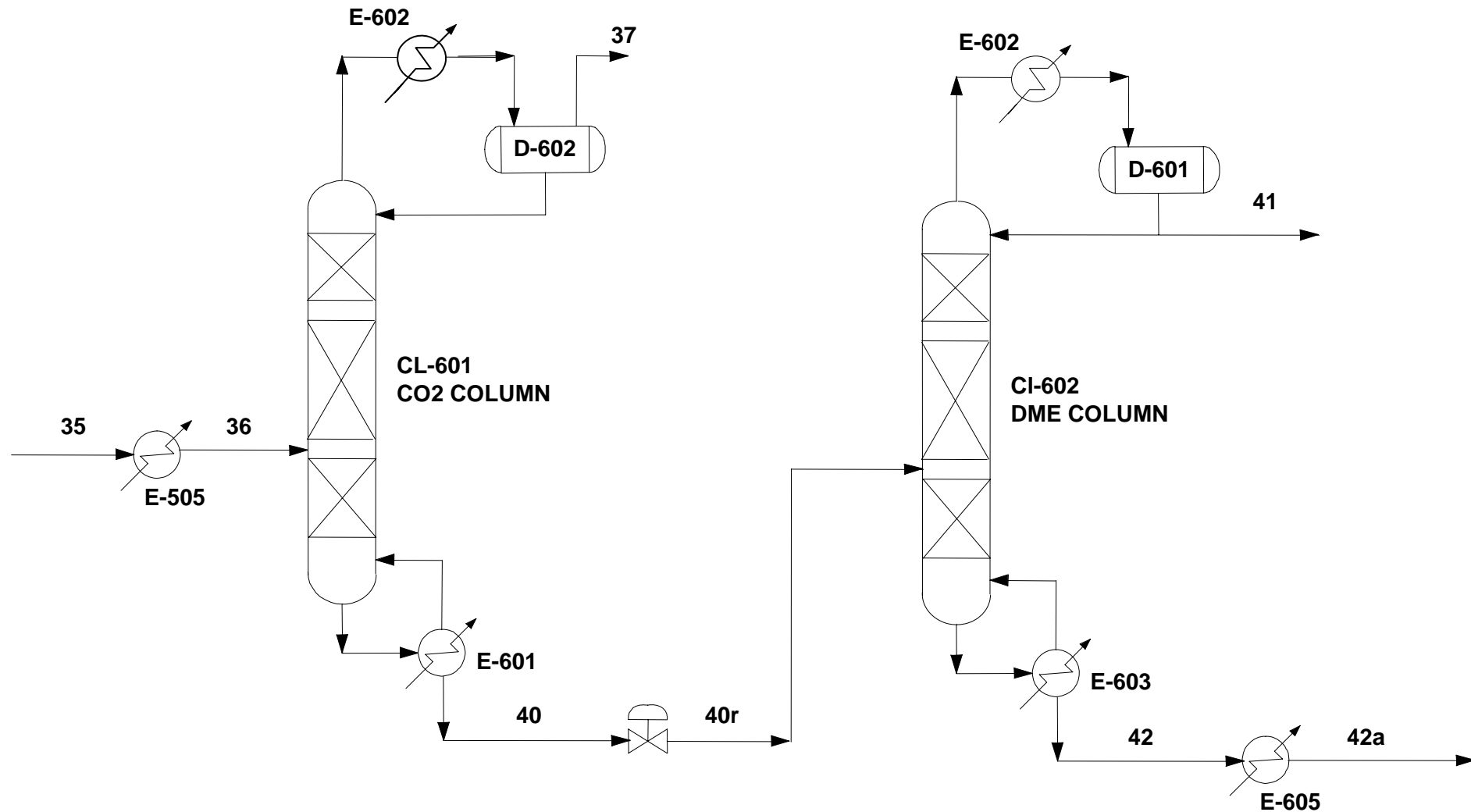


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# DME(10 TPD) Process Simulation for CO<sub>2</sub> Column & DME Column Using PRO/II with PROVISION

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Department of Chemical Engineering  
Dong Yang University

# Overall Flow Sheet for DME Production Unit



# Flowsheet for Toluene Recovery Process

Unit	Description
CL-601	CO2 Column
CL-602	DME Column
D-601	CO2 Column OVHD Drum
D-602	DME Column OVHD Drum
E-505	DME Liquid Recuperator
E-601	CO2 Column Reboiler
E-602	CO2 Column Overhead Condenser
E-603	DME Column Reboiler
E-604	DME Column Overhead Condenser
Stream	Description
36	CO2 Column Feed Stream
37	CO2 Column Overhead Vapor Stream
40	CO2 Column Bottom Liquid Stream
40r	DME Column Feed Stream
41	DME Column Overhead Product (Purified DME Product)
42	Wet Methanol to Dehydration Unit

# Objectives of This Unit

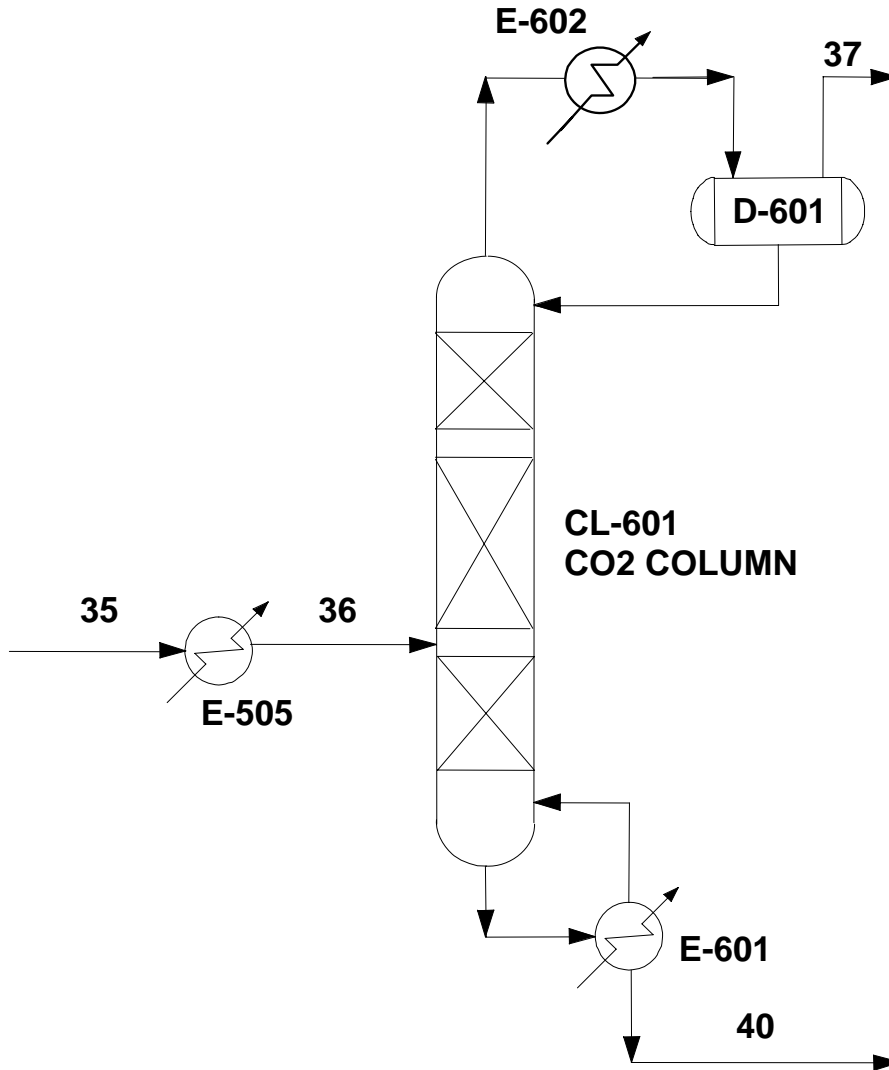
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- The primary objectives of this unit is to accept a mixed feed comprising mostly of DME and separating it away from the other constituents.
- The target is to produce DME of 99.9% purity but simultaneously limiting the methanol to under 100 ppm and water to under 500 ppm.

# Overall Material Balance: Design Case

	35	36	37	40	41	42
Temperature (°C)	-63.51	10.0	-8.565	109.3	35.89	130.3
Pressure (kPa, abs)	3000	3000	3000	3000	800	800
<b>Flow (k-mole/hr)</b>	<b>18.28</b>	<b>20.85</b>	<b>8.816</b>	<b>12.03</b>	<b>9.053</b>	<b>2.979</b>
<b>Total Kg/hr</b>	<b>803.1</b>	<b>887.9</b>	<b>378.4</b>	<b>509.5</b>	<b>417.1</b>	<b>92.39</b>
Component Molar Flow						
1. CO	0.4003	0.3732	0.3720	0.0000	0.0000	0.0000
2. H2O	0.0183	0.2189	0.0000	0.2189	0.0000	0.2184
3. CO2	8.2660	8.3360	8.3350	0.0000	0.0000	0.0000
4. H2	0.0640	0.0521	0.0511	0.0000	0.0000	0.0000
5. Methanol	0.7070	2.7610	0.0000	2.7600	0.0000	2.7600
6. DME	8.7690	9.0550	0.0018	9.0510	9.0530	0.0000
7. CH4	0.0494	0.0480	0.0485	0.0000	0.0000	0.0000
8. N2	0.0073	0.0063	0.0071	0.0000	0.0000	0.0000
9. O2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

# CL-601 (CO2 Column)



# CO2 Column Simulation (CL-601)

- The CO2 column (CL-601) served to remove the CO2 from DME.
- The CO2 is taken from overhead in the vapor phase along with small quantities of non-condensable gas and the DME along with some methanol and water is taken from the bottom as a liquid.

# CO<sub>2</sub> Column Simulation (CL-601): *Continued*

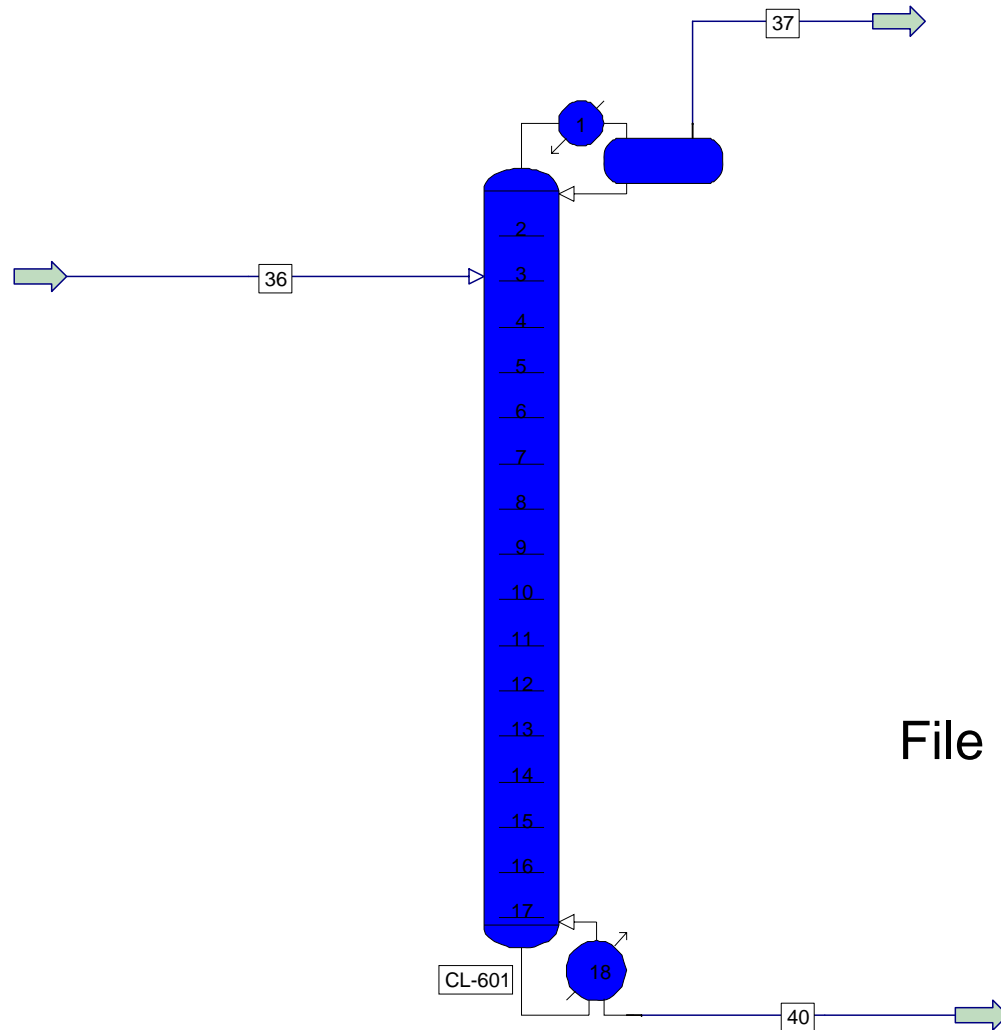
- Consider the following absorber column to absorb CO<sub>2</sub> contained in the feed stream using methanol as a solvent.
  - Feed: DME Reactor Outlet Stream (Refer to feedstock characterization)
  - CO<sub>2</sub> Column
    - 1) Number of Theoretical Stages: 18
    - 2) Column Type: Partial
    - 3) Overall Tray Efficiencies: ?
    - 4) Feed Tray Location: 3



# DME Column Simulation *Continued*

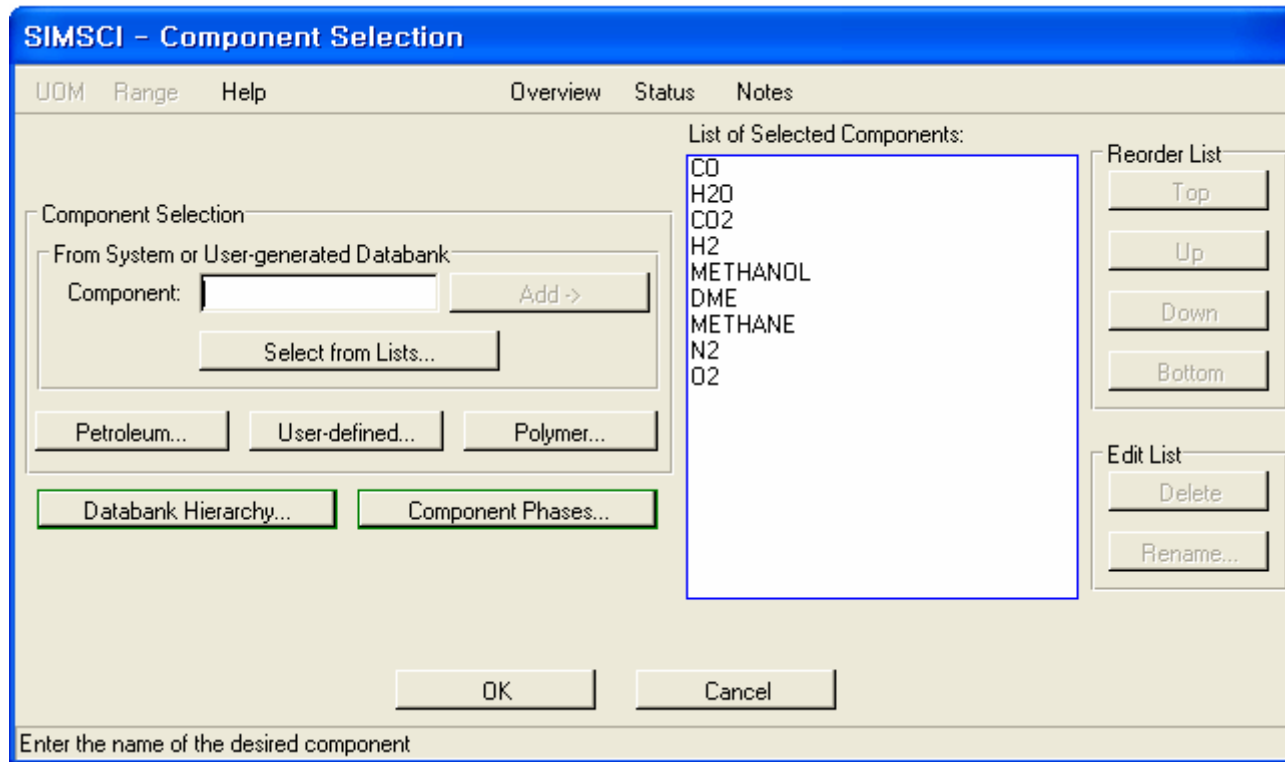
- Selection of appropriate thermodynamic model for the simulation of DME absorber using methanol as a solvent is very important.
  - NRTL (Non Random Two Liquid) activity coefficient model was chosen to explain non-ideal phase behavior of liquid mixture between H<sub>2</sub>O, DME, methanol and methanol.
  - Peng-Robinson equation of state method was used for the prediction of the vapor phase non-idealities since the system pressure is moderately high.
  - Henry's law option was also selected for the calculation of non-condensable supercritical gases like H<sub>2</sub>, CO, CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub> in a liquid mixture, especially methanol solvent.

# Flow Sheet Drawing Using PRO/II

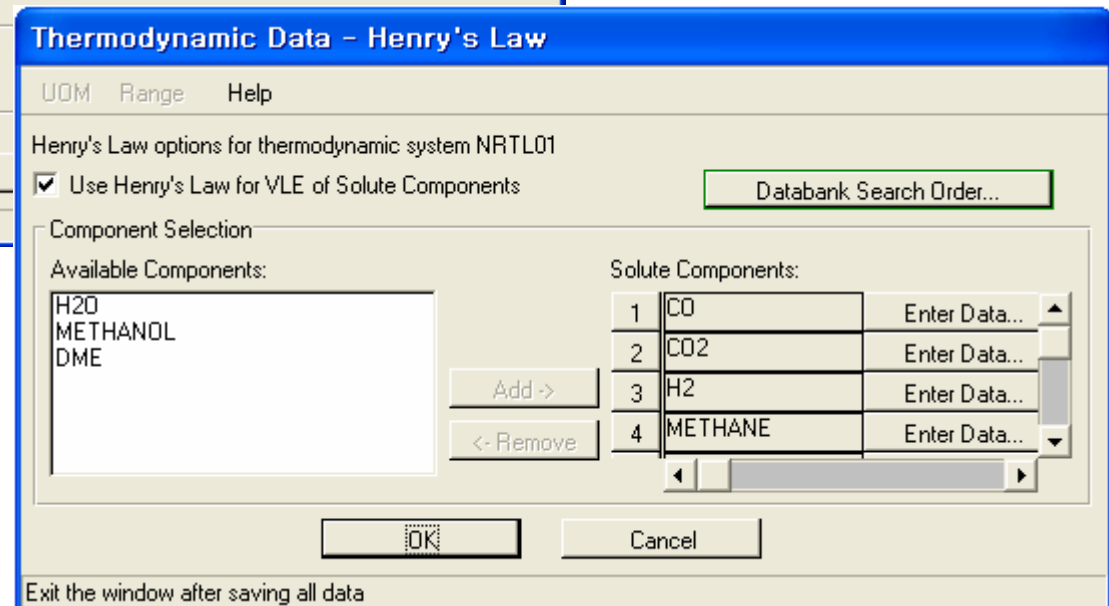
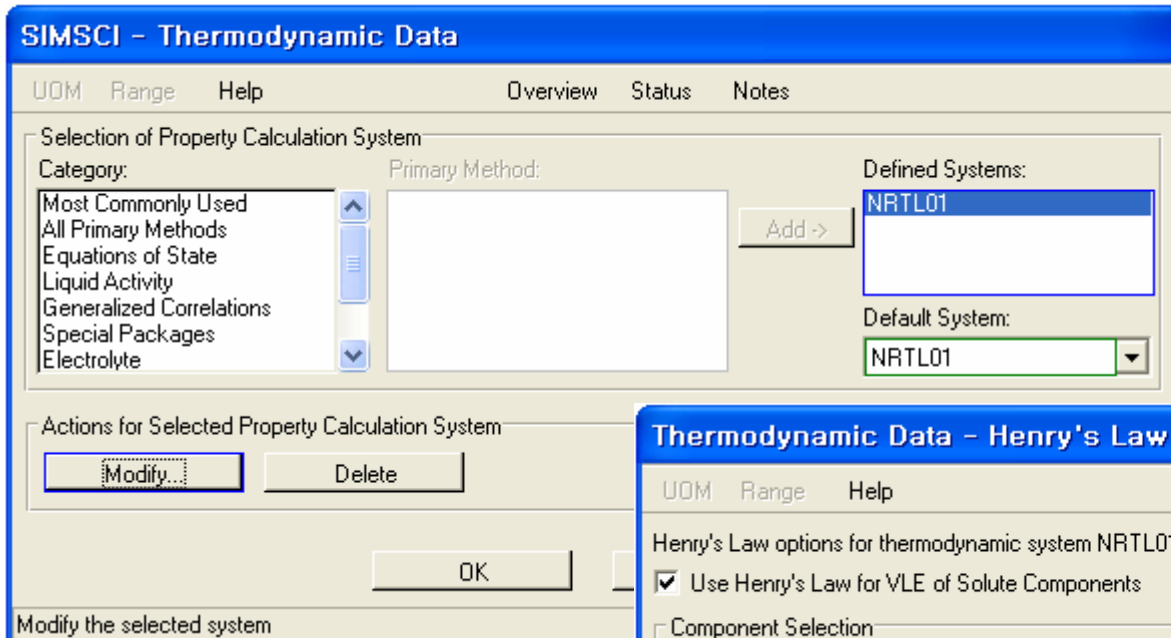


File Saved as: CL-601\_01.prz

# Component Data: Pure Component



# Thermodynamic Data: NRTL with Henry + PR EOS



# Thermodynamic Data: NRTL with Henry + PR EOS

**Thermodynamic Data - Modification**

UOM Range Help Overview

Modifying thermodynamic system NRTL01

Property:	Current Method:	Property-specific Data:
K-value (VLE)	NRTL	Enter Data...
K-value (LLE)	None	Enter Data...
K-value (SLE)	None	Enter Data...
Liquid Enthalpy	Library	Enter Data...
Vapor Enthalpy	Library	Enter Data...
Liquid Density	Library	Enter Data...
Vapor Density	Ideal	Enter Data...
Vapor Fugacity (Phi)	Peng-Robinson	Enter Data...
Liquid Entropy	None	Enter Data...
Vapor Entropy	None	Enter Data...

Enter property-specific data for vapor fugacity calculations

**Thermodynamic Data - Alpha Selection**

UOM Range Help

Specification of equation of state Alpha form for Peng-Robinson method for vapor fugacity in thermodynamic system NRTL01

Source of Equation of State Alphas

Acentric Factor Formulation  
 Alpha Databanks

Equation of State Alpha Databanks

Modifying alpha databank search order for NRTL01

Databank type: ALPHA

Databanks:

Current Search Order:

SIMSCI

Exit the window after saving all data

# NRTL(Non Random Two Liquid) Model

- NRTL. This model has up to 8 adjustable binary parameters that can be fitted to data.

$$\ln \gamma_i = \frac{\sum_j \tau_{ji} G_{ji} x_j}{\sum_k G_{ki} x_k} + \sum_j \frac{x_j G_{ij}}{\sum_k G_{kj} x_k} \left[ \tau_{ij} - \frac{\sum_l x_l \tau_{lj} G_{lj}}{\sum_k G_{kj} x_k} \right]$$

$$\tau_{ij} = a_{ij} + \frac{b_{ij}}{T} + \frac{c_{ij}}{T^2}$$

$$G_{ij} = \exp[-(\alpha_{ij} + \beta_{ij} T) \tau_{ij}]$$

# Henry's Law Option

- When using activity coefficient property methods for supercritical components, use Henry's law to better predict gas solubilities in the liquid phase.

$$K_i = \frac{y_i}{x_i} = \frac{H_{i,mix}}{P}$$

$H_{i,mix}$  is Henry's constant of component  $i$  in the mixture.

- $H_i$  is calculated from temperature-dependent (and also pressure-dependent) Henry's constants for each solute-solvent pair.

# Peng-Robinson Equation (1976)

- Peng-Robinson equation of state modified a functional form to fit better the liquid density so it is known to estimate well for midrange hydrocarbon ( $C_6$  to  $C_{10}$ ) systems.

$$P = \frac{RT}{V - b} - \frac{a_c(T_c) \cdot \alpha(T_r, \omega)}{V(V + b) + b(V - b)}$$



# Peng-Robinson Equation (1976)

- Changed the cubic from Redlich-Kwong slightly.
- Changed the constants in Soave's alpha slightly.

$$\alpha_i(T) = \left[ 1 + m_i \left( 1 - T_{ri}^{1/2} \right) \right]^2$$

$$m_i = 0.37464 + 1.54336\omega_i - 0.26992\omega_i^2$$

# Peng-Robinson Equation (1976)

- The pure component  $a_c$  &  $b_c$  are found from:

$$a = 0.45724 \frac{R^2 T_c^2}{P_c} \quad b = 0.07780 \frac{RT_c}{P_c}$$

- An alternative dimensionless form is given by:

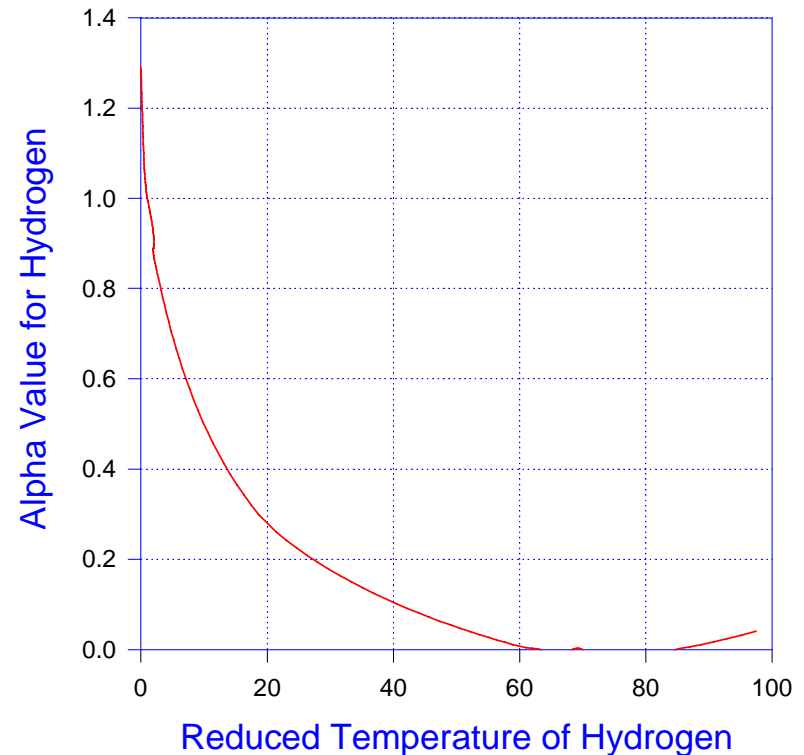
$$P_r = \frac{3.2573 T_r}{V_r - 0.2534} - \frac{4.8514 \alpha}{V_r^2 + 0.5068 V_r - 0.0642}$$

# Critical Compressibility Factors

- Experimental values for critical compressibility:
  - 0.2880 for  $\text{CH}_4$
  - 0.2840 for  $\text{C}_2\text{H}_6$  &
  - 0.2800 for  $\text{C}_3\text{H}_8$
  
- PR and SRK equation of state are still used to estimate phase equilibria calculation for non-ideal systems since what is the most important thing in the design of chemical process is K-values, *not the liquid densities.*

# Soave's Original Alpha form

- Good representation of liquid vapor pressure:  
*“Proper alpha form”*
- Soave's original alpha form is wrong since it increases again as reduced temperature of hydrogen,  $T_r$  approaches to infinity.



$$\alpha(T) = \left[ 1 + \left( 0.37464 + 1.54226 \omega_i - 0.26992 \omega_i^2 \right) \left( 1 - \sqrt{T_r} \right) \right]^2 \quad (11)$$

# Requirements for Alpha form

- Requirements for alpha form:
  - The  $\alpha$  function must be finite and positive for all temperature.
  - The  $\alpha$  function must equal unity at the critical point.
  - The  $\alpha$  function must approach a zero value as the temperature approaches infinity.
  
- The trend from now is to set the coefficients of alpha function component dependently by regressing the experimental vapor pressure data vs. temperatures.

# Several Alpha functions

$\alpha = \left[1 + C_1(1 - T_t^{0.5})\right]^2$	Soave (1972)
$\alpha = \left[C_1 + C_2(1 - T_t^{C_3})\right]^2$	Peng-Robinson (1980)
$\alpha = 1 + (1 - T_r) \left(C_1 + \frac{C_2}{T_r}\right)$	Soave (1979)
$\alpha = \exp\left[C_1(1 - T_r^{C_2})\right]$	Boston-Mathias (1980)
$\alpha = T_r^{2(C_2-1)} \exp\left[C_1(1 - T_r^{2C_2})\right]$	Twu (1988)
$\alpha = T_r^{C_3(C_2-1)} \exp\left[C_1(1 - T_r^{C_2C_3})\right]$	Twu-Bluck-Cunningham (1990) (Recommended by SimSci)

# New Alpha Form

- Since 1972, many alpha forms have been proposed, some better than others.
- PRO/II allows input of parameters for 11 different forms, including the SIMSCI (TBCC) alpha form.

$$\alpha(T) = T_r^{C_3(C_2-1)} \exp\left[C_1\left(1 - T_r^{C_2C_3}\right)\right]$$

- This 3 parameter form eliminates the 2 problems with the Soave alpha for defined components

# Mixing Rules

- The accuracy of correlating vapor-liquid equilibrium data using a cubic equation of state can be improved by choosing an appropriate mixing rule for calculating  $a$  and  $b$  for mixture.
- Expressions for mixing rules  $a$  and  $b$  are:

$$a = \sum_i \sum_j x_i x_j a_{ij}$$

$$b = \sum_i x_i b_i$$

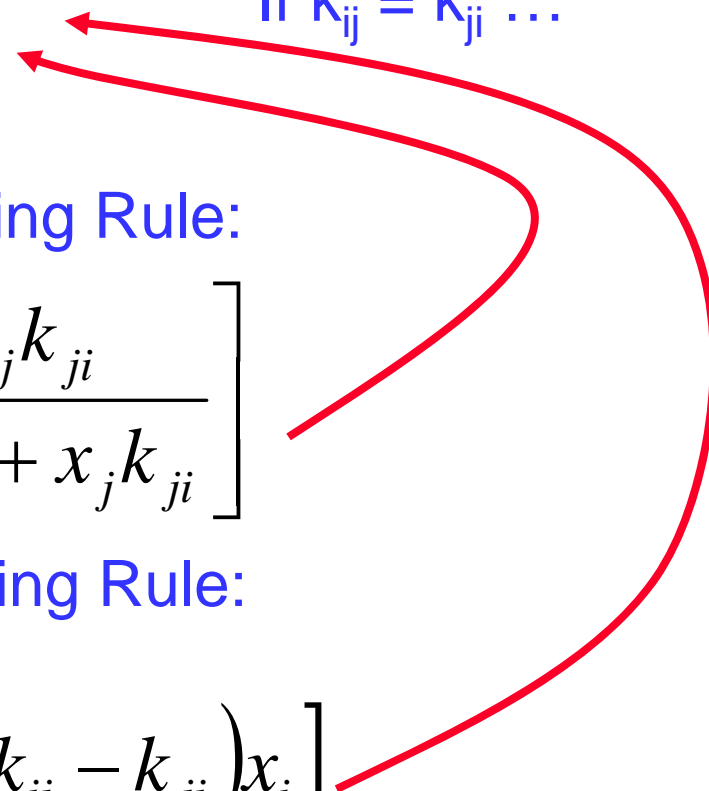


# Mixing Rules for 'a'

- Van der Waals Mixing Rule:

$$a_{ij} = \sqrt{a_i a_j} (1 - k_{ij})$$

If  $k_{ij} = k_{ji} \dots$



- Stryjek and Vera (1986) Mixing Rule:

$$a_{ij} = \sqrt{a_i a_j} \left[ 1 - \frac{k_{ij} k_{ji}}{x_i k_{ij} + x_j k_{ji}} \right]$$

- Panagiotopoulos (1985) Mixing Rule:

$$a_{ij} = \sqrt{a_i a_j} \left[ 1 - k_{ij} + (k_{ij} - k_{ji}) x_i \right]$$

# PRSV EOS in HYSYS Simulator

SIMULATION CASE14 - HYSYS 3.2 - [Fluid Package: Basis-1]

File Edit Basis Tools Window Help

Environment: Basis  
Mode: Steady State

Equation of State Interaction Parameters

	Methane	Ethane	Propane	i-Butane	n-Butane	i-Pentane	Nitrogen	CO	CO2	Hydrogen	H2O	Methanol	diM-Ether	Oxygen
Methane	...	-0.00020	0.01720	0.03880	0.00970	0.03390	0.03600	0.02100	0.10000	0.20230	0.48000	-0.03500	0.00000	0.00000
Ethane	-0.00020	...	-0.00360	-0.00460	0.01080	0.00792	0.05000	0.02540	0.13000	0.22330	0.50000	0.04500	0.00000	0.00000
Propane	0.01720	-0.00360	...	0.00480	0.00060	0.00730	0.08000	0.06130	0.13500	0.21420	0.50000	0.06000	0.00000	0.00000
i-Butane	0.03880	-0.00460	0.00480	...	-0.00150	0.00077	0.09500	0.00000	0.13000	0.20410	0.50000	0.06900	0.00000	0.00000
n-Butane	0.00970	0.01080	0.00060	-0.00150	...	0.00093	0.09000	0.00000	0.13000	0.19410	0.50000	0.06900	0.00000	0.00000
i-Pentane	0.03390	0.00792	0.00730	0.00077	0.00093	...	0.09500	0.00000	0.12500	0.29210	0.50000	0.06000	0.00000	0.00000
Nitrogen	0.03600	0.05000	0.08000	0.09500	0.09000	0.09500	...	0.01150	-0.02000	-0.03600	-0.31560	-0.21410	0.00000	-0.01200
CO	0.02100	0.02540	0.06130	0.00000	0.00000	0.00000	0.01150	...	-0.03140	0.02530	-0.38960	0.00000	0.00000	0.00000
CO2	0.10000	0.13000	0.13500	0.13000	0.13000	0.12500	-0.02000	-0.03140	...	0.12020	0.04450	0.04000	0.00000	0.09750
Hydrogen	0.20230	0.22330	0.21420	0.20410	0.19410	0.29210	-0.03600	0.02530	0.12020	...	-0.29980	0.00000	0.00000	0.00000
H2O	0.48000	0.50000	0.50000	0.50000	0.50000	0.50000	-0.31560	-0.38960	0.04450	-0.29980	...	-0.18000	0.00000	0.00000
Methanol	-0.03500	0.04500	0.06000	0.06900	0.06900	0.06000	-0.21410	0.00000	0.04000	0.00000	-0.18000	...	0.00000	0.00000
diM-Ether	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	...	0.00000
Oxygen	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.01200	0.00000	0.09750	0.00000	0.00000	0.00000	0.00000	...

- Number of components: 14
- Required pairs of BIP's:  $\frac{14 \times 13}{2!} = 91$
- Available pairs of BIP's built in HYSYS: 63 (69%)
- PRSV mixing rules have 2 adjustable parameters but....

# Henry's Constant Built-In PRO/II Library

HENRY COEFFICIENTS FOR SET 'NRTL01'

LN(H) = C1 + C2/T + C3\*LN(T) + C4\*P  
 TEMPERATURE IN K  
 PRESSURE IN KPA

HENRY COEFFICIENTS

SOLUTE	SOLVENT	C1	C2	C3	C4	FROM
1	2	166.6723	-7847.1602	-21.8994	9.8692E-07	SIMSCI BANK
<b>1</b>	<b>5</b>	<b>N/A</b>	<b>N/A</b>	<b>N/A</b>	<b>N/A</b>	<b>VAPOR PRESSURE</b>
<b>1</b>	<b>6</b>	<b>N/A</b>	<b>N/A</b>	<b>N/A</b>	<b>N/A</b>	<b>VAPOR PRESSURE</b>
3	2	154.9483	-8498.7197	-20.0841	7.3032E-06	SIMSCI BANK
<b>3</b>	<b>5</b>	<b>217.0283</b>	<b>-10620.0000</b>	<b>-30.1360</b>	<b>0.0000</b>	<b>SIMSCI BANK</b>
3	6	134.5983	-6535.3999	-18.2570	0.0000	SIMSCI BANK
4	2	116.4133	-4881.3198	-14.7884	3.5529E-06	SIMSCI BANK
4	5	15.5643	271.3300	-0.5485	0.0000	SIMSCI BANK
4	6	223.4183	-8787.0996	-31.9150	0.0000	SIMSCI BANK
7	2	169.8923	-8132.2300	-22.3559	1.4409E-06	SIMSCI BANK
7	5	-63.1517	2617.0000	11.5200	0.0000	SIMSCI BANK
<b>7</b>	<b>6</b>	<b>N/A</b>	<b>N/A</b>	<b>N/A</b>	<b>N/A</b>	<b>VAPOR PRESSURE</b>
8	2	158.2643	-7260.1401	-20.7005	1.4409E-06	SIMSCI BANK
8	5	27.7643	-598.8800	-2.2701	0.0000	SIMSCI BANK
8	6	225.6083	-9275.2002	-32.1410	0.0000	SIMSCI BANK
9	2	155.5533	-7442.2900	-20.2359	1.6186E-06	SIMSCI BANK
9	5	15.2813	-185.0300	-0.3951	0.0000	SIMSCI BANK
9	6	195.2183	-8362.7998	-27.4340	0.0000	SIMSCI BANK

# NRTL BIP's Built-In PRO/II Library

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
2	5	0.511068 0.736107	199.8540 -360.6920	0.00 0.00	0.2442 0.0000	DEG K SIMSCI VLEBANK
2	6	12.300150 -5.168679	-4019.6919 2145.8921	330053.91 74425.09	0.2000 0.0000	DEG K SIMSCI VLEBANK
5	6	0.000000 0.000000	653.0060 -18.9372	0.00 0.00	0.2951 0.0000	DEG K SIMSCI VLEBANK

2: H2O  
5: Methanol  
6: DME

# PR BIP's Built-In PRO/II Library

## PR INTERACTION PARAMETERS

$$K_{IJ} = A(I,J) + B(I,J)/T + C(I,J)/T^{*2}$$

I	J	KA(I,J)	KB(I,J)	KC(I,J)	UNITS	FROM
1	2	0.2000	0.00	0.00	DEG K	SIMSCI BANK
1	3	-0.0300	0.00	0.00	DEG K	SIMSCI BANK
1	4	0.0900	0.00	0.00	DEG K	SIMSCI BANK
1	7	0.0300	0.00	0.00	DEG K	SIMSCI BANK
1	8	0.0120	0.00	0.00	DEG K	SIMSCI BANK
2	3	0.2100	0.00	0.00	DEG K	SIMSCI BANK
2	4	0.5630	0.00	0.00	DEG K	SIMSCI BANK
2	5	-0.0789	0.00	0.00	DEG K	SIMSCI BANK
2	7	0.5000	0.00	0.00	DEG K	SIMSCI BANK
2	8	0.5080	0.00	0.00	DEG K	SIMSCI BANK
3	4	-0.1622	0.00	0.00	DEG K	SIMSCI BANK
<b>3</b>	<b>5</b>	<b>0.0421</b>	<b>0.00</b>	<b>0.00</b>	<b>DEG K</b>	<b>SIMSCI BANK, 3: CO2, 5: Methanol</b>
3	7	0.0919	0.00	0.00	DEG K	SIMSCI BANK
3	8	-0.0170	0.00	0.00	DEG K	SIMSCI BANK
4	7	0.0160	0.00	0.00	DEG K	SIMSCI BANK
4	8	-0.0300	0.00	0.00	DEG K	SIMSCI BANK
5	8	-0.2700	0.00	0.00	DEG K	SIMSCI BANK
7	8	0.0350	0.00	0.00	DEG K	SIMSCI BANK
7	9	0.0500	0.00	0.00	DEG K	MW CORRELATION
8	9	-0.0119	0.00	0.00	DEG K	SIMSCI BANK

# Coefficients in PR Alpha Form

## PR PURE COMPONENT DATA

COMP	CRITICAL TEMPERATURE DEG C	CRITICAL PRESSURE KPA	ALPHA TYPE	C1	C2	C3
1	-140.20	3495.71	6	0.0746	0.8722	2.2635
2	374.20	22119.20	6	0.3846	0.8700	1.9637
3	31.04	7381.52	5	0.2047	0.8197	N/A
4	-239.90	1296.96	6	0.9267	4.2324	0.1200
5	239.43	8095.87	6	0.7515	0.9320	1.6042
6	126.90	5370.22	6	0.1140	0.8996	3.7232
7	-82.60	4600.15	5	0.1195	0.9040	N/A
8	-146.90	3394.39	6	0.5764	0.9093	0.6765
9	-118.40	5076.38	6	1.8858	3.7551	0.0922

# Column Summary

## COLUMN SUMMARY

TRAY	TEMP DEG C	PRESSURE KPA	NET FLOW RATES			HEATER DUTIES M*KCAL/HR
			LIQUID	VAPOR	FEED PRODUCT	
			KG-MOL/HR			
1C	-8.6	3000.00	6.3			8.9V
2	2.0	3000.00	6.5	15.3		
3	18.1	3000.00	27.3	15.4	20.8M	
4	44.9	3000.00	27.2	15.4		
17	103.1	3000.00	33.2	22.1		
18R	107.1	3000.00		21.3		11.9L
						0.0664

## SPECIFICATIONS

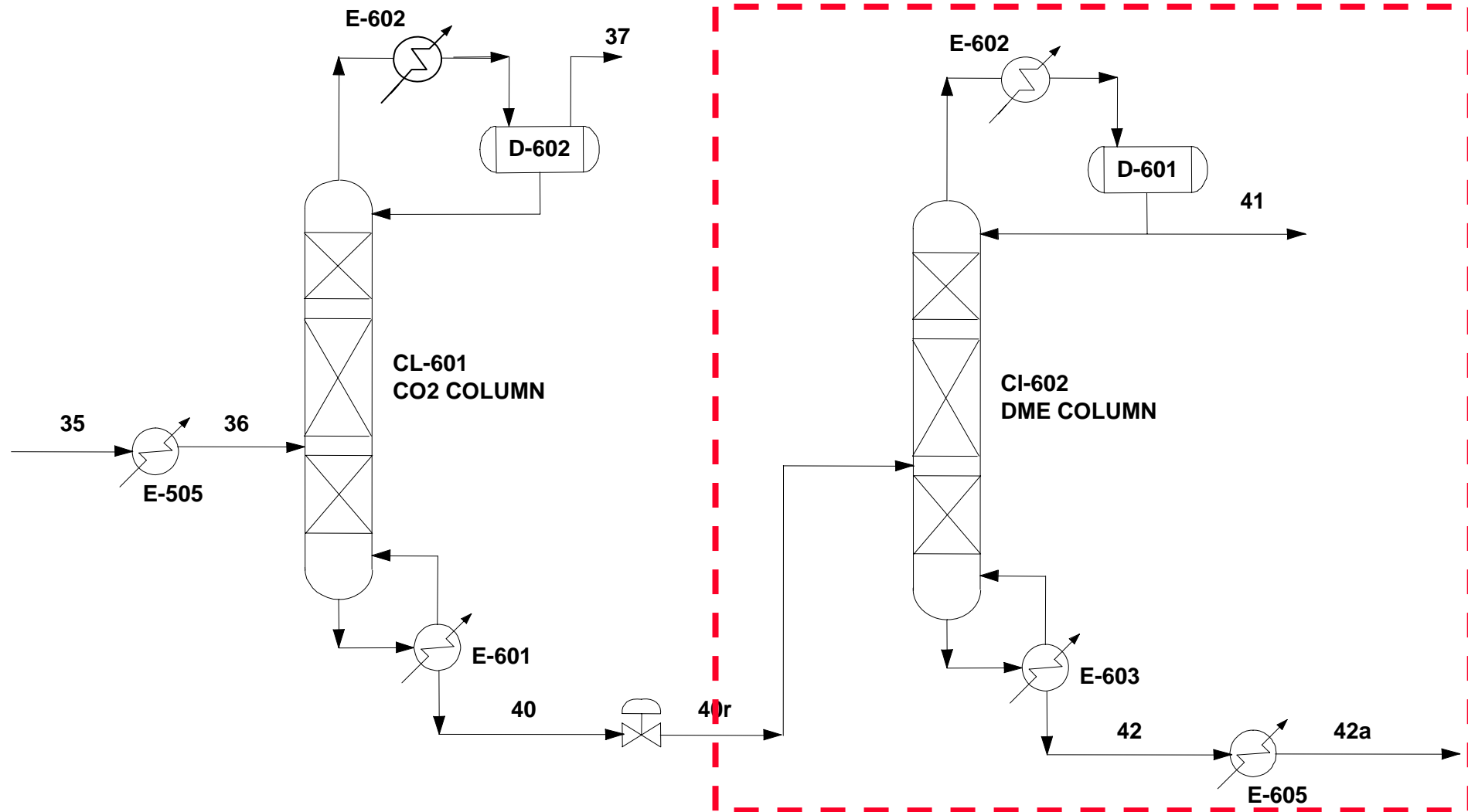
SPECIFICATION NUMBER	PARAMETER TYPE	TRAY NO	COMP NO	SPECIFICATION TYPE	SPECIFIED VALUE	CALCULATED VALUE
1 (ACTIVE)	TRAY LIQ	1		TEMPERATURE	-8.600E+00	-8.600E+00
2 (ACTIVE)	STRM 40	18	3	MOL PPM	1.000E+01	1.000E+01

# Stream Summary

STREAM ID		36	37	40
NAME				
PHASE		MIXED	VAPOR	LIQUID
FLUID RATES, KG-MOL/HR				
1	CO	0.3732	0.3732	0.0000
2	H2O	0.2189	6.7573E-10	0.2189
3	CO2	8.3358	8.3357	1.1908E-04
4	H2	0.0521	0.0521	8.9653E-17
5	METHANOL	2.7609	8.3293E-07	2.7609
6	DME	9.0548	0.1265	8.9283
7	METHANE	0.0480	0.0480	1.1908E-20
8	N2	6.2998E-03	6.2998E-03	7.0618E-18
9	O2	0.0000	0.0000	0.0000
TOTAL RATE, KG-MOL/HR		20.8500	8.9418	11.9082
TEMPERATURE, C		10.0000	-8.5996	107.0549
PRESSURE, KPA		3000.0000	3000.0000	3000.0000
ENTHALPY, M*KCAL/HR		9.9528E-03	0.0213	0.0370
MOLECULAR WEIGHT		42.5864	42.9654	42.3019
MOLE FRAC VAPOR		0.1111	1.0000	0.0000
MOLE FRAC LIQUID		0.8889	0.0000	1.0000



# DA-602 (DME Column)



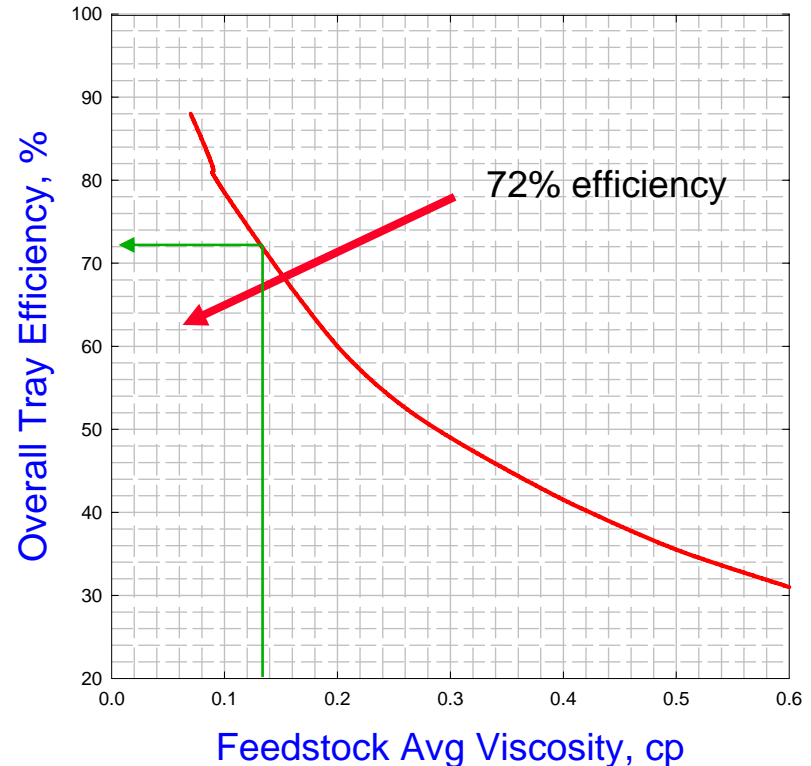
# Overall Tray Efficiencies: Method 1

## Method of Drickamer & Bradford <sup>1</sup>

Notes:

- 1) Based on 54 refinery columns.
- 2) Viscosity is average of feed as liquid at top & bottom temperatures of the column.
- 3) For Absorbers, use rich oil at exit temperature.
- 4) Efficiency is for key components.

1. Tran. Am. Inst. Chem. Engrs, 39, 319 (1943).



# Feedstock Average Viscosity

STREAM ID	<u>36</u>	37	40	40R
----- LIQUID -----				
RATE, KG-MOL/HR	9.950	N/A	11.908	6.469
K*KG/HR	0.412	N/A	0.504	0.257
M3/HR	0.676	N/A	1.069	0.385
GAL/MIN	2.977	N/A	4.708	1.693
STD LIQ RATE, M3/HR	0.571	N/A	0.725	0.362
SPECIFIC GRAVITY (H2O=1.0)	0.7226	N/A	0.6958	0.7123
MOLECULAR WEIGHT	41.457	N/A	42.302	39.789
ENTHALPY, KCAL/KG	31.130	N/A	73.429	26.945
CP, KCAL/KG-C	0.602	N/A	1.008	0.633
DENSITY, KG/M3	610.107	N/A	471.034	669.423
Z (FROM DENSITY)	0.0759	N/A	0.0852	0.0157
SURFACE TENSION, DYNE/CM	11.1912	N/A	5.6287	15.1811
THERMAL COND, KCAL/HR-M-C	0.10069	N/A	0.05962	0.10866
<u>VISCOSITY, CP</u>	<u>0.13607</u>	N/A	0.08042	0.20720

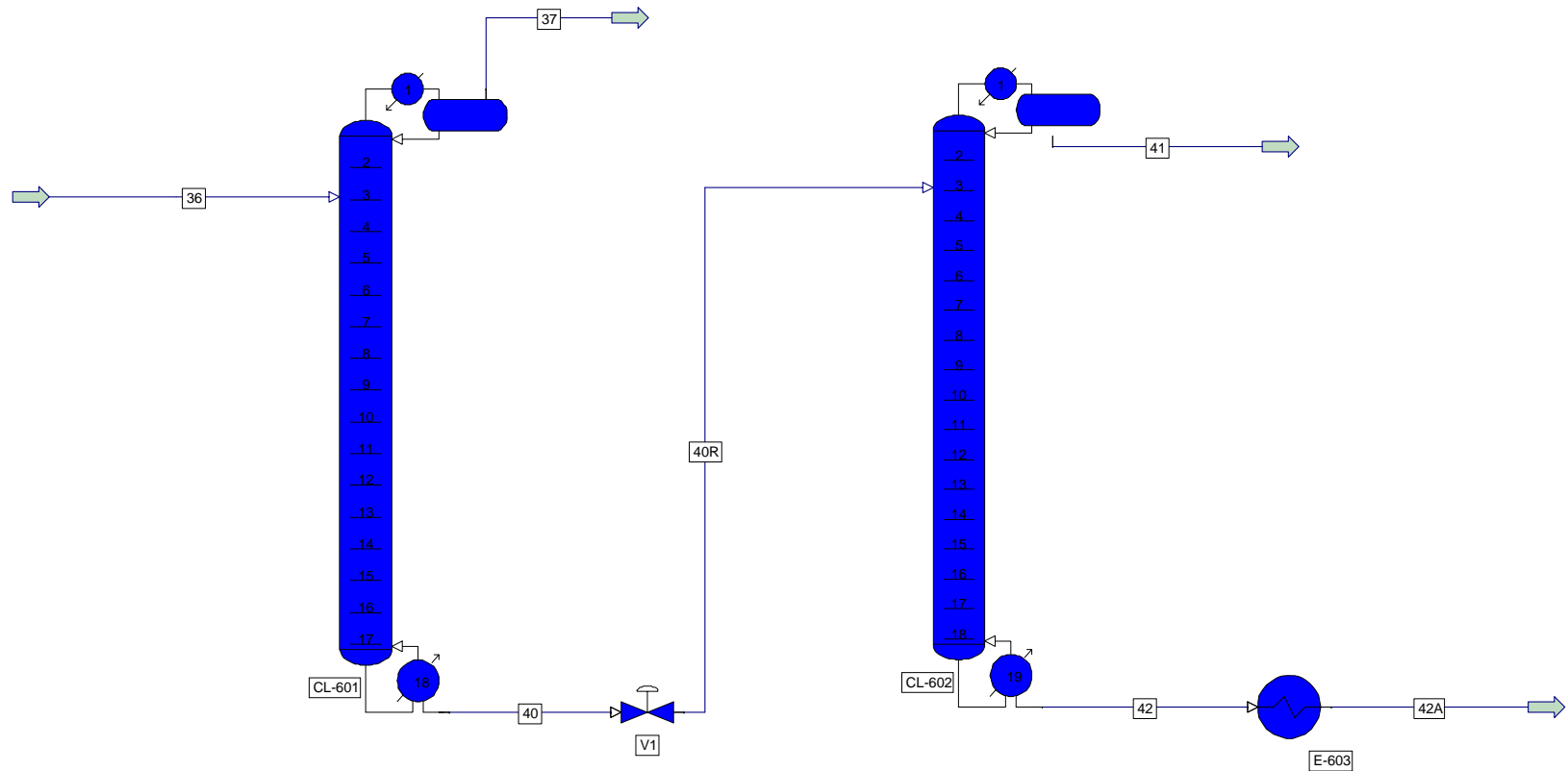
# DME Column Simulation

- The DME Column (CL-602) serves to purify the DME by removing the methanol and water.
- The DME product is taken from overhead as a liquid and the methanol and water are taken from the bottom as a liquid.
- The target is to produce DME of 99.9% purity but simultaneously limiting the methanol to under 100 ppm and water to under 500 ppm.

# Material Balance Around DME Column

	35	36	37	40	41	42
Temperature (°C)	-63.51	10.0	-8.565	109.3	35.89	130.3
Pressure (kPa, abs)	3000	3000	3000	3000	800	800
<b>Flow (k-mole/hr)</b>	<b>18.28</b>	<b>20.85</b>	<b>8.816</b>	<b>12.03</b>	<b>9.053</b>	<b>2.979</b>
<b>Total Kg/hr</b>	<b>803.1</b>	<b>887.9</b>	<b>378.4</b>	<b>509.5</b>	<b>417.1</b>	<b>92.39</b>
Component Molar Flow						
1. CO	0.4003	0.3732	0.3720	0.0000	0.0000	0.0000
2. H2O	0.0183	0.2189	0.0000	0.2189	0.0000	0.2184
3. CO2	8.2660	8.3360	8.3350	0.0000	0.0000	0.0000
4. H2	0.0640	0.0521	0.0511	0.0000	0.0000	0.0000
5. Methanol	0.7070	2.7610	0.0000	2.7600	0.0000	2.7600
6. DME	8.7690	9.0550	0.0018	9.0510	9.0530	0.0000
7. CH4	0.0494	0.0480	0.0485	0.0000	0.0000	0.0000
8. N2	0.0073	0.0063	0.0071	0.0000	0.0000	0.0000
9. O2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

# Flow Sheet Drawing Using PRO/II



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# DME Column (CL-602) Simulation

- Consider the following DME column to separate DME from methanol and water.
  - Feed: DME Column Feed
  - DME Column
    - 1) Number of Theoretical Stages: 19 including condenser & reboiler
    - 3) Overall Tray Efficiencies: Can be estimated by correlation
    - 4) Feed Tray Location: 6

# Optimization

UNIT 5, 'OP1'

BEST OBJECTIVE FUNCTION = 5.39788E-02 AT CYCLE NUMBER 6

\*\*\* FRACTIONAL RELATIVE CHANGE IN OBJECTIVE IS LESS THAN 5.0000E-03 \*\*\*

VARY INDEX	VARIABLE	INITIAL VALUE	OPTIMUM VALUE
1		3.00000E+00	6.04817E+00

OPTIMIZER HISTORY

VALUES	1	2	3	4	5
VARY 1	3.0000E+00	4.0000E+00	4.6830E+00	5.6830E+00	6.0579E+00
OBJECTIVE	5.8690E-01	1.7125E-01	1.1525E-01	6.7253E-02	5.4027E-02

VALUES	BEST - 6
VARY 1	6.0482E+00
OBJECTIVE	5.3979E-02



# Column Summary

## COLUMN SUMMARY

TRAY	TEMP DEG C	PRESSURE KPA	NET FLOW RATES			HEATER DUTIES M*KCAL/HR	
			LIQUID	VAPOR	FEED		PRODUCT
			KG-MOL/HR				
1C	30.0	700.00	8.5			8.9L	-0.0761
2	31.9	700.00	8.6	17.4			
3	32.0	700.00	8.5	17.5			
4	32.4	700.00	8.4	17.5			
5	34.0	700.00	7.9	17.3			
6	39.5	700.00	13.9	16.8	11.3M		
7	39.7	700.00	14.2	11.5	0.6M		
8	39.7	700.00	14.2	11.2			
9	39.7	700.00	14.2	11.2			
18	88.5	700.00	9.5	8.3			
19R	121.7	700.00		6.5		3.0L	0.0540

## SPECIFICATIONS

SPECIFICATION NUMBER	PARAMETER TYPE	TRAY NO	COMP NO	SPECIFICATION TYPE	SPECIFIED VALUE	CALCULATED VALUE
1 (ACTIVE)	STRM 41	1	6	MOL FRACTION	9.990E-01	9.990E-01
2 (ACTIVE)	STRM 42	19		MOL RATE	2.979E+00	2.979E+00

# Stream Summary

STREAM ID		41	42	42A
NAME				
PHASE		LIQUID	LIQUID	LIQUID
FLUID RATES, KG-MOL/HR				
1	CO	2.8857E-17	0.0000	0.0000
2	H2O	8.0640E-03	0.2108	0.2108
3	CO2	1.1908E-04	6.5429E-19	6.5429E-19
4	H2	5.2298E-16	0.0000	0.0000
5	METHANOL	7.4668E-04	2.7602	2.7602
6	DME	8.9203	7.9827E-03	7.9827E-03
7	METHANE	3.8289E-16	0.0000	0.0000
8	N2	4.3089E-16	3.7172E-20	3.7172E-20
9	O2	0.0000	0.0000	0.0000
TOTAL RATE, KG-MOL/HR		8.9292	2.9790	2.9790
TEMPERATURE, C		30.0000	121.7366	45.0000
PRESSURE, KPA		700.0000	700.0000	700.0000
ENTHALPY, M*KCAL/HR		7.1333E-03	7.7322E-03	2.5616E-03
MOLECULAR WEIGHT		46.0435	31.0869	31.0869
MOLE FRAC VAPOR		0.0000	0.0000	0.0000
MOLE FRAC LIQUID		1.0000	1.0000	1.0000

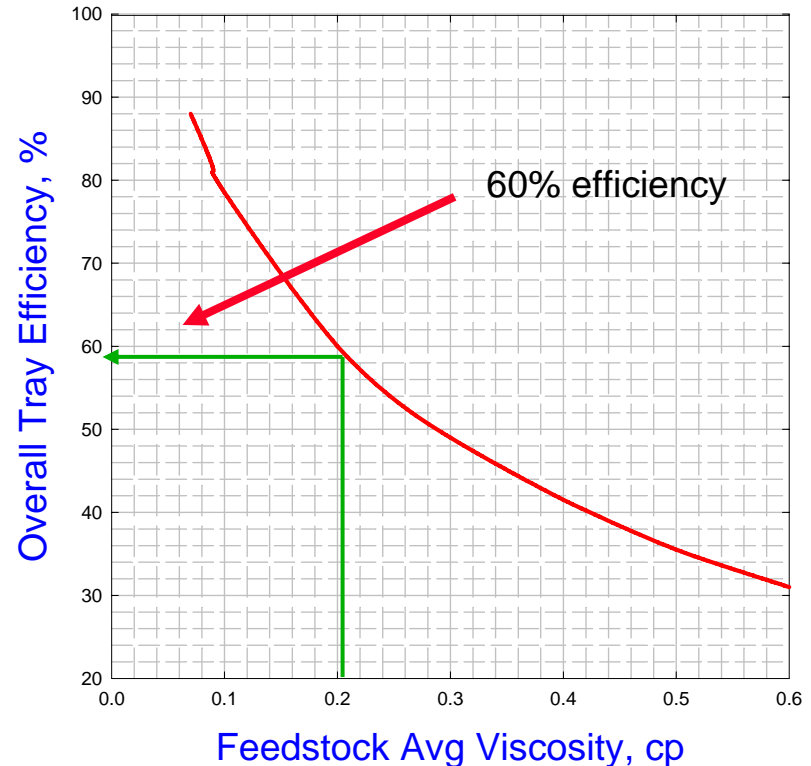
# Overall Tray Efficiencies: Method 1

## Method of Drickamer & Bradford <sup>1</sup>

Notes:

- 1) Based on 54 refinery columns.
- 2) Viscosity is average of feed as liquid at top & bottom temperatures of the column.
- 3) For Absorbers, use rich oil at exit temperature.
- 4) Efficiency is for key components.

1. Tran. Am. Inst. Chem. Engrs, 39, 319 (1943).



# Feedstock Average Viscosity

STREAM ID	36	37	40	<u>40R</u>
NAME				
PHASE	MIXED	VAPOR	LIQUID	MIXED
----- LIQUID -----				
RATE, KG-MOL/HR	18.534	N/A	11.908	6.470
K*KG/HR	0.793	N/A	0.504	0.257
M3/HR	1.056	N/A	1.069	0.385
GAL/MIN	4.650	N/A	4.709	1.693
STD LIQ RATE, M3/HR	1.074	N/A	0.725	0.362
SPECIFIC GRAVITY (H2O=1.0)	0.7391	N/A	0.6958	0.7123
MOLECULAR WEIGHT	42.793	N/A	42.302	39.789
ENTHALPY, KCAL/KG	5.883	N/A	73.428	26.945
CP, KCAL/KG-C	0.610	N/A	1.008	0.633
DENSITY, KG/M3	751.041	N/A	471.035	669.422
Z (FROM DENSITY)	0.0726	N/A	0.0852	0.0157
SURFACE TENSION, DYNE/CM	11.8660	N/A	5.6286	15.1810
THERMAL COND, KCAL/HR-M-C	0.10268	N/A	0.05962	0.10866
<u>VISCOSITY, CP</u>	0.15940	N/A	0.08042	<u>0.20720</u>

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The End....