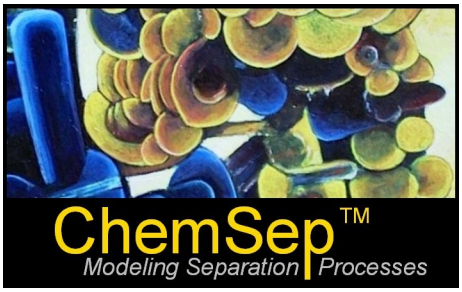

ChemSep™ - Exporting to Excel

New with Release 6.5 (December 15, 2009)
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ChemSep has long had the ability to export results to Microsoft Excel; but Version 6.5 takes the ability to export results to Excel to new levels of convenience. Here we describe how to get exactly what you want into Excel from ChemSep.

A few notes before we start the tutorial.

1. It is possible to create an unlimited number of different export formats.
2. The file that defines the output format must begin with the word *Export* and ends with *.def* and must be saved in the bin folder of *ChemSep*.
3. The export definition file is case sensitive.

Example 1: Getting Started

Here is just a simple exercise to see how easy it is to design your own export format.

1. Open a text editor (e.g. Notepad – whatever you do, don't use Word for this exercise)

2. Type what appears below (including the blank lines)

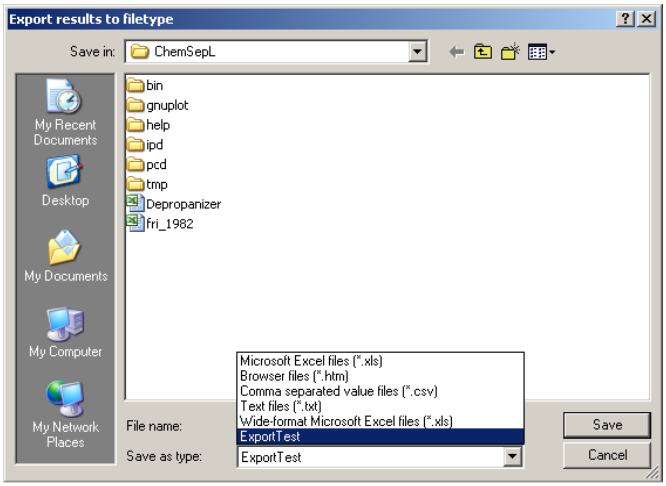
```
newsheet:
TabName
var:
stage

S
var:
Temperature
F
T
var:
Pressure
psia
p
newsheet:
Tab2
```

3. Save the above in a plain text file. The name of the file must begin with the word *Export*. The rest of the name is up to you (but we suggest that you don't stop with *Export*). The file extension must be *.def*.

4. Copy the saved file to the \chemsep\bin folder

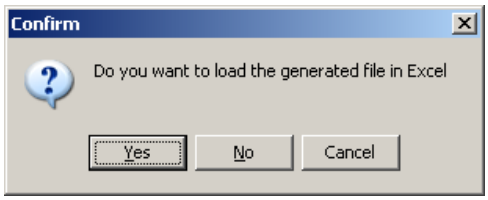
5. Start *ChemSep* and load any sep file.

6. Go to the *File* menu, select the *Export results* option and you will see a list that includes the name of the .def file file that you created in steps 2-4 above. In the illustration below you will see the name *ExportTest* because we created a file called *ExportTest.def* when we wrote this tutorial.

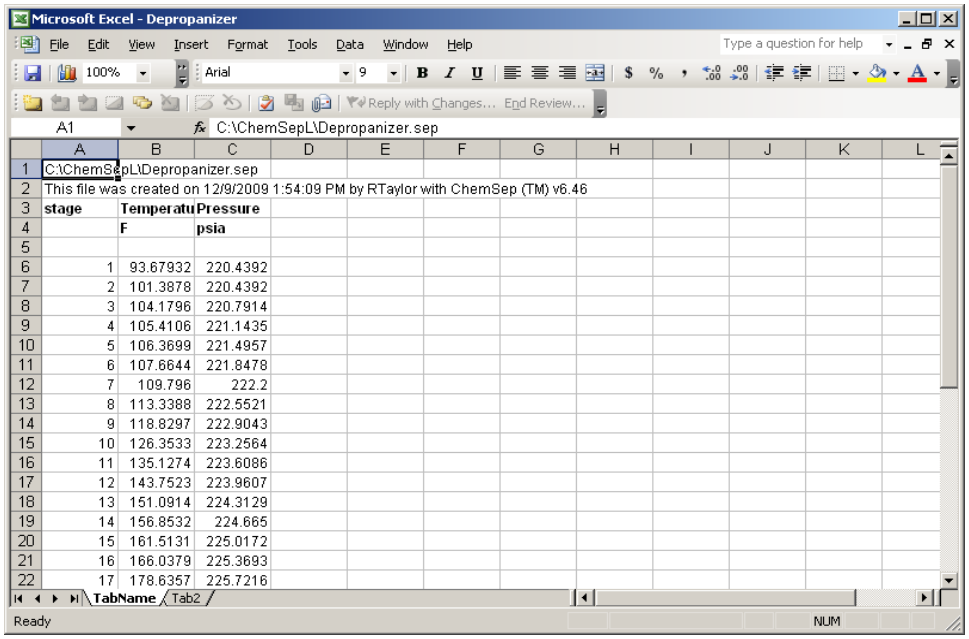


7. Select the export option that you have created and click on the *Save* button.

8. If the file name that you chose already exists you will be asked if you wish to overwrite it. You will also be asked the following question:



9. Click on yes to see the results of this exercise. The screen shot below shows what we have accomplished.



Now with that image before us we can see how the text file created above serves as the template for the Excel file we see in the screen shot.

The table below summarizes the meaning of each line of our export template. Items shown in bold in column 2 below are instructions and should not be changed.

Line	Text	Meaning
1	**`newsheet:`**	Instruction to create a new worksheet (tab sheet)
2	`TabName`	Name of the worksheet (tab sheet) created by the instruction above
3	**`var:`**	Instruction to populate a new column on the worksheet named on line 2
4	`stage`	Label that will appear on the top of the column (in row 3; rows 1 and 2 are reserved)
5		Line to enter the units to be used in the spreadsheet - empty because "stage" is dimensionless
6	`S`	Symbol for the stage index number
7	**`var:`**	Instruction to populate a new column on the worksheet
8	`Temperature`	Label that will appear on the top of the column (in row 3)
9	`F`	Units for the quantity to be displayed in this column
10	`T`	Symbol for temperature
11	**`var:`**	Instruction to populate a new column on the worksheet
12	`Pressure`	Label that will appear on the top of the column (in row 3)
13	`psia`	Units for the quantity to be displayed in this column
14	`p`	Symbol for the pressure
15	**`newsheet:`**	Instruction to create a new worksheet (tab sheet)
16	`Tab2`	Name of the worksheet (tab sheet)

It can be seen that each tab page is created by two lines and each column is characterized by four lines in our template text file. The first line of the block of four is the instruction *var:*. The second, third and fourth lines are text strings that specify, in order, the label to be written at the top of the column (2nd row of a block of four), the units to be used (3rd row), and the symbol (4th row) that denotes what *ChemSep* variable is to be written to the Excel file.

It is now straightforward to add columns with other variables; all we need to know are the variable names. A list of the main stage variables appears below.

Standard ChemSep stage variables:	
S	Stage number
x#	Liquid mole fraction for component #
xi#	Liquid interface mole fraction for component #
y#	Vapour mole fraction for component #
yi#	Vapour interface mole fraction for component #
K#	K-value for component #
T	Temperature [K]
Tb	Bubble point temperature [K]
TL	Liquid temperature [K]
Ti	Interface temperature [K]
TV	Vapour temperature [K]
Td	Dew point temperature [K]
p	Pressure [Pa]
L	Liquid flow [kmol/s]
V	Vapour flow [kmol/s]
HL	Liquid enthalpy [kJ/kmol]
HV	Vapour enthalpy [kJ/kmol]
SL	Liquid entropy [kJ/kmol/K]
SV	Vapour entropy [kJ/kmol/K]
SP	Entropy production [kJ/kmol/K]
R#	Reaction rate for component # [kmol/s]
N#	Mass transfer rate for component # [kmol/s]
C#	Conversion for component # [kmol/s]
M#	Murphree efficiency for component #
FE	Baur Efficiency
FA	Baur Efficiency Angle
Z	Stage height [m]
WF	Fraction of weeping
FF	Fraction of flooding

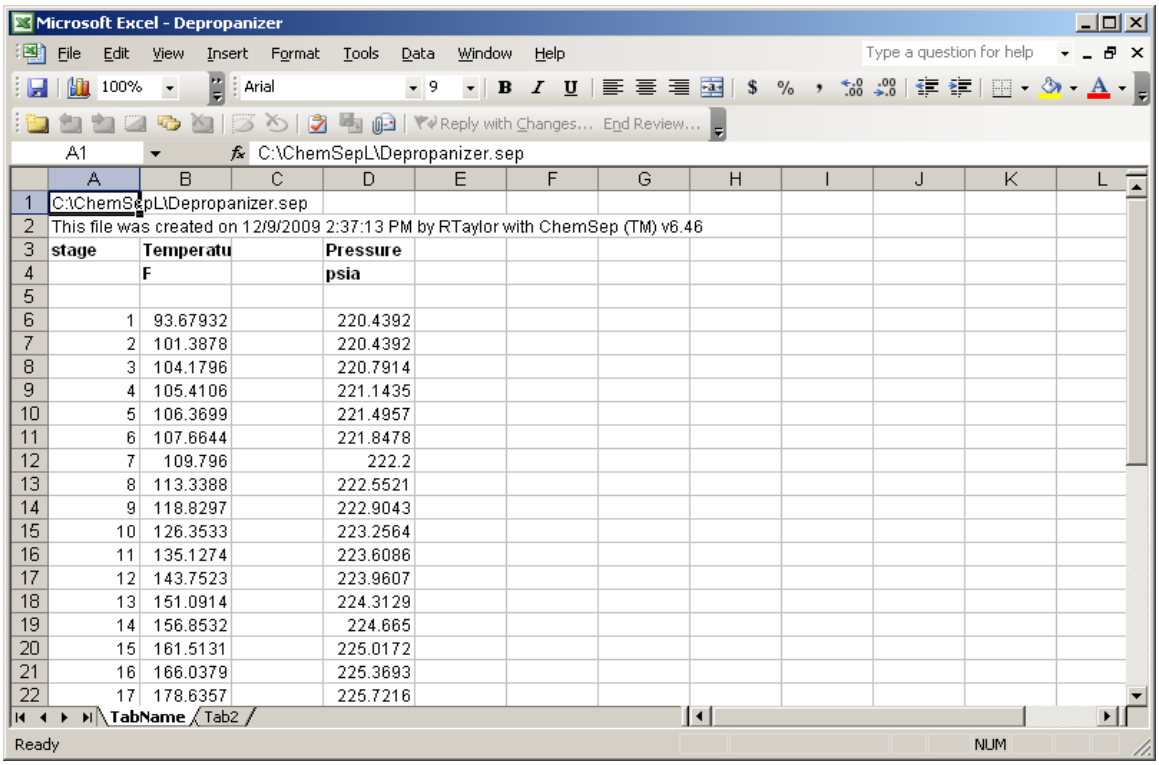
Exercise: Add columns for the *molar* flow rates of liquid and gas/vapor.

Exercise: Try changing the units as follows: Temperature (F to C to K), pressure (psia to bar to atm).

Example 2: Inserting an empty column

How can you modify the above to create a spreadsheet with an empty column between the columns for temperature and pressure?

Given how the template is constructed (the four lines per variable) we can see that adding four lines (the first of which says *var:* and the remaining three being empty) should accomplish our goal (as long as we insert the four lines in the right place). Here is what we see when we do this correctly:



Example 3: Calculating columns

The export mode is much more powerful than simply a means to print out the various things that are calculated during a *ChemSep* simulation. It is possible to combine quantities to compute something else that is of interest but that is not calculated directly. Mass flow rates are a case in point. *ChemSep* uses molar flows only while solving problems, very often it is the mass flows that are of more interest to the equipment designer. The mass flow rates can be obtained in Excel using the following additions to the template (again, in the appropriate place of course):

```
var:
Liquid flow rate
lb/h
L*$MwL
```

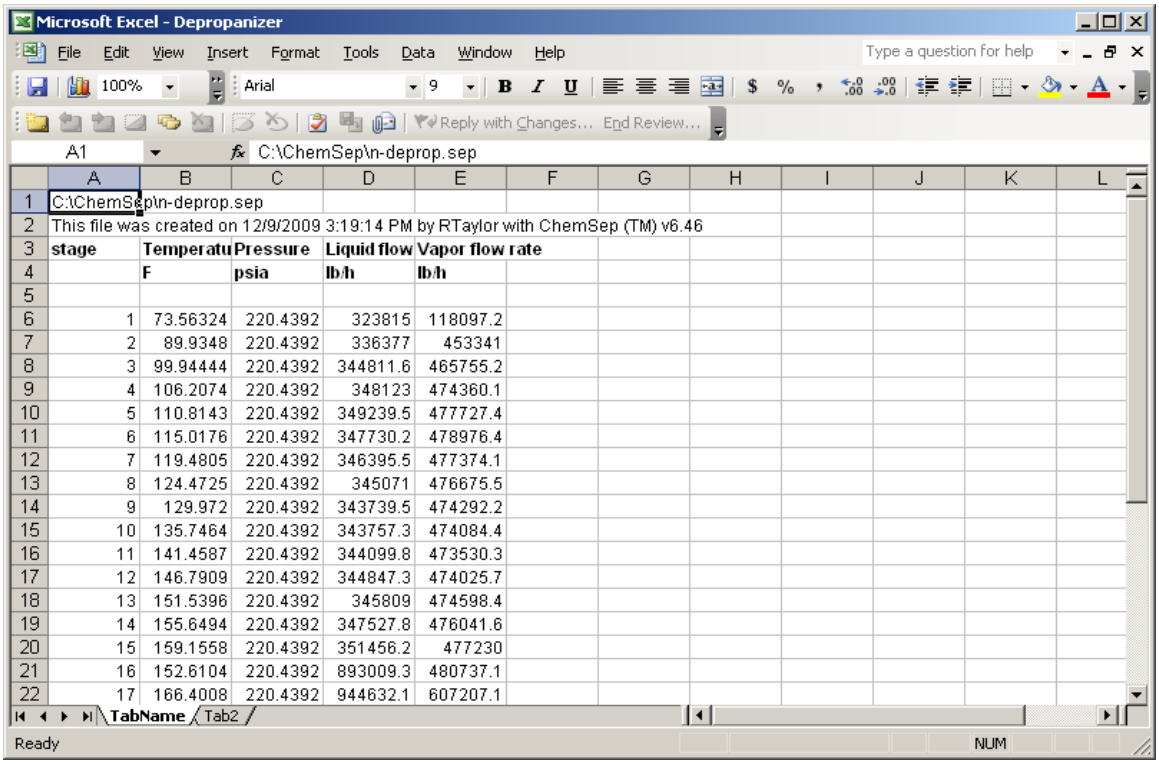
for the liquid phase, and

```
var:
Vapor flow rate
lb/h
V*$MwV
```

for the vapor phase.

Here the symbols for the vapor and liquid flow rates are simply multiplied by the molecular weights (symbols `$MwL` and `$MwV`). Note: the $ sign does *not* imply constancy of anything here; it is just part of the symbol we use to denote the molecular weight and the fact that the molecular weight changes along the column is most definitely taken into account.

The illustration below shows our table now that we have added the mass flows (and removed the empty column of the last exercise).



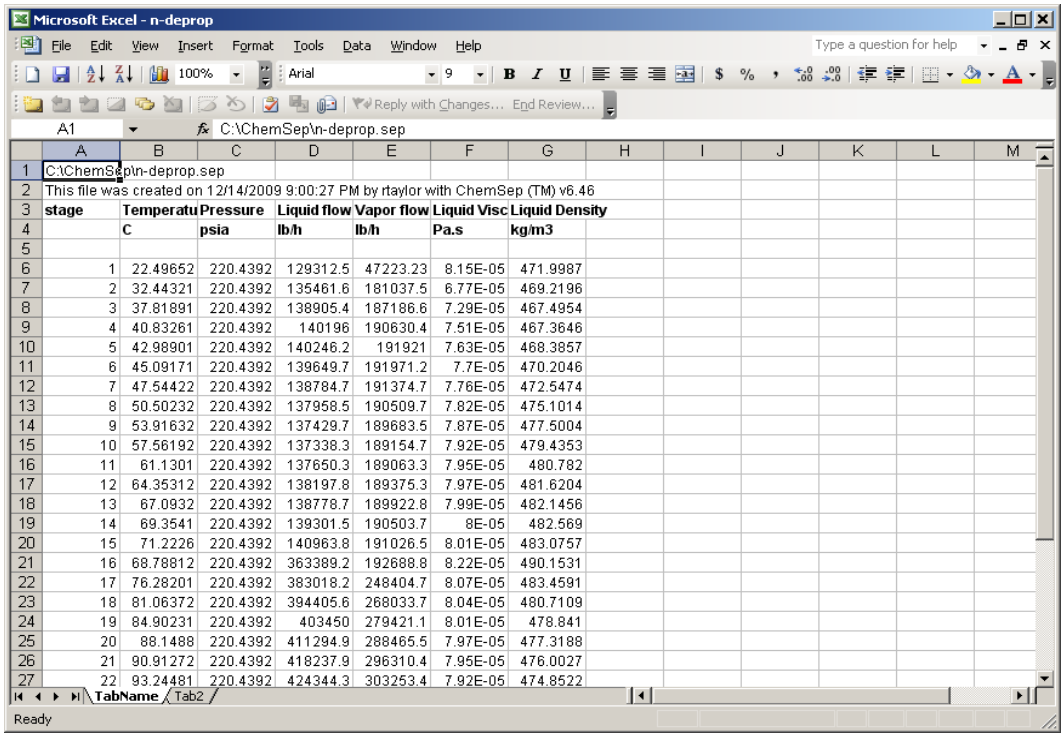
Hint: Remember that all of the variables listed in the tables that appear in this tutorial can be used in calculations to create new quantities.

Example 4: Physical Properties

We can also export physical properties as long as we use the proper key words: For example the following sequence:

```
var:
Liquid viscosity
Pa.s
$VisL
var:
Liquid density
kg/m3
$DsL
```

after the lines for the mass flow rates added above will give us:



We can now add columns for all of the mixture properties once we know their names; a list (and their SI units) is given below. Note that two not entirely interchangeable names are available for the properties; both names can be used after a simulation using the nonequilibrium, the second is the only option following a simulation with the equilibrium stage model. The name appearing second in this table should normally be enclosed within [].

ChemSep Export Names for Physical Properties

$DsL	RHOL	Liquid density [kg/m3]
$DsV	RHOV	Vapor density [kg/m3]
$Sigma	SIGMA	Surface tension [N/m]
$VisL	VISL	Liquid viscosity [Pa.s]
$VisV	VISV	Vapor viscosity [Pa.s]
$MwL	MWV	Liquid mole weight [kg/kmol]
$MwV	MWL	Vapor mole weight [kg/kmol]
$CpL	CPL	Liquid heat capacity [kJ/kmol]
$CpV	CPV	Vapor heat capacity [kJ/kmol]
$TcL	TCL	Liquid thermal conductivity [J/K/m/s]
$TcV	TCV	Vapor thermal conductivity [J/k/m/s]

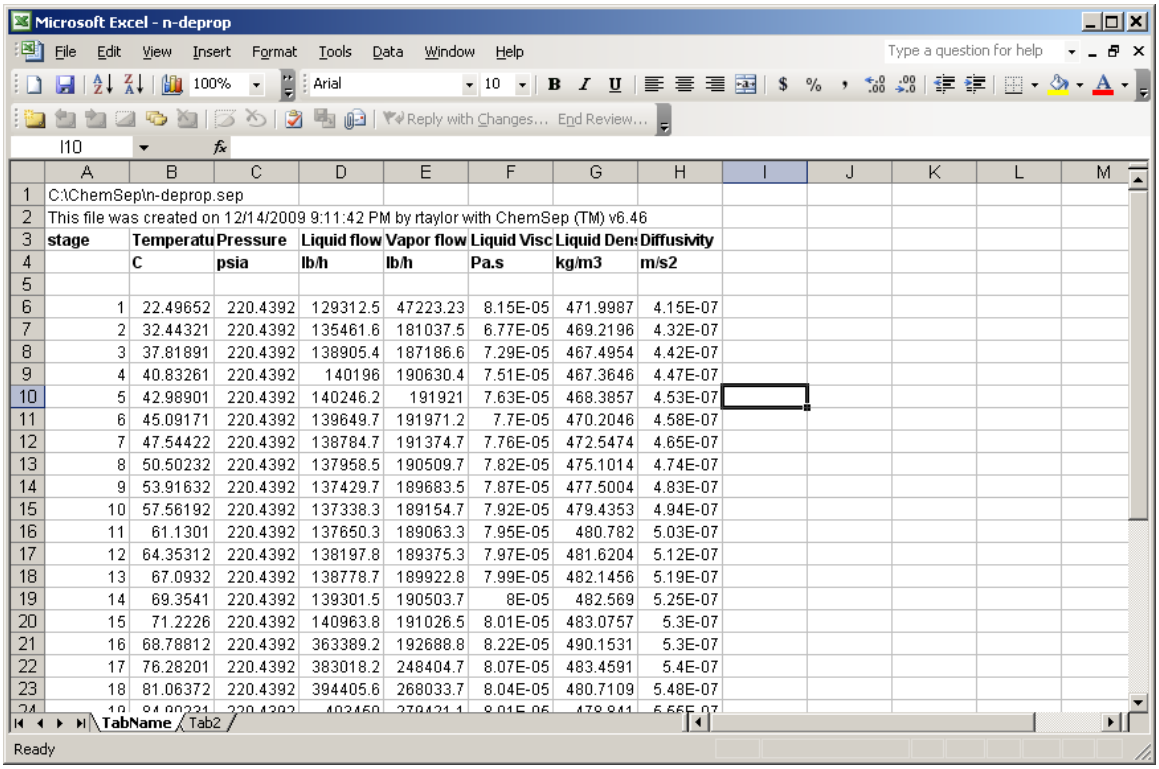
Example 5: Diffusion Coefficients

Diffusion coefficients must be handled differently because they are properties of a binary pair of compounds:

To illustrate consider the following sequence of lines to be added to our export definition file:

```
var:
Diffusivity
m/s2
$Dv1,3
```

Now we see:



	A	B	C	D	E	F	G	H	I	J	K	L	M
1	C:\ChemSep\n-deprop.sep												
2	This file was created on 12/14/2009 9:11:42 PM by rtaylor with ChemSep (TM) v6.46												
3	stage	Temperatu	Pressure	Liquid flow	Vapor flow	Liquid Visc	Liquid Den	Diffusivity					
4		C	psia	lb/h	lb/h	Pa.s	kg/m3	m/s2					
5													
6	1	22.49652	220.4392	129312.5	47223.23	8.15E-05	471.9987	4.15E-07					
7	2	32.44321	220.4392	135461.6	181037.5	6.77E-05	469.2196	4.32E-07					
8	3	37.81891	220.4392	138905.4	187186.6	7.29E-05	467.4954	4.42E-07					
9	4	40.83261	220.4392	140196	190630.4	7.51E-05	467.3646	4.47E-07					
10	5	42.98901	220.4392	140246.2	191921	7.63E-05	468.3857	4.53E-07					
11	6	45.09171	220.4392	139649.7	191971.2	7.7E-05	470.2046	4.58E-07					
12	7	47.54422	220.4392	138784.7	191374.7	7.76E-05	472.5474	4.65E-07					
13	8	50.50232	220.4392	137958.5	190509.7	7.82E-05	475.1014	4.74E-07					
14	9	53.91632	220.4392	137429.7	189683.5	7.87E-05	477.5004	4.83E-07					
15	10	57.56192	220.4392	137338.3	189154.7	7.92E-05	479.4353	4.94E-07					
16	11	61.1301	220.4392	137650.3	189063.3	7.95E-05	480.782	5.03E-07					
17	12	64.35312	220.4392	138197.8	189375.3	7.97E-05	481.6204	5.12E-07					
18	13	67.0932	220.4392	138778.7	189922.8	7.99E-05	482.1456	5.19E-07					
19	14	69.3541	220.4392	139301.5	190503.7	8E-05	482.569	5.25E-07					
20	15	71.2226	220.4392	140963.8	191026.5	8.01E-05	483.0757	5.3E-07					
21	16	68.78812	220.4392	363389.2	192688.8	8.22E-05	490.1531	5.3E-07					
22	17	76.28201	220.4392	383018.2	248404.7	8.07E-05	483.4591	5.4E-07					
23	18	81.06372	220.4392	394405.6	268033.7	8.04E-05	480.7109	5.48E-07					

where we have added a column that contains the diffusivity between species 1 and 3 in the gas/vapor phase.

Exercise: Add a column for gas/vapor diffusivity for species 2 and 3.

Exercise: Add a column for liquid diffusivity for species 2 and 3 (symbol `$DsL`).

Example 6: Key Components

The following illustrate how to find the key components. The output of each is a column containing a number of the designated key component that represents its position in the sequence of compounds.

```
var:
Light key

{LKEY}
var:
Heavy key

{HKEY}
```

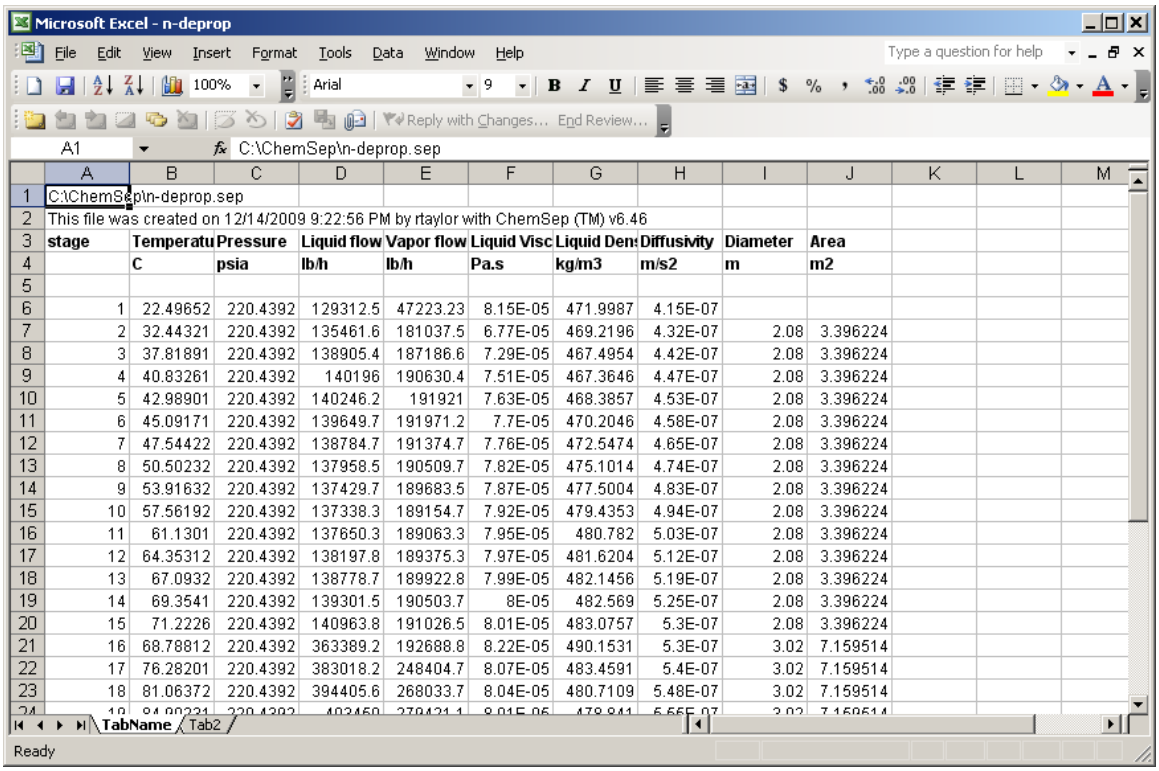
The symbols {LKEY} and {HKEY} may be used as subscripts to obtain the diffusivity of the key component pair, as in: `$Dv{LKEY},{HKEY}`

Example 7: Design Parameters

It is often desirable to output various equipment design parameters. We add the following lines to our export template:

```
var:
Diameter
m
{DS@P1}
var:
Area
m2
{DS@P1}^2*3.14/4
```

Now we see the diameter and the area appear in our spreadsheet.



It pays to spend some time to see how this was done:

Line	Text	Meaning
1	**`var:`**	Instruction to populate a new column in the worksheet
2	`Diameter`	Label that will appear on the top of the column
3	`m`	Line to enter the units to be used in the spreadsheet
4	`{DS@P1}`	Symbol for the first design parameter (this happens to be the diameter)
5	**`var:`**	Instruction to populate a new column on the worksheet
6	`Area`	Label that will appear on the top of the column
7	`m2`	Units for the quantity to be displayed in this column
8	`{DS@P1}^2*3.14`	Calculation of the area using the diameter (see line 4)

The symbol in line 4 is coded as follows: DS means Design Section, @ is a place holder for the column section number, and P1 means the first design parameter (and as noted this happens to be the diameter).

The conclusion we should draw from this exercise is that we can also output other design variables. What we get depends on what type of column internal we happen to have selected. That is: {DS@P4} for a sieve tray column is the liquid flow path length, whereas {DS@P4} for a column filled with some sort of random packing is the specific surface area of the packing. A complete list of the design parameters is given in the table below.

Internals Design Parameters in *ChemSep*

Design parameters – all packing types	
{DS@P1}	Column diameter
{DS@P2}	Height (of a stage)
~3	Name of packing
{DS@P4}	Specific packing surface
{DS@P5}	Void fraction
Design parameters – random packing	
{DS@P6}	Nominal size
{DS@P7}	Critical surface tension
{DS@P8}	Packing factor
Design parameters – structured packing	
{DS@P6}	Channel base
{DS@P7}	Crimp height
{DS@P8}	Channel side
{DS@P9}	Equivalent diameter
{DS@P10}	Channel flow angle
{DS@P11}	Packing factor
Design parameters – all trays	
{DS@P1}	Column diameter
{DS@P2}	Tray spacing
{DS@P3}	Number of passes
{DS@P4}	Liquid flow path length
{DS@P5}	Active area
{DS@P6}	Total hole area
{DS@P7}	Downcomer area
{DS@P8}	Hole diameter
{DS@P9}	Hole pitch
{DS@P10}	Weir length
{DS@P11}	Weir height
{DS@P12}	Weir type (1 = segmental
{DS@P13}	Notch depth or Weir diameter
{DS@P14}	Serration angle
{DS@P15}	Downcomer clearance
{DS@P16}	Deck thickness
{DS@P17}	Downcomer sloping
{DS@P18}	Downcomer length

Design model parameters (only if applicable)	
{SM@MTCP#}	Mass transfer coefficient parameter number #
{SM@VFP#}	Vapor flow model parameter number #
{SM@LFP#}	Liquid flow model parameter number #
{SM@PDP#}	Pressure drop model parameter number #
{SM@ENTP#}	Entrainment model parameter number #
{SM@HLDP#}	Holdup model parameter number #
{SM@DSNP#}	Design method parameter number #

Example 8: Internals Performance Parameters

In the course of its calculations *ChemSep* computes many other quantities that can be exported to Excel. Some examples are shown below:

```
var:
Flow parameter

$Flv
var:
C-factor
m/s
$Cs
```

There are many such possible performance variables. The illustration below shows a few of them:

Slope	F-factor	ave F	HETP	Ave HETP	HTU	Ave HTU
			ft	ft	ft	ft
0.279961	1.301995	1.300119	14.80015	3.673251	9.264678	2.617113
0.281857	1.349773	1.300119	10.95572	3.673251	6.973363	2.617113
0.282497	1.353693	1.300119	3.43523	3.673251	2.191808	2.617113
0.283023	1.353477	1.300119	3.601575	3.673251	2.300512	2.617113
0.28356	1.352823	1.300119	3.651686	3.673251	2.334934	2.617113
0.284125	1.3521	1.300119	3.656296	3.673251	2.340407	2.617113
0.284722	1.351344	1.300119	3.654439	3.673251	2.341896	2.617113
0.285355	1.350556	1.300119	3.651427	3.673251	2.342818	2.617113

In the partial screen shot above **slope** refers to the slope of the equilibrium line (symbol `FS`) and was obtained using this sequence:

```
var:
Slope

FS
```

The sequence below gives the HETP of each stage and the average section HETP

```
var:
HETP
ft
[HETP]

var:
Ave HETP
ft
{AHETP1}
```

Note the differences here: [HETP] reports the local (by stage) HETP; {AHETP#} reports the average HETP for column section #.

The other symbols used to create this screen shot appear in the more complete table below.

Column Performance Variables in ChemSep

FS	Slope of the equilibrium line
[FFAC]	Superficial F-factor [m/s (kg/m3)$^{0.5}$] (same as $Fs)
{AFFAC#}	Average F-factor for column section # [m/s (kg/m3)$^{0.5}$]
[HETP]	HETP [m]
{AHETP#}	Average HETP for column section # [m]
[HTU]	Height of an overall transfer unit [m]
{AHTU#}	Average HTU for column section # [m]
$Atot	Interfacial area [m2]
$Avap	Vapor interfacial area [m2]
$Aliq	Liquid interfacial area [m2]
$tV	Vapor residence time [s]
$tL	Liquid residence time [s]
$NTUv#,#	Vapor Number of Transfer Units for components #,#
$NTUl#,#	Liquid Number of Transfer Units for components #,#
$HTCv	Vapor Heat Transfer Coefficient [J/K/m2/s]
$HTCl	Liquid Heat Transfer Coefficient [J/K/m2/s]
$Ml	Liquid mass flow [kg/s]
$Mv	Vapor mass flow [kg/s]
$Qv	Vapor volumetric flow rate [m3/s]
$Ql	Liquid volumetric flow rate [m3/s]
$Uv	Vapor velocity [m/s]
$Ul	Liquid velocity [m/s]
$Flv	Flow parameter
$Vload	Vapor loading [m/s]
$Qlw	Weir loading [m3/s/m]
$Ud	Downcomer liquid velocity [m/s]
$Fs	Superficial F-factor [m/s (kg/m3)$^{0.5}$]
$Csf	Capacity factor
$Hwt	Wet liquid height [m]
$Hcl	Clear liquid height [m]
$Hr	Residual liquid height [m]
$Hd	Dry pressure drop liquid height [m]
$How	Height of liquid over the weir [m]
$Hg	Liquid height gradient [m]
$Hf	Height of the froth [m]
$Hdb	Clear downcomer backup height [m]
$PhiL	Fractional liquid entrainment
$PhiV	Fractional vapour entrainment

$Pd	Pressure drop (total) [Pa]
$Dyndp	Pressure drop (dynamic) [Pa]
$Statdp	Pressure drop (static) [Pa]
$Qmw	Minimum wetting rate [m/s]
$Ae	Liquid entrainment mass ratio
$Alpha	Vapour fraction on the tray
$Eps	Liquid fraction on the tray
$Tv	Vapour residence time on the tray
$Tl	Liquid residence time on the tray
$Uh	Hole velocity [m/s]
$Fr	Froude hole number
$Wflx	Weep flux [m3/s]
$AlphaD	Vapour fraction in the downcomer
$TimeD	Residence time of liquid in the downcomer
$ff	Fraction of flooding
$ffL	Fraction of flooding (Leva)
$ffK	Fraction of flooding (Kister)
$ffP	Fraction of flood (by packed design)
$fMOC	Fraction of max. capacity (IMTP packing only)
$WF	Fraction of Weeping
$Fp	Packing Factor
$KFp	Kister method packing Factor
$Cs	C-Factor
$Csult	Ultimate capacity
$YLevaN	GPDC capacity (Leva 1992)
$YKister	GPDC capacity (Strigle/Kister&Gill)
$YNorton	GPDC capacity (Norton)
SF	System Factor
$jetFF	Jet flood fraction
$bkupFF	Downcomer backup flood fraction
$dcckFF	Downcomer choke flood fraction
$dcvFF	Downcomer velcoity flood fraction
$dcrtFF	Downcomer residence time flood fraction
$wlFF	Weir load flood fraction
$Re	Reynolds number (packed columns)
$Dia	Diameter
$Area	Area
$SecHt	Section height
$Dp	Nominal size of packing
$Ap	Specific area of packing

Example 9: Conditional Columns

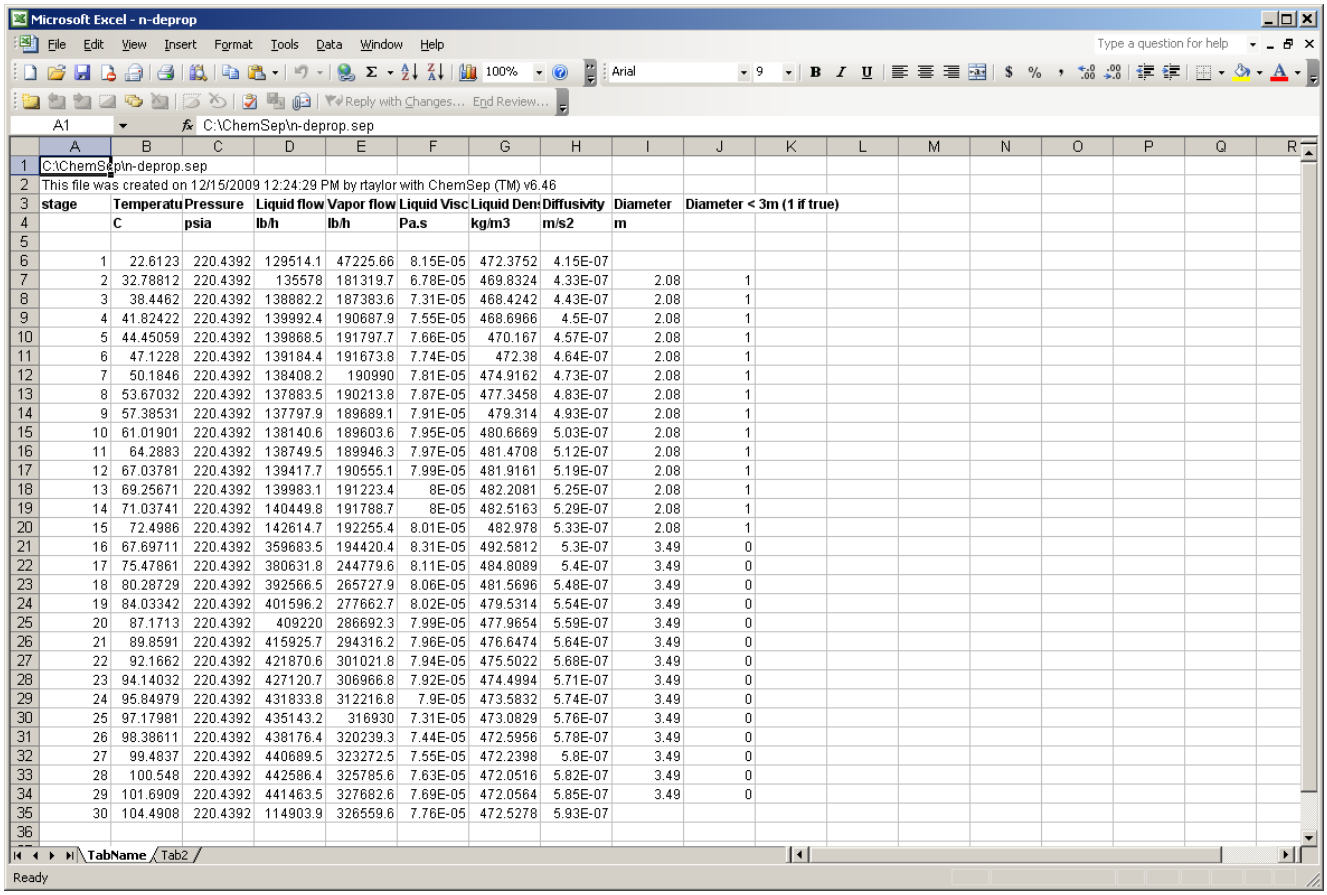
The Flexible Export feature permits some simple conditional tests to be carried out. Here is an example:

```
var:
Diameter < 3m (1 if true)

!a=(3.0);!b=(1);!c=(0);limit1({DS@P1})
```

The first line is the usual instruction for a new column. The second line is a text string that will appear at the top of the column. The third line is empty because there are no units associated with the result (it is either true – to be indicated by the display of a 1, or not true, in which case we will see a 0).

The fourth line is the "if" test. The partial statement !a=(3.0) assigns to a the cutoff value for the test (3m). The phrase !b=(1) assigns the value to appear if the test result is true, and !c=(0) assigns the value to appear if the test is false. Finally, the test is actually carried out with the logical function limit1.

Here is the result of this when added to our earlier example (which happens to be the depropanizer test case that comes with *ChemSep*). In this example we can see that the result of the test is true for the rectifying section and not true for the stripping section. We can also confirm that the test has been carried out correctly since the diameter appears in the second last column. Also note that the cells for stages 1 and 30 are empty – as they should be since they represent the condenser and the reboiler respectively.



Microsoft Excel - n-deprop

File Edit View Insert Format Tools Data Window Help

A1 C:\ChemSep\n-deprop.sep

	A	B	C	D	E	F	G	H	I	J	K
1	C:\ChemSep\n-deprop.sep										
2	This file was created on 12/15/2009 12:24:29 PM by rtaylor with ChemSep (TM) v6.46										
3	stage	Temperatu	Pressure	Liquid flow	Vapor flow	Liquid Visc	Liquid Den	Diffusivity	Diameter	Diameter < 3m (1 if true)	
4		C	psia	lb/h	lb/h	Pa.s	kg/m3	m/s2	m		
5											
6	1	22.6123	220.4392	129514.1	47225.66	8.15E-05	472.3752	4.15E-07			
7	2	32.78812	220.4392	135578	181319.7	6.78E-05	469.8324	4.33E-07	2.08	1	
8	3	38.4462	220.4392	138882.2	187383.6	7.31E-05	468.4242	4.43E-07	2.08	1	
9	4	41.82422	220.4392	139992.4	190687.9	7.55E-05	468.6966	4.5E-07	2.08	1	
10	5	44.45059	220.4392	139868.5	191797.7	7.66E-05	470.167	4.57E-07	2.08	1	
11	6	47.1228	220.4392	139184.4	191673.8	7.74E-05	472.38	4.64E-07	2.08	1	
12	7	50.1846	220.4392	138408.2	190990	7.81E-05	474.9162	4.73E-07	2.08	1	
13	8	53.67032	220.4392	137883.5	190213.8	7.87E-05	477.3458	4.83E-07	2.08	1	
14	9	57.38531	220.4392	137797.9	189689.1	7.91E-05	479.314	4.93E-07	2.08	1	
15	10	61.01901	220.4392	138140.6	189603.6	7.95E-05	480.6669	5.03E-07	2.08	1	
16	11	64.2883	220.4392	138749.5	189946.3	7.97E-05	481.4708	5.12E-07	2.08	1	
17	12	67.03781	220.4392	139417.7	190555.1	7.99E-05	481.9161	5.19E-07	2.08	1	
18	13	69.25671	220.4392	139983.1	191223.4	8E-05	482.2081	5.25E-07	2.08	1	
19	14	71.03741	220.4392	140449.8	191788.7	8E-05	482.5163	5.29E-07	2.08	1	
20	15	72.4986	220.4392	142614.7	192255.4	8.01E-05	482.978	5.33E-07	2.08	1	
21	16	67.69711	220.4392	359683.5	194420.4	8.31E-05	492.5812	5.3E-07	3.49	0	
22	17	75.47861	220.4392	380631.8	244779.6	8.11E-05	484.8089	5.4E-07	3.49	0	
23	18	80.28729	220.4392	392566.5	265727.9	8.06E-05	481.5696	5.48E-07	3.49	0	
24	19	84.03342	220.4392	401596.2	277662.7	8.02E-05	479.5314	5.54E-07	3.49	0	
25	20	87.1713	220.4392	409220	286692.3	7.99E-05	477.9654	5.59E-07	3.49	0	
26	21	89.8591	220.4392	415925.7	294316.2	7.96E-05	476.6474	5.64E-07	3.49	0	
27	22	92.1662	220.4392	421870.6	301021.8	7.94E-05	475.5022	5.68E-07	3.49	0	
28	23	94.14032	220.4392	427120.7	306966.8	7.92E-05	474.4994	5.71E-07	3.49	0	
29	24	95.84979	220.4392	431833.8	312216.8	7.9E-05	473.5832	5.74E-07	3.49	0	
30	25	97.17981	220.4392	435143.2	316930	7.31E-05	473.0829	5.76E-07	3.49	0	
31	26	98.38611	220.4392	438176.4	320239.3	7.44E-05	472.5956	5.78E-07	3.49	0	
32	27	99.4837	220.4392	440689.5	323272.5	7.55E-05	472.2398	5.8E-07	3.49	0	
33	28	100.548	220.4392	442586.4	325785.6	7.63E-05	472.0516	5.82E-07	3.49	0	
34	29	101.6909	220.4392	441463.5	327682.6	7.69E-05	472.0564	5.85E-07	3.49	0	
35	30	104.4908	220.4392	114903.9	326559.6	7.76E-05	472.5278	5.93E-07			
36											

TabName Tab2

Ready

Here is another example of a conditional column; in this case the test is slightly more sophisticated:

```
var:
Diameter 1:<2.0m 2:<3m 3:else

!a=(2.0);!b=(3);!c=(1);!d=(2);!e=(3);limit2({DS@P1})
```

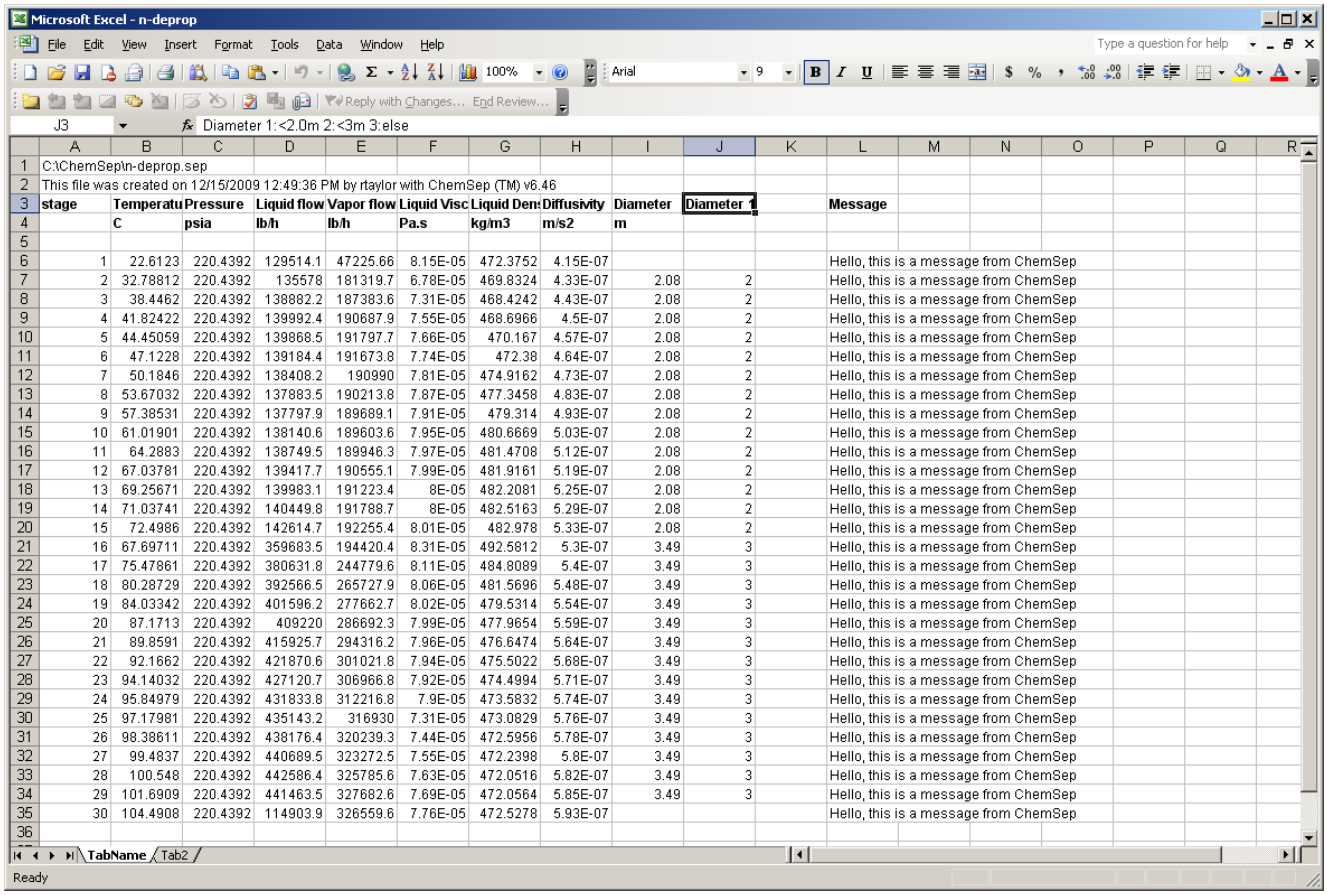
Note that this is a three-way test. Can you guess what the outcome will be (*Hint:* the second line above is a text string).

Example 10: Text Messages

Finally, the Flexible Export feature permits printing text strings simply by preceding them with a single opening quote mark. Here is an example:

```
var:
Message

'Hello, this is a message from ChemSep
```

The result is shown below (after adding this sequence to our export file and inserting an empty column before the message column).



Microsoft Excel - n-deprop

File Edit View Insert Format Tools Data Window Help

J3 Diameter 1:<2.0m 2:<3m 3:else

C:\ChemSep\n-deprop.sep

This file was created on 12/15/2009 12:49:36 PM by rtaylor with ChemSep (TM) v6.46

stage	Temperatu	Pressure	Liquid flow	Vapor flow	Liquid Visc	Liquid Den	Diffusivity	Diameter	Diameter 1		Message
	C	psia	lb/h	lb/h	Pa.s	kg/m3	m/s2	m			
1	22.6123	220.4392	129514.1	47225.66	8.15E-05	472.3752	4.15E-07				Hello, this is a message from ChemSep
2	32.78812	220.4392	135578	181319.7	6.78E-05	469.8324	4.33E-07	2.08	2		Hello, this is a message from ChemSep
3	38.4462	220.4392	138882.2	187383.6	7.31E-05	468.4242	4.43E-07	2.08	2		Hello, this is a message from ChemSep
4	41.82422	220.4392	139992.4	190687.9	7.55E-05	468.6966	4.5E-07	2.08	2		Hello, this is a message from ChemSep
5	44.45059	220.4392	139868.5	191797.7	7.66E-05	470.167	4.57E-07	2.08	2		Hello, this is a message from ChemSep
6	47.1228	220.4392	139184.4	191673.8	7.74E-05	472.38	4.64E-07	2.08	2		Hello, this is a message from ChemSep
7	50.1846	220.4392	138408.2	190990	7.81E-05	474.9162	4.73E-07	2.08	2		Hello, this is a message from ChemSep
8	53.67032	220.4392	137883.5	190213.8	7.87E-05	477.3458	4.83E-07	2.08	2		Hello, this is a message from ChemSep
9	57.38531	220.4392	137797.9	189689.1	7.91E-05	479.314	4.93E-07	2.08	2		Hello, this is a message from ChemSep
10	61.01901	220.4392	138140.6	189603.6	7.95E-05	480.6669	5.03E-07	2.08	2		Hello, this is a message from ChemSep
11	64.2883	220.4392	138749.5	189946.3	7.97E-05	481.4708	5.12E-07	2.08	2		Hello, this is a message from ChemSep
12	67.03781	220.4392	139417.7	190555.1	7.99E-05	481.9161	5.19E-07	2.08	2		Hello, this is a message from ChemSep
13	69.25671	220.4392	139983.1	191223.4	8E-05	482.2081	5.25E-07	2.08	2		Hello, this is a message from ChemSep
14	71.03741	220.4392	140449.8	191788.7	8E-05	482.5163	5.29E-07	2.08	2		Hello, this is a message from ChemSep
15	72.4986	220.4392	142614.7	192255.4	8.01E-05	482.978	5.33E-07	2.08	2		Hello, this is a message from ChemSep
16	67.69711	220.4392	359683.5	194420.4	8.31E-05	492.5812	5.3E-07	3.49	3		Hello, this is a message from ChemSep
17	75.47861	220.4392	380631.8	244779.6	8.11E-05	484.8089	5.4E-07	3.49	3		Hello, this is a message from ChemSep
18	80.28729	220.4392	392566.5	265727.9	8.06E-05	481.5696	5.48E-07	3.49	3		Hello, this is a message from ChemSep
19	84.03342	220.4392	401596.2	277662.7	8.02E-05	479.5314	5.54E-07	3.49	3		Hello, this is a message from ChemSep
20	87.1713	220.4392	409220	286692.3	7.99E-05	477.9654	5.59E-07	3.49	3		Hello, this is a message from ChemSep
21	89.8591	220.4392	415925.7	294316.2	7.96E-05	476.6474	5.64E-07	3.49	3		Hello, this is a message from ChemSep
22	92.1662	220.4392	421870.6	301021.8	7.94E-05	475.5022	5.68E-07	3.49	3		Hello, this is a message from ChemSep
23	94.14032	220.4392	427120.7	306966.8	7.92E-05	474.4994	5.71E-07	3.49	3		Hello, this is a message from ChemSep
24	95.84979	220.4392	431833.8	312216.8	7.9E-05	473.5832	5.74E-07	3.49	3		Hello, this is a message from ChemSep
25	97.17981	220.4392	435143.2	316930	7.31E-05	473.0829	5.76E-07	3.49	3		Hello, this is a message from ChemSep
26	98.38611	220.4392	438176.4	320239.3	7.44E-05	472.5956	5.78E-07	3.49	3		Hello, this is a message from ChemSep
27	99.4837	220.4392	440689.5	323272.5	7.55E-05	472.2398	5.8E-07	3.49	3		Hello, this is a message from ChemSep
28	100.548	220.4392	442586.4	325785.6	7.63E-05	472.0516	5.82E-07	3.49	3		Hello, this is a message from ChemSep
29	101.6909	220.4392	441463.5	327682.6	7.69E-05	472.0564	5.85E-07	3.49	3		Hello, this is a message from ChemSep
30	104.4908	220.4392	114903.9	326559.6	7.76E-05	472.5278	5.93E-07				Hello, this is a message from ChemSep

TabName Tab2

Ready

Example 11: Calculating the Efficiency of a Tray Column

The nonequilibrium model in *ChemSep* produces a great deal of information that can be used to calculate other things. Here we show how to set up a spreadsheet that will contain the results of a tray efficiency calculation.

The Murphree point efficiency for distillation in a tray column may be estimated from:

$$E_{oV} = 1 - \exp(-N_{oV})$$

where E_{oV} is the Murphree point efficiency and N_{oV} is the overall number of transfer units. The latter may be calculated from:

$$\frac{1}{N_{oV}} = \frac{1}{N_V} + \frac{\lambda}{N_L}$$

where N_V and N_L are the numbers of transfer units for the vapor and liquid phases respectively and where

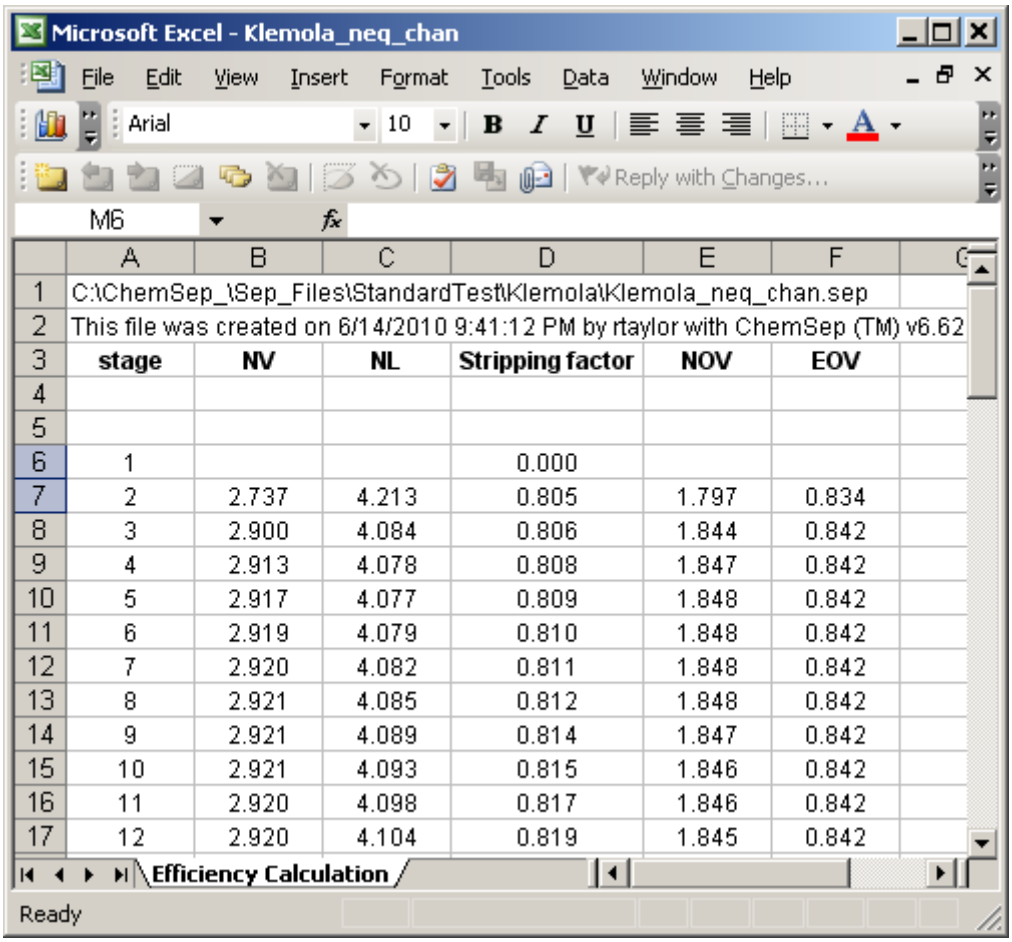
$$\lambda = mV/L$$

is the stripping factor with m the slope of the equilibrium line.

In the foregoing sections we have seen that the *ChemSep* rate-based model can export each of the quantities needed for the calculation of the point efficiency. The table below shows (in column 2) the contents of a .def file to compute the Murphree point efficiency for the two key components. Strictly speaking only the first two and last 4 lines of this table are necessary; the others are included to provide context for the final calculation. Note that the equations above apply as written only to binary systems. It is common, however, to use them for multicomponent systems using the properties of the pair of key components (as discussed in *Example 6* of this tutorial).

Line	Text	Meaning
1	`newsheet:`	
2	`Efficiency Calculation`	
3	`var:`	
4	`stage`	
5		
6	`S`	Symbol for the stage index number
7	`var:`	
8	`NV`	
9		
10	`$NTUv{LKEY},{HKEY}`	Number of vapor transfer units
11	`var:`	
12	`NL`	
13		
14	`$NTUl{LKEY},{HKEY}`	Number of liquid phase transfer units
15	`var:`	
16	`Stripping factor`	
17		
18	`FS`	Symbol for the stripping factor
19	`var:`	
20	`NOV`	
21		
22	`1/(1/$NTUv{LKEY},{HKEY} + FS / $NTUl{LKEY},{HKEY})`	Overall number of transfer units
23	`var:`	
24	`EOV`	
25		
26	`1-exp(-1/(1/$NTUv{LKEY},{HKEY} + FS / $NTUl{LKEY},{HKEY}))`	Murphree point efficiency

The screen image below shows the result of the application of this example .def file to the calculation of the point efficiency for an industrial C4 splitter.



Microsoft Excel - Klemola_neq_chan

File Edit View Insert Format Tools Data Window Help

Arial 10 B I U

Reply with Changes...

M6

	A	B	C	D	E	F
1	C:\ChemSep_\Sep_Files\StandardTest\Klemola\Klemola_neq_chan.sep					
2	This file was created on 6/14/2010 9:41:12 PM by rtaylor with ChemSep (TM) v6.62					
3	**stage**	**NV**	**NL**	**Stripping factor**	**NOV**	**EOV**
4						
5						
6	1			0.000		
7	2	2.737	4.213	0.805	1.797	0.834
8	3	2.900	4.084	0.806	1.844	0.842
9	4	2.913	4.078	0.808	1.847	0.842
10	5	2.917	4.077	0.809	1.848	0.842
11	6	2.919	4.079	0.810	1.848	0.842
12	7	2.920	4.082	0.811	1.848	0.842
13	8	2.921	4.085	0.812	1.848	0.842
14	9	2.921	4.089	0.814	1.847	0.842
15	10	2.921	4.093	0.815	1.846	0.842
16	11	2.920	4.098	0.817	1.846	0.842
17	12	2.920	4.104	0.819	1.845	0.842

Efficiency Calculation

Ready

Exercise: Extend this example in order to calculate the **Murphree *tray efficiency***.

Example 12: Calculating the HETP of a Packed Column

The HETP of a packed column can be calculated from:

$$HETP = H_{OV} \frac{\ln \lambda}{\lambda - 1}$$

where H_{OV} is the overall height of a transfer unit and is obtained from

$$H_{OV} = H_V + \lambda H_L$$

with H_V and H_L the Heights of transfer units of the gas/vapor and liquid phases respectively. These quantities are defined by:

$$H_V = u_V / k_V a' \qquad H_L = u_L / k_L a'$$

where u_V and u_V are the superficial velocities of the respective phases, k_V and k_L are the mass transfer coefficients of the vapor and liquid phases (units m/s), and a' is the interfacial area density (units m^2/m^3).

The numbers of transfer units are defined as:

$$N_V = k_V a' t_V \qquad N_L = k_L a' t_L$$

The above allow the calculation of the heights of transfer units:

$$H_V = Z / N_V \qquad H_L = Z / N_L$$

where Z is the height of packing.

The table below shows (in column 2) the contents of a .def file to compute the Murphree point efficiency for the two key components. Strictly speaking only the first two and last 4 lines of this table are necessary; the others are included to provide context for the final calculation. Note that the equations above apply as written only to binary systems. It is common, however, to use them for multicomponent systems using the properties of the pair of key components (as discussed in *Example 6* of this tutorial).

Line	Text	Meaning
1	`newsheet:`	
2	`HETP Calculation`	
3	`var:`	
4	`stage`	
5		
6	`S`	Symbol for the stage index number
7	`var:`	
8	`HV`	
9		
10	`Z/$NTUv{LKEY},{HKEY}`	Height of vapor phasetransfer units
11	`var:`	
12	`HL`	
13		
14	`Z/$NTUl{LKEY},{HKEY}`	Height of liquid phase transfer units
15	`var:`	
16	`Stripping factor`	
17		
18	`FS`	Symbol for the stripping factor
19	`var:`	
20	`HOV`	
21		
22	`(Z/$NTUv{LKEY},{HKEY} + FS*Z/$NTUl{LKEY},{HKEY})`	Overall height of transfer unit
23	`var:`	
24	`HETP`	
25		
26	`(Z/$NTUv{LKEY},{HKEY} + FS*Z/$NTUl{LKEY},{HKEY})*ln(FS)/(FS-1)`	HETP calculation