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APPENDIX

APPENDIX A: INITIAL TESTING OF STILL

A1: PROCESS INPUT FILE TO GENERATE DATA FROM DECHEMA PARAMETERS[56]

```
TITLE PROJECT=XY, PROBLEM=XY Data, *
     USER=BM,DATE=14/07/92
DIMEN SI,TIME=HR,WT=KG,TEMP=C,PRES=KPA,*
     ENER=KJ,WORK=KW,LIQV=M3,VAPV=M3,VISC=PAS,*
     COND=WMK,SURF=NM,XDEN=SPGR
*
COMPONENT DATA
     LIBID 1,ETOH/2,BENZENE
*
THERMODYNAMIC DATA

     METHOD SYSTEM=LACT,ENTHALPY=LIBRARY
          KVALUE SETNO=1
          WILSON 1,2,,,1136.0759,302.9235
*
STREAM DATA
     PROP STREAM=FEED,PRES=101,RATE(M)=100,LFRAC(M)=1,*
          COMP(M)=1,87/2,13,NOCHECK
*
UNIT OPERATIONS
*
PGEN UID=In1
BVLE COMP=1,2,PRESSURE=84.4,*
     POINTS=51,PLOT=XY
```

[56] This program merely instructs PROCESS to generate 51 T-x-y points at a pressure of 84.4 kPa and plot the data as well. The stream defined is never really used.

A2: DATA GENERATED

Computed T-x-y data at 844 mbar			
Number	Temperature (°C)	Ethanol fraction	
		x (mole)	y (mole)
1	74.3	0.00	0.0000
2	71.5	0.02	0.1008
3	69.6	0.04	0.1695
4	68.1	0.06	0.2191
5	67.1	0.08	0.2566
6	66.3	0.10	0.2857
7	65.7	0.12	0.3091
8	65.2	0.14	0.3283
9	64.8	0.16	0.3443
10	64.5	0.18	0.3580
11	64.2	0.20	0.3698
12	64.0	0.22	0.3801
13	63.8	0.24	0.3893
14	63.7	0.26	0.3976
15	63.6	0.28	0.4052
16	63.5	0.30	0.4121
17	63.4	0.32	0.4186
18	63.3	0.34	0.4247
19	63.3	0.36	0.4305
20	63.2	0.38	0.4361
21	63.2	0.40	0.4415
22	63.2	0.42	0.4468
23	63.2	0.44	0.4521
24	63.2	0.46	0.4573
25	63.2	0.48	0.4626
26	63.2	0.50	0.4679
27	63.2	0.52	0.4734
28	63.3	0.54	0.4790

29	63.3	0.56	0.4848
30	63.4	0.58	0.4909
31	63.4	0.60	0.4974
32	63.5	0.62	0.5042
33	63.6	0.64	0.5115
34	63.7	0.66	0.5193
35	63.8	0.68	0.5277
36	64.0	0.70	0.5369
37	64.1	0.72	0.5469
38	64.3	0.74	0.5580
39	64.6	0.76	0.5702
40	64.8	0.78	0.5838
41	65.1	0.80	0.5991
42	65.5	0.82	0.6165
43	65.9	0.84	0.6362
44	66.4	0.86	0.6589
45	67.0	0.88	0.6853
46	67.7	0.90	0.7162
47	68.5	0.92	0.7528
48	69.5	0.94	0.7968
49	70.6	0.96	0.8503
50	72.0	0.98	0.9165
51	73.7	1.00	1.0000

APPENDIX B: DATA AND REGRESS INPUT FILES

The output files from these regressions have not been reproduced because they are quite lengthy. Interaction paramters are given in tables in the relevant chapters.

B1: OCT1 MBK INPUT FILE

```
TITLE                USER=BM,   PROJECT=OCT1-MBK,PROBLEM=Regress,
DATE=APRIL-1993
DESCRIPTION Regression of 1-octene / 2-hexanone VLE data.
DIMENSION    SI, TEMPERATURE=C, PRESSURE=BAR
PRINT        INPUT=ALL, REGRESS=PART, OUTPUT=ALL
$
COMPONENT
  LIBID 1,OCT1/2,MBK
$
$  Pressure,  temperature,  1-octene  liquid  and  vapour  mole
fractions.
$
DATA
  SETNUMBER=1, TYPE=VLE
  FORMAT=PTXY
  0.835, 121.5, 0.000000, 0.000000
  0.838, 119.6, 0.046750, 0.099221
  0.839, 118.6, 0.096901, 0.176431
  0.836, 117.1, 0.155970, 0.239532
  0.836, 115.3, 0.270625, 0.348466
  0.837, 113.8, 0.350887, 0.407451
  0.836, 113.5, 0.370351, 0.425366
  0.837, 113.1, 0.417551, 0.459217
  0.837, 112.9, 0.479990, 0.506957
  0.837, 112.6, 0.517928, 0.538873
  0.836, 112.5, 0.569246, 0.583273
  0.836, 112.3, 0.662731, 0.661395
  0.836, 112.3, 0.762136, 0.751347
```

```
  0.839, 112.4, 0.824078, 0.812883
  0.838, 112.8, 0.881145, 0.870261
  0.835, 113.5, 0.946415, 0.941570
  0.835, 114.5, 1.000000, 1.000000
$
CALCULATION
$
$ Use the Wilson equation with the ideal vapour phase fugacity
method and
$ a Poynting correction term of 1.0.
$
  REGRESSION NAME=WILSON
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=WILSON, VFUG=IDEAL, MVOL=ZERO
$
$ Use Van Laar:
$
  REGRESSION NAME=VAN_LAAR
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=VANLAAR, VFUG=IDEAL, MVOL=ZERO
$
$ Use 3-parameter NRTL:
$
  REGRESSION NAME=NRTL
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=NRTL
$
$ Use UNIQUAC
$
  REGRESSION NAME=UNIQUAC
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=UNIQUAC, VFUG=IDEAL, MVOL=ZERO
END
```

B2: OCT1 METHANOL INPUT FILE

```
TITLE                USER=BM,   PROJECT=OCT1-MBK,PROBLEM=Regress,
DATE=APRIL-1993
DESCRIPTION Regression of 1-octene / methanol VLE data.
DIMENSION    SI, TEMPERATURE=C, PRESSURE=BAR
PRINT        INPUT=ALL, REGRESS=PART, OUTPUT=ALL
$
COMPONENT
  LIBID 1,OCT1/2,METHANOL
$
$  Pressure,  temperature,  1-octene  liquid  and  vapour  mole
fractions.
$
DATA
  SETNUMBER=1, TYPE=VLE
  FORMAT=PTXY
0.835,    114.4,         1,         1
0.838,     68.9, 0.966953, 0.361821
0.839,     58.6, 0.804204, 0.141341
0.838,     57.0, 0.696201, 0.140419
0.839,     56.9, 0.580585, 0.138906
0.839,     56.9, 0.473943, 0.138846
0.836,     56.8, 0.267058, 0.135142
0.836,     56.8 ,0.175076, 0.127150
0.835,     56.8, 0.149515, 0.123297
0.833,     56.6, 0.110533, 0.115662
0.833,     56.7, 0.079816, 0.104189
0.835,     56.8, 0.056265, 0.095863
0.833,     57.5, 0.020844, 0.051816
0.833,     57.5, 0.009089, 0.029220
0.835,     59.7,         0,         0
$
CALCULATION
$
$ Use the Wilson equation with the ideal vapour phase fugacity
method and
```

```
$ a Poynting correction term of 1.0.
$
  REGRESSION NAME=WILSON
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=WILSON, VFUG=IDEAL, MVOL=ZERO
$
$ Use Van Laar:
$
  REGRESSION NAME=VAN_LAAR
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=VANLAAR, VFUG=IDEAL, MVOL=ZERO
$
$ Use 3-parameter NRTL:
$
  REGRESSION NAME=NRTL
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=NRTL
$
$ Use UNIQUAC
$
  REGRESSION NAME=UNIQUAC
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=UNIQUAC, VFUG=IDEAL, MVOL=ZERO
END
```

B3: MBK METHANOL INPUT FILE

```
TITLE                USER=BM,   PROJECT=OCT1-MBK,PROBLEM=Regress,
DATE=APRIL-1993
DESCRIPTION Regression of 2-hexanone / methanol VLE data.
DIMENSION    SI, TEMPERATURE=C, PRESSURE=BAR
PRINT        INPUT=ALL, REGRESS=PART, OUTPUT=ALL
$
```

```
COMPONENT
  LIBID 1,MBK/2,METHANOL
$
$ Pressure, temperature, 2-hexanone liquid and vapour mole
fractions.
$
DATA
  SETNUMBER=1, TYPE=VLE
  FORMAT=PTXY
0.835,    121.6,        1,        1
0.839,    107.7, 0.960455, 0.618162
0.838,     85.8, 0.892508, 0.273013
0.838,     76.6, 0.787737, 0.227976
0.839,     71.7, 0.690839, 0.191747
0.836,     67.6, 0.591318, 0.150123
0.836,     65.0, 0.475671, 0.114838
0.835,     64.5, 0.401248, 0.092279
0.833,     63.0, 0.306125, 0.072779
0.833,     62.5, 0.230150, 0.055423
0.835,     62.3, 0.177237, 0.045059
0.833,     60.8, 0.038880, 0.013831
0.833,     60.5, 0.027469, 0.009797
0.835,     59.7,        0,        0
$
CALCULATION
$
$ Use the Wilson equation with the ideal vapour phase fugacity
method and
$ a Poynting correction term of 1.0.
$
  REGRESSION NAME=WILSON
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=WILSON, VFUG=IDEAL, MVOL=ZERO
$
$ Use Van Laar:
$
```

```
  REGRESSION NAME=VAN_LAAR
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=VANLAAR, VFUG=IDEAL, MVOL=ZERO
$
$ Use 3-parameter NRTL:
$
  REGRESSION NAME=NRTL
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=NRTL
$
$ Use UNIQUAC
$
  REGRESSION NAME=UNIQUAC
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=UNIQUAC, VFUG=IDEAL, MVOL=ZERO
END
```

B4: OCT1 DMF INPUT FILE

```
TITLE                USER=BM,   PROJECT=OCT1-MBK,PROBLEM=Regress,
DATE=APRIL-1993
DESCRIPTION Regression of 1-octene / DMF VLE data.
DIMENSION    SI, TEMPERATURE=C, PRESSURE=BAR
PRINT        INPUT=ALL, REGRESS=PART, OUTPUT=ALL
$
COMPONENT
  LIBID 1,OCT1/2,DMF
$
$ Pressure, temperature, 1-octene liquid and vapour mole
fractions.
$
DATA
  SETNUMBER=1, TYPE=VLE
  FORMAT=PTXY
```

```
 0.835,     114.4,         1,         1
 0.843,     113.1, 0.918373, 0.862277
 0.843,     111.8, 0.754099, 0.724056
 0.845,     111.5, 0.631083, 0.675661
 0.840,     111.4, 0.572051, 0.652383
 0.844,     111.9, 0.428334, 0.612310
 0.847,     112.4, 0.343523, 0.584490
 0.846,     112.9, 0.236637, 0.540293
 0.846,     113.6, 0.214281, 0.513306
 0.843,     119.8, 0.093731, 0.379957
 0.838,     120.8, 0.087968, 0.362214
 0.842,     131.2, 0.019036, 0.208506
 0.836,     132.3, 0.017886, 0.199318
 0.839,     140.7, 0.005157, 0.065531
$
CALCULATION
$
$ Use the Wilson equation with the ideal vapour phase fugacity
method and
$ a Poynting correction term of 1.0.
$
  REGRESSION NAME=WILSON
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=WILSON, VFUG=IDEAL, MVOL=ZERO
$
$ Use Van Laar:
$
  REGRESSION NAME=VAN_LAAR
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=VANLAAR, VFUG=IDEAL, MVOL=ZERO
$
$ Use 3-parameter NRTL:
$
  REGRESSION NAME=NRTL
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
```

```
  DATA SETNUMBER=1
  MODEL TYPE=NRTL
$
$ Use UNIQUAC
$
  REGRESSION NAME=UNIQUAC
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=UNIQUAC, VFUG=IDEAL, MVOL=ZERO
END
```

B5: MBK DMF INPUT FILE

```
TITLE                USER=BM,   PROJECT=OCT1-MBK,PROBLEM=Regress,
DATE=APRIL-1993
DESCRIPTION Regression of 2-hexanone/DMF VLE data.
DIMENSION    SI, TEMPERATURE=C, PRESSURE=BAR
PRINT        INPUT=ALL, REGRESS=PART, OUTPUT=ALL
$
COMPONENT
  LIBID 1,MBK/2,DMF
$
$ Pressure, temperature, 2-hexanone liquid and vapour mole
fractions.
$
DATA
  SETNUMBER=1, TYPE=VLE
  FORMAT=PTXY
0.835,     121.6,         1,         1
0.843,     122.4, 0.912307, 0.939957
0.843,     123.6, 0.818676, 0.873974
0.845,     125.8, 0.673190, 0.777738
0.840,     127.5, 0.548410, 0.681295
0.844,     128.1, 0.498729, 0.628903
0.847,     129.8, 0.400562, 0.547099
0.846,     132.1, 0.314157, 0.483194
0.846,     134.4, 0.227650, 0.432946
```

```
0.843,     137.1, 0.129228, 0.336487
0.838,     138.5, 0.092086, 0.277178
0.842,     141.4, 0.054217, 0.162472
0.836,     142.2, 0.048127, 0.130034
0.839,     144.7, 0.018835, 0.050084
$
CALCULATION
$
$ Use the Wilson equation with the ideal vapour phase fugacity
method and
$ a Poynting correction term of 1.0.
$
  REGRESSION NAME=WILSON
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=WILSON, VFUG=IDEAL, MVOL=ZERO
$
$ Use Van Laar:
$
  REGRESSION NAME=VAN_LAAR
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=VANLAAR, VFUG=IDEAL, MVOL=ZERO
$
$ Use 3-parameter NRTL:
$
  REGRESSION NAME=NRTL
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=NRTL
$
$ Use UNIQUAC
$
  REGRESSION NAME=UNIQUAC
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=UNIQUAC, VFUG=IDEAL, MVOL=ZERO
```

```
END
```

B6: OCT1 MXEA INPUT FILE

```
TITLE                USER=BM,   PROJECT=OCT1-MBK,PROBLEM=Regress,
DATE=APRIL-1993
DESCRIPTION Regression of 1-octene / 2-methoxyethanol VLE data.
DIMENSION    SI, TEMPERATURE=C, PRESSURE=BAR
PRINT        INPUT=ALL, REGRESS=PART, OUTPUT=ALL
$
COMPONENT
  LIBID 1,OCT1/2,MXEA
$
$  Pressure,  temperature,  1-octene  liquid  and  vapour  mole
fractions.
$
DATA
  SETNUMBER=1, TYPE=VLE
  FORMAT=PTXY
0.835,     114.4,         1,         1
0.842,     104.6, 0.896017, 0.698231
0.847,     102.5, 0.764312, 0.580572
0.841,     101.8, 0.609425, 0.524452
0.839,     101.7, 0.504234, 0.497408
0.839,     101.6, 0.419951, 0.465539
0.839,     101.7, 0.421492, 0.467449
0.833,     101.6, 0.324307, 0.444667
0.837,     102.5, 0.158852, 0.410051
0.839,     103.1, 0.115287, 0.397487
0.842,     105.1, 0.075627, 0.326250
0.842,     118.7,         0,         0
$
CALCULATION
$
$ Use the Wilson equation with the ideal vapour phase fugacity
method and
$ a Poynting correction term of 1.0.
```

```
$
  REGRESSION NAME=WILSON
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=WILSON, VFUG=IDEAL, MVOL=ZERO
$
$ Use Van Laar:
$
  REGRESSION NAME=VAN_LAAR
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=VANLAAR, VFUG=IDEAL, MVOL=ZERO
$
$ Use 3-parameter NRTL:
$
  REGRESSION NAME=NRTL
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=NRTL
$
$ Use UNIQUAC
$
  REGRESSION NAME=UNIQUAC
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=UNIQUAC, VFUG=IDEAL, MVOL=ZERO
END
```

B7: MBK MXEA INPUT FILE

```
TITLE                USER=BM,   PROJECT=OCT1-MBK,PROBLEM=Regress,
DATE=APRIL-1993
DESCRIPTION Regression of 2-hexanone / 2-methoxyethanol VLE data.
DIMENSION    SI, TEMPERATURE=C, PRESSURE=BAR
PRINT        INPUT=ALL, REGRESS=PART, OUTPUT=ALL
$
COMPONENT
```

```
  LIBID 1,MBK/2,MXEA
$
$ Pressure, temperature, 2-hexanone liquid and vapour mole
fractions.
$
DATA
  SETNUMBER=1, TYPE=VLE
  FORMAT=PTXY
0.835,     121.6,         1,         1
0.842,     118.9, 0.900673, 0.839515
0.847,     117.5, 0.784868, 0.700921
0.841,     116.4, 0.675267, 0.601664
0.839,     115.7, 0.580262, 0.526468
0.839,     115.4, 0.510362, 0.473018
0.839,     115.2, 0.419164, 0.406681
0.833,     115.0, 0.332745, 0.342817
0.839,     115.7, 0.185337, 0.222341
0.842,     116.1, 0.141713, 0.178440
0.837,     117.6, 0.042773, 0.063811
0.842,     118.7,         0,         0
$
CALCULATION
$
$ Use the Wilson equation with the ideal vapour phase fugacity
method and
$ a Poynting correction term of 1.0.
$
  REGRESSION NAME=WILSON
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=WILSON, VFUG=IDEAL, MVOL=ZERO
$
$ Use Van Laar:
$
  REGRESSION NAME=VAN_LAAR
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
```

```
  MODEL TYPE=VANLAAR, VFUG=IDEAL, MVOL=ZERO
$
$ Use 3-parameter NRTL:
$
  REGRESSION NAME=NRTL
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=NRTL
$
$ Use UNIQUAC
$
  REGRESSION NAME=UNIQUAC
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=UNIQUAC, VFUG=IDEAL, MVOL=ZERO
END
```

B8: OCT1 kerosol INPUT FILE

Note: This data set is not to be taken up into VLE compilations.

```
TITLE                USER=BM,   PROJECT=OCT1-MBK,PROBLEM=Regress,
DATE=APRIL-1993
DESCRIPTION Regression of 1-octene / kerosol 200 VLE data.
DIMENSION    SI, TEMPERATURE=C, PRESSURE=BAR
PRINT        INPUT=ALL, REGRESS=PART, OUTPUT=ALL
$
COMPONENT
  LIBID 1,OCT1/2,UNDC
$
$  Pressure,  temperature,  1-octene  liquid  and  vapour  mole
fractions.
$
DATA
  SETNUMBER=1, TYPE=VLE
  FORMAT=PTXY
```

```
0.835,     114.4,         1,         1
0.840,     115.3, 0.976219, 0.998226
0.841,     117.1, 0.915013, 0.992386
0.841,     119.9, 0.833684, 0.988042
0.840,     122.5, 0.770930, 0.981123
0.842,     126.1, 0.688743, 0.958229
0.837,     132.2, 0.550732, 0.930171
0.836,     134.9, 0.515955, 0.903823
0.840,     144.6, 0.376511, 0.831199
0.839,     153.8, 0.258359, 0.731232
0.837,     164.2, 0.136033, 0.541577
$
CALCULATION
$
$ Use the Wilson equation with the ideal vapour phase fugacity
method and
$ a Poynting correction term of 1.0.
$
  REGRESSION NAME=WILSON
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=WILSON, VFUG=IDEAL, MVOL=ZERO
$
$ Use Van Laar:
$
  REGRESSION NAME=VAN_LAAR
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=VANLAAR, VFUG=IDEAL, MVOL=ZERO
$
$ Use 3-parameter NRTL:
$
  REGRESSION NAME=NRTL
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=NRTL
$
```

```
$ Use UNIQUAC
$
  REGRESSION NAME=UNIQUAC
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=UNIQUAC, VFUG=IDEAL, MVOL=ZERO
END
```

B9: MBK kerosol INPUT FILE

Note: This data set is not to be taken up into VLE compilations.

```
TITLE                USER=BM,   PROJECT=OCT1-MBK,PROBLEM=Regress,
DATE=APRIL-1993
DESCRIPTION Regression of 2-hexanone / kerosol 200 VLE data.
DIMENSION    SI, TEMPERATURE=C, PRESSURE=BAR
PRINT        INPUT=ALL, REGRESS=PART, OUTPUT=ALL
$
COMPONENT
  LIBID 1,MBK/2,UNDC
$
$  Pressure,  temperature,  1-octene  liquid  and  vapour  mole
fractions.
$
DATA
  SETNUMBER=1, TYPE=VLE
  FORMAT=PTXY
0.835,     121.6,         1,         1
0.840,     122.5, 0.973306, 0.994996
0.841,     123.9, 0.916286, 0.981002
0.841,     124.2, 0.888574, 0.975811
0.840,     126.1, 0.816243, 0.961683
0.842,     127.1, 0.743876, 0.948567
0.837,     128.5, 0.667122, 0.939543
0.835,     130.3, 0.613403, 0.930931
0.836,     131.3, 0.569873, 0.898847
0.840,     132.4, 0.530606, 0.894123
```

```
0.839,     138.1, 0.404430, 0.874108
0.837,     154.4, 0.171413, 0.706662
$
CALCULATION
$
$ Use the Wilson equation with the ideal vapour phase fugacity
method and
$ a Poynting correction term of 1.0.
$
  REGRESSION NAME=WILSON
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=WILSON, VFUG=IDEAL, MVOL=ZERO
$
$ Use Van Laar:
$
  REGRESSION NAME=VAN_LAAR
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=VANLAAR, VFUG=IDEAL, MVOL=ZERO
$
$ Use 3-parameter NRTL:
$
  REGRESSION NAME=NRTL
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=NRTL
$
$ Use UNIQUAC
$
  REGRESSION NAME=UNIQUAC
  OBJECTIVE FUNCTION=1, ITERATIONS=50, TOLERANCE=1.0E-20
  DATA SETNUMBER=1
  MODEL TYPE=UNIQUAC, VFUG=IDEAL, MVOL=ZERO
END
```

APPENDIX C: ASEEK PROGRAM AND RESULTS

C1: RESULTS FROM ASEEK RUN

Results produced by ASEEK

Note: UNIFAC results are arranged into 6x3 matrices. The first row represents mixtures containing 2/3 mol solvent with solvent free percentages of component 1 of 1,20,40,60,80 and 99. Set two has component 1 and the solvent with increasing amounts of 1. The third set is component 2 with the solvent.

PRO 2 name	Chemical name	NBP (°C)	Infinite dilidilution selectivity Tassios	Weimer–F	MOSCED	Help–VW	
2MEAMIDE	2–METHACRYLAMIDE	214.9	6.03	5.39	13.47	2.14	
		11.64	31.09	158.39	3020.96	1252597.	2.7E+10
		18.99	21.42	17.56	14.59	12.65	11.45
		0.00	0.39	27.04	468.16	1839.51	3633.32
TBUTFORM	tert–BUTYLFORMAMIDE	202.00	2.84	2.66	4.19	1.36	
		15.70	45.05	248.59	6906.76	16877026	2.6E+10
		27.58	16.00	10.08	7.94	7.02	6.62
		0.00	0.29	31.39	529.72	1857.09	3421.17
NMF	N–METHYLFORMAMIDE	199.50	43.50	32.71	4.85	7.81	
		12.22	34.58	200.13	5155.98	5066324	2.6E+10
		12.46	12.35	10.47	9.10	8.22	7.69
		0.00	0.23	21.83	425.81	1716.62	3400.78
FRMD	FORMAMIDE	219.90	4222.20	2464.65	3.07	281.33	
		23.94	102.65	934.55	61830.97	8.7E+08	2.8E+10
		43.78	49.43	28.63	20.25	16.52	14.78
		0.00	0.14	31.04	1954.85	12640.69	30501.87
ACTAMIDE	ACETAMIDE	221.10	138.03	101.77	4.78	19.98	
		10.55	27.41	139.50	2859.90	1730862.	2.8E+10
		16.40	23.28	23.51	23.01	22.85	23.09
		0.00	0.38	38.74	823.02	3298.85	6521.40
ACRYAMDI	ACRYLAMIDE	192.60	254.46	214.78	3.38	36.11	
		12.34	31.11	155.64	2840.68	947047.13	1.2E+10
		12.75	20.05	20.78	19.95	19.46	19.57
		0.00	0.14	10.93	399.31	2307.11	5475.39
DCLACEAL	DICHLOROACETALDEHYDE	88.90	6.36	5.20	0.37	1.80	
		59.97	153.07	620.09	7009.67	928525.00	6.9E+09
		1.81	0.87	0.45	0.26	0.16	0.11
		0.00	0.01	1.13	9.86	32.82	61.72
H2O	WATER	100.00	1.8E+09	3.5E+08	0.29	6045863	
		13.19	9.84	6.99	4.94	3.49	2.50
		460626.59	4.74	0.46	0.13	0.05	0.02
		93.10	1.63	0.44	0.20	0.09	0.04
FORMALID	FORMANILIDE	271.00	4.39	4.13	0.32	1.88	
		37.26	121.88	488.27	4715.26	256560.19	78633152
		71.13	232.58	173.84	111.98	71.81	48.03
		0.00	0.81	65.51	1922.30	10390.69	24174.33
UREA	UREA	191.90	3415429.	1918245.	1.66	90643.97	
		1.33	1.25	1.17	1.09	1.02	0.95
		54.30	1015.97	2913.97	5327.69	8111.09	11024.28
		52.72	815.75	2144.46	3729.88	5484.90	7270.04
H2O2	HYDROGEN PEROXIDE	150.20	1407537.	467574.00	0.29	21291.96	
		1.94	1.70	1.47	1.28	1.10	0.96
		0.37	1.21	2.32	3.58	4.85	5.96
		0.23	0.92	1.93	3.15	4.46	5.66
N2H4	HYDRAZINE	113.50	72688.48	34113.37	0.29	1986.77	
		2.33	2.02	1.73	1.49	1.27	1.10
		0.21	0.49	0.78	1.02	1.22	1.38
		0.10	0.32	0.63	0.94	1.24	1.51
METHANOL	METHANOL	64.70	1198.13	660.82	4.06	62.42	
		5.27	4.60	4.00	3.48	3.04	2.69
		2.59	0.54	0.20	0.09	0.04	0.02
		0.29	0.18	0.12	0.09	0.08	0.07
HNO3	NITRIC ACID	83.00	231.70	130.14	0.29	17.76	
		1.55	1.43	1.32	1.21	1.12	1.03
		0.30	0.30	0.30	0.30	0.30	0.30
		0.23	0.23	0.24	0.24	0.25	0.25

EG	ETHYLENE GLYCOL	197.30	269.55	191.87	6.61	32.19	
		3.37	2.96	2.52	2.12	1.77	1.50
		746.31	253.19	33.19	7.46	2.10	0.63
		91.24	72.69	20.98	7.02	2.53	0.93
GLXL	GLYOXAL	50.40	106.71	69.70	5.70	10.36	
		16.85	12.63	9.23	6.73	4.89	3.60
		501.57	0.89	0.08	0.02	0.00	0.00
		5.63	0.20	0.05	0.02	0.02	0.02
PRPGLALC	PROPARGYL ALCOHOL	113.60	79.81	57.93	15.16	10.58	
		5.28	4.94	4.55	4.15	3.78	3.44
		6.25	2.82	1.30	0.61	0.25	0.08
		0.70	0.76	0.78	0.72	0.57	0.35
ETHANOL	ETHANOL	78.30	120.26	84.14	1.63	13.04	
		4.05	3.60	3.17	2.79	2.46	2.19
		2.63	0.87	0.36	0.16	0.07	0.03
		0.51	0.33	0.22	0.16	0.12	0.09
MEA	MONOETHANOLAMINE	171.00	93.50	69.23	3.63	13.54	
		5.31	4.98	4.50	3.99	3.51	3.10
		99.04	60.41	15.01	3.99	0.93	0.14
		11.05	9.49	6.23	3.67	1.92	0.84
ENIM	ETHYLENEIMINE	55.90	68.63	46.04	4.85	7.70	
		2.23	1.91	1.62	1.37	1.17	1.00
		0.13	0.11	0.11	0.12	0.13	0.15
		0.08	0.07	0.08	0.10	0.11	0.14
2BTYDIO	2–BUTYNE–1,4–DIOL	238.00	53.60	45.52	4.52	10.94	
		6.43	6.66	6.41	5.96	5.45	4.97
		339.17	2922.91	974.51	216.71	31.27	2.27
		23.74	80.27	124.03	116.95	69.92	26.89
NBF5	NIOBIUM PENTAFLUORIDE	228.90	60.49	47.70	0.29	11.07	
		1.33	1.25	1.17	1.09	1.02	0.95
		10.13	18.84	29.45	40.06	50.40	59.93
		9.52	16.17	23.66	30.86	37.68	43.84
LCNL	LACTONITRILE	183.90	48.32	38.59	3.38	8.82	
		9.09	9.04	8.10	6.99	5.95	5.09
		928.85	360.59	35.81	5.51	0.97	0.14
		19.36	17.08	9.78	5.38	2.84	1.40
HYAN	HYDRACRYLONITRILE	221.00	48.35	37.82	1.39	9.09	
		6.94	6.93	6.39	5.71	5.03	4.43
		400.92	463.68	93.44	19.75	3.98	0.67
		23.64	33.71	26.78	18.40	11.39	6.30
SUCAND	SUCCINIC ANHYDRIDE	263.40	48.24	36.81	8.31	9.31	
		5.09	4.85	4.37	3.85	3.36	2.93
		492.13	563.01	134.70	47.73	21.78	11.97
		38.70	69.76	61.70	51.66	44.13	39.01
PRLC	beta–PROPIOLACTONE	162.00	45.97	33.95	15.16	7.60	
		3.89	3.49	3.06	2.67	2.31	2.02
		26.02	8.55	3.65	2.14	1.48	1.14
		4.31	3.24	2.70	2.44	2.33	2.31
12PG	1,2–PROPYLENE GLYCOL	187.60	46.21	36.92	6.17	8.56	
		5.56	5.39	4.99	4.54	4.10	3.70
		179.96	183.94	42.21	8.84	1.45	0.13
		17.07	19.26	12.75	6.95	3.25	1.31
PRAA	3–AMINO–1–PROPANOL	187.50	34.06	28.12	12.16	6.97	
		4.35	4.12	3.79	3.43	3.08	2.78
		69.90	89.97	32.16	10.13	2.60	0.44
		11.59	13.65	11.38	7.92	4.69	2.29
ACH	ACETALDEHYDE	20.50	22.22	15.24	24.44	3.17	
		4.63	4.10	3.64	3.25	2.93	2.67
		0.08	0.04	0.02	0.02	0.01	0.02
		0.01	0.01	0.02	0.02	0.02	0.05
OAZL	OXAZOLE	69.50	38.00	27.77	3.63	5.53	
		2.67	2.26	1.90	1.60	1.35	1.15
		0.65	0.22	0.16	0.15	0.14	0.14
		0.18	0.15	0.14	0.14	0.13	0.14

13PG	1,3–PROPYLENE GLYCOL	214.40	40.98	33.10	5.24	8.16	
		5.50	5.35	4.97	4.53	4.09	3.70
		370.84	748.61	160.13	30.55	4.66	0.44
		28.76	51.00	37.02	20.75	9.92	4.16
MFOR	METHYL FORMATE	31.80	14.50	10.59	25.21	2.57	
		5.07	4.40	3.81	3.32	2.90	2.57
		0.23	0.08	0.04	0.02	0.02	0.03
		0.03	0.03	0.03	0.03	0.04	0.06
C2BTDIOL	cis–2–BUTENE–1,4–DIOL	235.00	28.35	24.24	0.90	6.63	
		4.90	4.83	4.59	4.28	3.96	3.66
		217.40	764.49	279.35	72.78	12.98	1.26
		25.65	58.18	59.85	45.00	26.93	13.12
T2BTDIOL	trans–2–BUTENE–1,4–DIO	236.90	28.12	24.07	0.46	6.61	
		4.90	4.83	4.59	4.28	3.96	3.66
		230.03	910.66	332.78	86.60	15.40	1.49
		26.19	66.08	69.74	52.85	31.77	15.54
IPA	ISOPROPANOL	82.30	24.86	19.52	16.61	4.45	
		3.37	3.04	2.74	2.46	2.21	2.00
		1.85	0.86	0.42	0.21	0.10	0.04
		0.49	0.35	0.25	0.19	0.14	0.11
AA	ALLYL ALCOHOL	97.10	29.63	22.69	5.82	5.07	
		3.71	3.39	3.08	2.79	2.52	2.29
		2.44	1.31	0.70	0.37	0.18	0.08
		0.54	0.48	0.42	0.36	0.30	0.24
ACEN	ACETONITRILE	81.60	43.39	29.35	2.14	5.80	
		6.14	5.45	4.78	4.17	3.64	3.19
		4.60	1.06	0.36	0.15	0.08	0.05
		0.41	0.31	0.25	0.21	0.20	0.19
NTRM	NITROMETHANE	101.20	38.13	26.51	1.66	5.60	
		6.15	5.67	5.14	4.64	4.18	3.77
		7.44	2.27	0.79	0.31	0.13	0.07
		0.68	0.57	0.48	0.42	0.37	0.33
GLOL	GLYCEROL	287.90	33.09	27.03	3.51	7.57	
		1.64	1.69	1.75	1.83	1.94	2.05
		26.39	121.27	260.29	427.50	616.09	800.02
		13.06	46.71	136.90	324.94	679.08	1251.04
13BZDIOL	1,3–BENZENEDIOL	276.50	11.44	11.17	1.75	3.92	
		12.58	15.38	15.76	15.21	14.35	13.45
		769.20	3560.31	920.55	269.80	84.51	26.66
		11.65	29.26	70.82	170.32	458.34	1426.21
CLEA	2–CHLOROETHANOL	128.60	30.43	23.10	4.85	5.40	
		4.41	4.10	3.75	3.42	3.12	2.85
		11.88	4.93	2.00	0.89	0.39	0.16
		1.74	1.45	1.18	0.95	0.75	0.60
2MERETOH	2–MERCAPTOETHANOL	157.80	25.27	19.68	1.63	5.02	
		1.38	1.29	1.20	1.12	1.04	0.97
		2.49	2.65	2.82	2.98	3.12	3.26
		2.19	2.28	2.37	2.45	2.54	2.61
ETLNCARB	ETHYLENE CARBONATE	238.00	30.91	24.39	3.10	6.57	
		4.08	3.73	3.28	2.85	2.45	2.12
		208.39	170.51	55.12	27.06	16.79	12.10
		26.00	36.43	32.34	28.60	26.18	24.75
ACRN	ACRYLONITRILE	77.40	12.64	9.61	15.16	2.63	
		5.53	5.04	4.56	4.14	3.76	3.45
		2.48	0.52	0.25	0.16	0.12	0.09
		0.14	0.17	0.21	0.24	0.25	0.24
MALONTRL	MALONONITRILE	218.40	23.67	18.16	4.86	5.07	
		1.34	1.26	1.18	1.10	1.02	0.95
		8.36	11.33	13.86	15.93	17.68	19.13
		7.80	9.94	11.66	13.02	14.15	15.07
ENDM	ETHYLENEDIAMINE	117.30	26.70	20.54	4.86	4.87	
		4.71	4.41	4.08	3.76	3.46	3.19
		7.37	3.10	1.29	0.59	0.29	0.15
		1.01	0.88	0.77	0.69	0.62	0.58

14BTD	1,4-BUTANEDIOL	228.00	24.32	21.31	4.47	5.98	
		4.65	4.53	4.26	3.94	3.61	3.31
		230.28	825.85	269.55	65.92	11.58	1.19
		27.79	66.64	60.83	40.68	22.36	10.47
PO	1,2-PROPYLENE OXIDE	34.50	5.83	4.49	19.11	1.50	
		2.23	1.94	1.67	1.45	1.25	1.09
		0.04	0.04	0.04	0.05	0.06	0.09
		0.02	0.03	0.03	0.04	0.05	0.08
IPAA	1-AMINO-2-PROPANOL	159.50	18.54	15.16	15.66	4.18	
		3.88	3.64	3.36	3.07	2.79	2.54
		23.93	20.58	9.51	3.65	1.07	0.18
		5.15	4.90	4.04	2.93	1.81	0.90
CLACCL	CHLOROACETYL CHLORIDE	106.00	19.29	15.87	5.70	4.02	
		2.77	2.69	2.62	2.58	2.55	2.55
		1.64	1.13	0.77	0.53	0.36	0.25
		0.43	0.46	0.50	0.54	0.59	0.62
GLUAN	GLUTARIC ANHYDRIDE	289.50	17.54	14.74	0.44	4.73	
		3.49	3.32	3.07	2.80	2.53	2.29
		168.90	581.41	293.06	150.57	85.81	54.90
		37.90	103.77	129.12	136.87	138.97	139.65
GLUAN	GLUTARIC ANHYDRIDE	289.50	17.54	14.74	0.44	4.73	
		3.49	3.32	3.07	2.80	2.53	2.29
		168.90	581.41	293.06	150.57	85.81	54.90
		37.90	103.77	129.12	136.87	138.97	139.65
13BTD	1,3-BUTANEDIOL	207.00	14.94	13.04	16.78	4.01	
		6.48	6.32	5.78	5.18	4.59	4.09
		833.05	1019.74	144.70	22.64	3.15	0.29
		31.65	52.80	32.82	16.34	7.18	2.85
PRH	n-PROPIONALDEHYDE	48.00	5.86	4.59	16.54	1.56	
		3.31	3.01	2.73	2.49	2.28	2.10
		0.20	0.13	0.09	0.07	0.06	0.06
		0.05	0.05	0.06	0.07	0.09	0.11
12BZDIOL	1,2-BENZENEDIOL	245.50	5.92	5.81	0.42	2.37	
		12.82	15.46	15.80	15.25	14.39	13.48
		308.23	425.15	118.79	37.45	12.01	3.59
		6.84	11.14	19.17	35.62	77.80	210.02
MICT	METHYL ISOCYANATE	38.90	21.01	15.04	0.40	3.31	
		1.23	1.24	1.25	1.26	1.27	1.28
		0.02	0.03	0.05	0.08	0.10	0.10
		0.02	0.03	0.04	0.06	0.07	0.09
23BTD	2,3-BUTANEDIOL	180.70	16.70	14.48	5.66	4.21	
		5.83	5.62	5.17	4.66	4.16	3.73
		241.09	220.98	40.54	7.28	1.08	0.09
		19.00	20.12	11.64	5.62	2.38	0.87
14BZDIOL	p-HYDROQUINONE	285.00	5.24	5.22	0.42	2.27	
		12.56	15.37	15.76	15.21	14.35	13.45
		934.59	3521.08	936.87	281.59	88.91	27.63
		13.50	36.29	86.48	200.05	511.42	1523.69
TMLPROP	TRIMETHYLOLPROPANE	288.90	12.66	11.91	4.67	4.12	
		5.86	5.80	5.50	5.12	4.72	4.35
		2523.54	39562.39	15044.84	2767.76	198.19	2.88
		92.28	991.68	1217.35	847.32	361.14	82.82
DEG	DIETHYLENE GLYCOL	245.00	16.02	14.57	4.31	4.58	
		5.78	5.73	5.40	4.99	4.55	4.16
		532.88	1860.92	488.09	93.45	12.12	0.82
		39.17	97.00	86.36	55.28	27.80	11.02
2PYRO	2-PYRROLIDONE	245.00	15.32	12.93	13.47	4.11	
		2.96	2.77	2.54	2.30	2.08	1.87
		56.40	98.04	60.75	38.50	26.47	19.83
		17.38	28.76	33.73	36.01	37.48	38.73
CLACETAL	CHLOROACETALDEHYDE	84.90	15.34	11.65	5.70	3.05	
		4.66	4.17	3.70	3.28	2.90	2.59
		2.17	0.79	0.40	0.23	0.13	0.08
		0.27	0.28	0.29	0.28	0.25	0.21

AMETEA	N–AMINOETHYL ETHANOLA	243.90	12.80	11.72	12.92	3.89	
		4.41	4.26	3.97	3.63	3.30	3.00
		218.56	1554.95	662.07	189.86	36.57	3.81
		30.91	106.29	129.29	105.01	61.89	24.86
MXEA	2–METHOXYETHANOL	124.40	10.05	8.20	10.57	2.56	
		2.96	2.69	2.43	2.18	1.95	1.76
		7.03	3.50	1.64	0.79	0.39	0.19
		2.18	1.59	1.12	0.78	0.54	0.37
PROPANOL	n–PROPANOL	97.20	23.55	18.48	0.97	4.38	
		3.23	2.93	2.65	2.39	2.15	1.95
		2.95	1.41	0.69	0.35	0.17	0.08
		0.81	0.59	0.43	0.32	0.25	0.19
SBA	sec–BUTANOL	99.60	8.95	7.61	10.76	2.39	
		2.82	2.59	2.36	2.16	1.97	1.81
		2.29	1.32	0.74	0.41	0.21	0.10
		0.78	0.60	0.46	0.36	0.28	0.23
HFOR	FORMIC ACID	100.60	10.14	5.46	7.11	1.65	
		15.21	11.99	9.00	6.72	5.02	3.79
		4855.43	2.62	0.40	0.15	0.07	0.04
		5.13	0.86	0.43	0.29	0.21	0.15
THDGLYCL	THIODIGLYCOL	282.00	11.43	10.45	8.64	3.68	
		5.89	5.49	4.83	4.18	3.59	3.10
		24158.16	13868.82	1587.59	215.68	22.53	1.13
		315.49	1075.76	437.90	148.25	42.76	9.95
THDGLYCL	THIODIGLYCOL	282.00	11.43	10.45	8.64	3.68	
		5.89	5.49	4.83	4.18	3.59	3.10
		24158.16	13868.82	1587.59	215.68	22.53	1.13
		315.49	1075.76	437.90	148.25	42.76	9.95
IPAM	ISOPROPYLAMINE	32.40	2.48	2.06	15.66	1.01	
		2.13	2.03	1.92	1.83	1.74	1.66
		0.05	0.04	0.04	0.04	0.05	0.07
		0.02	0.02	0.03	0.04	0.05	0.07
DEE	DIETHYL ETHER	34.40	1.26	1.11	16.78	0.88	
		1.77	1.57	1.38	1.21	1.07	0.94
		0.04	0.04	0.05	0.05	0.06	0.09
		0.04	0.03	0.03	0.04	0.04	0.07
ACRH	ACROLEIN	52.70	10.62	8.08	8.84	2.24	
		5.12	4.38	3.72	3.16	2.68	2.30
		1.10	0.25	0.10	0.06	0.04	0.04
		0.14	0.09	0.07	0.07	0.07	0.09
DCLACETA	DICHLOROACETIC ACID	194.00	11.40	9.79	5.70	3.19	
		5.95	5.78	5.32	4.79	4.27	3.82
		88.51	53.10	15.53	6.21	3.02	1.69
		7.31	7.44	7.30	7.31	7.49	7.80
2HMF	FURFURYL ALCOHOL	170.00	13.21	11.21	2.03	3.42	
		3.84	3.56	3.23	2.90	2.59	2.33
		38.89	23.06	8.47	3.49	1.48	0.60
		7.35	6.19	4.58	3.35	2.48	1.88
2HMF	FURFURYL ALCOHOL	170.00	13.21	11.21	2.03	3.42	
		3.84	3.56	3.23	2.90	2.59	2.33
		38.89	23.06	8.47	3.49	1.48	0.60
		7.35	6.19	4.58	3.35	2.48	1.88
C4NT	SUCCINONITRILE	267.00	12.95	11.02	4.49	3.72	
		5.90	5.87	5.48	4.97	4.44	3.97
		669.17	1845.46	408.03	92.29	21.51	4.99
		45.80	108.08	97.53	74.67	53.86	37.82
AEEA	1,4–AMINO–1–BUTANOL	243.70	11.36	10.33	2.49	3.53	
		4.42	4.26	3.97	3.64	3.30	3.00
		198.09	670.22	279.37	84.57	17.27	1.80
		30.16	72.35	75.28	57.07	32.44	12.50
MEETAM	METHYL ETHANOLAMINE	158.00	14.39	12.01	15.66	3.53	
		1.66	1.50	1.35	1.21	1.08	0.98
		3.62	3.30	3.06	2.93	2.88	2.89
		2.84	2.55	2.44	2.44	2.52	2.64

2MPRNIT	ISOBUTYRONITRILE	103.60	3.19	2.75	13.47	1.26	
		2.90	2.70	2.49	2.30	2.12	1.97
		1.62	1.08	0.72	0.48	0.33	0.24
		0.48	0.49	0.50	0.50	0.50	0.49
DEA	DIETHANOLAMINE	268.90	14.75	13.37	2.49	4.38	
		5.16	5.02	4.69	4.29	3.90	3.54
		1123.74	6213.61	1857.25	371.36	42.33	1.79
		72.72	362.87	331.98	196.77	80.93	21.37
3PHDIAM	m-PHENYLENEDIAMINE	286.90	6.67	6.04	0.58	2.46	
		10.50	10.73	9.42	7.92	6.56	5.46
		19455.22	5741.39	633.04	115.82	24.05	4.69
		86.44	192.55	151.09	114.45	82.44	53.73
THIOUREA	THIOUREA	262.90	13.03	11.27	3.07	3.79	
		1.33	1.25	1.17	1.09	1.02	0.95
		17.59	40.19	63.04	82.85	100.43	115.61
		16.87	34.64	51.19	64.97	76.89	86.98
ETCYNAC	ETHYL CYANOACETATE	206.00	12.71	11.74	3.71	3.76	
		4.46	4.34	4.07	3.75	3.43	3.13
		54.41	113.16	52.29	21.32	8.36	3.18
		8.63	13.74	17.36	18.33	16.99	14.10
NPAM	n-PROPYLAMINE	47.90	3.91	3.22	12.16	1.28	
		2.56	2.43	2.30	2.18	2.07	1.97
		0.15	0.11	0.09	0.08	0.07	0.09
		0.05	0.05	0.06	0.08	0.10	0.12
2CLP	ISOPROPYL CHLORIDE	35.70	1.59	1.36	14.20	0.88	
		1.02	1.04	1.07	1.11	1.17	1.24
		0.03	0.04	0.05	0.06	0.08	0.10
		0.04	0.03	0.03	0.04	0.05	0.08
EXEA	2-ETHOXYETHANOL	135.00	10.91	9.58	5.49	2.96	
		3.42	3.20	2.96	2.72	2.50	2.30
		8.60	5.09	2.56	1.21	0.52	0.19
		2.15	1.80	1.46	1.15	0.89	0.67
BUTR	n-BUTYRONITRILE	117.60	3.55	3.03	11.21	1.34	
		2.92	2.72	2.51	2.32	2.14	1.98
		2.61	1.67	1.08	0.71	0.48	0.34
		0.75	0.75	0.76	0.75	0.74	0.71
DMSO	DIMETHYL SULFOXIDE	190.90	12.86	10.41	3.27	3.27	
		4.84	4.56	4.12	3.66	3.22	2.84
		111.17	55.25	13.65	4.35	1.60	0.65
		14.40	11.31	7.32	4.86	3.35	2.43
15PNDIOL	1,5-PENTANEDIOL	239.00	11.24	10.38	3.78	3.54	
		4.07	3.96	3.74	3.49	3.23	2.99
		166.04	856.30	390.16	118.15	23.84	2.66
		27.61	78.60	85.52	66.35	41.40	21.51
BALD	n-BUTYRALDEHYDE	74.80	2.97	2.53	11.61	1.17	
		2.61	2.39	2.17	1.98	1.81	1.66
		0.47	0.34	0.26	0.20	0.17	0.16
		0.16	0.17	0.19	0.20	0.22	0.24
VFOR	VINYL FORMATE	46.90	10.49	8.16	4.52	2.25	
		5.63	4.89	4.21	3.64	3.14	2.74
		0.73	0.20	0.08	0.04	0.03	0.03
		0.08	0.06	0.05	0.05	0.05	0.07
EPCH	alpha-EPICHLOROHYDRIN	116.10	11.98	9.98	4.82	2.93	
		1.20	1.54	1.93	2.35	2.79	3.21
		1.07	0.94	0.87	0.83	0.82	0.81
		0.35	0.49	0.67	0.88	1.05	1.00
CRCN	ACROLEIN CYANOHYDRIN	188.00	8.63	7.32	2.22	2.56	
		6.07	5.84	5.30	4.68	4.09	3.57
		110.74	96.30	23.12	6.37	1.85	0.51
		10.96	10.30	8.11	6.12	4.45	3.08
TBTAMINE	tert-BUTYLAMINE	44.40	1.28	1.13	12.92	0.89	
		1.68	1.50	1.34	1.19	1.06	0.95
		0.07	0.07	0.07	0.08	0.09	0.11
		0.05	0.05	0.05	0.06	0.06	0.09

CLPA	2,3-DICHLOROPROPYL ALC	182.00	9.60	8.50	5.82	2.87	
		3.65	3.49	3.28	3.05	2.83	2.63
		21.86	21.61	12.35	6.34	2.98	1.24
		4.81	5.41	5.70	5.68	5.38	4.91
ALLAMINE	ALLYLAMINE	53.30	7.42	5.91	8.03	1.85	
		1.83	1.87	1.91	1.93	1.95	1.96
		0.17	0.14	0.12	0.12	0.12	0.13
		0.06	0.08	0.09	0.11	0.13	0.15
ETCLFORM	ETHYL CHLOROFORMATE	92.90	9.09	7.81	3.10	2.42	
		6.19	5.12	4.16	3.37	2.72	2.22
		22.45	1.45	0.40	0.20	0.12	0.08
		1.40	0.53	0.32	0.24	0.20	0.17
VEE	ETHYL VINYL ETHER	35.60	1.78	1.51	11.96	0.90	
		1.95	1.85	1.75	1.66	1.58	1.50
		0.05	0.05	0.05	0.05	0.06	0.08
		0.03	0.03	0.04	0.04	0.06	0.09
ACCN	ACETONE CYANOHYDRIN	189.90	8.21	7.14	11.21	2.53	
		5.30	5.07	4.70	4.29	3.89	3.52
		30.19	30.50	12.29	3.94	1.01	0.17
		4.33	4.26	3.80	3.09	2.23	1.37
NMAMIDE	N-METHYLACETAMIDE	205.00	13.39	11.15	3.52	3.52	
		0.52	0.59	0.70	0.85	1.07	1.40
		4.95	6.88	10.12	14.79	19.81	21.11
		8.29	8.16	8.57	9.57	10.95	12.46
IBUH	ISOBUTYRALDEHYDE	64.10	2.69	2.29	10.35	1.10	
		2.70	2.48	2.28	2.10	1.94	1.81
		0.31	0.23	0.18	0.14	0.11	0.11
		0.11	0.11	0.12	0.13	0.15	0.18
NEOC5GLY	NEOPENTYL GLYCOL	209.90	8.13	7.63	7.65	2.77	
		4.07	3.94	3.72	3.47	3.21	2.98
		89.58	324.49	147.99	44.44	8.88	0.97
		16.46	30.68	31.75	24.26	14.96	7.68
VACT	VINYL ACETATE	72.50	3.29	2.82	9.36	1.24	
		3.29	2.92	2.58	2.28	2.02	1.79
		0.83	0.41	0.24	0.16	0.12	0.10
		0.22	0.19	0.17	0.16	0.16	0.17
DMS	DIMETHYL SULFIDE	37.30	3.86	3.09	10.15	1.23	
		0.02	0.13	0.43	0.92	1.48	2.00
		0.00	0.02	0.07	0.13	0.19	0.24
		0.02	0.03	0.04	0.05	0.07	0.10
CLAC	TRICHLOROACETALDEHYDE	97.70	7.85	6.92	4.31	2.26	
		5.41	4.82	4.21	3.66	3.17	2.76
		20.01	3.62	0.80	0.21	0.06	0.03
		2.80	1.08	0.48	0.25	0.15	0.11
2M2B	2-METHYL-2-BUTANOL	102.00	3.98	3.58	8.73	1.49	
		2.53	2.33	2.15	1.97	1.81	1.68
		1.94	1.27	0.79	0.46	0.25	0.12
		0.78	0.62	0.50	0.39	0.31	0.25
MECYAC	METHYL CYANOACETATE	205.10	7.12	6.27	4.52	2.35	
		5.50	5.33	4.91	4.42	3.93	3.50
		98.03	95.45	29.26	9.71	3.37	1.17
		10.98	12.89	12.10	10.24	8.04	5.89
MANH	MALEIC ANHYDRIDE	202.00	10.33	8.39	12.16	2.83	
		1.41	1.41	1.42	1.42	1.42	1.42
		5.72	7.34	9.28	11.38	13.48	15.13
		4.04	5.25	7.17	10.01	13.67	16.67
PFOCTANE	PERFLUOROOCTANE	103.60	1.89	1.96	5.03	1.16	
		3.80	4.65	6.13	8.82	14.14	25.12
		6.05	3.22	1.36	0.45	0.10	0.02
		0.65	0.42	0.40	0.45	0.55	0.67
PTT2	trans-2-PENTENE	36.30	1.02	0.90	11.50	1.03	
		1.04	0.97	0.91	0.85	0.79	0.73
		0.04	0.04	0.05	0.06	0.08	0.11
		0.06	0.04	0.04	0.03	0.04	0.06

DGA	2-AMINOETHOXYETHANOL	240.90	7.13	6.47	12.92	2.50	
		4.75	4.61	4.30	3.95	3.59	3.26
		126.48	295.92	114.91	34.08	7.40	0.95
		18.52	30.90	30.92	24.11	15.08	7.23
4PHDIAM	p-PHENYLENEDIAMINE	266.90	3.33	3.23	0.58	1.61	
		10.51	10.73	9.42	7.92	6.56	5.46
		14449.91	4560.94	488.13	87.44	17.97	3.51
		64.23	133.28	107.02	82.33	60.06	39.61
FRAN	FURAN	31.40	4.51	3.57	8.31	1.32	
		3.05	2.62	2.24	1.92	1.65	1.42
		0.07	0.05	0.04	0.04	0.04	0.06
		0.02	0.02	0.03	0.03	0.05	0.07
DEAM	DIETHYLAMINE	55.50	1.69	1.49	10.75	0.93	
		1.56	1.39	1.23	1.09	0.97	0.86
		0.12	0.11	0.12	0.12	0.14	0.16
		0.11	0.09	0.09	0.09	0.10	0.13
IPAC	ISOPROPYL ACETATE	88.50	1.59	1.45	10.45	0.96	
		2.14	1.94	1.74	1.57	1.41	1.27
		0.68	0.51	0.40	0.32	0.27	0.24
		0.35	0.32	0.30	0.29	0.29	0.30
2M1B	2-METHYL-1-BUTANOL	128.70	5.50	4.95	7.12	1.88	
		2.40	2.23	2.06	1.91	1.76	1.63
		3.93	2.84	1.85	1.13	0.63	0.31
		1.66	1.40	1.16	0.96	0.78	0.64
2PNA	2-PENTANOL	119.00	4.32	3.91	8.03	1.60	
		2.44	2.26	2.09	1.93	1.78	1.65
		3.14	2.16	1.38	0.83	0.46	0.23
		1.30	1.08	0.88	0.72	0.58	0.47
VANILLIN	VANILLIN	284.90	4.10	3.98	0.30	1.87	
		6.49	6.92	7.12	7.28	7.51	7.86
		2797.05	13392.90	2582.19	458.68	68.11	7.11
		54.00	225.07	246.08	222.56	197.87	181.16
3M1B	3-METHYL-1-BUTANOL	131.20	4.66	4.21	7.50	1.70	
		2.39	2.23	2.06	1.91	1.76	1.64
		4.19	3.03	1.98	1.21	0.68	0.34
		1.77	1.50	1.25	1.03	0.85	0.70
3PNALC	3-PENTANOL	115.30	4.40	3.96	7.65	1.61	
		2.45	2.27	2.10	1.93	1.78	1.65
		2.83	1.93	1.23	0.74	0.40	0.20
		1.17	0.96	0.78	0.63	0.51	0.41
16HXDIOL	1,6-HEXANEDIOL	243.00	7.10	6.78	24.44	2.62	
		3.65	3.54	3.35	3.14	2.93	2.73
		119.11	833.56	510.28	186.90	42.86	5.18
		25.17	80.12	103.33	92.56	65.54	38.01
CRTA	trans-CROTONALDEHYDE	104.10	6.30	5.25	6.05	1.85	
		3.06	2.78	2.51	2.27	2.05	1.86
		2.14	1.11	0.66	0.43	0.30	0.23
		0.57	0.51	0.48	0.45	0.44	0.44
11CE	1,1-DICHLOROETHYLENE	31.60	3.10	2.54	8.46	1.11	
		0.99	1.48	2.09	2.75	3.44	4.09
		0.03	0.03	0.04	0.05	0.06	0.09
		0.01	0.02	0.03	0.05	0.07	0.08
3M2B	3-METHYL-2-BUTANOL	111.50	3.91	3.54	7.78	1.50	
		2.49	2.31	2.13	1.96	1.80	1.67
		2.52	1.69	1.06	0.64	0.35	0.17
		1.02	0.84	0.68	0.55	0.45	0.37
MERPRO	3-MERCAPTOPROPIONIC A	227.90	8.06	7.18	1.10	2.65	
		2.86	2.67	2.45	2.24	2.03	1.85
		33.34	43.57	31.06	23.36	18.99	16.48
		10.02	15.00	19.26	22.86	26.14	29.10
VALNITRL	VALERONITRILE	141.30	2.46	2.22	8.83	1.17	
		2.48	2.33	2.18	2.03	1.89	1.76
		3.82	2.88	2.08	1.48	1.04	0.73
		1.43	1.45	1.46	1.46	1.45	1.40

DIKT	DIKETENE	126.10	6.90	5.71	4.49	2.00	
		5.48	5.02	4.47	3.95	3.47	3.05
		20.40	5.86	1.77	0.66	0.28	0.13
		2.35	1.57	1.10	0.82	0.64	0.52
1BTO	1,2-EPOXYBUTANE	63.40	2.40	2.04	9.66	1.04	
		1.05	1.03	1.02	1.02	1.01	1.02
		0.12	0.14	0.16	0.18	0.20	0.22
		0.15	0.13	0.12	0.12	0.13	0.16
PF2MP	PERFLUORO-2-METHYLPE	57.50	2.18	2.16	7.43	1.15	
		5.78	6.41	7.39	8.92	11.33	15.06
		1.50	0.61	0.22	0.07	0.02	0.01
		0.12	0.08	0.08	0.09	0.12	0.16
PF2MP	PERFLUORO-2-METHYLPE	57.50	2.18	2.16	7.43	1.15	
		5.78	6.41	7.39	8.92	11.33	15.06
		1.50	0.61	0.22	0.07	0.02	0.01
		0.12	0.08	0.08	0.09	0.12	0.16
PFHP	PERFLUOROHEPTANE	82.60	2.01	2.05	3.15	1.16	
		4.56	5.31	6.55	8.59	12.11	18.24
		3.41	1.59	0.62	0.20	0.05	0.01
		0.33	0.21	0.20	0.23	0.27	0.33
BRCLM	BROMOCHLOROMETHANE	68.10	8.78	6.83	1.0E+18	2.07	
		2.37	2.43	2.49	2.54	2.58	2.62
		0.33	0.24	0.19	0.17	0.15	0.16
		0.08	0.10	0.14	0.18	0.22	0.23
IBA	ISOBUTANOL	107.70	8.80	7.52	0.73	2.40	
		2.29	2.08	1.89	1.71	1.55	1.41
		2.22	1.39	0.87	0.55	0.34	0.19
		1.01	0.79	0.61	0.48	0.37	0.30
EVANILLN	ETHYL VANILLIN	293.90	4.24	4.21	0.46	1.96	
		5.26	5.61	5.90	6.23	6.68	7.30
		1238.05	21401.17	6684.67	1568.44	291.10	39.18
		46.73	305.45	491.99	600.51	684.73	767.38
PFHX	PERFLUOROHEXANE	57.10	2.09	2.07	0.84	1.13	
		5.76	6.37	7.34	8.84	11.20	14.85
		1.52	0.62	0.22	0.07	0.02	0.01
		0.12	0.08	0.08	0.10	0.12	0.16
ADIPNTRL	ADIPONITRILE	295.00	6.11	5.80	0.58	2.43	
		4.25	4.19	3.99	3.74	3.46	3.20
		299.76	1542.23	782.83	295.10	92.45	24.49
		48.83	163.13	210.20	214.34	194.17	162.19
MECLFORM	METHYL CHLOROFORMATE	70.90	7.91	6.36	5.70	2.00	
		4.22	3.68	3.19	2.76	2.39	2.08
		1.46	0.45	0.21	0.12	0.09	0.07
		0.23	0.18	0.16	0.14	0.14	0.14
PFNONANE	PERFLUORONONANE	125.40	1.84	1.95	0.45	1.18	
		9.07	9.24	9.23	9.11	8.93	8.73
		10.22	6.41	2.94	1.00	0.21	0.03
		0.70	0.75	0.83	0.96	1.17	1.56
PYRR	PYRROLE	129.90	11.93	9.47	2.22	2.83	
		1.80	1.59	1.39	1.21	1.05	0.93
		2.68	1.62	1.24	1.09	1.02	1.00
		1.77	1.30	1.07	0.95	0.88	0.85
DIPE	DIISOPROPYL ETHER	68.30	1.37	1.30	9.97	0.95	
		1.16	1.05	0.94	0.85	0.76	0.69
		0.18	0.19	0.19	0.20	0.21	0.22
		0.26	0.19	0.16	0.13	0.12	0.13
SBTAMINE	sec-BUTYLAMINE	63.00	1.79	1.58	9.28	0.95	
		1.97	1.78	1.61	1.46	1.31	1.19
		0.19	0.17	0.16	0.15	0.15	0.16
		0.11	0.11	0.12	0.13	0.14	0.17
PFLRDECN	PERFLUORODECANE	144.30	1.70	1.83	0.40	1.17	
		8.76	9.11	9.23	9.23	9.17	9.06
		15.27	11.44	5.74	2.00	0.40	0.03
		1.13	1.22	1.37	1.63	2.12	3.18

DMEN	1,2-DIMETHOXYETHANE	84.10	1.72	1.53	8.64	0.95	
		3.19	2.88	2.58	2.31	2.07	1.86
		1.31	0.69	0.39	0.24	0.16	0.12
		0.36	0.31	0.28	0.26	0.24	0.24
AC2O	ACETIC ANHYDRIDE	139.60	4.92	4.29	6.90	1.71	
		1.34	1.30	1.26	1.23	1.19	1.15
		1.49	1.57	1.66	1.76	1.86	1.94
		1.17	1.26	1.37	1.48	1.60	1.70
SALAL	SALICYLALDEHYDE	196.50	5.94	5.42	1.51	2.13	
		5.52	6.08	6.76	7.70	9.12	11.27
		172.10	87.02	21.22	5.88	1.53	0.31
		10.70	8.53	6.83	6.08	5.92	6.13
GBLAC	gamma-BUTYROLACTONE	204.00	7.97	6.65	3.44	2.41	
		3.51	3.30	3.03	2.74	2.47	2.23
		35.14	29.04	14.39	7.68	4.45	2.80
		8.38	8.94	8.62	8.14	7.69	7.33
DBRM	DIBROMOMETHANE	97.00	13.74	10.85	0.24	2.98	
		1.04	1.23	1.52	1.96	2.69	3.88
		0.30	0.38	0.48	0.59	0.67	0.67
		0.12	0.23	0.38	0.56	0.77	0.99
2PHDIAM	o-PHENYLENEDIAMINE	251.90	2.01	2.02	1.75	1.23	
		10.53	10.74	9.42	7.92	6.56	5.46
		7544.52	2188.70	242.31	44.53	9.30	1.80
		49.63	77.00	59.08	44.35	31.75	20.58
DMF	N,N-DIMETHYLFORMAMIDE	153.00	11.14	9.21	0.78	2.89	
		4.03	3.73	3.39	3.04	2.72	2.44
		21.82	8.90	3.40	1.54	0.78	0.43
		3.72	3.01	2.36	1.83	1.42	1.12
OETHANLN	o-PHENETIDINE	230.70	5.82	5.70	0.34	2.32	
		3.98	3.89	3.70	3.47	3.23	3.01
		56.33	103.57	60.62	29.35	12.35	4.41
		11.43	17.77	22.43	24.86	25.02	23.01
12CE	1,2-DICHLOROETHANE	83.40	4.78	3.95	6.35	1.51	
		2.32	2.19	2.06	1.94	1.82	1.72
		0.69	0.41	0.31	0.27	0.26	0.26
		0.21	0.23	0.26	0.28	0.31	0.33
FMCH	PERFLUOROMETHYLCYCLO	76.40	1.63	1.75	3.55	1.12	
		5.01	5.68	6.74	8.40	11.11	15.48
		2.63	1.14	0.44	0.15	0.04	0.02
		0.23	0.16	0.16	0.19	0.24	0.29
IHPTANOL	ISOHEPTANOL	172.00	2.09	2.05	0.21	1.18	
		9.54	9.57	8.85	7.93	7.02	6.21
		100.34	100.44	28.63	6.01	0.76	0.03
		6.22	6.58	6.06	4.75	2.75	0.76
MEBU	METHYL n-BUTYRATE	102.80	1.70	1.56	8.76	0.98	
		1.77	1.61	1.46	1.31	1.19	1.08
		0.85	0.71	0.61	0.54	0.48	0.44
		0.58	0.52	0.48	0.46	0.45	0.45
NMP	N-METHYL-2-PYRROLIDO	202.00	6.71	5.99	8.83	2.28	
		3.09	2.98	2.84	2.68	2.52	2.37
		26.34	24.09	13.66	7.83	4.71	3.02
		7.48	7.85	7.87	7.94	8.16	8.51
TCLE	1,1,2-TRICHLOROETHANE	113.90	11.60	10.29	0.40	3.04	
		2.23	2.33	2.43	2.53	2.62	2.70
		1.60	1.10	0.84	0.69	0.61	0.55
		0.40	0.50	0.63	0.77	0.91	1.00
TEG	TRIETHYLENE GLYCOL	288.40	5.30	5.20	3.15	2.26	
		5.31	5.27	5.02	4.69	4.34	4.01
		627.38	4128.95	1800.42	457.81	62.24	3.18
		56.99	227.64	270.72	222.37	134.95	57.10
TLDA	TOLUENEDIAMINE	284.00	3.95	3.94	0.20	1.87	
		6.12	6.17	5.85	5.41	4.95	4.53
		741.90	2756.32	794.71	218.70	54.59	11.18
		40.29	132.54	159.45	155.90	141.76	124.89

MACA	METHYL ACRYLATE	80.20	3.55	3.02	6.71	1.30	
		2.58	2.43	2.29	2.16	2.03	1.92
		0.69	0.45	0.31	0.23	0.18	0.16
		0.21	0.22	0.23	0.24	0.24	0.24
MACA	METHYL ACRYLATE	80.20	3.55	3.02	6.71	1.30	
		2.58	2.43	2.29	2.16	2.03	1.92
		0.69	0.45	0.31	0.23	0.18	0.16
		0.21	0.22	0.23	0.24	0.24	0.24
PFDCLN	PERFLUORODECALIN	141.90	1.91	2.00	0.47	1.19	
		8.16	8.36	8.31	8.13	7.88	7.61
		13.13	8.06	3.80	1.39	0.35	0.06
		1.07	1.15	1.28	1.49	1.89	2.75
PHHYDRZN	PHENYLHYDRAZINE	243.50	6.42	5.84	1.75	2.33	
		3.49	3.24	2.92	2.59	2.29	2.03
		94.15	112.72	50.58	27.10	16.60	11.27
		21.25	29.45	28.45	26.94	26.00	25.62
PTBUCAT	p-tert-BUTYLCATECHOL	284.90	2.18	2.23	0.28	1.32	
		5.76	6.49	7.17	7.90	8.81	9.97
		84.83	572.55	584.36	389.63	196.35	75.34
		8.11	21.00	65.20	207.62	716.51	2740.07
BAMN	n-BUTYLAMINE	77.40	2.33	2.04	7.72	1.06	
		2.19	2.04	1.89	1.76	1.64	1.53
		0.42	0.34	0.28	0.23	0.20	0.19
		0.18	0.19	0.20	0.22	0.23	0.25
TBA	tert-BUTANOL	82.40	7.22	6.17	0.73	2.03	
		2.94	2.68	2.44	2.21	2.02	1.84
		1.37	0.76	0.42	0.22	0.11	0.05
		0.45	0.34	0.26	0.19	0.15	0.12
FALD	FURFURAL	161.70	8.39	7.16	2.03	2.46	
		4.11	3.81	3.44	3.07	2.73	2.43
		25.68	12.31	4.66	2.03	0.98	0.51
		5.06	3.70	2.78	2.22	1.87	1.63
MDEA	METHYL DIETHANOLAMINE	247.00	5.34	5.05	7.43	2.13	
		4.19	4.07	3.84	3.57	3.30	3.05
		221.37	862.58	380.42	105.75	16.86	1.08
		35.92	91.31	88.00	59.90	30.42	11.09
ETLACT	ETHYL LACTATE	154.50	3.16	2.99	5.61	1.42	
		3.99	3.78	3.51	3.24	2.98	2.74
		15.73	10.20	4.96	2.20	0.82	0.23
		3.16	2.94	2.57	2.13	1.65	1.19
CE12	cis-1,2-DICHLOROETHYLE	60.50	4.78	3.92	5.70	1.46	
		2.06	1.99	1.91	1.83	1.74	1.66
		0.24	0.14	0.12	0.12	0.14	0.16
		0.08	0.09	0.10	0.12	0.14	0.18
14DCY2B	1,4-DICYANO-2-BUTENE	273.90	4.65	4.37	0.17	1.96	
		4.93	4.87	4.60	4.25	3.88	3.53
		299.88	1538.72	583.76	170.23	42.92	9.45
		37.65	107.28	125.20	115.64	95.23	72.56
12PRODAM	1,2-PROPANEDIAMINE	119.30	6.66	5.68	15.66	2.00	
		3.15	2.93	2.71	2.49	2.30	2.12
		3.79	2.25	1.29	0.74	0.42	0.25
		0.99	0.92	0.84	0.76	0.66	0.57
MXET	2-METHOXYETHYL ACETAT	144.50	3.15	2.93	6.12	1.39	
		2.90	2.73	2.55	2.37	2.20	2.04
		6.65	4.51	2.73	1.63	0.95	0.55
		1.95	1.89	1.79	1.64	1.44	1.22
PRNT	PROPIONITRILE	97.40	9.80	7.71	1.39	2.34	
		3.60	3.30	3.00	2.72	2.47	2.26
		1.99	1.02	0.58	0.36	0.24	0.17
		0.41	0.41	0.41	0.41	0.41	0.40
DIPRPGLY	DIPROPYLENE GLYCOL	231.80	4.80	4.66	4.67	2.01	
		4.43	4.33	4.12	3.85	3.58	3.33
		124.62	349.51	172.31	55.86	10.75	0.87
		20.82	40.62	42.89	34.57	22.01	10.60

13PO	1,3-PROPYLENE OXIDE	47.90	8.50	6.44	16.54	1.91	
		0.80	0.88	1.02	1.21	1.51	1.96
		0.05	0.06	0.08	0.11	0.13	0.15
		0.05	0.05	0.06	0.07	0.10	0.13
HXG	HEXYLENE GLYCOL	197.50	4.04	3.84	4.67	1.71	
		3.70	3.57	3.37	3.16	2.94	2.74
		46.96	82.83	45.49	17.20	4.19	0.49
		10.99	14.61	14.17	11.18	7.32	3.91
NTRETH	NITROETHANE	114.10	9.64	7.66	1.01	2.39	
		3.96	3.69	3.40	3.12	2.86	2.63
		3.83	2.00	1.06	0.59	0.34	0.20
		0.70	0.69	0.68	0.67	0.66	0.65
PFCH	PERFLUOROCYCLOHEXANE	52.60	1.02	0.97	7.43	1.07	
		6.44	6.81	7.41	8.34	9.75	11.78
		1.14	0.43	0.15	0.05	0.02	0.01
		0.08	0.06	0.06	0.07	0.10	0.13
EACR	ETHYL ACRYLATE	99.50	2.13	1.93	7.08	1.06	
		2.22	2.10	1.99	1.88	1.77	1.68
		1.04	0.78	0.59	0.45	0.36	0.29
		0.41	0.43	0.44	0.44	0.44	0.43
EACR	ETHYL ACRYLATE	99.50	2.13	1.93	7.08	1.06	
		2.22	2.10	1.99	1.88	1.77	1.68
		1.04	0.78	0.59	0.45	0.36	0.29
		0.41	0.43	0.44	0.44	0.44	0.43
NBA	n-BUTANOL	117.70	10.49	8.93	0.73	2.73	
		2.40	2.24	2.09	1.94	1.80	1.67
		3.11	2.18	1.35	0.78	0.41	0.20
		1.35	1.07	0.84	0.66	0.52	0.42
MOXYPHL	3-METHOXYPHENOL	242.90	3.34	3.32	0.28	1.63	
		3.53	3.90	4.45	5.27	6.58	8.65
		121.73	263.75	115.58	46.64	17.32	5.58
		16.80	23.72	28.92	36.36	47.26	61.12
PMEOXPHN	p-METHOXYPHENOL	242.90	3.34	3.32	0.31	1.63	
		3.53	3.90	4.45	5.27	6.58	8.65
		121.73	263.75	115.58	46.64	17.32	5.58
		16.80	23.72	28.92	36.36	47.26	61.12
IBFT	ISOBUTYL FORMATE	98.10	1.68	1.54	7.31	0.98	
		2.30	2.13	1.97	1.82	1.68	1.56
		0.99	0.75	0.57	0.44	0.35	0.28
		0.42	0.41	0.41	0.42	0.42	0.43
DEGMME	2-(2-METHOXYETHOXY) ETHANOL	193.60	2.76	2.61	5.29	1.34	
		3.98	3.84	3.62	3.38	3.12	2.89
		40.68	52.44	25.37	9.88	3.13	0.74
		8.39	9.84	9.43	7.99	6.15	4.37
SBACTAT	sec-BUTYL ACETATE	112.00	1.19	1.13	7.88	0.95	
		1.82	1.67	1.52	1.39	1.26	1.15
		1.22	1.01	0.84	0.70	0.60	0.52
		0.78	0.70	0.65	0.61	0.59	0.57
MCLA	METHYL CHLOROACETATE	129.80	6.02	5.21	4.82	1.92	
		3.37	3.08	2.78	2.50	2.25	2.03
		6.41	2.94	1.52	0.91	0.60	0.43
		1.37	1.24	1.12	1.01	0.91	0.83
BFORMATE	n-BUTYL FORMATE	106.10	1.97	1.80	6.94	1.04	
		2.25	2.09	1.93	1.78	1.65	1.53
		1.24	0.95	0.73	0.56	0.44	0.35
		0.55	0.53	0.52	0.52	0.53	0.53
GUAIACOL	GUAIACOL	205.00	3.27	3.03	0.28	1.47	
		3.62	3.98	4.53	5.36	6.69	8.81
		57.78	52.02	22.06	9.00	3.33	1.03
		8.05	7.66	7.72	8.49	9.93	11.90
DETM	DIETHYLENE TRIAMINE	207.10	5.67	5.22	12.92	2.10	
		2.96	2.82	2.65	2.46	2.29	2.12
		23.57	28.11	17.90	9.90	5.08	2.49
		7.38	8.85	9.29	8.90	7.97	6.76

2M1PNALC	2-METHYL-1-PENTANOL	148.00	3.05	2.87	5.98	1.38	
		2.15	2.02	1.88	1.75	1.63	1.52
		5.21	4.41	3.25	2.17	1.30	0.69
		2.55	2.34	2.07	1.80	1.54	1.30
AACETAT	ALLYL ACETATE	104.00	2.00	1.80	6.77	1.03	
		2.52	2.30	2.08	1.88	1.69	1.54
		1.60	1.03	0.69	0.49	0.37	0.29
		0.61	0.56	0.51	0.48	0.46	0.44
DIPA	DIISOPROPANOLAMINE	248.80	4.36	4.20	3.55	1.89	
		4.02	3.88	3.65	3.39	3.13	2.89
		178.78	941.60	521.90	169.19	28.15	1.43
		32.76	94.26	108.00	83.93	45.34	14.98
DIPA	DIISOPROPANOLAMINE	248.80	4.36	4.20	3.55	1.89	
		4.02	3.88	3.65	3.39	3.13	2.89
		178.78	941.60	521.90	169.19	28.15	1.43
		32.76	94.26	108.00	83.93	45.34	14.98
DIPA	DIISOPROPANOLAMINE	248.80	4.36	4.20	3.55	1.89	
		4.02	3.88	3.65	3.39	3.13	2.89
		178.78	941.60	521.90	169.19	28.15	1.43
		32.76	94.26	108.00	83.93	45.34	14.98
CAPNTRL	HEXANENITRILE	163.60	1.36	1.28	7.11	0.96	
		2.19	2.07	1.95	1.83	1.71	1.60
		5.44	4.77	3.83	2.94	2.17	1.57
		2.48	2.58	2.67	2.75	2.78	2.75
DEXM	DIETHOXYMETHANE	88.00	1.05	0.98	7.43	0.99	
		2.02	1.85	1.68	1.52	1.38	1.26
		0.63	0.50	0.40	0.33	0.28	0.24
		0.35	0.32	0.30	0.29	0.29	0.29
TBUTHYPR	t-BUTYL HYDROPEROXIDE	132.40	6.79	6.04	4.47	2.15	
		1.42	1.32	1.23	1.14	1.06	0.98
		1.36	1.37	1.40	1.42	1.44	1.46
		1.15	1.16	1.16	1.17	1.17	1.18
MEACACT	METHYL ACETOACETATE	171.70	3.54	3.22	4.94	1.48	
		2.75	2.60	2.43	2.26	2.09	1.94
		12.02	9.31	5.86	3.69	2.36	1.54
		3.76	3.89	3.87	3.70	3.40	3.01
THFA	TETRAHYDROFURFURYL ALCOHOL	178.00	5.36	4.77	8.76	1.91	
		3.18	3.01	2.81	2.61	2.41	2.23
		19.82	16.53	9.07	4.52	2.03	0.79
		5.54	5.43	4.85	4.12	3.37	2.69
IBAC	ISOBUTYL ACETATE	116.60	1.43	1.36	7.18	0.97	
		1.56	1.47	1.38	1.30	1.22	1.16
		1.15	1.07	0.96	0.84	0.70	0.56
		0.88	0.79	0.73	0.68	0.66	0.64
4CLPHNOL	p-CHLOROPHENOL	220.00	2.57	2.56	0.17	1.38	
		4.76	5.08	5.40	5.75	6.21	6.81
		24.23	30.04	22.08	14.87	9.79	6.49
		2.50	4.84	9.64	18.12	31.50	50.19
MMAC	METHYL METHACRYLATE	100.30	3.14	2.83	5.45	1.30	
		2.21	2.08	1.94	1.82	1.70	1.60
		1.03	0.77	0.58	0.45	0.36	0.29
		0.43	0.43	0.43	0.43	0.41	0.40
2E1BALC	2-ETHYL-1-BUTANOL	146.50	2.72	2.54	5.65	1.28	
		2.16	2.02	1.88	1.75	1.63	1.52
		5.02	4.12	2.98	1.98	1.18	0.62
		2.46	2.22	1.94	1.67	1.41	1.19
ACCL	ACETYL CHLORIDE	50.80	5.71	4.46	3.80	1.53	
		3.44	3.17	2.91	2.68	2.47	2.29
		0.24	0.15	0.10	0.08	0.06	0.07
		0.05	0.06	0.07	0.08	0.10	0.13
3MOXYNIT	3-METHOXYPROPIONITRILE	165.90	4.30	3.78	11.21	1.62	
		4.52	4.29	3.98	3.64	3.31	3.01
		22.66	13.76	5.95	2.59	1.11	0.47
		3.61	3.54	3.30	2.93	2.43	1.88

DPRE	DI-n-PROPYL ETHER	90.10	1.06	1.01	7.36	1.00	
		1.32	1.20	1.09	0.98	0.89	0.81
		0.43	0.42	0.40	0.39	0.38	0.38
		0.47	0.39	0.33	0.30	0.27	0.26
PHOH	PHENOL	181.80	3.61	3.68	1.75	1.69	
		5.93	6.10	6.16	6.17	6.19	6.25
		18.24	13.28	7.69	4.79	3.17	2.21
		1.32	2.15	3.59	6.06	10.30	17.15
2CLPHNOL	o-CHLOROPHENOL	174.40	2.13	2.16	0.27	1.24	
		5.08	5.37	5.67	6.04	6.54	7.22
		10.69	8.36	5.48	3.50	2.21	1.40
		0.86	1.66	2.90	4.78	7.54	11.29
CPTN	CYCLOPENTANONE	130.60	3.74	3.26	4.89	1.42	
		2.16	1.99	1.82	1.66	1.51	1.39
		2.37	1.79	1.39	1.13	0.95	0.83
		1.09	1.09	1.08	1.09	1.09	1.09
DMOT	DIMETHYL OXALATE	163.50	4.35	3.92	6.71	1.67	
		4.34	4.07	3.72	3.37	3.03	2.73
		28.39	14.37	5.45	2.40	1.16	0.60
		4.22	3.86	3.31	2.74	2.23	1.80
3CLPHNOL	m-CHLOROPHENOL	213.90	2.34	2.33	0.17	1.30	
		4.79	5.11	5.42	5.77	6.23	6.84
		21.85	24.95	17.98	12.00	7.84	5.15
		2.20	4.20	8.13	14.92	25.48	40.15
EBE	n-BUTYL ETHYL ETHER	92.20	1.05	1.00	7.26	1.01	
		1.31	1.20	1.08	0.98	0.89	0.81
		0.47	0.45	0.43	0.42	0.41	0.40
		0.51	0.42	0.36	0.32	0.29	0.28
BROMFORM	TRIBROMOMETHANE	149.20	3.99	3.51	1.0E+18	1.52	
		4.94	4.64	4.24	3.82	3.42	3.06
		22.66	9.42	3.34	1.32	0.56	0.25
		3.10	2.55	2.04	1.62	1.28	1.00
R114B2	1,2-DIBROMOTETRAFLUOR	47.30	1.12	1.02	0.02	0.94	
		9.01	8.25	7.51	6.83	6.22	5.70
		1.14	0.36	0.12	0.04	0.01	0.01
		0.07	0.06	0.06	0.07	0.08	0.10
CL2M	DICHLOROMETHANE	39.80	8.85	6.68	0.81	1.93	
		3.87	3.46	3.08	2.75	2.47	2.23
		0.06	0.05	0.06	0.06	0.08	0.10
		0.01	0.02	0.04	0.07	0.11	0.15
PROPINM	PROPYLENEIMINE	60.90	6.83	5.37	0.53	1.75	
		1.90	1.65	1.43	1.24	1.07	0.93
		0.16	0.14	0.14	0.14	0.15	0.17
		0.12	0.10	0.10	0.11	0.13	0.15
2BEA	2-BUTOXYETHANOL	171.30	2.53	2.43	5.19	1.28	
		2.63	2.49	2.34	2.19	2.04	1.90
		10.78	9.69	6.70	4.00	2.02	0.82
		4.04	4.00	3.75	3.38	2.93	2.45
DEOE	ACETAL (1,1-DIETHOXYETH	103.60	1.11	1.06	6.85	0.98	
		1.78	1.64	1.51	1.38	1.27	1.16
		0.90	0.77	0.64	0.54	0.45	0.39
		0.58	0.54	0.50	0.46	0.44	0.42
MRPN	MORPHOLINE	128.00	4.75	4.09	4.01	1.63	
		2.17	1.98	1.79	1.61	1.46	1.32
		2.55	1.78	1.31	1.03	0.85	0.73
		1.20	1.10	1.03	0.98	0.94	0.91
1122TBRE	1,1,2,2-TETRABROMOETHA	243.50	3.47	3.30	3.51	1.60	
		4.66	4.58	4.32	3.99	3.65	3.34
		109.36	212.53	91.85	32.71	10.38	2.97
		18.57	29.09	31.49	29.17	24.24	18.28
1BRPRPAN	1-BROMOPROPANE	71.00	2.01	1.74	6.12	0.98	
		1.89	1.75	1.61	1.48	1.37	1.27
		0.27	0.23	0.21	0.20	0.20	0.21
		0.15	0.16	0.16	0.18	0.19	0.21

DECARB	DIETHYL CARBONATE	126.80	1.89	1.76	6.28	1.05	
		1.43	1.33	1.24	1.15	1.06	0.99
		1.16	1.16	1.17	1.17	1.17	1.17
		0.98	0.98	0.98	0.98	0.98	0.98
OEBT	ETHYL ACETOACETATE	180.80	2.46	2.34	4.65	1.26	
		3.16	3.02	2.84	2.66	2.47	2.30
		16.17	14.77	8.96	4.96	2.62	1.36
		4.54	4.81	4.85	4.73	4.51	4.25
DIIM	DIIODOMETHANE	182.00	5.62	4.84	0.22	1.92	
		1.57	1.62	1.68	1.77	1.87	1.99
		3.90	4.34	4.85	5.39	5.93	6.38
		1.89	2.59	3.62	5.07	7.04	9.49
OMANILIN	o-ANISIDINE	220.50	2.64	2.66	0.20	1.41	
		5.63	5.53	5.15	4.68	4.22	3.80
		131.47	158.90	51.46	17.68	6.05	1.92
		12.83	17.94	18.90	17.46	14.83	11.81
CPLT	CAPROLACTONE	215.00	5.02	4.65	3.65	1.95	
		2.38	2.25	2.11	1.95	1.81	1.67
		26.80	41.94	35.95	27.63	20.90	16.14
		11.67	17.23	21.37	24.43	26.86	28.80
DMEETAM	DIMETHYLETHANOLAMINE	134.00	6.08	5.40	10.75	1.99	
		1.16	1.12	1.08	1.04	1.01	0.98
		1.32	1.37	1.43	1.50	1.57	1.63
		1.35	1.27	1.21	1.19	1.17	1.17
TETM	TRIETHYLENE TETRAMINE	266.50	3.25	3.25	3.15	1.63	
		4.00	4.02	3.95	3.84	3.70	3.56
		123.03	546.99	374.12	167.55	53.22	11.75
		23.59	61.51	90.00	107.85	116.89	118.19
ALCN	VINYLACETONITRILE	118.50	4.66	3.86	4.49	1.54	
		3.57	3.30	3.01	2.74	2.49	2.28
		4.55	2.28	1.19	0.66	0.39	0.24
		1.00	0.89	0.81	0.74	0.69	0.65
PNAMINE	n-PENTYLAMINE	104.50	1.86	1.71	5.76	1.02	
		1.94	1.79	1.65	1.51	1.39	1.28
		0.92	0.78	0.66	0.56	0.49	0.43
		0.51	0.51	0.51	0.51	0.51	0.51
PYRO	PYRROLIDINE	86.60	4.00	3.38	4.48	1.39	
		1.57	1.40	1.23	1.09	0.96	0.85
		0.40	0.37	0.35	0.34	0.34	0.34
		0.38	0.31	0.27	0.26	0.26	0.28
12PR	1,2-DICHLOROPROPANE	96.40	1.81	1.61	5.82	0.97	
		1.73	1.65	1.57	1.50	1.42	1.35
		0.65	0.55	0.49	0.46	0.44	0.44
		0.35	0.37	0.39	0.42	0.44	0.46
112TRBRE	1,1,2-TRIBROMOETHANE	188.40	3.82	3.50	5.70	1.59	
		3.94	3.76	3.49	3.20	2.91	2.65
		30.74	25.24	11.71	5.34	2.45	1.14
		6.29	6.53	6.19	5.56	4.81	4.05
T4MCHXNL	trans-4-METHYLCYCLOHE	171.00	3.56	3.35	3.98	1.54	
		2.09	1.96	1.84	1.71	1.60	1.49
		8.32	8.29	6.63	4.68	2.94	1.63
		4.27	4.30	4.09	3.76	3.38	3.02
22M1	2,2-DIMETHYL-1-PROPAN	113.10	4.97	4.46	4.19	1.73	
		2.46	2.28	2.10	1.94	1.78	1.65
		2.68	1.81	1.14	0.68	0.37	0.18
		1.10	0.90	0.72	0.58	0.46	0.36
25DHYFUR	2,5-DIHYDROFURAN	65.90	5.18	4.18	4.52	1.52	
		2.50	2.37	2.25	2.13	2.01	1.91
		0.38	0.22	0.16	0.14	0.14	0.15
		0.10	0.11	0.13	0.15	0.17	0.20
T3MCHXNL	trans-3-METHYLCYCLOHE	168.00	3.39	3.17	3.99	1.48	
		2.09	1.97	1.84	1.72	1.60	1.49
		7.79	7.59	6.00	4.21	2.63	1.45
		3.98	3.95	3.72	3.40	3.04	2.70

2NANL	o-NITROANILINE	284.90	2.80	2.83	0.42	1.51	
		5.29	4.96	4.34	3.69	3.11	2.64
		1552.49	2354.59	521.35	151.88	48.81	15.70
		93.16	242.01	193.46	144.60	96.73	51.10
C4MCHXNL	cis-4-METHYLCYCLOHEXA	171.00	3.62	3.40	3.77	1.55	
		2.09	1.96	1.84	1.71	1.60	1.49
		8.24	8.21	6.58	4.65	2.92	1.63
		4.23	4.25	4.04	3.72	3.35	2.99
C3MCHXNL	cis-3-METHYLCYCLOHEXA	168.00	3.29	3.09	4.03	1.46	
		2.09	1.97	1.84	1.72	1.60	1.49
		7.98	7.89	6.27	4.41	2.76	1.53
		4.08	4.09	3.88	3.55	3.18	2.83
EGDIACT	ETHYLENE GLYCOL DIACET	190.50	2.03	1.96	4.53	1.16	
		2.97	2.82	2.63	2.43	2.24	2.07
		23.22	23.24	13.18	6.82	3.48	1.81
		7.42	7.49	6.86	6.08	5.34	4.74
DEOXLAT	DIETHYL OXALATE	185.70	1.78	1.72	4.64	1.09	
		3.02	2.87	2.69	2.50	2.32	2.15
		16.87	15.11	9.39	5.52	3.18	1.84
		4.93	5.35	5.50	5.41	5.13	4.72
1MCHXNOL	1-METHYLCYCLOHEXANOL	157.00	3.06	2.87	4.19	1.39	
		2.05	1.93	1.80	1.68	1.57	1.47
		5.77	5.26	4.13	2.92	1.84	1.01
		3.03	2.88	2.65	2.38	2.10	1.83
CYHPEROX	CYCLOHEXYL PEROXIDE	216.90	5.22	4.89	7.88	2.03	
		1.34	1.26	1.17	1.09	1.02	0.95
		8.26	13.44	19.60	25.76	31.77	37.31
		7.70	11.57	15.88	20.02	23.96	27.52
THDPYRAN	TETRAHYDROPYRAN	88.40	1.87	1.67	5.58	0.99	
		1.51	1.36	1.21	1.09	0.97	0.87
		0.41	0.39	0.37	0.37	0.37	0.37
		0.38	0.33	0.30	0.29	0.29	0.29
CDCY2BT	cis-DICYANO-1-BUTENE	227.90	5.25	4.81	0.17	2.01	
		1.34	1.25	1.17	1.09	1.02	0.95
		9.98	16.57	23.69	30.41	36.73	42.42
		9.37	14.35	19.35	23.90	28.07	31.75
T2MCHXNL	trans-2-METHYLCYCLOHE	166.50	3.32	3.11	3.85	1.46	
		2.09	1.97	1.84	1.72	1.60	1.49
		7.98	7.89	6.27	4.41	2.76	1.53
		4.08	4.09	3.88	3.55	3.18	2.83
TCEE	TRICHLOROETHYLENE	87.00	2.39	2.09	4.31	1.08	
		2.99	2.75	2.52	2.31	2.12	1.96
		0.38	0.36	0.35	0.35	0.36	0.37
		0.11	0.16	0.25	0.37	0.54	0.74
EDBR	1,2-DIBROMOETHANE	131.40	4.28	3.73	2.80	1.55	
		3.05	2.81	2.56	2.33	2.12	1.93
		4.80	2.71	1.59	1.01	0.68	0.48
		1.28	1.22	1.15	1.09	1.02	0.96
BVETHER	BUTYL VINYL ETHER	93.80	1.18	1.11	5.86	0.94	
		1.58	1.45	1.33	1.22	1.12	1.03
		0.52	0.48	0.45	0.43	0.41	0.39
		0.40	0.38	0.37	0.36	0.35	0.34
C2MCHXNL	cis-2-METHYLCYCLOHEXA	165.00	3.20	2.99	3.82	1.43	
		2.10	1.98	1.85	1.72	1.60	1.50
		7.32	6.60	5.00	3.43	2.11	1.14
		3.73	3.55	3.23	2.87	2.51	2.18
DIMA	N,N-DIMETHYLACETAMIDE	166.10	4.07	3.59	3.95	1.56	
		0.97	0.85	0.73	0.63	0.54	0.46
		13.61	9.71	5.30	2.79	1.44	0.74
		64.53	11.52	3.60	1.65	0.87	0.48
DMMALATE	DIMETHYL MALEATE	205.00	2.45	2.34	3.65	1.28	
		3.10	3.03	2.93	2.80	2.67	2.53
		24.35	28.99	18.87	10.80	5.84	3.09
		6.84	8.43	9.67	10.33	10.26	9.43

12DFETHN	1,2–DIFLUOROETHANE	30.50	5.87	4.29	6.35	1.42	
		1.47	1.47	1.47	1.47	1.48	1.48
		0.01	0.01	0.01	0.02	0.03	0.05
		0.00	0.01	0.01	0.01	0.02	0.04
DAA	DIACETONE ALCOHOL	167.90	3.13	2.97	0.64	1.43	
		3.98	3.82	3.60	3.37	3.14	2.92
		18.76	15.15	7.99	3.51	1.21	0.29
		4.01	3.92	3.61	3.14	2.55	1.94
PRANHYD	PROPIONIC ANHYDRIDE	167.00	1.85	1.77	5.23	1.09	
		1.31	1.23	1.15	1.08	1.01	0.95
		3.06	3.32	3.58	3.82	4.05	4.25
		2.85	2.97	3.07	3.14	3.20	3.23

C2: ASEEK PROGRAM

```
Program ASeek;

{-------------------------------------------------------------------------
    ASEEK Version: 3.0

    Date: March 1993
    Last update (DD/MM/YY): 1/4/93

    (c) BJ van der Merwe

    Requirements:
      - The program must have access its database file: AGENTS.INF.
      - The computer must be a 286 or later with a maths coprocessor.
      - Access to the PRO/II BATCH system must have been arranged.
        (If this is a problem, alter the program to submit only one
         input file at a time using the FEED.BAT P2 xxx or LANP2
         commands instead of BATCH.EXE.)
-------------------------------------------------------------------------}

{Use extra 286 instructions to improve code:}
{$G+}

{Force far calls:}
{$F+}

{Align data:}
{$A+}

{Enable input/output checking:}
{$I+}

{Enable range checking:}
{$R+}

{Enable stack checking:}
{$S+}

{Use the math coprocessor and do not emulate it:}
{$N+,E-}
{Change this to $N+,E+ if you do not have a mah coprocessor.}

{Set memory so that sub-processes (EXEC) can be used:}
{$M 16384,0,81920}

{Use the standard CRT and DOS units for screen IO and Exec:}

Uses Overlay,
     CRT,
     DOS,

     ASEEKU,     {Some basic definitions and variable declarations.}
     ASEEKU1,    {Overlay units.}
     ASEEKU2,
```

```
     ASEEKU3;

{$O DOS}
{$O ASEEKU1}
{$O ASEEKU2}
{$O ASEEKU3}

Var c: char;          {A character read from the keyboard.}
    i: integer;
    we1,we2,we3,we4,we5,wt: rtype;    {Weights for the different models
                                         when sorting results.}

{Calculate r1^r2}
Function Power (r1,r2: rtype): rtype;
  Begin
    If r1=0.0 then Power:=0                    {0^x=0 but ln(0) is not
allowed!}
              else Power:=exp(r2*ln(r1));  {x^y=exp(y*ln(x))}
end {Power};

{Determine those MOSCED parameters which depend on one component only.}
{(According to the formulas of Thomas and Eckert, p.203)}

Procedure Do_MOSCED (var cc: param; il:any);
  Var nd: rtype;          {Refractive index}
      i: integer;
      Ct,Ca,Cb: rtype;    {Adjustable parameters.}
  Begin

    {Unable to handle water:}

    If cc.p2name='H2O       ' then il[27]:=' ';

    {Are MOSCED parameters available?:}

    If il[27]=' ' then    {No data for MOSCED model}
       cc.OK:=false
    else begin

       cc.OK:=true;

      {Get the refractive index:}

      Val (copy(il,27,4),nd,i);

      {Compute the dispersion parameter:}

      case il[3] of
           'p','c': Begin
                      cc.disp:=10.3*(nd*nd-1)/(nd*nd+2)+3.02;
{non-aromatic}
                    end;
           'a':     Begin
                      cc.disp:=19.5*(nd*nd-1)/(nd*nd+2)+2.79;
{Aromatic}
                    end;
```

```
end;

{Get the induction parameter:}

Val (copy(il,a_q,4),cc.q,i);

{Get the classification code:}

cc.mc:=il[a_c];

{Number of carbon atoms:}

If il[a_nc]=' ' then cc.nc:=ord(il[a_nc+1])-48
                else Val (copy(il,a_nc,2),cc.nc,i);

{Assume everything is OK:}

cc.warn:=0;

Case cc.mc of
     '0':  Begin              {alkanes}
             Ct:=0.0;
             Ca:=0.0;
             Cb:=0.0;
           end;
     '1':  Begin              {chlorides}
             Ct:=2.69;
             Ca:=0.42;
             Cb:=0.25;
           end;
     '2':  Begin              {bromides}
             Ct:=2.47;
             Ca:=0.39;
             Cb:=0.38;
           end;
     '3':  Begin              {iodides}
             Ct:=2.02;
             Ca:=0.37;
             Cb:=0.30;
           end;
     '4':  Begin              {nitriles}
             Ct:=5.84;
             Ca:=0.33;
             Cb:=4.00;
           end;
     '5':  Begin              {nitroalkanes}
             Ct:=5.87;
             Ca:=0.35;
             Cb:=2.66;
           end;
     '6':  Begin              {alcohols}
             Ct:=1.65;
             Ca:=7.49;
             Cb:=7.49;
           end;
     '7':  Begin              {esters}
```

```
                    Ct:=4.03;
                    Ca:=0.00;
                    Cb:=4.64;
                  end;
          '8':    Begin              {ketones}
                    Ct:=3.93;
                    Ca:=0.00;
                    Cb:=4.87;
                  end;
          '9':    Begin              {Other}
                    cc.warn:=1;       {Component is not in a standard
class.}
                                     {Warn the user.}
                    Ct:=3.00;        {Guessed!}
                    Ca:=0.30;        {Guessed!}
                    Cb:=0.30;        {Guessed!}
                  end;
      end;

      {Get the normal boiling point, °C:}

      If il[21]=' ' then Val (copy(il,22,4),cc.nbp,i)
                    else Val (copy(il,21,5),cc.nbp,i);

      {Compute the group approach parameters}

      cc.t:=power((293/(cc.nbp+273.15)),0.4) *
            ( Ct*4.5/ (3.5+cc.nc) * (1+(cc.nc-1)/100) );

      cc.a:=power((293/(cc.nbp+273.15)),0.8) *
            ( Ca*4.5/ (3.5+cc.nc) * (1+(cc.nc-1)/100) );

      cc.b:=power((293/(cc.nbp+273.15)),0.8) *
            ( Cb*4.5/ (3.5+cc.nc) * (1+(cc.nc-1)/100) );

      {q already computed. Find other parameters:}

      cc.pol:=(sqr(cc.q)*sqr(cc.q))*
              (1.15-1.15*exp(-0.020*cc.t*cc.t*cc.t))+1;

      cc.phii:=cc.pol+0.011*cc.a*cc.b;

      cc.eps:=0.68*(cc.pol-1)+
              power(
                 (3.4-2.4*exp(
                    power(
                       (
                       ( Ca*4.5/ (3.5+cc.nc) * (1+(cc.nc-1)/100) ) *
                       ( Cb*4.5/ (3.5+cc.nc) * (1+(cc.nc-1)/100) )
                    ),1.5)
                    *(-0.23))
                 )
              ,sqr(293/(cc.nbp+273.15)));

      {Use special parameters for specific compounds at 20°C:}
```

```
      For i:=1 to nat20 do begin
        If cc.p2name=MOSCED20[i].p2name then begin
          cc.warn:=2;                          {Used published values}
          cc.disp:=MOSCED20[i].ds;
          cc.t   :=MOSCED20[i].t;
          cc.a   :=MOSCED20[i].a;
          cc.b   :=MOSCED20[i].b;
        end;
      end;

      {Correct parameters at 20° to boiling point:}

      If cc.warn=2 then begin
         cc.t:=cc.t*power((293/(cc.nbp+273.15)),0.4);
         cc.a:=cc.a*power((293/(cc.nbp+273.15)),0.8);
         cc.b:=cc.b*power((293/(cc.nbp+273.15)),0.8);

        cc.pol:=(sqr(cc.q)*sqr(cc.q))*
                (1.15-1.15*exp(-0.020*cc.t*cc.t*cc.t))+1;

        cc.phii:=cc.pol+0.011*cc.a*cc.b;

        cc.eps:=0.68*(cc.pol-1)+
                power(
                   (3.4-2.4*exp(
                      power(
                         (
                         ( Ca*4.5/ (3.5+cc.nc) * (1+(cc.nc-1)/100) )
*
                         ( Cb*4.5/ (3.5+cc.nc) * (1+(cc.nc-1)/100) )
                      ),1.5)
                      *(-0.23))
                   )
                ,sqr(293/(cc.nbp+273.15)));
      end;

    end;
end {MOSCED};

{Process an output file.}
{This procedure reads in data from a PRO/II output file. It then
computes
 the parameters which depend on one component only.}

Procedure Process (fn:any;          {File name}
                   var cc:param;    {Component parameters}
                   il:any);         {Line from AGENTS.INF}

  Var f1: text;           {The output file.}
      cont: boolean;      {Is the output file in order. OK to continue?}
      s3,
      s2,
      s1: any;            {A line or part of a line of text from
                           PRO/II the output file.}
      ts1,ts2: rtype;     {Hold temporary values.}
      i,j:integer;
```

```
Begin

  cc.cok:=false;     {Assume an error.}

  {Open the output file:}

  assign (f1,fn);
  reset (f1);

  {Assume the output file has no warnings or errors:}

  cont:=true;

  {Check that it is indeed the case:}

  repeat
    readln (f1,s1);
  until (eof(f1)) or (copy (s1,6,8)='RUN STAT');

  {If RUN STATISTICS can not be found, then do not process the file.
   It a dummy file or something/someone unusual affected PRO/II.}

  If eof(f1) then cont:=false;

  {Check for NO errors and NO warnings.}

  If cont then begin
    readln (f1,s1);
    If copy(s1,44,2)<>'NO' then cont:=false;
    readln (f1,s1);
    If copy(s1,44,2)<>'NO' then cont:=false;
  end;

  {If no errors or warnings were found, continue: }

  If cont then begin

    cc.cok:=True;    {Output is ok}

    {Get flash alpha values:}
    {Get the first set:}

    For j:=1 to 6 do begin
      repeat
        readln (f1,s1);
      until (copy(s1,2,17)='VAPOR-LIQUID COMP');
      readln (f1,s1);
      readln (f1,s1);
      readln (f1,s1);
      readln (f1,s1);
      readln (f1,s2);
      Val (copy(s1,49,10),ts1,i);
      Val (copy(s2,49,10),ts2,i);
      cc.alpha[j]:=ts1/ts2;
    end;
```

```
{Get the second set:}

For j:=7 to 12 do begin
  repeat
    readln (f1,s1);
  until (copy(s1,2,17)='VAPOR-LIQUID COMP');
  readln (f1,s1);
  readln (f1,s1);
  readln (f1,s1);
  readln (f1,s1);
  readln (f1,s2);
  readln (f1,s2);
  Val (copy(s1,49,10),ts1,i);
  Val (copy(s2,49,10),ts2,i);
  cc.alpha[j]:=ts1/ts2;
end;

{Get the third set:}

For j:=13 to 18 do begin
  repeat
    readln (f1,s1);
  until (copy(s1,2,17)='VAPOR-LIQUID COMP');
  readln (f1,s1);
  readln (f1,s1);
  readln (f1,s1);
  readln (f1,s1);
  readln (f1,s1);
  readln (f1,s2);
  Val (copy(s1,49,10),ts1,i);
  Val (copy(s2,49,10),ts2,i);
  cc.alpha[j]:=ts1/ts2;
end;

{Get the nbp:}

s1:=copy(il,a_nbp,5);
If s1[1]=' ' then s1:=copy (s1,2,length(s1)-1);
Val(s1,cc.nbp,i);

{Compute dHv:}

{Skip to the first 'REQUESTED STREAM PROPERTIES':}

repeat
  readln (f1,s1);
until copy(s1,27,16)='REQUESTED STREAM';
readln (f1,s1);
readln (f1,s1);
readln (f1,s1);
readln (f1,s1);
readln (f1,s1);
readln (f1,s1);
readln (f1,s1);
readln (f1,s1);
readln (f1,s1);
```

```
s2:=copy(s1,32,9);
If s2[1]=' ' then s2:=copy(s2,2,length(s2)-1);
If s2[1]=' ' then s2:=copy(s2,2,length(s2)-1);
If s2[1]=' ' then s2:=copy(s2,2,length(s2)-1);
Val (s2,ts1,i);
s2:=copy(s1,45,9);
If s2[1]=' ' then s2:=copy(s2,2,length(s2)-1);
If s2[1]=' ' then s2:=copy(s2,2,length(s2)-1);
If s2[1]=' ' then s2:=copy(s2,2,length(s2)-1);
Val (s2,ts2,i);

{Convert K*KJ/KG-MOL to cal/gmol:}

cc.dHv:=(ts2-ts1)/4.1868*1000;

{Compute dU = dHv - RT, equation 22 :}
{R=1.9872 cal/deg.mol}

cc.dU:=cc.dHv-1.987*(cc.nbp+273.15);

readln (f1,s1);
readln (f1,s1);
readln (f1,s2);

{Molar volume, (g/mol) / (g/cc),  mw/density :}

s2:=copy(s2,33,8);
If s2[1]=' ' then s2:=copy(s2,2,length(s2)-1);

Val (s2,ts2,i);
Val (copy(s1,35,6),ts1,i);

cc.mV:=ts2/ts1;

{Reduced temperature:}

readln (f1,s1);
readln (f1,s1);
readln (f1,s1);

Val (copy(s1,48,6),cc.Tr,i);

{Nonpolar solubility parameter:}

GetNonPolar (cc,il);

{Polar solubility parameter:}

cc.psp:=sqrt(abs(cc.dU/cc.mV-sqr(cc.npsp)));

{Put in the names:}

cc.p2name:=copy(il,a_p2name,10);
cc.cname :=copy(il,a_cname,length(il)-a_cname+1);

Do_MOSCED (cc,il);
```

```
    end {processing the output file};

    close (f1);

end {Process};

{Estimate the selectivities etc. using the parameters calculated by
 the Process procedure. cc contains the parameters for the agent and
 c1 & c2 those for the two components. The results are returned in cc:}

Procedure Compute (Var cc: param);
  Var g1,g2: rtype;     {Gammas for components 1 & 2 in the solvent.}
  Begin

    {Tassios: (solvent tau)^2*(Vj-Vi) }

    cc.Ts:=exp(sqr(cc.psp)*(c1.Mv-c2.Mv)/1.987/(cc.nbp+273.15));

    {Weimer-Prausnitz:}
    {Equation tested OK:}

                c c . W P s : = e x p ( (
c1.mV*sqr(cc.npsp-c1.npsp)-c2.mV*sqr(cc.npsp-c2.npsp)+
                    1.987*(cc.nbp+273.15)*
                    ( ln(c1.mV/c2.mV)+(c2.mV-c1.mV)/cc.mV )+
                    2*(c2.mV*c2.phi-c1.mV*c2.phi)+
                    sqr(cc.psp)*(c1.mV-c2.mV)
                  ) / 1.987/(cc.nbp+273.15)
                );

    {Helpinstill & Van Winkle, equation 21 on page 214:}

                    g 1 : = e x p (
c1.Mv*(sqr(c1.npsp-cc.npsp)+sqr(cc.psp-c1.psp)-2*c1.phiHV)
                  /1.987/(cc.nbp+273.15)
                    + (ln(c1.Mv/cc.Mv)+1-c1.Mv/cc.Mv)
                );

                    g 2 : = e x p (
c2.Mv*(sqr(c2.npsp-cc.npsp)+sqr(cc.psp-c1.psp)-2*c2.phiHV)
                  /1.987/(cc.nbp+273.15)
                    + (ln(c2.Mv/cc.Mv)+1-c2.Mv/cc.Mv)
                );

    cc.HVs:=g1/g2;

    {MOSCED equations:}

    {Do not use MOSCED if any parameters are missing:}

    If not(c1.ok) then cc.ok:=false;
    If not(c2.ok) then cc.ok:=false;

    If cc.ok then begin

       {Calculate aa:}
```

```
        c1.aa:=0.953-0.00968*(sqr(c1.t)+c1.a*c1.b);
        c2.aa:=0.953-0.00968*(sqr(c2.t)+c2.a*c2.b);

        {Combinatorial term, d12:}

                                  c 1 . d 1 2 : = l n
(power(c1.mV/cc.mV,c1.aa))+1-power(c1.mV/cc.mV,c1.aa);
                                  c 2 . d 1 2 : = l n
(power(c2.mV/cc.mV,c2.aa))+1-power(c2.mV/cc.mV,c2.aa);

        {Activity coefficients, p.197 eq 14 of Thomas & Eckert:}

        g1:=exp( c1.mV/1.987/(cc.nbp+273.15)*
                 ( sqr(cc.disp-c1.disp) +
                   sqr(c1.q)*sqr(cc.q)*sqr(cc.t-c1.t)/cc.phii+
                   (cc.a-c1.a)*(cc.b-c1.b)/cc.eps
                 ) + c1.d12
               );

        g2:=exp( c2.mV/1.987/(cc.nbp+273.15)*
                 ( sqr(cc.disp-c2.disp) +
                   sqr(c2.q)*sqr(cc.q)*sqr(cc.t-c2.t)/cc.phii+
                   (cc.a-c2.a)*(cc.b-c2.b)/cc.eps
                 ) + c2.d12
               );

        {Selectivity is the ratio of the activity coefficients:}

        cc.Ms:=g1/g2;

    end;

end {Compute};

{Test one specific agent:}

Procedure Test_One;
  Var il: any;          {The correct parameter line from AGENTS.INF.}
      c: char;
      found: boolean;   {Is the agent chosen in AGENTS.INF?}
      i: integer;
      ns: any;  {Name of component to test.}

  Begin
    ClrScr;
    Gotoxy (12,10); write ('Please enter the first PRO/II library name
of the agent:');
    Gotoxy (30,14);
    readln (ns);
    ns:=ns+' ';
    For i:=1 to length(ns) do ns[i]:=upcase(ns[i]);
    Gotoxy   (15,18);   write   ('Looking   for   data   on   ',ns,'in
AGENTS.INF...');

    assign (fs,'AGENTS.INF');
    reset (fs);
```

```
    found:=false;
    repeat
      readln (fs,il);
      if ns=copy(il,10,length(ns)) then found:=true;
    until (found) or (eof(fs));
    If not found then begin
      Gotoxy (15,20); write (ns,'is not in AGENTS.INF!    Press any
key.');
      c:=Readkey;
    end;

    close (fs);

    If found then begin
      ClrScr;
      writeln;
      writeln ('Found data on ',ns,'in AGENTS.INF.');
      writeln ('Creating the PRO/II input (ASEEK1.INP) file ...');
      MakeInput ('ASEEK1.INP',il);
      writeln ('OK');
      writeln ('Submitting the input file:');

      {Erase the old output files:}

      {$I-}
      assign (fd,'ASEEK1.OUT');
      erase (fd);
      i:=IOResult;
      {$I+}

      {Send the input file and for an output:}

      Exec ('W:\UTILS\BATCH.EXE','-st -5 d:\simsci\hardp2\ramp2 ASEEK1
/B');
      writeln ('OK.');
      write ('Waiting for the PRO/II output file ...');
      Waitfor ('ASEEK1.OUT');
      writeln;
      writeln ('OK');
      writeln ('Processing the output file.');
      Process ('ASEEK1.OUT',cc1,il);
      writeln ('OK');

      {Compute selectivities:}
      writeln ('Calculating selectivities.');
      Compute (cc1);

      writeln ('OK');
      ClrScr;

      {Show the results:}

      writeln ('Results after testing ',ns,'on ',c1name,' & ',c2name,'
:');
      writeln ('(',ns,'is ',cc1.cname,' with nbp ',cc1.nbp:5:1,' °C)');
      writeln;
```

```
      writeln ('Tassios selectivity:                    ',cc1.Ts :7:2);
      writeln ('Weimer-Prausnitz selectivity:           ',cc1.WPs:7:2);
      writeln ('Helpinstill-Van Winkle selectivity:     ',cc1.HVs:7:2);

      If not cc1.ok then begin
        writeln ('All the parameters required by MOSCED for this system
could not');
        writeln ('be located in AGENTS.INF. Please add the missing
information.');
      end else begin
        If (cc1.warn=0) or (cc1.warn=2)
          then writeln ('MOSCED selectivity:                    ',cc1.Ms
:7:2);
        If cc1.warn=1 then writeln ('This solvent does not belong to
any MOSCED group.');
        If cc1.warn=2 then writeln ('(Special regressed parameters are
available for the solvent.)');
      end;

      writeln;

      writeln ('UNIFAC model:');
      writeln ('Alpha values at 2/3 mole fraction solvent with solvent
free percentages');
      writeln   ('for   component   1   of   1,20,40,60,80   and   99
respectively:');
      writeln  (cc1.alpha[1]:7:3,'          ',cc1.alpha[2]:7:3,'
',cc1.alpha[3]:7:3);
      writeln  (cc1.alpha[4]:7:3,'          ',cc1.alpha[5]:7:3,'
',cc1.alpha[6]:7:3);
      writeln;
      writeln ('Alpha values for increasing component 1 and the
solvent:');
      writeln  (cc1.alpha[ 7]:7:3,'         ',cc1.alpha[ 8]:7:3,'
',cc1.alpha[ 9]:7:3);
      writeln  (cc1.alpha[10]:7:3,'         ',cc1.alpha[11]:7:3,'
',cc1.alpha[12]:7:3);
      writeln;
      writeln ('Alpha values for increasing component 2 and the
solvent:');
      writeln  (cc1.alpha[13]:7:3,'         ',cc1.alpha[14]:7:3,'
',cc1.alpha[15]:7:3);
      writeln  (cc1.alpha[16]:7:3,'         ',cc1.alpha[17]:7:3,'
',cc1.alpha[18]:7:3);

      writeln;
      write ('Please press any key for parameters used ...');
      While keypressed do c:=Readkey;
      c:=Readkey;
      clrscr;
      writeln ('Properties for components ',c1name,', ',c2name,' and
solvent ',ns,' :');
      writeln;

      writeln ('Molar volumes (cc/gmol):');
      writeln (c1.mV:6:2,'     ',c2.mV:6:2,'     ',cc1.mV:6:2);
```

```
      writeln;

      writeln ('Selected Weimer-Prausnitz & Tassios parameters:');
      writeln ('Nonpolar solubility parameters (cal/cc)^0.5:');
      writeln (c1.npsp:6:1,'     ',c2.npsp:6:1,'     ',cc1.npsp:6:1);

      writeln ('Polar solubility parameters (cal/cc)^0.5:');
      writeln (c1.psp:6:1,'     ',c2.psp:6:1,'     ',cc1.psp:6:1);
      writeln;

      If (not cc1.ok) or (cc1.warn=1) then begin

        writeln ('(For reasons already indicated, MOSCED parameters
will not be shown.)');

      end else begin

        writeln ('Selected MOSCED parameters.');
        writeln ('Dispersion parameters (cal/cc)^0.5:');
        writeln (c1.disp:6:2,'     ',c2.disp:6:2,'     ',cc1.disp:6:2);

        writeln ('Polar parameters (cal/cc)^0.5:');
        writeln (c1.t:6:2,'     ',c2.t:6:2,'     ',cc1.t:6:2);

        writeln ('Acidity, basicity and induction parameters:');
        writeln (c1.a:6:2,'     ',c2.a:6:2,'     ',cc1.a:6:2);
        writeln (c1.b:6:2,'     ',c2.b:6:2,'     ',cc1.b:6:2);
        writeln (c1.q:6:2,'     ',c2.q:6:2,'     ',cc1.q:6:2);

        writeln ('Polar assymetry and hydrogen bonding assymetry
factors:');
        writeln (c1.phii:6:3,'     ',c2.phii:6:3,'     ',cc1.phii:6:3);
        writeln (c1.eps:6:3,'     ',c2.eps:6:3,'     ',cc1.eps:6:3);
        writeln;
      end;

      write ('Please press any key to return to the main menu ...');
      c:=Readkey;
    end;

end {Test_One};

{Compute an index showing how good the agent is:}

Procedure GetIndex (ca: param; Var index: rtype);
  Var uin: rtype;     {An average value for UNIFAC}
  Begin

    {Average UNIFAC value:}

    uin:=(ca.alpha[1]+ca.alpha[2]+ca.alpha[3]+
          ca.alpha[4]+ca.alpha[5]+ca.alpha[6]) / 6;

    {Compute index, depending on the sort option chosen:}
    {Use MOSCED if values could be calculated, else exclude it.}
```

```
    Case sort of
      '1': Begin
             If ca.ok then index:=(uin+ca.Ts+ca.WPs+ca.Ms+ca.HVs)/5
                      else index:=(uin+ca.Ts+ca.WPs+ca.HVs)/4;
             If index<1 then index:=1/index;
           end;
      '2': Begin
                                    I f    c a . o k    t h e n
index:=(uin+2*ca.Ts+2*ca.WPs+2*ca.Ms+2*ca.HVs)/9
                      else index:=(uin+2*ca.Ts+2*ca.WPs+2*ca.HVs)/7;
             If index<1 then index:=1/index;
           end;
      '3': Begin
                                   I f    c a . o k    t h e n
index:=(2*uin+ca.Ts+ca.WPs+3*ca.Ms+2*ca.HVs)/9
                      else index:=(2*uin+ca.Ts+ca.WPs+2*ca.HVs)/6;
             If index<1 then index:=1/index;
           end;
      '4': Begin
             If ca.ok then

index:=(we1*ca.Ts+we2*ca.WPs+we3*ca.HVs+we4*ca.Ms+we5*uin)/wt
               else

index:=(we1*ca.Ts+we2*ca.WPs+we3*ca.HVs+we5*uin)/(wt-we4);
             If index<1 then index:=1/index;
           end;
    end;
end {GetIndex};

{The results from an agent just tested by Test_All are in cc. Check if
it
 belongs in the top topsize and if so add it.}

Procedure SortAdd (cc:param);
  Var int,                          {Index for last agent in the top list}
      ina: rtype;                   {Index for new agent}
      w,i: integer;
  Begin

    {Get an index for the new agent:}
    GetIndex (cc,ina);

    {Get one for the worst member of the top list:}
    GetIndex (top[topsize]^,int);

    {If the new agent better?}

    If ina>int then begin

      {Yes. Now find its rightful position in the top list:}

      w:=topsize;
      Repeat
        GetIndex (top[w]^,int);
        If int<ina then dec(w);
```

```
      until (w=0) or (not(int<ina));
      inc(w);

      {Make room for the new agent:}

      For i:=topsize downto (w+1) do
        top[i]^:=top[i-1]^;

      {Store it in the top list:}

      top[w]^:=cc;
    end;

end {SortAdd};

{Test all the agents known:}

Procedure Test_All;
  Var i,j: integer;
      nn: integer;      {Count the agents}
      fs: text;         {Source file.}
      inn: rtype;       {Index}
      il1,il2: any;     {A line from AGENTS.INF}
      cc: char;

  Begin

  ClrScr;
  writeln;
  writeln ('Test All Agents.');
  writeln;
  writeln ('(Resetting the current top list.)');

  {Reset the top list by filling it with dummy agents with unity
values:}

  For i:=1 to topsize do begin
    top[i]^.p2name:='dummy';
    top[i]^.cname :='dummy';
    top[i]^.Ts:=1;
    top[i]^.WPs:=1;
    top[i]^.HVs:=1;
    top[i]^.Ms:=1;
    For j:=1 to 18 do
      top[i]^.Alpha[j]:=1.0;
  end;

  writeln;

  writeln ('Which sorting criterium would you like to be used ?');
  writeln;
  writeln ('The following options are available:');
  writeln ('  1: Compute the average of the methods, compensating for
values below unity.');
  writeln ('    2: This is a separation of two highly nonpolar
components.');
```

```
  writeln ('   3: This is a separation of polar or polar-nonpolar
components.');
  writeln ('  4: Specify relative weights for the different models.');
  writeln;
  write ('Which option do you want (1,2,3 or 4) ? ');
  repeat
    sort:=readkey;
  until sort in ['1','2','3','4'];

  If sort='4' then begin
    writeln;
    writeln;
    writeln ('There are five models. Please supply the weights (eg:
1,1,2,2,1):');
    write ('Weight for Tassios:                ');  readln (we1);
    write ('Weight for Weimer-Prausnitz:       ');  readln (we2);
    write ('Weight for Helpinstill-Van Winkle: ');  readln (we3);
    write ('Weight for MOSCED:                 ');  readln (we4);
    write ('Weight for UNIFAC:                 ');  readln (we5);
    wt:=we1+we2+we3+we4+we5;
  end;

  assign (fs,'AGENTS.INF');
  reset (fs);

  repeat
    readln (fs,il1);
  until il1[1]<>';';

  clrscr;
  writeln;
  writeln (' Starting to test all agents:');
  writeln;
  writeln (' (Press X to stop prematurely.)');
  writeln (' (Press I to see the top 20 agents.)');
  writeln;

  nn:=0;   {Start counting}
  cc:=' ';

  {Keep reading and testing agents until there are no more:}

  repeat

    {Delete the old output files:}

    {$I-}
    assign (fd,'ASEEK1.OUT');
    erase (fd);
    assign (fd,'ASEEK2.OUT');
    erase (fd);
    i:=IOResult;
    {$I+}

    {Read one name and send it:}
```

```
    readln (fs,il1);
    MakeInput ('ASEEK1.INP',il1);
    Exec ('W:\UTILS\BATCH.EXE','-st -5 d:\simsci\hardp2\ramp2 ASEEK1
/B');

    {Write out the name on the screen:}

    inc(nn);
    writeln ('Processing agent number: ',nn:4,' which is ',
             copy(il1,a_p2name,10));

    {If not yet done, send another as two PRO/II machines can work
     at one time.}

    If not eof(fs) then begin
      readln (fs,il2);
      MakeInput ('ASEEK2.INP',il2);
      Exec ('W:\UTILS\BATCH.EXE','-st -5 d:\simsci\hardp2\ramp2 ASEEK2
/B');

      inc(nn);
      writeln ('Processing agent number: ',nn:4,' which is ',
               copy(il2,a_p2name,10));
    end;

    {Wait for the output files from PRO/II:}

    Waitfor ('ASEEK1.OUT');
    If not eof(fs) then Waitfor ('ASEEK2.OUT');

    {Handle the first file:}

    Process ('ASEEK1.OUT',cc1,il1);
    Compute (cc1);
    SortAdd (cc1);

    {and the second if it existed:}

    If not eof(fs) then begin
      Process ('ASEEK2.OUT',cc2,il2);
      Compute (cc2);
      SortAdd (cc2);
    end;

    {Save the results every now and again:}

    If ((nn div 20) * 20)=nn then begin
      SaveIt;
    end;

    If keypressed then cc:=upcase(Readkey);

    If cc='I' then begin     {Print out the top 20 agents.}
      writeln;
      writeln ('The top 20 agents are: ');
      writeln;
```

```
      For i:=1 to 20 do begin
        GetIndex (top[i]^,inn);
        writeln (top[i]^.cname:20,'  with index ',inn:6:2);
      end;
      writeln;
      writeln ('Press any key to continue...');
      c:=readkey;
      c:=' ';
    end;

    If cc='X' then begin     {Stop testing agents.}
      SaveIt;
      writeln;
      writeln ('Program interrupted by user. Results saved to disk.');
      writeln ('Press any key to proceed.');
      cc:=Readkey;
      cc:='X';
    end;

  until eof(fs) or (cc='X');

  close (fs);

  SaveIt;

  clrscr;
  writeln;
  writeln (' Finished testing the agents.');
  writeln;
  writeln (' The results have been written to the file ASEEK.RES');
  writeln (' Use the / File Import Numbers command in LOTUS 1-2-3 to
import the file.');
  writeln;
  writeln (' Press any key to return to the main menu.');
  While keypressed do cc:=readkey;   {Flush buffer}
  cc:=readkey;

end {Test_All};

{Get the parameters for components 1 and 2:}

Procedure Get12Param;
  Var il1,il2: any;        {Text lines from AGENTS.INF.}

    {Retrieve the line from AGENTS.INF which matches the PRO/II name
given:}

    Procedure GetLine (name:any;     {PRO/II name}
                       Var il:any);
      Var fs:text;
          found: boolean;       {Has the name been found?}
      Begin
        assign (fs,'AGENTS.INF');
        reset (fs);
        found:=false;
        repeat
```

```
          readln (fs,il);
          if (name+' ')=copy(il,10,length(name)+1) then found:=true;
        until (found) or (eof(fs));
        close (fs);
        If not found then begin
          ClrScr;
          writeln ('SEVERE ERROR:');
          writeln;
          writeln ('The name (',name,') given for one of the components
to be');
          writeln ('separated can not be found in AGENTS.INF.');
          writeln ('Unable to proceed. Program operation suspended.');
          writeln;
          halt (1);
        end;

    end {GetLine};

  Begin;

    {Get the lines from AGENTS.INF:}

    GetLine (c1name,il1);
    GetLine (c2name,il2);

    {Write the input files:}

    writeln ('Writing input files.');
    MakeInput ('ASEEK1.INP',il1);
    MakeInput ('ASEEK2.INP',il2);

    {Erase old output files:}

    {$I-}
    assign (fd,'ASEEK1.OUT');
    erase (fd);
    assign (fd,'ASEEK2.OUT');
    erase (fd);
    i:=IOResult;
    {$I+}

    {Submit them and wait for the output:}

    writeln ('Sending input files to PRO/II:');
    Exec ('W:\UTILS\BATCH.EXE','-st -5 d:\simsci\hardp2\ramp2 ASEEK1
/B');

    {If an error occurs, report it:}

    If (Doserror<>0) then begin
      writeln;
      writeln ('Unable to use EXEC to call BATCH.EXE.');
      writeln ('DOSError number: ',doserror:2,':');
      Case Doserror of
          8  : writeln ('Not enough memory.');
          2,3: writeln ('Could not find some files. (BATCH?)');
```

```
      end;
      writeln;
      writeln ('ASEEK halted.');
      halt (1);
    end;

    Exec ('W:\UTILS\BATCH.EXE','-st -5 d:\simsci\hardp2\ramp2 ASEEK2
/B');
    write ('Waiting for the PRO/II output files ...');
    Waitfor ('ASEEK1.OUT');
    Waitfor ('ASEEK2.OUT');
    writeln;

    {Process the output files:}

    writeln ('Processing the output.');
    Process ('ASEEK1.OUT',c1,il1);
    Process ('ASEEK2.OUT',c2,il2);

    c12ok:=true;

end {Get12Param};

{Write a string with a letter highlighted:}

Procedure SWrite (ss: any);
  Var i:integer;
  Begin
    i:=1;
    repeat
      If ss[i]='_' then begin   {Highlight letter}
        TextColor (White);
        write (ss[i+1]);
        inc (i);
        TextColor (Yellow);
      end else begin
        write (ss[i]);
      end;
      inc (i);
    until i>length(ss);
end {SWrite};

Begin

  ClrScr;
  writeln ('ASEEK 3.0 starting...');

  {Start overlay management:}

  writeln ('Setting up overlays...');

  OvrInit('ASEEK.OVR');

  If ovrresult<>0 then begin
    ClrScr;
    writeln ('Overlay manager error number: ',ovrresult:2);
```

```
    writeln ('ASEEK aborted.');
  end;

  OvrInitEMS;

  {Set up top list}

  writeln ('Allocating memory...');
  For i:=1 to topsize do New (top[i]);

  {Default case:}

  c1name:='OCT1';
  c2name:='MBK';

  {Parameters are not yet available for the two components to be
separated:}

  c12ok:=false;

  {Prevent network messages from PRO/II to halt the program:}

  Exec ('Z:\PUBLIC\CASTOFF.EXE','');

  {Now present a simple menu and execute the choice exercised.}

  Repeat

    TextColor (Yellow);
    TextBackground (Blue);
    ClrScr;

    TextColor (White); TextBackground (Red);
    Gotoxy (35,4); Write('┌─────────┐');
    Gotoxy (35,5); Write('│ ASEEK │');
    Gotoxy (35,6); Write('└─────────┘');
    TextColor (Yellow); TextBackground (Blue);
    Gotoxy (25, 9); Write('Please choose an option:');
    Gotoxy (25,11); SWrite('_1. _General information.');
    Gotoxy (25,12); SWrite('_2. Test _One specific agent.');
    Gotoxy (25,13); SWrite('_3. Test _All known agents.');
    Gotoxy (25,14); SWrite('_4. _Choose the system to study.');
    Gotoxy (25,15); SWrite('_5. Component _Name search.');
    Gotoxy (25,16); SWrite('_6. _Boiling point search.');
    Gotoxy (25,17); SWrite('_7. _Exit this program.');
    Gotoxy (21,19); Write('Please press a letter of your choice: ');

    c:=upcase(readkey);

    If (c in ['2','O','3','A']) and (not c12ok) then begin
      ClrScr;
      writeln;
                        w   r   i   t   e   l   n         (   '
┌──────────────────────────────────────────────────────────────────────┐');
      writeln (' |    Before any agents can be tested, parameters MUST
first be    |');
```

```
      writeln (' | determined for the components to be separated. This
needs to be |');
      writeln (' |       done ONCE only every time a new system is
configured.      |');
                        w   r   i   t   e   l   n           (   '
└──────────────────────────────────────────────────────────────────┘');
      writeln ('             (Please wait. This should take 2 to 3
minutes.)');
      writeln ('   (Use the time to check if both PRO/II machines are
operating.)');
      writeln;
      Get12Param;
    end;

    case c of
        '1','I','G': Begin
                       GenInfo;
                     end;
        '2','O':     Begin
                       Test_One;
                     end;
        '3','A':     Begin
                       Test_All;
                       c:=' ';
                     end;
        '4','C':     Begin
                       Config;
                     end;
        '5','N':     Begin
                       NameSearch;
                     end;
        '6','B':     Begin
                       BoilSearch;
                     end;
    end;

  until c in ['7','E','X',#13,#32,#27];

  TextColor (White); TextBackground (Black);
  ClrScr;

  {Accept network messages from now on.}

  Exec ('Z:\PUBLIC\CASTON.EXE','');

  writeln;
  writeln;

  writeln ('Thank you for using ASEEK.');
  writeln;

end.


Unit ASEEKU;
```

```
{This unit has some basic definitions which is used by many other
units.}

{$F+}

{$N+,E-}

{$D-}
{$L-}

Interface

{Where in a line from AGENTS.INF can items be found?}

Const a_p2name = 10;    {The PRO/II name.}
      a_nc     = 33;    {The number of carbon atoms.}
      a_cname  = 36;    {The full chemical name.}
      a_nbp    = 21;    {The normal boiling point.}
      a_q      = 5;     {The induction parameter q.}
      a_c      = 1;     {The MOSCED code.}

      topsize = 300;    {The size of the top hits.}

      {R=1.987 cal/degK/gmol}

Type rtype = single;    {The real type used.}
     any   = string;    {Any string}

     param=record     {Model parameters for an agent.}

             p2name: string[10];  {The PRO/II library name.}
             cname: string[40];   {The full chemical name.}

             nbp: rtype;          {Normal boiling point, °C}

             cok: boolean;        {True if the output file is OK.}
                                  {If false, parameters are rubbish.
                                   Do not give output.}

             {Tassios and Weimer-Prausnitz parameters:}

             Ts: rtype;          {Tassios selectivity}

             WPs: rtype;         {Weimer Prausnitz selectivity}

             dHv: rtype;         {Enthalpy of evaporation, cal/gmol.}
             dU : rtype;          {Change in internal energy, cal/gmol
}
             mV : rtype;         {Molar volume V, cc/gmol }
             Tr : rtype;         {Reduced temperature.}
             npsp:  rtype;           {Nonpolar solubility parameter,
sqrt(cal/cc)}
             psp:  rtype;                {Polar solubility paramete,
sqrt(cal/cc)}
             phi: rtype;           {Induction energy: 0.396,0.415 or
0.450}
```

```
            {Helpinstill & Van Winkle:}

            phihv: rtype;          {Induction energy: 0.399,0.415 or
0.447}
            HVs: rtype;          {Selectivity}

            {MOSCED parameters:}

            ok: boolean;             {True if MOSCED parameters are
available.}
                                   {If not, then ignore this model.}
            Ms: rtype;             {MOSCED selectivity.}
            disp: rtype;           {Dispersion parameter, sqrt(cal/cc)}
            q: rtype;              {Induction parameter.}
            mc: char;            {Code: 0= alkane, 1=chloride, 2=bromide
etc.}
            nc: integer;           {Number of carbon atoms.}
            warn: integer;         {If 0 then no problem.}
                                   {If 1 then non-standard class.}
                                   {If 2 then used params at 20°C.}
            t,                     {Polar parameter}
            a,                     {Acidity parameter}
            b: rtype;              {Basicity parameter}

            POL,                   {See p. 203, Thomas & Eckert}
            phii,                  {Polar assymetry parameter}
            eps: rtype;            {Hydrogen bonding assymetry factor}

            aa: rtype;             {exponent in d12}
            d12: rtype;            {Combinatorial term.}

            {UNIFAC parameters:}

            alpha: array [1..18] of rtype;    { 1- 6: c1 & c2 with
agent}
                                                { 7-12: c1 & agent only}
                                                {13-18: c2 & agent only}
          end;

     topt=array [1..topsize] of ^param;    {Top topsize agents}

Var c1name,              {The PRO/II library names of the two components}
    c2name: any;         {to be separated.}
    c12ok: boolean;      {Have parameters been obtained for components 1
& 2 ?}

    sort: char;          {The sorting option chosen.}

    top: topt;         {The top topsize agents.}

    fd,                  {Used to delete old output files.}
    fs: text;            {The AGENTS.INF source file.}
    cc1,cc2,             {Parameters for agents being processed.}
    c1,c2: param;          {Parameters for the two components to be
separated.}
```

```
Implementation

end.


Unit ASEEKU1;

{$N+,E-}

{$F+}
{$O+}

{$D-}
{$R-}
{$L-}

Interface

Uses CRT,ASEEKU;

Procedure SaveIt;

Procedure GetNonPolar (var cc: param;  {Component parameters:}
                       il: any);       {Line from AGENTS.INF.}

Procedure Waitfor (fn: any);

Procedure GenInfo;

Function Inter5 (xx, x0,x1,x2,x3,x4,
                     y0,y1,y2,y3,y4:rtype): rtype;
Function Inter7 (xx, x0,x1,x2,x3,x4,x5,x6,
                     y0,y1,y2,y3,y4,y5,y6:rtype): rtype;


Implementation

{Save the results to a file.}

Procedure SaveIt;
  Var fsr:text;          {The output file.}
      i,j: integer;
  Begin
    assign (fsr,'ASEEK.RES');
    rewrite (fsr);
    writeln ('Saving results to ASEEK.RES ...');

    writeln (fsr,'"ASEEK 3.0 study."');
    writeln (fsr,'');
    writeln   (fsr,'"Component   1   is   ',c1.cname,'   and   2   is
',c2.cname,'"');
    writeln (fsr,'');
    writeln (fsr,'"Properties of the components:"');
    writeln (fsr,'');
    writeln (fsr,'"Molar volumes (cc/gmol)"');
    writeln (fsr,c1.mv,',',c2.mv);
```

```
    writeln (fsr,'');
    writeln (fsr,'"Weimer-Prausnitz & Tassios parameters:"');
    writeln (fsr,'"Nonpolar solubility parameters (cal/cc)^0.5:"');
    writeln (fsr,c1.npsp,',',c2.npsp);
    writeln (fsr,'');
    writeln (fsr,'"Polar solubility parameters (cal/cc)^0.5:"');
    writeln (fsr,c1.psp,',',c2.psp);
    writeln (fsr,'');
    If (not c1.ok) or (not c2.ok) then begin
      writeln (fsr,'"MOSCED parameters are not shown because some
parameters are missing."');
      writeln (fsr,'');
    end else begin
      writeln (fsr,'"MOSCED parameters:"');
      writeln (fsr,'"Dispersion parameters (cal/cc)^0.5:"');
      writeln (fsr,c1.disp,',',c2.disp);
      writeln (fsr,'');

      writeln (fsr,'"Polar parameters (cal/cc)^0.5:"');
      writeln (fsr,c1.t,',',c2.t);
      writeln (fsr,'');

      writeln (fsr,'"Acidity, basicity and induction parameters:"');
      writeln (fsr,c1.a,',',c2.a);
      writeln (fsr,c1.b,',',c2.b);
      writeln (fsr,c1.q,',',c2.q);
      writeln (fsr,'');

      writeln (fsr,'"Polar assymetry and hydrogen bonding assymetry
factors:"');
      writeln (fsr,c1.phii,',',c2.phii);
      writeln (fsr,c1.eps,',',c2.eps);
      writeln(fsr,'');
    end;

    writeln (fsr,'"The 3x6 matrices contain three sets of flashes using
UNIFAC."');
    writeln (fsr,'"Set one has 2/3 mol solvent with solvent free
percentages of component 1"');
    writeln (fsr,'"of 1,20,40,60,80 and 99. Set two has component 1
with the solvent with"');
    writeln (fsr,'"increasing amounts of 1. The third set is component
2 with the agent."');
    writeln (fsr,'');

    writeln (fsr,'"The values for the top agents are:"');
    writeln (fsr,'');

                              w     r     i     t     e     l     n
(fsr,'"P2","Chemical","NBP","Tassios","Weimer-P","MOSCED","Help-VW');
     writeln    (fsr,'"name","name","(°C)","Infinite","dilution
selectivity"');
    writeln (fsr,'');

    For i:=1 to topsize do begin
      write (fsr,'"',top[i]^.p2name,'","',top[i]^.cname,'",');
```

```
      write (fsr,top[i]^.nbp:5:1,',');
                                    w    r    i    t    e    l    n
(fsr,top[i]^.Ts,',',top[i]^.WPs,',',top[i]^.Ms,',',top[i]^.HVs);
      write (fsr,'"","",');
      For j:=1 to 5 do begin
        write (fsr,top[i]^.alpha[j],',');
      end;
      writeln (fsr,top[i]^.alpha[6]);
      For j:=7 to 11 do begin
        write (fsr,top[i]^.alpha[j],',');
      end;
      writeln (fsr,top[i]^.alpha[12]);
      For j:=13 to 17 do begin
        write (fsr,top[i]^.alpha[j],',');
      end;
      writeln (fsr,top[i]^.alpha[18]);
    end;

    close (fsr);
end {SaveIt};

{Interpolate the nonpolar solubility parameter from Mv and Tr.
 Used for the Weimer Prausnitz model.}

Procedure GetNonPolar (var cc: param;  {Component parameters:}
                       il: any);       {Line from AGENTS.INF.}

  Var n1,n2,n3,n4,n5,n6,n7: rtype;    {Parameter for mV at different
Tr's}
  Begin
    Case il[3] of
      'p': Begin  {Paraffin}    {Molar volume}      {Parameter²}
             n1:=Inter5(cc.Mv,  60,80,100,120,140,  53,50,49,48,47);
             n2:=Inter5(cc.Mv,  60,80,100,120,140,  56,53,52,50,49);
             n3:=Inter5(cc.Mv,  60,80,100,120,140,  59,57,56,54,52);
             n4:=Inter5(cc.Mv,  60,80,100,120,140,  63,60,59,58,57);
             n5:=Inter5(cc.Mv,  60,80,100,120,140,  68,65,63,62,61);
             n6:=Inter5(cc.Mv,  60,80,100,120,140,  72,70,70,69,68);
             n7:=Inter5(cc.Mv,  60,80,100,120,140,  79,79,78,77,77);
             cc.phi  :=0.396;
             cc.phihv:=0.399;
           end;
      'c': Begin  {Cycloparaffin}
             n1:=Inter5(cc.Mv,  60,70,80,100,120,    69,65,63,59,53);
             n2:=Inter5(cc.Mv,  60,70,80,100,120,    71,69,66,61,57);
             n3:=Inter5(cc.Mv,  60,70,80,100,120,    76,73,69,63,60);
             n4:=Inter5(cc.Mv,  60,70,80,100,120,    81,77,73,68,65);
             n5:=Inter5(cc.Mv,  60,70,80,100,120,    88,82,79,72,69);
             n6:=Inter5(cc.Mv,  60,70,80,100,120,    95,90,86,79,77);
             n7:=Inter5(cc.Mv,  60,70,80,100,120,   102,98,92,87,81);
             cc.phi  :=0.415;
             cc.phihv:=0.415;
           end;
      'a': Begin  {Aromatic}
             n1:=Inter5(cc.Mv,  90,100,110,130,160,  70,66,62,58,54);
             n2:=Inter5(cc.Mv,  90,100,110,130,160,  73,70,66,61,59);
```

```
              n3:=Inter5(cc.Mv,  90,100,110,130,160,  78,73,70,66,61);
              n4:=Inter5(cc.Mv,  90,100,110,130,160,  83,78,74,70,68);
              n5:=Inter5(cc.Mv,  90,100,110,130,160,  88,83,80,75,73);
              n6:=Inter5(cc.Mv,  90,100,110,130,160,  95,90,87,82,78);
              n7:=Inter5(cc.Mv,  90,100,110,130,160, 105,98,94,90,88);
              cc.phi  :=0.450;
              cc.phihv:=0.447;
            end;
    end;
    cc.npsp:=sqrt(Inter7(cc.Tr, 0.40,0.45,0.50,0.55,0.60,0.65,0.70,
                                n7,  n6,  n5,  n4,  n3,  n2,  n1));

end {GetNonPolar};

{Wait for a certain output file name to appear. If it does not appear
 within the 15 minutes allowed, a dummy file is created to allow the
 program to proceed.}

Procedure Waitfor (fn: any);
  Var f1:text;                  {The file}
      i: integer;               {Timer}
  Begin
    assign (f1,fn);
    i:=1;
    repeat
      inc (i);
      delay (1000);             {Wait one second}
      {$I-}
      reset (f1);               {Try to open the file}
      {$I+}
    until (IOResult=0) or (i=900); {Wait for file to exist or 10
minutes.}

    {If 15 minutes passed and output appeared, a dummy file is
created.}

    If (i=900) then begin
      writeln ('  -> Error: Fifteen minutes passed and no output file
appeared.');
      writeln ('  -> A dummy file will be created !');
      rewrite (f1);
      writeln (f1,'This is a dummy file to allow processing to continue
!');
      writeln (f1,'Something unusual happened to PRO/II.');
    end;
    close (f1);
end {Waitfor};

{Provide some general information:}

Procedure GenInfo;
  Var c:char;
  Begin
    ClrScr;
    TextColor (White); TextBackground (Red);
    Gotoxy (2,2); Write('General information on ASEEK.');
```

```
    TextColor (Yellow); TextBackground (Blue);
    writeln;writeln;

    writeln ('ASEEK was developed to test components for their
potential as extractive or');
    writeln ('or azeotropic distillation solvents.');
    writeln ('It supports five different models. (For more information
on the models');
    writeln ('and their limitations, see chapters 4 & 3 of the related
M thesis.)');
    writeln ('ASEEK uses the ascii text file AGENTS.INF as a source of
solvents. Solvents');
    writeln ('are identified according to their first PRO/II library
name.');
    writeln;
    Textcolor (White);
    writeln ('The following summary of the models may be of use:');
    Textcolor (Yellow);
    writeln;
    writeln ('Tassios: Good for nonpolar binaries separated by a polar
solvent.');
    writeln;
    writeln ('Weimer-Prausnitz: A more advanced equation with similar
applications.');
    writeln;
    writeln ('Helpinstill & Van Winkle: Able to handle polar and
nonpolar binaries as well.');
    writeln;
    writeln ('MOSCED: Usually very accurate for most systems.');
    writeln;
    writeln ('UNIFAC: Very good for polar-polar, excellent for
nonpolar-nonpolar and');
    writeln ('        fair for polar-nonpolar combinations.');
    writeln;
    Textcolor (White);
    write ('Press any key to proceed...');
    Textcolor (Yellow);

    c:=Readkey;

end {GenInfo};

{Interpolate linearly, (Mathews, 175):}
Function Inter5 (xx, x0,x1,x2,x3,x4,
                    y0,y1,y2,y3,y4:rtype): rtype;
  Begin
    If (xx<=x1)
      then Inter5:=y0*(xx-x1)/(x0-x1)+y1*(xx-x0)/(x1-x0);
    If (xx<=x2) and (xx>x1) then
      Inter5:=y1*(xx-x2)/(x1-x2)+y2*(xx-x1)/(x2-x1);
    If (xx<=x3) and (xx>x2) then
      Inter5:=y2*(xx-x3)/(x2-x3)+y3*(xx-x2)/(x3-x2);
    If (xx>x3)
      then Inter5:=y3*(xx-x4)/(x3-x4)+y4*(xx-x3)/(x4-x3);
end {Inter5};
```

```
Function Inter7 (xx, x0,x1,x2,x3,x4,x5,x6,
                    y0,y1,y2,y3,y4,y5,y6:rtype): rtype;
  Begin
    If (xx<=x1)
      then Inter7:=y0*(xx-x1)/(x0-x1)+y1*(xx-x0)/(x1-x0);
    If (xx<=x2) and (xx>x1) then
      Inter7:=y1*(xx-x2)/(x1-x2)+y2*(xx-x1)/(x2-x1);
    If (xx<=x3) and (xx>x2) then
      Inter7:=y2*(xx-x3)/(x2-x3)+y3*(xx-x2)/(x3-x2);
    If (xx<=x4) and (xx>x3) then
      Inter7:=y3*(xx-x4)/(x3-x4)+y4*(xx-x3)/(x4-x3);
    If (xx<=x5) and (xx>x4) then
      Inter7:=y4*(xx-x5)/(x4-x5)+y5*(xx-x4)/(x5-x4);
    If (xx>x5)
      then Inter7:=y5*(xx-x6)/(x5-x6)+y6*(xx-x5)/(x6-x5);
end {Inter7};


end.


Unit ASEEKU2;

{$N+,E-}

{$F+}
{$O+}

{$D-}
{$R-}
{$L-}

Interface

Uses CRT,ASEEKU;

Const nat20 = 114;      {Number of data sets for MOSCED at 20°C}
                        {Taken fromThomas and Eckert, 1984:200}

      MOSCED20 : array [1..nat20] of record
                   p2name: string[10];  {PRO/II name}
                   ds,                  {Dispersion parameter}
                   t,                   {Polar parameter}
                   a,                   {Acidity parameter at 20°C}
                   b: single;           {Basicity parameter at 20°C}
                 end= (

                 (p2name:'CS2           '; ds:9.80; t:0.30; a:0.29;
b:0.16),
                 (p2name:'CCL4          '; ds:8.58; t:0.87; a:0.58;
b:0.15),
                 (p2name:'BRTRICLM    '; ds:9.05; t:1.00; a:0.70;
b:0.10),
                 (p2name:'CLFR          '; ds:8.43; t:1.95; a:3.05;
b:0.06),
```

```
                (p2name:'CL2M          '; ds:8.20; t:2.79; a:2.49;
b:0.38),
                (p2name:'DBRM          '; ds:9.41; t:2.90; a:2.00;
b:0.10),
                (p2name:'METHANOL     '; ds:7.14; t:2.55; a:7.45;
b:7.45),
                (p2name:'NTRM          '; ds:7.73; t:6.24; a:1.30;
b:2.40),
                (p2name:'CH3I          '; ds:9.30; t:1.95; a:0.35;
b:0.29),
                (p2name:'ACEN          '; ds:7.43; t:5.99; a:0.86;
b:3.98),
                (p2name:'1TCE          '; ds:8.35; t:1.40; a:0.50;
b:0.20),
                (p2name:'TCLE          '; ds:8.70; t:2.40; a:1.50;
b:0.20),
                (p2name:'12TE          '; ds:8.42; t:3.13; a:0.79;
b:0.51),
                (p2name:'11C2          '; ds:8.12; t:2.20; a:1.00;
b:0.30),
                (p2name:'NTRETH       '; ds:7.85; t:4.85; a:0.29;
b:2.20),
                (p2name:'EIOD          '; ds:9.12; t:1.66; a:0.31;
b:0.27),
                (p2name:'ETBR          '; ds:8.20; t:2.04; a:0.32;
b:0.23),
                (p2name:'ETHANOL      '; ds:7.51; t:1.36; a:6.19;
b:6.19),
                (p2name:'PRNT          '; ds:7.57; t:4.82; a:0.38;
b:3.31),
                (p2name:'DMK           '; ds:7.49; t:4.10; a:0.00;
b:4.87),
                (p2name:'ETFO          '; ds:7.50; t:3.32; a:0.00;
b:3.83),
                (p2name:'MEAC          '; ds:7.52; t:3.32; a:0.00;
b:3.83),
                (p2name:'1NTRPR       '; ds:7.96; t:4.15; a:0.25;
b:1.88),
                (p2name:'DMF           '; ds:8.26; t:4.62; a:0.65;
b:10.30),
                (p2name:'2NIP          '; ds:7.88; t:4.13; a:0.23;
b:1.85),
                (p2name:'1CLP          '; ds:7.81; t:1.90; a:0.30;
b:0.18),
                (p2name:'PROPANE      '; ds:6.70; t:0.00; a:0.00;
b:0.00),
                (p2name:'PROPANOL     '; ds:7.79; t:1.16; a:5.28;
b:5.28),
                (p2name:'MEK           '; ds:7.71; t:3.25; a:0.00;
b:4.05),
                (p2name:'MOPR          '; ds:7.69; t:2.84; a:0.00;
b:3.28),
                (p2name:'THF           '; ds:8.02; t:2.30; a:0.00;
b:4.58),
                (p2name:'PRFO          '; ds:7.69; t:2.84; a:0.00;
b:3.28),
```

```
                (p2name:'EOAC          '; ds:7.64; t:2.84; a:0.00;
b:3.28),
                (p2name:'DOXN          '; ds:8.08; t:3.32; a:0.00;
b:4.14),
                (p2name:'2CLB          '; ds:7.91; t:1.62; a:0.25;
b:0.15),
                (p2name:'1CLB          '; ds:7.96; t:1.66; a:0.26;
b:0.16),
                (p2name:'TBCL          '; ds:7.79; t:1.60; a:0.25;
b:0.15),
                (p2name:'BUTANE        '; ds:7.20; t:0.00; a:0.00;
b:0.00),
                (p2name:'NBA           '; ds:7.93; t:1.02; a:4.62;
b:4.62),
                (p2name:'PYRI          '; ds:8.57; t:3.16; a:0.68;
b:6.70),
                (p2name:'TPND          '; ds:8.27; t:0.58; a:0.00;
b:0.37),
                (p2name:'IPRN          '; ds:8.18; t:0.52; a:0.00;
b:0.34),
                (p2name:'CP            '; ds:8.01; t:0.00; a:0.00;
b:0.00),
                (p2name:'PTC2          '; ds:7.76; t:0.26; a:0.00;
b:0.21),
                (p2name:'PNT1          '; ds:7.62; t:0.25; a:0.00;
b:0.20),
                (p2name:'MIPK          '; ds:7.81; t:2.50; a:0.00;
b:3.20),
                (p2name:'CYPNTNOL      '; ds:8.51; t:1.10; a:4.50;
b:4.50),
                (p2name:'DEK           '; ds:7.86; t:2.77; a:0.00;
b:3.43),
                (p2name:'MPK           '; ds:7.83; t:2.77; a:0.00;
b:3.43),
                (p2name:'PROA          '; ds:7.77; t:2.48; a:0.00;
b:2.86),
                (p2name:'EPRT          '; ds:7.77; t:2.48; a:0.00;
b:2.86),
                (p2name:'PENTANE       '; ds:7.48; t:0.00; a:0.00;
b:0.00),
                (p2name:'2MB           '; ds:7.43; t:0.00; a:0.00;
b:0.00),
                (p2name:'PNTA          '; ds:8.05; t:0.90; a:4.12;
b:4.12),
                (p2name:'NITBNZ        '; ds:8.95; t:3.78; a:0.63;
b:1.36),
                (p2name:'CLBZ          '; ds:8.71; t:1.84; a:0.75;
b:0.45),
                (p2name:'BNZN          '; ds:8.49; t:1.95; a:0.22;
b:0.56),
                (p2name:'PHOH          '; ds:8.94; t:2.16; a:16.20;
b:1.64),
                (p2name:'ANLN          '; ds:9.25; t:4.22; a:3.81;
b:2.13),
                (p2name:'CHEN          '; ds:8.44; t:0.28; a:0.00;
b:0.25),
```

```
b:4.82),
b:0.18),
b:0.00),
b:0.18),
b:0.18),
b:0.00),
b:0.18),
b:4.00),
b:2.55),
b:0.00),
b:0.00),
b:0.00),
b:0.00),
b:0.00),
b:3.73),
b:4.98),
b:2.94),
b:0.93),
b:0.60),
b:1.60),
b:0.00),
b:0.22),
b:0.00),
b:2.69),
b:0.00),
b:0.00),
b:0.00),
b:0.00),
```

```
(p2name:'CHON          '; ds:8.48; t:3.05; a:0.00;
(p2name:'4PN1          '; ds:7.85; t:0.23; a:0.00;
(p2name:'CH            '; ds:8.22; t:0.00; a:0.00;
(p2name:'HXE1          '; ds:7.81; t:0.23; a:0.00;
(p2name:'2M1P          '; ds:7.75; t:0.23; a:0.00;
(p2name:'MCP           '; ds:8.05; t:0.00; a:0.00;
(p2name:'2PN2          '; ds:7.95; t:0.23; a:0.00;
(p2name:'CHXA          '; ds:8.65; t:0.90; a:4.00;
(p2name:'BACT          '; ds:7.85; t:2.21; a:0.00;
(p2name:'HEXANE        '; ds:7.67; t:0.00; a:0.00;
(p2name:'23MB          '; ds:7.67; t:0.00; a:0.00;
(p2name:'3MP           '; ds:7.68; t:0.00; a:0.00;
(p2name:'22MB          '; ds:7.60; t:0.00; a:0.00;
(p2name:'2MP           '; ds:7.63; t:0.00; a:0.00;
(p2name:'HXA           '; ds:8.14; t:0.82; a:3.73;
(p2name:'TEAM          '; ds:7.52; t:0.53; a:0.00;
(p2name:'BNZNITRL      '; ds:8.73; t:3.30; a:0.64;
(p2name:'BNZLCL        '; ds:8.84; t:2.71; a:0.74;
(p2name:'TOLU          '; ds:8.45; t:1.56; a:0.15;
(p2name:'MPHE          '; ds:8.64; t:2.77; a:0.28;
(p2name:'MCH           '; ds:8.19; t:0.00; a:0.00;
(p2name:'HPT1          '; ds:7.94; t:0.24; a:0.00;
(p2name:'CHP           '; ds:8.40; t:0.00; a:0.00;
(p2name:'EBK           '; ds:8.00; t:2.17; a:0.00;
(p2name:'HEPTANE       '; ds:7.81; t:0.00; a:0.00;
(p2name:'3MHX          '; ds:7.82; t:0.00; a:0.00;
(p2name:'22MP          '; ds:7.75; t:0.00; a:0.00;
(p2name:'24MP          '; ds:7.74; t:0.00; a:0.00;
```

```
                (p2name:'ACPH          '; ds:8.79; t:3.02; a:0.86;
b:3.13),
                (p2name:'EBZN          '; ds:8.49; t:1.28; a:0.05;
b:0.50),
                (p2name:'PXYL          '; ds:8.44; t:1.27; a:0.07;
b:0.74),
                (p2name:'OXYL          '; ds:8.58; t:1.65; a:0.04;
b:0.90),
                (p2name:'COCT          '; ds:8.56; t:0.00; a:0.00;
b:0.00),
                (p2name:'OCT1          '; ds:8.04; t:0.23; a:0.00;
b:0.21),
                (p2name:'ECH           '; ds:8.30; t:0.00; a:0.00;
b:0.00),
                (p2name:'224P          '; ds:7.84; t:0.00; a:0.00;
b:0.00),
                (p2name:'OCTANE        '; ds:7.91; t:0.00; a:0.00;
b:0.00),
                (p2name:'OCTA          '; ds:8.26; t:0.69; a:3.13;
b:3.13),
                (p2name:'QUINOLIN     '; ds:9.60; t:2.80; a:0.34;
b:3.10),
                (p2name:'BZLACTAT     '; ds:8.69; t:3.26; a:0.23;
b:2.51),
                (p2name:'DBK           '; ds:8.15; t:1.78; a:0.00;
b:2.21),
                (p2name:'DIBK          '; ds:8.07; t:1.60; a:0.00;
b:2.40),
                (p2name:'NONANE        '; ds:8.00; t:0.00; a:0.00;
b:0.00),
                (p2name:'TRPAMINE     '; ds:7.63; t:0.45; a:0.00;
b:3.30),
                (p2name:'1BRNAPH      '; ds:9.85; t:1.95; a:0.57;
b:0.38),
                (p2name:!BBNZ          '; ds:8.43; t:1.00; a:0.05;
b:0.40),
                (p2name:'CISD          '; ds:8.80; t:0.00; a:0.00;
b:0.00),
                (p2name:'BCH           '; ds:8.38; t:0.00; a:0.00;
b:0.00),
                (p2name:'DEC1          '; ds:8.17; t:0.21; a:0.00;
b:0.19),
                (p2name:'DECA          '; ds:8.07; t:0.00; a:0.00;
b:0.00),
                (p2name:'DALC          '; ds:8.34; t:0.60; a:2.72;
b:2.72),
                (p2name:'DDEC          '; ds:8.17; t:0.00; a:0.00;
b:0.00),
                (p2name:'HDC1          '; ds:8.38; t:0.10; a:0.00;
b:0.11),
                (p2name:'HXDC          '; ds:8.32; t:0.00; a:0.00;
b:0.00));

Procedure MakeInput (ss,          {The input file name.}
                     il: any);    {A line from AGENTS.INF.}
```

```
Procedure Config;

Implementation

{Generate an input file named ss for the agent contained in the line
obtained
 from AGENTS2.TXT earlier.}

Procedure MakeInput (ss,          {The input file name.}
                     il: any);    {A line from AGENTS.INF.}

  Var f2: text;                   {The input file generated.}
      s1: any;                    {A line of text.}
      s2: any;                    {Normal boiling point+-delta string.}
      nbp: rtype;                 {Agent normal boiling point.}
      i: integer;                 {String<=>number conversion code.}

  Begin

     {Get the normal boiling point:}

     s2:=copy(il,a_nbp,5);
     If s2[1]=' ' then s2:=copy (s2,2,length(s2)-1);

     Val(s2,nbp,i);

     If (i<>0) then begin
       writeln ('Error reading NBP from:');
       writeln (il);
       halt(1);
     end;

    {Write the input file:}

    assign(f2,ss);
    rewrite (f2);

    writeln (f2,'TITLE        PROJECT=ASEEK3,PROBLEM=Get_Data,*');
    writeln (f2,'             USER=BM,DATE=16/3/93');
    writeln (f2,'$');
    writeln  (f2,'DESCRIPTION    Generate source data for agent
evaluation.');
    writeln (f2,'$');
        w r i t e l n   ( f 2 , ' D I M E N S I O N
SI,TIME=HR,WT=KG,TEMPERATUE=K,PRESSURE=KPA,*');
     writeln   (f2,'
ENERGY=KJ,WORK=KW,LIQV=M3,VAPV=M3,VISC=PAS,*');
    writeln (f2,'             COND=WMK,SURF=NM,XDEN=SPGR');
    writeln (f2,'$');
    writeln (f2,'OUTDIMENSION SI');
    writeln (f2,'$');
    writeln (f2,'$ Reduce tolerances:');
    writeln (f2,'$');
    writeln (f2,'TOLERANCE    TEMP=-0.01,PRES=0.0001');
    writeln (f2,'$');
```

```
        w r i t e l n    ( f 2 , ' P R I N T
RATE=WT,FRACTION=M,STREAM=NONE,INPUT=ALL');
    writeln (f2,'$');
    writeln (f2,'COMPONENT DATA');
          w r i t e l n     ( f 2 , '          L I B I D
1,',c1name,'/2,',c2name,'/3,',copy(il,a_p2name,10));
    writeln (f2,'$');
    writeln (f2,'THERMODYNAMIC DATA');
    writeln (f2,'*');
    writeln (f2,'  METHOD SYSTEM=IDEAL,SET=SET01,DEFAULT');
    writeln (f2,'*');
    writeln (f2,'  METHOD KVALUE(VLE)=NRTL,PHI=IDEAL,ENTH(V)=PURE,*');
         w r i t e l n    ( f 2 , '
ENTH(L)=PURE,DENS(V)=SRK,DENS(L)=SRK,SET=SET02');
    writeln (f2,'          KVALUE FILL=UNIFAC');
    writeln (f2,'*');
    writeln (f2,'STREAM DATA');
    writeln (f2,'*');
    writeln (f2,'$ Used to compute dHv:');

    writeln (f2,'$');
    writeln (f2,'  PROPERTY STREAM=PURE3A,PRES(KPA)=84.4,PHASE=L*');
    writeln (f2,'           COMPOSITION(M)=3,1,RATE(M,KGM/H)=1');
    writeln (f2,'$');
    writeln (f2,'  PROPERTY STREAM=PURE3B,PRES(KPA)=84.4,PHASE=V*');
    writeln (f2,'           COMPOSITION(M)=3,1,RATE(M,KGM/H)=1');
    writeln (f2,'$');
    writeln (f2,'$ Ternary streams.');
    writeln (f2,'$');
       w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F T 1 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=1, 1/2,99/3,200,NORMALIZE');
    writeln (f2,'*');
       w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F T 2 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=1,20/2,80/3,200,NORMALIZE');
    writeln (f2,'*');
       w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F T 3 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=1,40/2,60/3,200,NORMALIZE');
    writeln (f2,'*');
       w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F T 4 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=1,60/2,40/3,200,NORMALIZE');
    writeln (f2,'*');
       w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F T 5 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=1,80/2,20/3,200,NORMALIZE');
    writeln (f2,'*');
       w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F T 6 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=1,99/2, 1/3,200,NORMALIZE');
    writeln (f2,'$');
    writeln (f2,'$ Binary streams: Component 1 & agent.');
    writeln (f2,'$');
```

```
      w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F B 1 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=1, 1/3,99,NORMALIZE');
    writeln (f2,'*');
      w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F B 2 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=1,20/3,80,NORMALIZE');
    writeln (f2,'*');
      w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F B 3 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=1,40/3,60,NORMALIZE');
    writeln (f2,'*');
      w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F B 4 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=1,60/3,40,NORMALIZE');
    writeln (f2,'*');
      w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F B 5 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=1,80/3,20,NORMALIZE');
    writeln (f2,'*');
      w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F B 6 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=1,99/3, 1,NORMALIZE');
    writeln (f2,'$');
    writeln (f2,'$ Component 2 & agent.');
    writeln (f2,'$');
      w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F B 7 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=2, 1/3,99,NORMALIZE');
    writeln (f2,'*');
      w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F B 8 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=2,20/3,80,NORMALIZE');
    writeln (f2,'*');
      w r i t e l n    ( f 2 , '        P R O P    S T R E A M = F B 9 ,
PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=2,40/3,60,NORMALIZE');
    writeln (f2,'*');
        w r i t e l n    ( f 2 , '          P R O P
STREAM=FB10,PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=2,60/3,40,NORMALIZE');
    writeln (f2,'*');
        w r i t e l n    ( f 2 , '          P R O P
STREAM=FB11,PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=2,80/3,20,NORMALIZE');
    writeln (f2,'*');
        w r i t e l n    ( f 2 , '          P R O P
STREAM=FB12,PRES=85.5,PHASE=M,RATE(WT)=1000,LFRAC(M)=1, *');
    writeln (f2,'       COMP(M)=2,99/3, 1,NORMALIZE');
    writeln (f2,'$');
    writeln (f2,' OUTPUT STREAMS=PURE3A,PURE3B,PURE3C,FORMAT=FMT1');
    writeln   (f2,'      FORMAT   IDNO=FMT1,TITLE=REQUESTED   STREAM
PROPERTIES,*');
       w r i t e l n    ( f 2 , '
PHASE,TEMPERATURE(K),PRESSURE(KPA),ENTHALPY(M),RATE(M)*');
```

```
          w r i t e l n    ( f 2 , '
DENSITY(G/CM3),MW,TC(K),PC(KPA),TR,PR,ACENTRIC,*');
    writeln (f2,'          NBP(M,K),TVP(KPA)');
    writeln (f2,'$');
    writeln (f2,'UNIT OPERATIONS');
    writeln (f2,'$');
    writeln (f2,'$ Binary flashes:');
    writeln (f2,'$');
    writeln (f2,'FLASH UID=T1,KPRINT');
    writeln (f2,'  FEED FT1');
    writeln (f2,'  PROD V=FTV1,L=FTL1');
    writeln (f2,'  BUBB PRES(ATM)=1.0');
    writeln (f2,'  METHOD SET=SET02');
    writeln (f2,'*');
    writeln (f2,'FLASH UID=T2,KPRINT');
    writeln (f2,'  FEED FT2');
    writeln (f2,'  PROD V=FTV2,L=FTL2');
    writeln (f2,'  BUBB PRES(ATM)=1.0');
    writeln (f2,'  METHOD SET=SET02');
    writeln (f2,'*');
    writeln (f2,'FLASH UID=T3,KPRINT');
    writeln (f2,'  FEED FT3');
    writeln (f2,'  PROD V=FTV3,L=FTL3');
    writeln (f2,'  BUBB PRES(ATM)=1.0');
    writeln (f2,'  METHOD SET=SET02');
    writeln (f2,'*');
    writeln (f2,'FLASH UID=T4,KPRINT');
    writeln (f2,'  FEED FT4');
    writeln (f2,'  PROD V=FTV4,L=FTL4');
    writeln (f2,'  BUBB PRES(ATM)=1.0');
    writeln (f2,'  METHOD SET=SET02');
    writeln (f2,'*');
    writeln (f2,'FLASH UID=T5,KPRINT');
    writeln (f2,'  FEED FT5');
    writeln (f2,'  PROD V=FTV5,L=FTL5');
    writeln (f2,'  BUBB PRES(ATM)=1.0');
    writeln (f2,'  METHOD SET=SET02');
    writeln (f2,'*');
    writeln (f2,'FLASH UID=T6,KPRINT');
    writeln (f2,'  FEED FT6');
    writeln (f2,'  PROD V=FTV6,L=FTL6');
    writeln (f2,'  BUBB PRES(ATM)=1.0');
    writeln (f2,'  METHOD SET=SET02');
    writeln (f2,'*');
    writeln (f2,'FLASH UID=B1,KPRINT');
    writeln (f2,'  FEED FB1');
    writeln (f2,'  PROD V=FBV1,L=FBL1');
    writeln (f2,'  BUBB PRES(ATM)=1.0');
    writeln (f2,'  METHOD SET=SET02');
    writeln (f2,'*');
    writeln (f2,'FLASH UID=B2,KPRINT');
    writeln (f2,'  FEED FB2');
    writeln (f2,'  PROD V=FBV2,L=FBL2');
    writeln (f2,'  BUBB PRES(ATM)=1.0');
    writeln (f2,'  METHOD SET=SET02');
    writeln (f2,'*');
```

```
writeln (f2,'FLASH UID=B3,KPRINT');
writeln (f2,'  FEED FB3');
writeln (f2,'  PROD V=FBV3,L=FBL3');
writeln (f2,'  BUBB PRES(ATM)=1.0');
writeln (f2,'  METHOD SET=SET02');
writeln (f2,'*');
writeln (f2,'FLASH UID=B4,KPRINT');
writeln (f2,'  FEED FB4');
writeln (f2,'  PROD V=FBV4,L=FBL4');
writeln (f2,'  BUBB PRES(ATM)=1.0');
writeln (f2,'  METHOD SET=SET02');
writeln (f2,'*');
writeln (f2,'FLASH UID=B5,KPRINT');
writeln (f2,'  FEED FB5');
writeln (f2,'  PROD V=FBV5,L=FBL5');
writeln (f2,'  BUBB PRES(ATM)=1.0');
writeln (f2,'  METHOD SET=SET02');
writeln (f2,'*');
writeln (f2,'FLASH UID=B6,KPRINT');
writeln (f2,'  FEED FB6');
writeln (f2,'  PROD V=FBV6,L=FBL6');
writeln (f2,'  BUBB PRES(ATM)=1.0');
writeln (f2,'  METHOD SET=SET02');
writeln (f2,'*');
writeln (f2,'FLASH UID=B7,KPRINT');
writeln (f2,'  FEED FB7');
writeln (f2,'  PROD V=FBV7,L=FBL7');
writeln (f2,'  BUBB PRES(ATM)=1.0');
writeln (f2,'  METHOD SET=SET02');
writeln (f2,'*');
writeln (f2,'FLASH UID=B8,KPRINT');
writeln (f2,'  FEED FB8');
writeln (f2,'  PROD V=FBV8,L=FBL8');
writeln (f2,'  BUBB PRES(ATM)=1.0');
writeln (f2,'  METHOD SET=SET02');
writeln (f2,'*');
writeln (f2,'FLASH UID=B9,KPRINT');
writeln (f2,'  FEED FB9');
writeln (f2,'  PROD V=FBV9,L=FBL9');
writeln (f2,'  BUBB PRES(ATM)=1.0');
writeln (f2,'  METHOD SET=SET02');
writeln (f2,'*');
writeln (f2,'FLASH UID=B10,KPRINT');
writeln (f2,'  FEED FB10');
writeln (f2,'  PROD V=FBV10,L=FBL10');
writeln (f2,'  BUBB PRES(ATM)=1.0');
writeln (f2,'  METHOD SET=SET02');
writeln (f2,'*');
writeln (f2,'FLASH UID=B11,KPRINT');
writeln (f2,'  FEED FB11');
writeln (f2,'  PROD V=FBV11,L=FBL11');
writeln (f2,'  BUBB PRES(ATM)=1.0');
writeln (f2,'  METHOD SET=SET02');
writeln (f2,'*');
writeln (f2,'FLASH UID=B12,KPRINT');
writeln (f2,'  FEED FB12');
```

```
    writeln (f2,'  PROD V=FBV12,L=FBL12');
    writeln (f2,'  BUBB PRES(ATM)=1.0');
    writeln (f2,'  METHOD SET=SET02');
    writeln (f2,'*');

    close (f2);

end {MakeInput};

{Configure the program:}

Procedure Config;
  Var c: char;
      fs:text;              {AGENTS.INF file}
      found: boolean;       {Is the name known.}
      il: any;              {A line from AGENTS.INF}
      i: integer;
  Begin
    ClrScr;
    writeln;
    writeln ('ASEEK Configuration');
    writeln;
    writeln ('The current components selected are (PRO/II library
names): ');
    writeln;
    writeln ('      Component 1: ',c1name);
    writeln ('      Component 2: ',c2name);

    {Get the chemical names of the components:}

    writeln;
    writeln ('     or (searching AGENTS.INF) ... ');
    writeln;
    assign (fs,'AGENTS.INF');
    reset (fs);
    found:=false;
    repeat
      readln (fs,il);
      if (c1name+' ')=copy(il,10,length(c1name)+1) then found:=true;
    until (found) or (eof(fs));
    If found then write ('     ',copy(il,a_cname,40));
    If  il[a_c]<>'  '  then  writeln  ('  (with  MOSCED  parameters
available.)')
                  else  writeln  ('  (with  no  MOSCED  parameters
found.)');
    reset (fs);
    found:=false;
    repeat
      readln (fs,il);
      if (c2name+' ')=copy(il,10,length(c2name)+1) then found:=true;
    until (found) or (eof(fs));
    If found then write ('     ',copy(il,a_cname,40));
    If  il[a_c]<>'  '  then  writeln  ('  (with  MOSCED  parameters
available.)')
                  else  writeln  ('  (with  no  MOSCED  parameters
found.)');
```

```
    writeln ('     (Parameters are available for the other models.)');
    close (fs);

    {Is this the default case?}

    writeln;
    If (c1name='OCT1') and (c2name='MBK') then begin
      writeln ('     (This is the default case.)');
      writeln;
    end;

    {Allow the selection of other components:}

    write ('Do you wish to select other components (yY/nN) ?');
    c:=upcase(Readkey);
    writeln;
    writeln;
    If c='Y' then begin
      Repeat
        c12ok:=false;  {Must compute new parameters.}
        writeln ('     Please enter the FIRST PRO/II library names:');
        writeln;
        write ('     Component 1 is: '); readln (c1name);
        write ('     Component 2 is: '); readln (c2name);
        writeln;
        For i:=1 to length(c1name) do c1name[i]:=upcase(c1name[i]);
        For i:=1 to length(c2name) do c2name[i]:=upcase(c2name[i]);

        {Check if the components are in AGENTS.INF:}

        writeln ('Checking if the names are in AGENTS.INF ...');
        writeln;

        reset (fs);
        found:=false;
        repeat
          readln (fs,il);
          if    (c1name+'    ')=copy(il,10,length(c1name)+1)    then
found:=true;
        until (found) or (eof(fs));
        reset (fs);
        If found then begin
          found:=false;
          repeat
            readln (fs,il);
            if    (c2name+'    ')=copy(il,10,length(c2name)+1)    then
found:=true;
          until (found) or (eof(fs));
        end;
        close (fs);

        If not found then begin
          writeln ('===> Both names are not in the file. Use the
correct names.');
          writeln;
        end;
```

```
      until found;
    end;
end {Config};


end.


Unit ASEEKU3;

{$N+,E-}

{$F+}
{$O+}

{$D-}
{$R-}
{$L-}

Interface

Uses CRT,ASEEKU;

Procedure NameSearch;
Procedure BoilSearch;

Implementation

Procedure NameSearch;  {Search for a given string inside AGENTS.INF.}
  Var f2: text;                    {The file.}
      s2,                          {String to search for}
      s1: any;                     {A line of text from AGENTS.INF.}
      i: integer;                  {Counter.}
      c: char;
  Begin
    ClrScr;
    writeln;
    writeln (' Please enter a short string or substring of text to scan
for:');
    writeln;
    write (' ');
    readln (s2);
    For i:=1 to length(s2) do s2[i]:=upcase(s2[i]);
    writeln;
    writeln (' Looking for your string ...');
    writeln (' (Use any key to stop the search.)');
    writeln;
    assign (f2,'AGENTS.INF');
    reset (f2);
    repeat
      readln (f2,s1);
      If Pos(s2,s1)>0 then begin
        write (copy(s1,a_nbp,5),' °C: ');
          writeln    (copy(s1,a_p2name,10),'    used    for
',copy(s1,a_cname,30));
        delay (500);
```

```
      end;
    until (eof(f2)) or keypressed;
    while keypressed do c:=readkey;

    close (f2);

    writeln;
    writeln (' Press any key to return to the main menu.');
    c:=readkey;

end {NameSearch};

Procedure BoilSearch;  {Search for solvent with a certain nbp range.}
  Var f2: text;                {The file.}
      bp,                      {A boiling point.}
      bp1,bp2: rtype;          {Search in the range bp1 to bp2.}
      s1,s2: any;              {A line of text from AGENTS.INF.}
      i: integer;              {Counter.}
      c: char;
  Begin
    ClrScr;
    writeln;
    writeln (' This option will provide a list of solvents which boil
in a certain range.');
    writeln;
    write (' Please enter low boiling point limit (°C)  : ');
    readln (bp1);
    write (' Please enter high boiling point limit (°C) : ');
    readln (bp2);

    writeln;
    writeln (' Looking ...');
    writeln (' (Use any key to stop the search.)');
    writeln;
    assign (f2,'AGENTS.INF');
    reset (f2);
    repeat
      readln (f2,s1);
    until s1[1]<>';';
    repeat
      readln (f2,s1);
      s2:=copy(s1,a_nbp,5);
      While s2[1]=' ' do s2:=copy(s2,2,length(s2)-1);
      Val (s2,bp,i);
      If (bp>=bp1) and (bp<=bp2) then begin
        write (bp:5:1,' °C: ');
          writeln   (copy(s1,a_p2name,10),'   used   for
',copy(s1,a_cname,30));
        delay (500);
      end;
    until (eof(f2)) or keypressed;
    while keypressed do c:=readkey;

    close (f2);

    writeln;
```

```
    writeln (' Press any key to return to the main menu.');
    c:=readkey;

end {BoilSearch};


end.
```

C3: ASEEK DATABASE FILE

This page contains the first page of the database file AGENTS.INF. The entire file is not printer because it contains over 1100 entries.

```
;
;
;       Agents database for ASEEK 3
;       ASCII format.
;
;       Latest update: 3/93
;
;
;
; Sources of information:
; ----------------------
;
; - PRO/II 3.01 Dataprep for names and normal boiling points only.
; - Riddick, Organic Solvents -  Physical Properties, 1986, ML882150
; - Thomas & Eckert, Ind.Eng.Chem.Process.Des.Dev. Vol. 23, No. 2, 1984
;
; Contents:
; ---------
;
; 1) MOSCED code: 0=alkane,1=chloride,2=bromide,3=iodide,4=nitrile,
;                 5=nitroalkane,6=alcohol,7=ester,8=ketone,9=other
; 2) Homomorph code: p=paraffin, c=cycloparaffin, a=aromatic
; 3) MOSCED q parameter: 1.0=saturated compounds.
;                        0.9=aromatics
;                        or 1.0-0.5*(no of C=C bonds)/(no of C atoms)
;                        (induction parameter)
; 4) PRO/II library name
; 5) Normal boiling point NBP, °C
; 6) Refractive index, nd
; 7) Assigned number of carbon atoms
; 8) Full chemical name
;
; 3 5    10          21    27    33 36
; | |    |           |     |     |  |
1 p 1.00 BRTRICLM   104.9 1.506  1 BROMOTRICHLOROMETHANE
1 p 1.00 CCL4        76.6 1.460  1 CARBON TETRACHLORIDE
  p      BROMFORM   149.2          TRIBROMOMETHANE
1 p 1.00 CLFR        61.2 1.446  1 CHLOROFORM
  p      BRCLM       68.1          BROMOCHLOROMETHANE
2 p 1.00 DBRM        97.0 1.542  1 DIBROMOMETHANE
0 p 1.00 PROPANE    -42.1 1.290  3 PROPANE
0 p 1.00 BUTANE      -0.5 1.333  4 n-BUTANE
9 p 0.90 PNT1        30.0 1.371  5 1-PENTENE
0 p 1.00 2MB         27.9 1.354  5 ISOPENTANE
1 p 1.00 CL2M        39.8 1.424  1 DICHLOROMETHANE
  p      DIIM       182.0          DIIODOMETHANE
9 p 1.00 HFOR       100.6 1.371  1 FORMIC ACID
  p      METCLSI     66.4          METHYL TRICHLOROSILANE
3 p 1.00 CH3I        42.4 1.513  1 METHYL IODIDE
8 p 1.00 FRMD       219.9 1.448  1 FORMAMIDE
```

5 p 1.00 NTRM 101.2 1.381 1 NITROMETHANE

APPENDIX D: SIMULATION RESULTS

Output from these simulation input files have not been reproduced here due their length. Essential results can be found in the relevant chapters.

These files are input files for the PRO/II simulation program version 3.3.

D1: Methanol alternative

```
TITLE       PROJECT=VLE_Data, PROBLEM=Azeotropic,USER=BM,DATE=24/9/93
DIMENSION    SI,TIME=HR,WT=KG,TEMPERATUE=C,PRESSURE=BAR,*
             ENERGY=KJ,WORK=KW,LIQV=M3,VAPV=M3,VISC=PAS,*
             COND=WMK,SURF=NM,XDEN=SPGR

OUTDIMENSION SI,TEMPERATUE=C,PRESSURE=BAR,ENERGY=CAL
PRINT INPUT=ALL

COMPONENT DATA
  LIBID 1,OCT1/2,MBK/3,METHANOL
  VANDERWALLS 2,3.956,4.59657

$
$ Use this section for special interaction parameters:
$

THERMODYNAMIC DATA
  METHOD SYSTEM(VLE)=UNIQUAC, TRANSPORT=PETRO, DEFAULT
  KVALUE(VLE) FILL=UNIFAC
$ OCT1-MBK:
  UNIQUAC(K) 1,2,-119.016,209.751

$ OCT1-METHANOL:
  UNIQUAC(K) 1,3,637.841,5.390
$ MBK-METHANOL:
```

```
  UNIQUAC(K) 2,3,581.608,-127.926

STREAM DATA
  PROP STREAM=FEED,PRES(BAR)=0.84,RATE(M)=60,LFRAC(M)=1, *
       COMP(M)=1,71.9/2,28.1,NOCHECK

  PROP STREAM=SOLV,PRES(BAR)=0.84,RATE(M)=385.86,LFRAC(M)=1, *
       COMP(M)=3,100,NOCHECK

UNIT OPERATIONS

COLUMN UID=COL1,NAME=AZEO
  PARAMETER TRAY=35,CHEMDIST=70,ERRINC=100,DAMP=0.5
  FEED FEED,10/SOLV,4
  PROD OVHD=ATOP,431,BTMS=ABOT
  DUTY 1,1/2,35
  VARY DUTY=1,2
  PRES(BAR) 1,0.844/35,0.900
  PRINT PROP=ALL,COMP=WT,KVALUE
  ESTI MODEL=CHEM,RRATIO=2
  PLOT PROFILE,XCOMP=1,1/2,2/3,3
  CONDENSER TYPE=BUBB
  SPEC RRATIO, VALUE=2.0
  SPEC STREAM=ATOP,RATE(M),VALUE=429
  PACKING SECTION(1)=2,34,SULZER=M250X,HETP(M)=0.3,CAPACITY=80
```

D2: DMF alternative

```
TITLE       PROJECT=VLE_Data, PROBLEM=Azeotropic,USER=BM,DATE=24/9/93
DIMENSION    SI,TIME=HR,WT=KG,TEMPERATUE=C,PRESSURE=BAR,*
             ENERGY=KJ,WORK=KW,LIQV=M3,VAPV=M3,VISC=PAS,*
             COND=WMK,SURF=NM,XDEN=SPGR

OUTDIMENSION SI,TEMPERATUE=C,PRESSURE=BAR,ENERGY=CAL
PRINT INPUT=ALL

COMPONENT DATA
```

```
  LIBID 1,OCT1/2,MBK/3,DMF
  VANDERWALLS 2,3.956,4.59657

$
$ Use this section for special interaction parameters:
$

THERMODYNAMIC DATA
  METHOD SYSTEM(VLE)=UNIQUAC, TRANSPORT=PETRO, DEFAULT
  KVALUE(VLE) FILL=UNIFAC
$ OCT1-MBK:
  UNIQUAC(K) 1,2,-119.016,209.751

$ OCT1-DMF:
  UNIQUAC(K) 1,3,105.238,104.229
$ MBK-DMF:
  UNIQUAC(K) 2,3,-15.397,84.614

STREAM DATA
  PROP STREAM=FEED,PRES(BAR)=0.84,RATE(M)=60,LFRAC(M)=1, *
       COMP(M)=1,71.9/2,28.1,NOCHECK

  PROP STREAM=SOLV,PRES(BAR)=0.84,RATE(M)=74,LFRAC(M)=1, *
       COMP(M)=3,100,NOCHECK

UNIT OPERATIONS

COLUMN UID=COL1,NAME=AZEO
  PARAMETER TRAY=65,CHEMDIST=70,ERRINC=100,DAMP=0.5
  FEED FEED,52/SOLV,4
  PROD OVHD=ATOP,58,BTMS=ABOT
  DUTY 1,1/2,65
  VARY DUTY=1,2
  PRES(BAR) 1,0.844/65,0.900
  PRINT PROP=ALL,COMP=WT,KVALUE
  ESTI MODEL=CHEM,RRATIO=2
  PLOT PROFILE,XCOMP=1,1/2,2/3,3
```

```
  CONDENSER TYPE=BUBB
  SPEC RRATIO, VALUE=2.0
  SPEC STREAM=ATOP,RATE(M),VALUE=57.9
  PACKING SECTION(1)=2,64,SULZER=M250X,HETP(M)=0.3,CAPACITY=80
```

D3: 2-methoxyethanol alternative

```
TITLE       PROJECT=VLE_Data, PROBLEM=Azeotropic,USER=BM,DATE=24/9/93
DIMENSION    SI,TIME=HR,WT=KG,TEMPERATUE=C,PRESSURE=BAR,*
             ENERGY=KJ,WORK=KW,LIQV=M3,VAPV=M3,VISC=PAS,*
             COND=WMK,SURF=NM,XDEN=SPGR

OUTDIMENSION SI,TEMPERATUE=C,PRESSURE=BAR,ENERGY=CAL
PRINT INPUT=ALL

COMPONENT DATA
  LIBID 1,OCT1/2,MBK/3,MXEA
  VANDERWALLS 2,3.956,4.59657

$
$ Use this section for special interaction parameters:
$

THERMODYNAMIC DATA
  METHOD SYSTEM(VLE)=UNIQUAC, TRANSPORT=PETRO, DEFAULT
  KVALUE(VLE) FILL=UNIFAC
$ OCT1-MBK:
  UNIQUAC(K) 1,2,-119.016,209.751

$ OCT1-MXEA:
  UNIQUAC(K) 1,3,125.182,100.937
$ MBK-MXEA:
  UNIQUAC(K) 2,3,50.634,25.320

STREAM DATA
  PROP STREAM=FEED,PRES(BAR)=0.84,RATE(M)=60,LFRAC(M)=1, *
       COMP(M)=1,71.9/2,28.1,NOCHECK
```

```
$RATE used to be 126:
  PROP STREAM=SOLV,PRES(BAR)=0.84,RATE(M)=156,LFRAC(M)=1, *
       COMP(M)=3,100,NOCHECK

UNIT OPERATIONS

COLUMN UID=COL1,NAME=AZEO
$48 used to be 42:
  PARAMETER TRAY=48,CHEMDIST=70,ERRINC=100,DAMP=0.5
  FEED FEED,35/SOLV,4
  PROD OVHD=ATOP,88.6,BTMS=ABOT
  DUTY 1,1/2,48
  VARY DUTY=1,2
  PRES(BAR) 1,0.844/48,0.900
  PRINT PROP=ALL,COMP=WT,KVALUE
  ESTI MODEL=CHEM,RRATIO=2
  PLOT PROFILE,XCOMP=1,1/2,2/3,3
  CONDENSER TYPE=BUBB
  SPEC RRATIO, VALUE=2.0
  SPEC STREAM=ATOP,RATE(M),VALUE=88.69
  PACKING SECTION(1)=2,47,SULZER=M250X,HETP(M)=0.3,CAPACITY=80
```

D4: kerosol alternatives

This section contains three input files for the different ratios of kerosol.

```
TITLE        PROJECT=Extractive, PROBLEM=Undecane,USER=BM,DATE=24/9/93
DIMENSION     SI,TIME=HR,WT=KG,TEMPERATUE=C,PRESSURE=BAR,*
              ENERGY=KJ,WORK=KW,LIQV=M3,VAPV=M3,VISC=PAS,*
              COND=WMK,SURF=NM,XDEN=SPGR

OUTDIMENSION SI,TEMPERATUE=C,PRESSURE=BAR,ENERGY=CAL
PRINT INPUT=ALL

COMPONENT DATA
  LIBID 1,OCT1/2,MBK/3,UNDC
```

```
  VANDERWALLS 2,3.956,4.59657
$ For UNDC (kersol 200):
  VANDERWALLS 3,6.556,7.87146

$
$ Use this section for special interaction parameters:
$

THERMODYNAMIC DATA
  METHOD SYSTEM(VLE)=UNIQUAC, TRANSPORT=PETRO
  KVALUE(VLE) FILL=UNIFAC

$ OCT1-MBK:
  UNIQUAC(K) 1,2,-119.016,209.751

$ OCT1-kerosol:
  UNIQUAC(K) 1,3,-9.240,-9.240
$ MBK-kerosol:
  UNIQUAC(K) 2,3,-20.360,87.449


STREAM DATA

$ Feed stream with OCT1 and MBK only, at its boiling point:

  PROP STREAM=FEED,PRES(BAR)=0.910,RATE(M)=60,LFRAC(M)=1, *
       COMP(M)=1,71.9/2,28.1,NOCHECK

$ Extractive stream, at 60 °C:

  PROP STREAM=EXTR,TEMP(C)=60,PRES(BAR)=0.910,RATE(M)=180,*
       COMP(M)=3,100,NOCHECK

UNIT OPERATIONS

$ The extractive column:
```

```
COLUMN UID=COL1,NAME=COL1
  PARAMETER TRAY=93,CHEMDIST=60,ERRINC=100,DAMP=0.6
  FEED FEED,31/EXTR,4
  PROD OVHD=TOP1,20,BTMS=BOT1
  DUTY 1,1/2,93
  VARY DUTY=1,2
  PRES(BAR) 1,0.844/93,0.900
  PRINT PROP=ALL,COMP=WT,KVALUE
  ESTI MODEL=CHEM,RRATIO=20
  PLOT PROFILE,XCOMP=1,1/2,2/3,3
  CONDENSER TYPE=BUBB
  SPEC RRATIO, VALUE=10.0
  SPEC STREAM=TOP1,RATE(M),VALUE=18
  PACKING SECTION(1)=2,92,SULZER=M250X,HETP(M)=0.3,CAPACITY=80

COLUMN UID=COL2,NAME=COL2
  PARAMETER TRAY=20,CHEMDIST=60,ERRINC=100,DAMP=0.6
  FEED BOT1,8
  PROD OVHD=TOP2,42,BTMS=BOT2
  DUTY 1,1/2,20
  VARY DUTY=1,2
  PRES(BAR) 1,0.844/20,0.900
  PRINT PROP=ALL,COMP=WT,KVALUE
  ESTI MODEL=CHEM,RRATIO=20
  PLOT PROFILE,XCOMP=1,1/2,2/3,3
  CONDENSER TYPE=BUBB
  SPEC RRATIO, VALUE=10.0
  SPEC STREAM=TOP2,RATE(M),VALUE=42
  PACKING SECTION(1)=2,19,SULZER=M250X,HETP(M)=0.3,CAPACITY=80

TITLE       PROJECT=Extractive, PROBLEM=Undecane,USER=BM,DATE=24/9/93
DIMENSION    SI,TIME=HR,WT=KG,TEMPERATUE=C,PRESSURE=BAR,*
             ENERGY=KJ,WORK=KW,LIQV=M3,VAPV=M3,VISC=PAS,*
             COND=WMK,SURF=NM,XDEN=SPGR

OUTDIMENSION SI,TEMPERATUE=C,PRESSURE=BAR,ENERGY=CAL
PRINT INPUT=ALL
```

```
COMPONENT DATA
  LIBID 1,OCT1/2,MBK/3,UNDC
  VANDERWALLS 2,3.956,4.59657
$ For UNDC (kersol 200):
  VANDERWALLS 3,6.556,7.87146

$
$ Use this section for special interaction parameters:
$

THERMODYNAMIC DATA
  METHOD SYSTEM(VLE)=UNIQUAC, TRANSPORT=PETRO
  KVALUE(VLE) FILL=UNIFAC

$ OCT1-MBK:
  UNIQUAC(K) 1,2,-119.016,209.751

$ OCT1-kerosol:
  UNIQUAC(K) 1,3,-9.240,-9.240
$ MBK-kerosol:
  UNIQUAC(K) 2,3,-20.360,87.449


STREAM DATA

$ Feed stream with OCT1 and MBK only, at its boiling point:

  PROP STREAM=FEED,PRES(BAR)=0.910,RATE(M)=60,LFRAC(M)=1, *
       COMP(M)=1,71.9/2,28.1,NOCHECK

$ Extractive stream, at 60 °C:

  PROP STREAM=EXTR,TEMP(C)=60,PRES(BAR)=0.910,RATE(M)=240,*
       COMP(M)=3,100,NOCHECK

UNIT OPERATIONS
```

```
$ The extractive column:

COLUMN UID=COL1,NAME=COL1
   PARAMETER TRAY=81,CHEMDIST=60,ERRINC=100,DAMP=0.6
   FEED FEED,24/EXTR,4
   PROD OVHD=TOP1,20,BTMS=BOT1
   DUTY 1,1/2,81
   VARY DUTY=1,2
   PRES(BAR) 1,0.844/81,0.900
   PRINT PROP=ALL,COMP=WT,KVALUE
   ESTI MODEL=CHEM,RRATIO=20
   PLOT PROFILE,XCOMP=1,1/2,2/3,3
   CONDENSER TYPE=BUBB
   SPEC RRATIO, VALUE=10.0
   SPEC STREAM=TOP1,RATE(M),VALUE=18
   PACKING SECTION(1)=2,80,SULZER=M250X,HETP(M)=0.3,CAPACITY=80

COLUMN UID=COL2,NAME=COL2
   PARAMETER TRAY=20,CHEMDIST=60,ERRINC=100,DAMP=0.6
   FEED BOT1,8
   PROD OVHD=TOP2,42,BTMS=BOT2
   DUTY 1,1/2,20
   VARY DUTY=1,2
   PRES(BAR) 1,0.844/20,0.900
   PRINT PROP=ALL,COMP=WT,KVALUE
   ESTI MODEL=CHEM,RRATIO=20
   PLOT PROFILE,XCOMP=1,1/2,2/3,3
   CONDENSER TYPE=BUBB
   SPEC RRATIO, VALUE=10.0
   SPEC STREAM=TOP2,RATE(M),VALUE=42
   PACKING SECTION(1)=2,19,SULZER=M250X,HETP(M)=0.3,CAPACITY=80

TITLE       PROJECT=Extractive, PROBLEM=Undecane,USER=BM,DATE=24/9/93
DIMENSION    SI,TIME=HR,WT=KG,TEMPERATUE=C,PRESSURE=BAR,*
             ENERGY=KJ,WORK=KW,LIQV=M3,VAPV=M3,VISC=PAS,*
             COND=WMK,SURF=NM,XDEN=SPGR
```

```
OUTDIMENSION SI,TEMPERATUE=C,PRESSURE=BAR,ENERGY=CAL
PRINT INPUT=ALL

COMPONENT DATA
  LIBID 1,OCT1/2,MBK/3,UNDC
  VANDERWALLS 2,3.956,4.59657
$ For UNDC (kersol 200):
  VANDERWALLS 3,6.556,7.87146

$
$ Use this section for special interaction parameters:
$

THERMODYNAMIC DATA
  METHOD SYSTEM(VLE)=UNIQUAC, TRANSPORT=PETRO
  KVALUE(VLE) FILL=UNIFAC

$ OCT1-MBK:
  UNIQUAC(K) 1,2,-119.016,209.751

$ OCT1-kerosol:
  UNIQUAC(K) 1,3,-9.240,-9.240
$ MBK-kerosol:
  UNIQUAC(K) 2,3,-20.360,87.449


STREAM DATA

$ Feed stream with OCT1 and MBK only, at its boiling point:

  PROP STREAM=FEED,PRES(BAR)=0.910,RATE(M)=60,LFRAC(M)=1, *
       COMP(M)=1,71.9/2,28.1,NOCHECK

$ Extractive stream, at 60 °C:

  PROP STREAM=EXTR,TEMP(C)=60,PRES(BAR)=0.910,RATE(M)=300,*
       COMP(M)=3,100,NOCHECK
```

```
UNIT OPERATIONS

$ The extractive column:

COLUMN UID=COL1,NAME=COL1
  PARAMETER TRAY=72,CHEMDIST=60,ERRINC=100,DAMP=0.6
  FEED FEED,19/EXTR,4
  PROD OVHD=TOP1,20,BTMS=BOT1
  DUTY 1,1/2,72
  VARY DUTY=1,2
  PRES(BAR) 1,0.844/72,0.900
  PRINT PROP=ALL,COMP=WT,KVALUE
  ESTI MODEL=CHEM,RRATIO=20
  PLOT PROFILE,XCOMP=1,1/2,2/3,3
  CONDENSER TYPE=BUBB
  SPEC RRATIO, VALUE=10.0
  SPEC STREAM=TOP1,RATE(M),VALUE=18
  PACKING SECTION(1)=2,71,SULZER=M250X,HETP(M)=0.3,CAPACITY=80

COLUMN UID=COL2,NAME=COL2
  PARAMETER TRAY=20,CHEMDIST=60,ERRINC=100,DAMP=0.6
  FEED BOT1,8
  PROD OVHD=TOP2,42,BTMS=BOT2
  DUTY 1,1/2,20
  VARY DUTY=1,2
  PRES(BAR) 1,0.844/20,0.900
  PRINT PROP=ALL,COMP=WT,KVALUE
  ESTI MODEL=CHEM,RRATIO=20
  PLOT PROFILE,XCOMP=1,1/2,2/3,3
  CONDENSER TYPE=BUBB
  SPEC RRATIO, VALUE=10.0
  SPEC STREAM=TOP2,RATE(M),VALUE=42
  PACKING SECTION(1)=2,19,SULZER=M250X,HETP(M)=0.3,CAPACITY=80
```

D5: Methanol test on a synthetic stream

```
TITLE PROJECT=C8_Methanol, Problem=Azeotropic,*
```

```
      USER=BM, DATE=5/10/93
DESC  Investigate effect of methanol on C8.
DIMEN SI,time=hr,wt=kg,temp=k,pres=kpa,*
      ener=kj,work=kw,liqv=m3,vapv=m3,visc=pas,*
      cond=wmk,surf=nm,xden=spgr
OUTDIMENSION SI,TEMPERATUE=C,PRESSURE=BAR,ENERGY=CAL
PRINT RATE=m,wt,FRACTION=wt,STREAM=all,INPUT=all
DBASE DATA=all,PC1

COMPONENT DATA
      LIBID 1,oct1/2,oct2/3,2eh1/4,octn/5,4mhept/6,2m3epn/*
            7,dipk/8,dibe/9,mbk/10,nba/11,2m1b/12,2pna/13,meoh
      VANDERWALLS 9,3.956,4.59657

THERMODYNAMIC DATA
  METHOD SYSTEM(VLE)=NRTL, TRANSPORT=PETRO, DEFAULT
  KVALUE(VLE) FILL=UNIFAC

$ OCT1-MBK:
  NRT3(K) 1,9,-4.728832,345.7976,0.8192004
$ OCT1-METHANOL:
  NRT3(K) 1,13,337.6995,646.4594,0.2372091
$ MBK-METHANOL:
  NRT3(K) 9,13,501.7869,232.4536,0.7436261

STREAM DATA
  PROP STREAM=C8F,   PRES(BAR)=0.84,RATE(M)=60, LFRAC(M)=1,*
       COMP(M)=1,67/2,1/3,9/4,9/5,1/6,1/7,3/8,2/9,4/10,1/11,1/*
       12,1,NORMALIZE
  PROP STREAM=METH, PRES(BAR)=0.84,RATE(M)=395, LFRAC(M)=1,*
       COMP(M)=13,100,NORMALIZE

UNIT OPERATIONS

COLUMN UID=COL1,NAME=COL1
  PARAMETER TRAY=35,CHEMDIST=70,ERRINC=100,DAMP=0.5
  FEED C8F,10/METH,4
```

```
PROD OVHD=TOP,446,BTMS=BOT
DUTY 1,1/2,35
VARY DUTY=1,2
PRES(BAR) 1,0.84/35,0.9
PRINT PROP=ALL,COMP=WT,KVALUE
ESTI MODEL=CHEM,RRATIO=2
PLOT PROFILE,XCOMP=1,1/9,9/13,13
CONDENSER TYPE=BUBB
SPEC RRATIO, VALUE=2.0
SPEC STREAM=TOP,RATE(M),VALUE=447
PACKING SECTION(1)=2,34,SULZER=M250X,HETP(M)=0.3,CAPACITY=80
```