CPI COLOM DATA FILE FORMAT

General Information

All current data files follow a common style, which is designed to allow easy inclusion of new data items.

Basic principles:-

- Case insensitive
- Order insensitive
- Column insensitive
- Any missing data supplied by program (sensible defaults)

Data is stored in the form of:

Item_name = value, value, value, …

The data items are delimited by commas (",")
The line will be ignored if the data items are missing or not the correct type (real, character etc.)
All values must be on the same line as the "Item-name"

Character data – spaces & special characters. Preceding and following spaces are ignored by the system e.g.

Process_name = 1,   primary distillation tower   , summer operation

Would return the values
1
"primary distillation tower"
"summer operation"

Some characters have special meaning to the system so they cannot be used directly in character data. Any special characters are converted into an equivalent token.
Below is a list of special characters with their meanings, and the equivalent tokens

To use ;   Type
"," (comma)   = "~ " (space)   Delimiter
";"   = "~#"   Inline comment   … value, value   ; this is a comment
"!"   = "~@"   Entire line is commented   !item_name = value , value
"~"   = "~~"   Token identifier

The data file has an identifier header and two sections delimited by the two keywords [COUNTERS] & [DATA]

Identifier header

This must be the first line in the file e.g.

2.0 [UMIST SDF Data File Version Number 02/11/1998 10:34:00]

2.0 = data file version number
[UMIST SDF Data File Version Number 02/11/1998 10:34:00] = optional information (ignored by program)

[COUNTERS]

This must precede the [DATA] section.

This gives summary information as to the size of the problem contained within the file.

It is used to check that the program can accommodate the problem and used to initialise the default data areas.

Any "item_name" which should be in the [DATA] section will be ignored

[DATA]

This must follow the [COUNTERS] section. Any "item_name" which should be in the [COUNTERS] section will be ignored.

This is the main information for the program. As data items are read in they overwrite any default information.

Miscellaneous items

The data file may contain information that is ignored by the system

[### ….] = these are treated as comment and are ignored
" "   Blank lines
"!"   This is a comment line
";"   Inline comment   … value, value   ; this is a comment
[EOF] End of File marker – ignored by program

Colom Item Names

Identifier Header

4.0 [UMIST COL Data File Version Number]

Counters Section

CSM_Present = <n>
Presence flag for simulator section of the data file
<n> = 1 : simulator data is present in the file
<n> = 0 : simulator data is not present

CSM_NumSections = <n>
<n> = number of sections in the column. If in doubt select n = 2, and the program will calculate the number of sections.

Data Section

CSM_VersNo = 2.1
Version number of simulator data file format. Currently at 2.1.

CSM_Date = <dd/mm/yy>
<dd/mm/yy> Date of creation of simulator data. Max 11 characters

CSM_ColName = <column name>
<column name> = Text description of the column. Max 25 characters

CSM_NumComponents = <n>
<n> = number of components present in the column.

CSM_NumStages = <n>
<n> = number of stages in the column.

CSM_NumFeeds = <n>
<n> = number of feed streams to the column.

CSM_NumProducts = <n>
<n> = number of product streams from column.

CSM_NumPumpArounds = <n>
<n> = number of pump-arounds on the column.

CSM_CompName = <n>, <name>
<n> = component number
<name> = component name. Max 25 characters

Units
All information is exported to the Colom data file in whichever units are being used during the simulation ("local" units). In addition, text descriptions of these

units are required, and the necessary conversion factors required to convert to Colom's own units ("internal" units).

Unit Names

CSM_FlowUnit = <flow unit>
<flow unit> = text description of the units being used for all flow based simulator data. Max 30 characters.

CSM_TempUnit = <temperature unit>
<temperature unit> = text description of the units being used for all temperatures in simulator data. Max 30 characters.

CSM_PressureUnit = <pressure unit>
<pressure unit> = text description of the units being used for all pressures in simulator data. Max 30 characters.

CSM_EnthalpyUnit = <enthalpy unit>
<enthalpy unit> = text description of the units being used for all enthalpies in simulator data. Max 30 characters.

CSM_EntropyUnit = <entropy unit>
<entropy unit> = text description of the units being used for all entropies in simulator data. Max 30 characters.

CSM_HeatFlowUnit = <heatflow unit>
<heatflow unit> = text description of the units being used for all heat flows in simulator data. Max 30 characters.

Unit Conversions

CSM_FlowConv = <n> ; (mol/sec)
<n> = value to multiply all simulator flows by to convert to mol/sec

CSM_TempConv = <n> ;(C)
<n> = value to multiply all simulator temperatures by to convert to C (see also CSM_TempOffset)

CSM_PressureConv = <n> ; (N/m^2)
<n> = value to multiply all simulator pressures by to convert to N/m^2 (see also CSM_PressOffset)

CSM_EnthalpyConv = <n> ; (J/mol)
<n> = value to multiply all simulator enthalpies by to convert to J/mol

CSM_EntropyConv = <n> ; (J/mol-C)
<n> = value to multiply all simulator entropies by to convert to J/mol-C

CSM_HeatFlowConv = <n> ; (J/sec)
<n> = value to multiply all simulator heat flows by to convert to J/sec

CSM_TempOffset = <n>

<n> = temperature offset to convert simulator temperatures to C. The offset is applied before the scaling factor
e.g. simulator temperatures are in Rankine
CSM_TempOffset = -491.67
CSM_TempConv = 0.555555

So Temp(C) = [Temp(R) - 491.67] * 0.55555

CSM_PressOffset = <n>
<n> = pressure offset to convert simulator temperatures to N/m^2 (Absolute). The offset is applied before the scaling factor

Heat Duty Information

CSM_HeatDuty = <stage>, <heatflow / duty>
<stage> = stage number (1 = top stage)
<heatflow/duty> = Total heat duty for the stage. Positive values indicate heat flow in e.g. reboiler, negative values indicate heat flow out, e.g. condenser. If pump-arounds are present the pump-around heat duty should be included in the pump-around return stage duty (see later)

Feed Information Section

CSM_FeedName = <n>, <feedname>
<n> = feed number
<feedname> = name of feed. Max 25 characters

CSM_FeedTempPress = <nfeed>, <nstage>, <temperature>, <pressure>
<nfeed> = feed number
<nstage> = stage number of the feed (1 = top stage)
<temperature> = temperature of the feed stream.
<pressure> = pressure of the feed stream.

CSM_FeedLFlowVFlow = <nfeed>, <nstage>, <liquid flow>, <vapour flow>
<nfeed> = feed number
<nstage> = stage number of the feed (1 = top stage)
<liquid flow> = liquid molar flow rate of the feed
<vapour flow> = vapour molar flow rate of the feed

CSM_FeedLVEnthalpy = <nfeed>, <nstage>, <liquid enthalpy>, <vapour enthalpy>
<nfeed> = feed number
<nstage> = stage number of the feed (1 = top stage)
<liquid enthalpy> = liquid specific molar enthalpy of the feed
<vapour enthalpy> = vapour specific molar enthalpy of the feed

CSM_FeedLVEntropy = <nfeed>, <nstage>, <liquid entropy>, <vapour entropy>
<nfeed> = feed number
<nstage> = stage number of the feed (1 = top stage)
<liquid entropy> = liquid specific molar entropy of the feed
<vapour entropy> = vapour specific molar entropy of the feed

CSM_FeedCompn = <nfeed>, <ncomp>, <liquid fraction>, <vapour fraction>
<nfeed> = feed number
<ncomp> = component number
<liquid fraction> = liquid fraction of this component in this feed
<vapour fraction> = vapour fraction of this component in this feed

Product Information Section

CSM_ProdName = <nprod>, <prod name>
<nprod> = product number
<prod name> = name of the product

CSM_ProdTempPress = <nprod>, <nstage>, <temperature>, <pressure>
<nprod> = product number
<nstage> = stage number of the product (1 = top stage)
<temperature> = temperature of the product
<pressure> = pressure of the product

CSM_ProdLFlowVFlow = <nproduct>, <nstage>, <liquid flow>, <vapour flow>
<nproduct> = product number
<nstage> = stage number of the product (1 = top stage)
<liquid flow> = liquid molar flow rate of the product
<vapour flow> = vapour molar flow rate of the product

CSM_ProdLVEnthalpy = <nproduct>, <nstage>, <liquid enthalpy>, <vapour enthalpy>
<nproduct> = product number
<nstage> = stage number of the product (1 = top stage)
<liquid enthalpy> = liquid specific molar enthalpy of the product
<vapour enthalpy> = vapour specific molar enthalpy of the product

CSM_ProdLVEntropy = <nproduct>, <nstage>, <liquid entropy>, <vapour entropy>
<nproduct> = product number
<nstage> = stage number of the product (1 = top stage)
<liquid entropy> = liquid specific molar entropy of the product
<vapour entropy> = vapour specific molar entropy of the product

CSM_ProdCompn = <nproduct>, <ncomp>, <liquid fraction>, <vapour fraction>
<nproduct> = product number
<ncomp> = component number
<liquid fraction> = liquid fraction of this component in this product
<vapour fraction> = vapour fraction of this component in this product

Pump Around Information

CSM_P/AName = <npa>, <pa name>
<npa> = pump around number
<pa name> = name of pump around. Max 25 characters

CSM_P/ADrawTempPress = <npa>, <nstage>, <temperature>, <pressure>

<npa> = pump around number
<nstage> = stage number of the pump around draw
<temperature> = temperature at the pump around draw
<pressure> = pressure at the pump around draw

CSM_P/ADrawLFlowVFlow = <npa>, <nstage>, <liquid flow>, <vapour flow>
<npa> = pump around number
<nstage> = stage number of the pump around draw
<liquid flow> = liquid molar flow rate of the pump around draw
<vapour flow> = vapour molar flow rate of the pump around draw

CSM_P/ADrawLVEnthalpy = <npa>, <nstage>, <liquid enthalpy>, <vapour enthalpy>
<npa> = pump around number
<nstage> = stage number of the pump around draw
<liquid enthalpy> = liquid specific enthalpy at the pump around draw
<vapour enthalpy> = vapour specific enthalpy at the pump around draw

CSM_P/ADrawLVEntropy = <npa>, <nstage>, <liquid entropy>, <vapour entropy>
<npa> = pump around number
<nstage> = stage number of the pump around draw
<liquid entropy> = liquid specific entropy at the pump around draw
<vapour entropy> = vapour specific entropy at the pump around draw

CSM_P/AReturnTempPress = <npa>, <nstage>, <temperature>, <pressure>
<npa> = pump around number
<nstage> = stage number of the pump around return
<temperature> = temperature at the pump around return
<pressure> = pressure at the pump around return

CSM_P/AReturnLFlowVFlow = <npa>, <nstage>, <liquid flow>, <vapour flow>
<npa> = pump around number
<nstage> = stage number of the pump around return
<liquid flow> = liquid molar flow rate of the pump around return
<vapour flow> = vapour molar flow rate of the pump around return

CSM_P/AReturnLVEnthalpy = <npa>, <nstage>, <liquid enthalpy>, <vapour enthalpy>
<npa> = pump around number
<nstage> = stage number of the pump around return
<liquid enthalpy> = liquid specific enthalpy at the pump around return
<vapour enthalpy> = vapour specific enthalpy at the pump around return

CSM_P/AReturnLVEntropy = <npa>, <nstage>, <liquid entropy>, <vapour entropy>
<npa> = pump around number
<nstage> = stage number of the pump around return
<liquid entropy> = liquid specific entropy at the pump around return
<vapour entropy> = vapour specific entropy at the pump around return

Stage By Stage Information

CSM_StgByStgTempPress = <nstage>, <nstage>, <temperature>, <pressure>
<nstage> = stage number (two entries required)
<temperature> = temperature at the stage
<pressure> = pressure at the stage

CSM_StgByStgLFlowVFlow = <nstage>, <nstage>, <liquid flow>, <vapour flow>
<nstage> = stage number (two entries required)
<liquid flow> = liquid molar flow rate at the stage
<vapour flow> = vapour molar flow rate at the stage

CSM_StgByStgLVEnthalpy = <nstage>, <nstage>, <liquid enthalpy>, <vapour enthalpy>
<nstage> = stage number (two entries required)
<liquid enthalpy> = liquid specific enthalpy at the stage
<vapour enthalpy> = vapour specific enthalpy at the stage

CSM_StgByStgLVEntropy = <nstage>, <nstage>, <liquid entropy>, <vapour entropy>
<nstage> = stage number (two entries required)
<liquid entropy> = liquid specific entropy at the stage
<vapour entropy> = vapour specific entropy at the stage

CSM_StgByStgLVDensity = <nstage>, <nstage>, <liq. mol. density>, <vap. mol. density>
<nstage> = stage number (two entries required)
<liq. mol. density> = liquid molar density at the stage ($kmol/m^3$)
<vap. mol. density> = vapour molar density at the stage ($kmol/m^3$)

CSM_StgByStgLVMoleMass = <nstage>, <nstage>, <liq. mol. mass>, <vap. mol. mass>
<nstage> = stage number (two entries required)
<liq. mol. mass> = liquid molar mass at the stage (kg/kmol)
<vap. mol. mass> = vapour molar mass at the stage (kg/kmol)

CSM_StgByStgSurfaceTen = <nstage>, <nstage>, <surface tension>
<nstage> = stage number (two entries required)
<liq. mol. mass> = surface tension of liquid on the stage (dyne/cm)

CSM_StageComposition = <nstage>, <ncomp>, <liquid fraction>, <vapour fraction>
<nstage> = stage number
<ncomp> = component number
<liquid fraction> = liquid fraction of this component at this stage
<vapour fraction> = vapour fraction of this component at this stage

Miscellanous Information

CSM_LightKey = <n>
<n> = component number specified as the light key during the simulation

CSM_HeavyKey = \<n\>
\<n\> = component number specified as the heavy key during the simulation

CSM_FeedConvention = \<nfeed\> \<n\>
\<nfeed\> = feed number
\<n\> = flash condition of the feed
\<n\> = 1 : liquid and vapour feeds to same stage
\<n\> = 0 : vapour feed on tray above liquid feed

CSM_AnalysisType = \<n\>
\<n\> = analysis method used to calculate profiles
\<n\> = 1 : light/heavy key
\<n\> = 2 : grouped key
\<n\> = 3 : driving force (Henke)

CSM_DrivingForce = \<n\>
\<n\> = minimum driving force during Henke calculations

CSM_ColumnType = \<n\>
\<n\> = column type
\<n\> = 1 : Simple column (1 feed, 2 products)
\<n\> = 2 : multi-feed (multiple feeds, 2 products)
\<n\> = 3 : multi-products (1 feed, multiple products)
\<n\> = 4 : side-columns (simple column with side columns)

CSM_MainFeedStage = \<n\>
\<n\> = for multi-feed columns, the stage that divides the column into a stripping section and rectifying section. This is used to determine whether to add a side reboiler or side condenser during the Henke driving force analysis.

CSM_Section_LightKey = \<nsect\>, \<light key\>
\<nsect\> = section number
\<light key\> = number of the light key component in the section

CSM_Section_HeavyKey = \<nsect\>, \<heavy key\>
\<nsect\> = section number
\<heavy key\> = number of the heavy key component in the section