Simulation of a steady state flash

Description: Stationary flash simulation of an Ethanol(1) - Water(2) - mixture
With following assumptions:

- Apart from heater and mass flows, no energy is transferred across the system boundary.
- Liquid and vapor phase are each ideally mixed. Liquid and vapor phase are in equilibrium.
- The vapor phase behaves as an ideal gas and the liquid as an incompressible fluid.
- VLE described by extended Raoult's law.
- Vapor pressure calculation by Antoine.
- Evaporation enthalpy calculation by PPDS12.
- Real fluid behavior of the liquid phase is expressed through Wilson's gE model.
- Excess variables neglected.

Wilson and Antoine parameter are taken from: Gmehling, Kolbe;
PPDS12 parameter are taken from: www.ddbst.de;

Equation System: 86383: statFlash.moseqs
IndexSpecification: e[0]86383.NC = 2

Variable Specification: 86386: IV_statFlash.mosvar
Parameter Specification: none.
Results Specification: 86388: RE_statFlash_CBzzMath_Orig.mosvar

Hierarchical view of equations:

Equation System: 86383: statFlash.moseqs

Description: Stationary flash with following additional assumption to basicFlash:

1. Apart from heater and mass flows, no energy is transferred across the system boundary.
2. flash geometry is cylindric.

Connected Equations:

- Eq: 86378: StatEnergyBalance.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Energy balance (stationary)

$$0 = F^{F,n} \cdot h^{F,n} - h^{B,n} \cdot F^{B,n} - h^{D,n} \cdot F^{D,n} + Q \tag{1}$$

- Eq: 86379: StatComponentBalance.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Component balance (stationary)

$$0 = x_i^F \cdot F^{F,n} - x_i^B \cdot F^{B,n} - y_i^D \cdot F^{D,n} \tag{2}$$

Connected EQ-Systems:

- 86375: basicFlash.moseqs
- 86384: tankGeometry.moseqs

Connection Level (1) – EQ-Systems connected to 86383: statFlash.moseqs:

Equation System: 86375: basicFlash.moseqs

Description: basic model of a flash with following assumptions:

1. liquid and vapor phase are each ideally mixed. Liquid and vapor phase are in equilibrium.
2. The vapor phase behaves as an ideal gas and the liquid as an incompressible fluid.
3. VLE description by extended Raoult's law
4. Vapor pressure calculation by Antoine
5. Acitivity calculations in the liquid phase by Wilson's g^E-Model

Connected Equations:

- Eq: 86350: sumRelationVapor.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar summation relation (vapor)

$$1 = \sum_{i=1}^{NC} y_i^D \tag{3}$$

- Eq: 86353: molarEnthalpyVapor.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar enthalpy (vapor)

$$h^{D,n} = \sum_{i=1}^{NC} y_i^D \cdot h_i^{D,n} + h^{E,D,n} \tag{4}$$

- Eq: 86356: molarEnthalpyFeed.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar enthalpy (feed)

$$h^{F,n} = \sum_{i=1}^{NC} x_i^F \cdot h_i^{F,n} + h^{E,F,n} \tag{5}$$

- Eq: 86364: molarEvapEnthalpyLiquid.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar evaporation enthalpy (liquid, pure component), source: www.ddbonline.ddbst.de

$$\begin{aligned} h_i^{B,LV,n} = R \cdot T_i^c \cdot (A_{PPDS12,i} \cdot (1 - \frac{T}{T_i^c})^{\frac{1}{3}} + B_{PPDS12,i} \cdot (1 - \frac{T}{T_i^c})^{\frac{2}{3}} \\ + C_{PPDS12,i} \cdot (1 - \frac{T}{T_i^c}) + D_{PPDS12,i} \cdot (1 - \frac{T}{T_i^c})^2 \\ + E_{PPDS12,i} \cdot (1 - \frac{T}{T_i^c})^6) \end{aligned} \tag{6}$$

- Eq: 86368: molarEnthalpyComponentVapor.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar enthalpy (vapor, pure component), assumptions:
  - ideal gas

$$\begin{aligned} h_i^{D,n} = h_i^{o,n} + A_{cp,i} \cdot (T - T_i^o) + \frac{B_{cp,i}}{2} \cdot ((T)^2 - (T_i^o)^2) \\ + \frac{C_{cp,i}}{3} \cdot ((T)^3 - (T_i^o)^3) + \frac{D_{cp,i}}{4} \cdot ((T)^4 - (T_i^o)^4) \end{aligned} \tag{7}$$

- Eq: 86367: molarEnthalpyComponentFeed.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar enthalpy (feed, pure component), assumptions:

  - incompressible fluid
  - ideal gas behavior of corresponding vapor phase (pressure independency of h in V-phase)

$$\begin{aligned} h_i^{F,n} = h_i^{o,n} + A_{cp,i} \cdot (T^F - T_i^o) + \frac{B_{cp,i}}{2} \cdot ((T^F)^2 - (T_i^o)^2) \\ + \frac{C_{cp,i}}{3} \cdot ((T^F)^3 - (T_i^o)^3) + \frac{D_{cp,i}}{4} \\ \cdot ((T^F)^4 - (T_i^o)^4) + v_i^{L,n} \cdot (p^F - p_i^{F,LV}) - h_i^{F,LV,n} \end{aligned} \tag{8}$$

- Eq: 86374: activityCoeffWilsonParameterLiquid.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Parameter calculation (liquid) based on Wilson's g^E-model (liquid), source: Gmehling, Kolbe S.239

$$\alpha_i^B = \frac{\sum_{i=1}^{NC} v_i^{L,n} - v_i^{L,n}}{v_i^{L,n}} \cdot \exp(\frac{-\lambda_i}{T}) \tag{9}$$

- Eq: 86372: volumeFlowLiquid.mosequ (using Nota: 86349: not_-flash.mosnot)
  Desc.: Volume flow (liquid)

$$F^{B,n} = F^{B,v} \cdot \rho^{B,n} \tag{10}$$

- Eq: 86363: pressureDrop.mosequ (using Nota: 86349: not_-flash.mosnot)
  Desc.: Pressure drop (Feed $->$ flash)

$$\Delta p = p^F - p \tag{11}$$

- Eq: 86361: volumeLiquid.mosequ (using Nota: 86349: not_-flash.mosnot)
  Desc.: Volume in flash (liquid)

$$HU^{L,v} = (\sum_{i=1}^{NC} v_i^{L,n} \cdot x_i^B + v^{L,n,E}) \cdot HU^{L,n} \cdot 1000 \tag{12}$$

- Eq: 86351: sumRelationLiquid.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar summation relation (liquid)

$$1 = \sum_{i=1}^{NC} x_i^B \tag{13}$$

- Eq: 86352: molarEnthalpyLiquid.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar enthalpy (liquid)

$$h^{B,n} = \sum_{i=1}^{NC} x_i^B \cdot h_i^{B,n} + h^{B,n,E} \tag{14}$$

- Eq: 86359: molarHoldupComponent.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar component holdup within flash

$$HU_i^n = x_i^B \cdot HU^{L,n} + y_i^D \cdot HU^{V,n} \tag{15}$$

- Eq: 86357: levelLiquid.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Liquid level calculation

$$L^L = 4 \cdot \frac{HU^{L,v}}{\pi \cdot (d)^2} \tag{16}$$

- Eq: 86369: vaporPressureAntoineLiquid.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Vapor pressure by Antoine equation (liquid, pure component), source: Kolbe, Mehling p.59

$$p_i^{LV,B} = (10)^3 \cdot (10)^{A_{Antoine,i} - \frac{B_{Antoine,i}}{C_{Antoine,i} + (T - 273.15)}} \tag{17}$$

- Eq: 86371: molarDensityLiquid.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar density with no excess volume (liquid)

$$1 = \rho^{B,n} \cdot \sum_{i=1}^{NC} x_i^B \cdot v_i^{L,n} \tag{18}$$

- Eq: 86370: vaporPressureAntoineFeed.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Vapor pressure by Antoine equation (feed, pure component), source: Kolbe, Mehling p.59

$$p_i^{LV,F} = (10)^3 \cdot (10)^{A_{Antoine,i} - \frac{B_{Antoine,i}}{C_{Antoine,i} + (T^F - 273.15)}} \tag{19}$$

- Eq: 86362: volume.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Volume of flash

$$HU^v = HU^{L,v} + HU^{V,v} \tag{20}$$

- Eq: 86365: molarEvapEnthalpyFeed.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar evaporation enthalpy (feed, pure component), source: www.ddbonline.ddbst.de

$$\begin{aligned} h_i^{F,LV,n} = R \cdot T_i^c \cdot (A_{PPDS12,i} \cdot (1 - \frac{T^F}{T_i^c})^{\frac{1}{3}} + B_{PPDS12,i} \\ \cdot (1 - \frac{T^F}{T_i^c})^{\frac{2}{3}} + C_{PPDS12,i} \cdot (1 - \frac{T^F}{T_i^c}) + D_{PPDS12,i} \\ \cdot (1 - \frac{T^F}{T_i^c})^2 + E_{PPDS12,i} \cdot (1 - \frac{T^F}{T_i^c})^6) \end{aligned} \tag{21}$$

- Eq: 86358: internalEnergy.mosequ (using Nota: 86349: not_-flash.mosnot)
  Desc.: Internal energy within flash

$$\begin{aligned} & U \\ & = \frac{HU^{L,n} \cdot (h^{B,n} - p \cdot (\sum_{i=1}^{NC} x_i^B \cdot v_i^{L,n} + v^{L,n,E})) + HU^{V,n} \cdot (h^{D,n} - R \cdot T \cdot z)}{(10)^6} \end{aligned} \tag{22}$$

- Eq: 86360: volumeVapor.mosequ (using Nota: 86349: not_-flash.mosnot)
  Desc.: Volume in flash (vapor)

$$HU^{V,v} = \frac{HU^{V,n} \cdot R \cdot T \cdot z}{p} \cdot 1000 \tag{23}$$

- Eq: 86354: sumRelationFeed.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar summation relation (feed)

$$1 = \sum_{i=1}^{NC} x_i^F \tag{24}$$

- Eq: 86373: activityCoeffWilsonLiquid.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Activity coefficient calculations by Wilson's g^E-model (liquid)

$$\begin{aligned} \gamma_i^B = & \frac{1}{x_i^B + \alpha_i^B \cdot (1 - x_i^B)} \\ & \cdot \exp((1 - x_i^B) \cdot (\frac{\alpha_i^B}{x_i^B + \alpha_i^B \cdot (1 - x_i^B)} \\ & - \frac{\sum_{i=1}^{NC} \alpha_i^B - \alpha_i^B}{(\sum_{i=1}^{NC} \alpha_i^B - \alpha_i^B) \cdot x_i^B + (1 - x_i^B)})) \end{aligned} \tag{25}$$

- Eq: 86355: VLEextendedRaoult.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Extended Raoult's law for VLE in flash

$$y_i^D = x_i^B \cdot \frac{p_i^{B,LV} \cdot \gamma_i^B}{p} \tag{26}$$

- Eq: 86366: molarEnthalpyComponentLiquid.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: Molar enthalpy (liquid, pure component), assumptions:
  - incompressible fluid
  - ideal gas behavior of corresponding vapor phase (pressure independency of h in V-phase)

$$\begin{aligned} h_i^{B,n} = & h_i^{o,n} + A_{cp,i} \cdot (T - T_i^o) + \frac{B_{cp,i}}{2} \cdot ((T)^2 - (T_i^o)^2) \\ & + \frac{C_{cp,i}}{3} \cdot ((T)^3 - (T_i^o)^3) + \frac{D_{cp,i}}{4} \\ & \cdot ((T)^4 - (T_i^o)^4) + v_i^{L,n} \cdot (p - p_i^{B,LV}) - h_i^{B,LV,n} \end{aligned} \tag{27}$$

Equation System: 86384: tankGeometry.moseqs

Description: Tank geometry

Connected Equations:

- Eq: 86381: volumeTank.mosequ (using Nota: 86349: not_-flash.mosnot)
  Desc.: Flash's volume

$$HU^{v} = A \cdot L \tag{28}$$

- Eq: 86382: ratioDiameterLengthTank.mosequ (using Nota: 86349: not_flash.mosnot)
  Desc.: diameter to height ratio of tank

$$r^{D,L} = \frac{d}{L} \tag{29}$$

- Eq: 86380: crossSectionArea.mosequ (using Nota: 86349: not_-flash.mosnot)
  Desc.: Flash's cross section area

$$A = \frac{\pi}{4} \cdot (d)^{2} \tag{30}$$

Equation instances:

Eq: 86378: StatEnergyBalance.mosequ (using Nota: 86349: not_flash.mosnot). Description: Energy balance (stationary).

$$0 = e0.F^{F,n} \cdot e0.h^{F,n} - e0.h^{B,n} \cdot e0.F^{B,n} - e0.h^{D,n} \cdot e0.F^{D,n} + e0.Q \tag{31}$$

Eq: 86379: StatComponentBalance.mosequ (using Nota: 86349: not_flash.mosnot). Description: Component balance (stationary).

$$0 = e0.x^{F}_{i=1} \cdot e0.F^{F,n} - e0.x^{B}_{i=1} \cdot e0.F^{B,n} - e0.y^{D}_{i=1} \cdot e0.F^{D,n} \tag{32}$$

$$0 = e0.x^{F}_{i=2} \cdot e0.F^{F,n} - e0.x^{B}_{i=2} \cdot e0.F^{B,n} - e0.y^{D}_{i=2} \cdot e0.F^{D,n} \tag{33}$$

Eq: 86350: sumRelationVapor.mosequ (using Nota: 86349: not_flash.mosnot). Description: Molar summation relation (vapor).

$$1 = (e0.y^{D}_{i=1} + e0.y^{D}_{i=2}) \tag{34}$$

Eq: 86351: sumRelationLiquid.mosequ (using Nota: 86349: not_flash.mosnot). Description: Molar summation relation (liquid).

$$1 = (e0.x^B_{i=1} + e0.x^B_{i=2}) \tag{35}$$

Eq: 86354: sumRelationFeed.mosequ (using Nota: 86349: not_flash.mosnot). Description: Molar summation relation (feed).

$$1 = (e0.x^F_{i=1} + e0.x^F_{i=2}) \tag{36}$$

Eq: 86355: VLEextendedRaoult.mosequ (using Nota: 86349: not_flash.mosnot). Description: Extended Raoult's law for VLE in flash.

$$e0.y^D_{i\ =1} = e0.x^B_{i=1} \cdot \frac{e0.p^{B,LV}_{i=1} \cdot e0.\gamma^B_{i=1}}{e0.p} \tag{37}$$

$$e0.y^D_{i\ =2} = e0.x^B_{i=2} \cdot \frac{e0.p^{B,LV}_{i=2} \cdot e0.\gamma^B_{i=2}}{e0.p} \tag{38}$$

Eq: 86352: molarEnthalpyLiquid.mosequ (using Nota: 86349: not_flash.mosnot). Description: Molar enthalpy (liquid).

$$e0.h^{B,n} = (e0.x^B_{i=1} \cdot e0.h^{B,n}_{i=1} + e0.x^B_{i=2} \cdot e0.h^{B,n}_{i=2}) + e0.h^{B,E,n} \tag{39}$$

Eq: 86353: molarEnthalpyVapor.mosequ (using Nota: 86349: not_flash.mosnot). Description: Molar enthalpy (vapor).

$$e0.h^{D,n} = (e0.y^D_{i=1} \cdot e0.h^{D,n}_{i=1} + e0.y^D_{i=2} \cdot e0.h^{D,n}_{i=2}) + e0.h^{D,E,n} \tag{40}$$

Eq: 86356: molarEnthalpyFeed.mosequ (using Nota: 86349: not_flash.mosnot). Description: Molar enthalpy (feed).

$$e0.h^{F,n} = (e0.x^F_{i=1} \cdot e0.h^{F,n}_{i=1} + e0.x^F_{i=2} \cdot e0.h^{F,n}_{i=2}) + e0.h^{E,F,n} \tag{41}$$

Eq: 86357: levelLiquid.mosequ (using Nota: 86349: not_flash.mosnot). Description: Liquid level calculation.

$$e0.L^L = 4 \cdot \frac{e0.HU^{L,v}}{e0.\pi \cdot (e0.d)^{(2)}} \tag{42}$$

Eq: 86358: internalEnergy.mosequ (using Nota: 86349: not_flash.mosnot). Description: Internal energy within flash.

$$e0.U = \frac{e0.HU^{L,n} \cdot (e0.h^{B,n} - e0.p \cdot ((e0.x^B_{i=1} \cdot e0.v^{L,n}_{i=1} + e0.x^B_{i=2} \cdot e0.v^{L,n}_{i=2}) + e0.v^{E,L,n})) + e0.HU^{V,n} \cdot (e0.h^{D,n} -}{(10)^{(6)}} \tag{43}$$

Eq: 86359: molarHoldupComponent.mosequ (using Nota: 86349: not_flash.mosnot). Description: Molar component holdup within flash.

$$e0.HU^n_{i\ =1} = e0.x^B_{i=1} \cdot e0.HU^{L,n} + e0.y^D_{i=1} \cdot e0.HU^{V,n} \tag{44}$$

$$e0.HU^{n}_{i=2} = e0.x^{B}_{i=2} \cdot e0.HU^{L,n} + e0.y^{D}_{i=2} \cdot e0.HU^{V,n} \tag{45}$$

Eq: 86360: volumeVapor.mosequ (using Nota: 86349: not_flash.mosnot). Description: Volume in flash (vapor).

$$e0.HU^{V,v} = \frac{e0.HU^{V,n} \cdot e0.R \cdot e0.T \cdot e0.z}{e0.p} \cdot 1000 \tag{46}$$

Eq: 86361: volumeLiquid.mosequ (using Nota: 86349: not_flash.mosnot). Description: Volume in flash (liquid).

$$e0.HU^{L,v} = ((e0.v^{L,n}_{i=1} \cdot e0.x^{B}_{i=1} + e0.v^{L,n}_{i=2} \cdot e0.x^{B}_{i=2}) + e0.v^{E,L,n}) \cdot e0.HU^{L,n} \cdot 1000 \tag{47}$$

Eq: 86362: volume.mosequ (using Nota: 86349: not_flash.mosnot). Description: Volume of flash.

$$e0.HU^{v} = e0.HU^{L,v} + e0.HU^{V,v} \tag{48}$$

Eq: 86363: pressureDrop.mosequ (using Nota: 86349: not_flash.mosnot). Description: Pressure drop (Feed $->$ flash).

$$e0.\Delta p = e0.p^{F} - e0.p \tag{49}$$

Eq: 86364: molarEvapEnthalpyLiquid.mosequ (using Nota: 86349: not_flash.mosnot).
Description: Molar evaporation enthalpy (liquid, pure component), source: www.ddbonline.ddbst.de.

$$\begin{aligned} e0.h^{B,LV,n}_{i=1} = {} & e0.R \cdot e0.T^{c}_{i=1} \cdot (e0.A_{PPDS12,i=1} \cdot (1 - \frac{e0.T}{e0.T^{c}_{i=1}})^{(\frac{1}{3})} \\ & + e0.B_{PPDS12,i=1} \cdot (1 - \frac{e0.T}{e0.T^{c}_{i=1}})^{(\frac{2}{3})} + e0.C_{PPDS12,i=1} \\ & \cdot (1 - \frac{e0.T}{e0.T^{c}_{i=1}}) + e0.D_{PPDS12,i=1} \cdot (1 - \frac{e0.T}{e0.T^{c}_{i=1}})^{(2)} \\ & + e0.E_{PPDS12,i=1} \cdot (1 - \frac{e0.T}{e0.T^{c}_{i=1}})^{(6)}) \end{aligned} \tag{50}$$

$$\begin{aligned} e0.h^{B,LV,n}_{i=2} = {} & e0.R \cdot e0.T^{c}_{i=2} \cdot (e0.A_{PPDS12,i=2} \cdot (1 - \frac{e0.T}{e0.T^{c}_{i=2}})^{(\frac{1}{3})} \\ & + e0.B_{PPDS12,i=2} \cdot (1 - \frac{e0.T}{e0.T^{c}_{i=2}})^{(\frac{2}{3})} + e0.C_{PPDS12,i=2} \\ & \cdot (1 - \frac{e0.T}{e0.T^{c}_{i=2}}) + e0.D_{PPDS12,i=2} \cdot (1 - \frac{e0.T}{e0.T^{c}_{i=2}})^{(2)} \\ & + e0.E_{PPDS12,i=2} \cdot (1 - \frac{e0.T}{e0.T^{c}_{i=2}})^{(6)}) \end{aligned} \tag{51}$$

Eq: 86365: molarEvapEnthalpyFeed.mosequ (using Nota: 86349: not_flash.mosnot).
Description: Molar evaporation enthalpy (feed, pure component), source: www.ddbonline.ddbst.de.

$$e0.h^{F,LV,n}_{i\ =1} = e0.R \cdot e0.T^{c}_{i=1} \cdot (e0.A_{PPDS12,i=1} \cdot (1 - \frac{e0.T^{F}}{e0.T^{c}_{i=1}})^{(\frac{1}{3})} + e0.B_{PPDS12,i=1} \cdot (1 - \frac{e0.T^{F}}{e0.T^{c}_{i=1}})^{(\frac{2}{3})} + e0.C_{PPDS12,i=1} \cdot (1 - \frac{e0.T^{F}}{e0.T^{c}_{i=1}}) + e0.D_{PPDS12,i=1} \cdot (1 - \frac{e0.T^{F}}{e0.T^{c}_{i=1}})^{(2)} + e0.E_{PPDS12,i=1} \cdot (1 - \frac{e0.T^{F}}{e0.T^{c}_{i=1}})^{(6)}) \quad (52)$$

$$e0.h^{F,LV,n}_{i\ =2} = e0.R \cdot e0.T^{c}_{i=2} \cdot (e0.A_{PPDS12,i=2} \cdot (1 - \frac{e0.T^{F}}{e0.T^{c}_{i=2}})^{(\frac{1}{3})} + e0.B_{PPDS12,i=2} \cdot (1 - \frac{e0.T^{F}}{e0.T^{c}_{i=2}})^{(\frac{2}{3})} + e0.C_{PPDS12,i=2} \cdot (1 - \frac{e0.T^{F}}{e0.T^{c}_{i=2}}) + e0.D_{PPDS12,i=2} \cdot (1 - \frac{e0.T^{F}}{e0.T^{c}_{i=2}})^{(2)} + e0.E_{PPDS12,i=2} \cdot (1 - \frac{e0.T^{F}}{e0.T^{c}_{i=2}})^{(6)}) \quad (53)$$

Eq: 86366: molarEnthalpyComponentLiquid.mosequ (using Nota: 86349: not_flash.mosnot). Description: Molar enthalpy (liquid, pure component), assumptions:

- incompressible fluid
- ideal gas behavior of corresponding vapor phase (pressure independency of h in V-phase)

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$$e0.h^{B,n}_{i\ =1} = e0.h^{n,o}_{i=1} + e0.A_{cp,i=1} \cdot (e0.T - e0.T^{o}_{i=1}) + \frac{e0.B_{cp,i=1}}{2} \cdot ((e0.T)^{(2)} - (e0.T^{o}_{i=1})^{(2)}) + \frac{e0.C_{cp,i=1}}{3} \cdot ((e0.T)^{(3)} - (e0.T^{o}_{i=1})^{(3)}) + \frac{e0.D_{cp,i=1}}{4} \cdot ((e0.T)^{(4)} - (e0.T^{o}_{i=1})^{(4)}) + e0.v^{L,n}_{i=1} \cdot (e0.p - e0.p^{B,LV}_{i=1}) - e0.h^{B,LV,n}_{i=1} \quad (54)$$

$$e0.h^{B,n}_{i\ =2} = e0.h^{n;o}_{i=2} + e0.A_{cp,i=2} \cdot (e0.T - e0.T^{o}_{i=2}) + \frac{e0.B_{cp,i=2}}{2} \cdot ((e0.T)^{(2)} - (e0.T^{o}_{i=2})^{(2)}) + \frac{e0.C_{cp,i=2}}{3} \cdot ((e0.T)^{(3)} - (e0.T^{o}_{i=2})^{(3)}) + \frac{e0.D_{cp,i=2}}{4} \cdot ((e0.T)^{(4)} - (e0.T^{o}_{i=2})^{(4)}) + e0.v^{L,n}_{i=2} \cdot (e0.p - e0.p^{B,LV}_{i=2}) - e0.h^{B,LV,n}_{i=2} \tag{55}$$

Eq: 86368: molarEnthalpyComponentVapor.mosequ (using Nota: 86349: not_-flash.mosnot). Description: Molar enthalpy (vapor, pure component), assumptions:

- ideal gas

.

$$e0.h^{D,n}_{i\ =1} = e0.h^{n;o}_{i=1} + e0.A_{cp,i=1} \cdot (e0.T - e0.T^{o}_{i=1}) + \frac{e0.B_{cp,i=1}}{2} \cdot ((e0.T)^{(2)} - (e0.T^{o}_{i=1})^{(2)}) + \frac{e0.C_{cp,i=1}}{3} \cdot ((e0.T)^{(3)} - (e0.T^{o}_{i=1})^{(3)}) + \frac{e0.D_{cp,i=1}}{4} \cdot ((e0.T)^{(4)} - (e0.T^{o}_{i=1})^{(4)}) \tag{56}$$

$$e0.h^{D,n}_{i\ =2} = e0.h^{n;o}_{i=2} + e0.A_{cp,i=2} \cdot (e0.T - e0.T^{o}_{i=2}) + \frac{e0.B_{cp,i=2}}{2} \cdot ((e0.T)^{(2)} - (e0.T^{o}_{i=2})^{(2)}) + \frac{e0.C_{cp,i=2}}{3} \cdot ((e0.T)^{(3)} - (e0.T^{o}_{i=2})^{(3)}) + \frac{e0.D_{cp,i=2}}{4} \cdot ((e0.T)^{(4)} - (e0.T^{o}_{i=2})^{(4)}) \tag{57}$$

Eq: 86367: molarEnthalpyComponentFeed.mosequ (using Nota: 86349: not_-flash.mosnot). Description: Molar enthalpy (feed, pure component), assumptions:

- incompressible fluid
- ideal gas behavior of corresponding vapor phase (pressure independency of h in V-phase)

.

$$e0.h^{F,n}_{i\ =1} = e0.h^{n,o}_{i=1} + e0.A_{cp,i=1} \cdot (e0.T^{F} - e0.T^{o}_{i=1}) + \frac{e0.B_{cp,i=1}}{2} \cdot ((e0.T^{F})^{(2)} - (e0.T^{o}_{i=1})^{(2)}) + \frac{e0.C_{cp,i=1}}{3} \cdot ((e0.T^{F})^{(3)} - (e0.T^{o}_{i=1})^{(3)}) + \frac{e0.D_{cp,i=1}}{4} \cdot ((e0.T^{F})^{(4)} - (e0.T^{o}_{i=1})^{(4)}) + e0.v^{L,n}_{i=1} \cdot (e0.p^{F} - e0.p^{F,LV}_{i=1}) - e0.h^{F,LV,n}_{i=1} \tag{58}$$

$$
\begin{aligned}
e0.h^{F,n}_{i\ =2} = {} & e0.h^{n,o}_{i=2} + e0.A_{cp,i=2} \cdot (e0.T^{F} - e0.T^{o}_{i=2}) + \frac{e0.B_{cp,i=2}}{2} \\
& \cdot ((e0.T^{F})^{(2)} - (e0.T^{o}_{i=2})^{(2)}) + \frac{e0.C_{cp,i=2}}{3} \cdot ((e0.T^{F})^{(3)} - (e0.T^{o}_{i=2})^{(3)}) \\
& + \frac{e0.D_{cp,i=2}}{4} \cdot ((e0.T^{F})^{(4)} - (e0.T^{o}_{i=2})^{(4)}) \\
& + e0.v^{L,n}_{i=2} \cdot (e0.p^{F} - e0.p^{F,LV}_{i=2}) - e0.h^{F,LV,n}_{i=2}
\end{aligned} \tag{59}
$$

Eq: 86369: vaporPressureAntoineLiquid.mosequ (using Nota: 86349: not_flash.mosnot). Description: Vapor pressure by Antoine equation (liquid, pure component), source: Kolbe, Mehling p.59.

$$
e0.p^{B,LV}_{i\ =1} = (10)^{(3)} \cdot (10)^{\left(e0.A_{Antoine,i=1} - \frac{e0.B_{Antoine,i=1}}{e0.C_{Antoine,i=1} + (e0.T - 273.15)}\right)} \tag{60}
$$

$$
e0.p^{B,LV}_{i\ =2} = (10)^{(3)} \cdot (10)^{\left(e0.A_{Antoine,i=2} - \frac{e0.B_{Antoine,i=2}}{e0.C_{Antoine,i=2} + (e0.T - 273.15)}\right)} \tag{61}
$$

Eq: 86370: vaporPressureAntoineFeed.mosequ (using Nota: 86349: not_flash.mosnot). Description: Vapor pressure by Antoine equation (feed, pure component), source: Kolbe, Mehling p.59.

$$
e0.p^{F,LV}_{i\ =1} = (10)^{(3)} \cdot (10)^{\left(e0.A_{Antoine,i=1} - \frac{e0.B_{Antoine,i=1}}{e0.C_{Antoine,i=1} + (e0.T^{F} - 273.15)}\right)} \tag{62}
$$

$$
e0.p^{F,LV}_{i\ =2} = (10)^{(3)} \cdot (10)^{\left(e0.A_{Antoine,i=2} - \frac{e0.B_{Antoine,i=2}}{e0.C_{Antoine,i=2} + (e0.T^{F} - 273.15)}\right)} \tag{63}
$$

Eq: 86371: molarDensityLiquid.mosequ (using Nota: 86349: not_flash.mosnot). Description: Molar density with no excess volume (liquid).

$$
1 = e0.\rho^{B,n} \cdot (e0.x^{B}_{i=1} \cdot e0.v^{L,n}_{i=1} + e0.x^{B}_{i=2} \cdot e0.v^{L,n}_{i=2}) \tag{64}
$$

Eq: 86372: volumeFlowLiquid.mosequ (using Nota: 86349: not_flash.mosnot). Description: Volume flow (liquid).

$$
e0.F^{B,n} = e0.F^{B,v} \cdot e0.\rho^{B,n} \tag{65}
$$

Eq: 86373: activityCoeffWilsonLiquid.mosequ (using Nota: 86349: not_flash.mosnot). Description: Activity coefficient calculations by Wilson's g^{E}-model (liquid).

$$
\begin{aligned}
e0.\gamma^{B}_{i\ =1} = {} & \frac{1}{e0.x^{B}_{i=1} + e0.\alpha^{B}_{i=1} \cdot (1 - e0.x^{B}_{i=1})} \\
& \cdot \exp\Bigg((1 - e0.x^{B}_{i=1}) \cdot (\frac{e0.\alpha^{B}_{i=1}}{e0.x^{B}_{i=1} + e0.\alpha^{B}_{i=1} \cdot (1 - e0.x^{B}_{i=1})} \\
& - \frac{(e0.\alpha^{B}_{i=1} + e0.\alpha^{B}_{i=2}) - e0.\alpha^{B}_{i=1}}{((e0.\alpha^{B}_{i=1} + e0.\alpha^{B}_{i=2}) - e0.\alpha^{B}_{i=1}) \cdot e0.x^{B}_{i=1} + (1 - e0.x^{B}_{i=1})})\Bigg)
\end{aligned} \tag{66}
$$

$$e0.\gamma^B_{i=2} = \frac{1}{e0.x^B_{i=2} + e0.\alpha^B_{i=2} \cdot (1 - e0.x^B_{i=2})} \cdot \exp\left((1 - e0.x^B_{i=2}) \cdot (\frac{e0.\alpha^B_{i=2}}{e0.x^B_{i=2} + e0.\alpha^B_{i=2} \cdot (1 - e0.x^B_{i=2})} - \frac{(e0.\alpha^B_{i=1} + e0.\alpha^B_{i=2}) - e0.\alpha^B_{i=2}}{((e0.\alpha^B_{i=1} + e0.\alpha^B_{i=2}) - e0.\alpha^B_{i=2}) \cdot e0.x^B_{i=2} + (1 - e0.x^B_{i=2})})\right) \tag{67}$$

Eq: 86374: activityCoeffWilsonParameterLiquid.mosequ (using Nota: 86349: not_flash.mosnot). Description: Parameter calculation (liquid) based on Wilson's g^E-model (liquid), source: Gmehling, Kolbe S.239.

$$e0.\alpha^B_{i=1} = \frac{(e0.v^{L,n}_{i=1} + e0.v^{L,n}_{i=2}) - e0.v^{L,n}_{i=1}}{e0.v^{L,n}_{i=1}} \cdot \exp\left(\frac{-e0.\lambda_{i=1}}{e0.T}\right) \tag{68}$$

$$e0.\alpha^B_{i=2} = \frac{(e0.v^{L,n}_{i=1} + e0.v^{L,n}_{i=2}) - e0.v^{L,n}_{i=2}}{e0.v^{L,n}_{i=2}} \cdot \exp\left(\frac{-e0.\lambda_{i=2}}{e0.T}\right) \tag{69}$$

Eq: 86380: crossSectionArea.mosequ (using Nota: 86349: not_flash.mosnot). Description: Flash's cross section area.

$$e0.A = \frac{e0.\pi}{4} \cdot (e0.d)^{(2)} \tag{70}$$

Eq: 86381: volumeTank.mosequ (using Nota: 86349: not_flash.mosnot). Description: Flash's volume.

$$e0.HU^v = e0.A \cdot e0.L \tag{71}$$

Eq: 86382: ratioDiameterLengthTank.mosequ (using Nota: 86349: not_flash.mosnot). Description: diameter to height ratio of tank.

$$e0.r^{D,L} = \frac{e0.d}{e0.L} \tag{72}$$

Variable Specs '86386: IV_statFlash.mosvar'

Design variables

$e0.A_{Antoine,i=1}$	=	7.2371
$e0.A_{Antoine,i=2}$	=	7.19621
$e0.A_{PPDS12,i=1}$	=	9.1919
$e0.A_{PPDS12,i=2}$	=	5.6297
$e0.A_{cp,i=1}$	=	9.008
$e0.A_{cp,i=2}$	=	32.22
$e0.B_{Antoine,i=1}$	=	1592.86
$e0.B_{Antoine,i=2}$	=	1730.63

$$
\begin{aligned}
e0.B_{PPDS12,i=1} &= 2.8118\\
e0.B_{PPDS12,i=2} &= 13.962\\
e0.B_{cp,i=1} &= 0.2139\\
e0.B_{cp,i=2} &= 0.0019225\\
e0.C_{Antoine,i=1} &= 226.184\\
e0.C_{Antoine,i=2} &= 233.426\\
e0.C_{PPDS12,i=1} &= 8.6931\\
e0.C_{PPDS12,i=2} &= -11.673\\
e0.C_{cp,i=1} &= -8.3846E-5\\
e0.C_{cp,i=2} &= 1.0548E-5\\
e0.D_{PPDS12,i=1} &= -11.776\\
e0.D_{PPDS12,i=2} &= 2.1784\\
e0.D_{cp,i=1} &= 1.3723E-9\\
e0.D_{cp,i=2} &= -3.594E-9\\
e0.E_{PPDS12,i=1} &= -31.745\\
e0.E_{PPDS12,i=2} &= -0.31666\\
e0.F^{F,n} &= 1.75\\
e0.L &= 0.5\\
e0.L^{L} &= 0.25\\
e0.R &= 8.314\\
e0.T &= 353.15\\
e0.T^{F} &= 353.15\\
e0.T^{c}_{i=1} &= 516.2\\
e0.T^{o}_{i=1} &= 298.15\\
e0.T^{c}_{i=2} &= 647.3\\
e0.T^{o}_{i=2} &= 298.15\\
e0.\Delta p &= 25000.0\\
e0.\lambda_{i=1} &= 95.68\\
e0.\lambda_{i=2} &= 506.7\\
e0.\pi &= 3.14159265359\\
e0.d &= 0.16\\
e0.h^{B,E,n} &= 0.0\\
e0.h^{D,E,n} &= 0.0\\
e0.h^{E,F,n} &= 0.0\\
e0.h^{n,o}_{i=1} &= -234800.0\\
e0.h^{n,o}_{i=2} &= -241820.0\\
e0.p &= 75000.0\\
e0.v^{E,L,n} &= 0.0\\
e0.v^{L,n}_{i=1} &= 5.869E-5\\
e0.v^{L,n}_{i=2} &= 1.807E-5\\
e0.x^{F}_{i=1} &= 0.15\\
e0.z &= 1.0
\end{aligned}
$$

Iteration variables

$$
e0.A = 1.0
$$

$$
\begin{aligned}
e0.F^{B,n} &= 1.0\\
e0.F^{B,v} &= 1.0\\
e0.F^{D,n} &= 1.0\\
e0.HU^{L,n} &= 1.0\\
e0.HU^{L,v} &= 1.0\\
e0.HU^{V,n} &= 1.0\\
e0.HU^{V,v} &= 1.0\\
e0.HU^{v} &= 1.0\\
e0.HU^{n}_{i=1} &= 1.0\\
e0.HU^{n}_{i=2} &= 1.0\\
e0.Q &= 1.0\\
e0.U &= 1.0\\
e0.\alpha^{B}_{i=1} &= 1.0\\
e0.\alpha^{B}_{i=2} &= 1.0\\
e0.\gamma^{B}_{i=1} &= 1.0\\
e0.\gamma^{B}_{i=2} &= 1.0\\
e0.\rho^{B,n} &= 1.0\\
e0.h^{B,n} &= 1.0\\
e0.h^{D,n} &= 1.0\\
e0.h^{F,n} &= 1.0\\
e0.h^{B,LV,n}_{i=1} &= 1.0\\
e0.h^{B,n}_{i=1} &= 1.0\\
e0.h^{D,n}_{i=1} &= 1.0\\
e0.h^{F,LV,n}_{i=1} &= 1.0\\
e0.h^{F,n}_{i=1} &= 1.0\\
e0.h^{B,LV,n}_{i=2} &= 1.0\\
e0.h^{B,n}_{i=2} &= 1.0\\
e0.h^{D,n}_{i=2} &= 1.0\\
e0.h^{F,LV,n}_{i=2} &= 1.0\\
e0.h^{F,n}_{i=2} &= 1.0\\
e0.p^{F} &= 1.0\\
e0.p^{B,LV}_{i=1} &= 1.0\\
e0.p^{F,LV}_{i=1} &= 1.0\\
e0.p^{B,LV}_{i=2} &= 1.0\\
e0.p^{F,LV}_{i=2} &= 1.0\\
e0.r^{D,L} &= 1.0\\
e0.x^{B}_{i=1} &= 1.0\\
e0.x^{B}_{i=2} &= 1.0\\
e0.x^{F}_{i=2} &= 1.0\\
e0.y^{D}_{i=1} &= 1.0\\
e0.y^{D}_{i=2} &= 1.0
\end{aligned}
$$

Results '86388: RE_statFlash_CBzzMath_Orig.mosvar'

Design variables

$e0.A_{Antoine,i=1}$	=	7.2371
$e0.A_{Antoine,i=2}$	=	7.19621
$e0.A_{PPDS12,i=1}$	=	9.1919
$e0.A_{PPDS12,i=2}$	=	5.6297
$e0.A_{cp,i=1}$	=	9.008
$e0.A_{cp,i=2}$	=	32.22
$e0.B_{Antoine,i=1}$	=	1592.86
$e0.B_{Antoine,i=2}$	=	1730.63
$e0.B_{PPDS12,i=1}$	=	2.8118
$e0.B_{PPDS12,i=2}$	=	13.962
$e0.B_{cp,i=1}$	=	0.2139
$e0.B_{cp,i=2}$	=	0.0019225
$e0.C_{Antoine,i=1}$	=	226.184
$e0.C_{Antoine,i=2}$	=	233.426
$e0.C_{PPDS12,i=1}$	=	8.6931
$e0.C_{PPDS12,i=2}$	=	-11.673
$e0.C_{cp,i=1}$	=	$-8.3846E-5$
$e0.C_{cp,i=2}$	=	$1.0548E-5$
$e0.D_{PPDS12,i=1}$	=	-11.776
$e0.D_{PPDS12,i=2}$	=	2.1784
$e0.D_{cp,i=1}$	=	$1.3723E-9$
$e0.D_{cp,i=2}$	=	$-3.594E-9$
$e0.E_{PPDS12,i=1}$	=	-31.745
$e0.E_{PPDS12,i=2}$	=	-0.31666
$e0.F^{F,n}$	=	1.75
$e0.L$	=	0.5
$e0.L^{L}$	=	0.25
$e0.R$	=	8.314
$e0.T$	=	353.15
$e0.T^{F}$	=	353.15
$e0.T^{c}_{i=1}$	=	516.2
$e0.T^{o}_{i=1}$	=	298.15
$e0.T^{c}_{i=2}$	=	647.3
$e0.T^{o}_{i=2}$	=	298.15
$e0.\Delta p$	=	25000.0
$e0.\lambda_{i=1}$	=	95.68
$e0.\lambda_{i=2}$	=	506.7
$e0.\pi$	=	3.14159265359
$e0.d$	=	0.16
$e0.h^{B,E,n}$	=	0.0
$e0.h^{D,E,n}$	=	0.0
$e0.h^{E,F,n}$	=	0.0

$e0.h^{n,o}_{i=1} = -234800.0$
$e0.h^{n,o}_{i=2} = -241820.0$
$e0.p = 75000.0$
$e0.v^{E,L,n} = 0.0$
$e0.v^{L,n}_{i=1} = 5.869E-5$
$e0.v^{L,n}_{i=2} = 1.807E-5$
$e0.x^{F}_{i=1} = 0.15$
$e0.z = 1.0$

Iteration variables

$e0.A = 0.020106192982976$
$e0.F^{B,n} = 1.410014354560068$
$e0.F^{B,v} = 3.0446040035E-5$
$e0.F^{D,n} = 0.3399856454399321$
$e0.HU^{L,n} = 0.2327890645957856$
$e0.HU^{L,v} = 0.005026548245744$
$e0.HU^{V,n} = 1.283990729133E-4$
$e0.HU^{V,v} = 0.005026548245744$
$e0.HU^{v} = 0.010053096491488$
$e0.HU^{n}_{i=1} = 0.0202412820423757$
$e0.HU^{n}_{i=2} = 0.2126761816263232$
$e0.Q = 13780.540133376764$
$e0.U = -0.065334452684665$
$e0.\alpha^{B}_{i=1} = 0.2348168850216206$
$e0.\alpha^{B}_{i=2} = 0.773534640352742$
$e0.\gamma^{B}_{i=1} = 3.2920349140807814$
$e0.\gamma^{B}_{i=2} = 1.0208621837932104$
$e0.\rho^{B,n} = 46311.9129101942$
$e0.h^{B,n} = -280525.9122197867$
$e0.h^{D,n} = -236247.8265326519$
$e0.h^{F,n} = -279798.2702724677$
$e0.h^{B,LV,n}_{i=1} = 39069.479076511685$
$e0.h^{B,n}_{i=1} = -270032.46712301427$
$e0.h^{D,n}_{i=1} = -230961.0311094514$
$e0.h^{F,LV,n}_{i=1} = 39069.479076511685$
$e0.h^{F,n}_{i=1} = -270030.9998730143$
$e0.h^{B,LV,n}_{i=2} = 41564.186300811496$
$e0.h^{B,n}_{i=2} = -281522.35797531245$
$e0.h^{D,n}_{i=2} = -239958.67281428122$
$e0.h^{F,LV,n}_{i=2} = 41564.186300811496$
$e0.h^{F,n}_{i=2} = -281521.90622531244$
$e0.p^{F} = 100000.0$
$e0.p^{B,LV}_{i=1} = 108343.6198873657$

$e0.p_{i=1}^{F,LV}$	=	108343.6198873657
$e0.p_{i=2}^{B,LV}$	=	47266.75261408215
$e0.p_{i=2}^{F,LV}$	=	47266.75261408215
$e0.r^{D,L}$	=	0.32
$e0.x_{i=1}^{B}$	=	0.0867236920119577
$e0.x_{i=2}^{B}$	=	0.9132763079880423
$e0.x_{i=2}^{F}$	=	0.85
$e0.y_{i=1}^{D}$	=	0.4124243222129412
$e0.y_{i=2}^{D}$	=	0.5875756777870588

Notation '86349: not_flash.mosnot'

Base line symbols

A	Area [m]; Parameter
B	Parameter
C	Parameter
D	Parameter
E	Parameter
F	Flow[mol/s]
HU	Holdup
I	Integral (by time)
K	Equilibrium constant [1]; Control constant
L	Height [m]
M	Molar mass [g/mol]
Q	Heat flow [W]
R	Ideal gas constant [J/mol/K]
T	Temperature [K]; Time constant [s]
U	Internal Energy [J]
ΔF	Flow difference
ΔL	Level difference [m]
ΔQ	Heat flow difference [J/s]
ΔT	Temperature difference [K]
Δp	Pressure difference [Pa]
α	Wilson Parameter [1]
γ	Activity coefficient [1]
λ	Interaction parameter (Wilson Modell)
π	Natural constant π [1]
ρ	Density [mol/m]
d	Diameter [m]
h	Specific enthalpy[J/mol];
p	Pressure [Pa]
r	ratio [1]
t	Time [s]

v	Specific molar volume [mol/m]
x	Mol fraction (liquid) [1]
y	Mol fraction (vapor) [1]
z	Compressibility factor [1]

Superscripts

B	Bottom
D	Distillate
E	Excess
F	Feed
L	Liquid; Height
LV	Liquid/Vapor
V	Vapor
c	Critical
max	Maximum
n	Molar
o	Reference
v	volumetric

Subscripts

$Antoine$	Antoine equation
$PPDS12$	PPDS12 equation (http://www.ddbst.de)
cp	molar heat capacity

Indices

i	$1..NC$	Komponentenindex