Informationen

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Reaktor_Ester_v2.8.mcdx

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Projekt

Reaktor-Modell - Verersterung

Kurzbeschreibung

Nomenklatur

Stoffdaten

Molmasse:

$M_{N2} := 28.0135 \frac{gm}{mol}$ Molmasse N2

$M_A := 102.09 \frac{gm}{mol}$ Molmasse A = Essigsäureanhydrid

$M_B := 32.04 \frac{gm}{mol}$ Molmasse B = Methanol

$M_C := 74.08 \frac{gm}{mol}$ Molmasse C = Essigssäuremethylester

$M_D := 60.06 \frac{gm}{mol}$ Molmasse D = Essigsäure

Uni. Gaskonstante:

$R := 8.314 \frac{J}{mol\,K}$

kritische Daten:

kritische Temperatur

$T_{krit\_A} := 606.05\,K$ $T_{krit\_B} := 513.38\,K$ $T_{krit\_C} := 506.55\,K$ $T_{krit\_D} := 591.95\,K$

kritischer Druck

$p_{krit\_A} := 40\,bar$ $p_{krit\_B} := 82.16\,bar$ $p_{krit\_C} := 47.5\,bar$ $p_{krit\_D} := 57.86\,bar$

kritischer Dichte

$\rho_{krit\_A} := 352 \frac{kg}{m^3}$ $\rho_{krit\_B} := 282 \frac{kg}{m^3}$ $\rho_{krit\_C} := 334 \frac{kg}{m^3}$ $\rho_{krit\_D} := 325 \frac{kg}{m^3}$

Dichte:

$\rho_A(Temp) := \text{linterp}\left(\begin{bmatrix}\vdots \\ 60\,°C \\ \vdots\end{bmatrix}, \begin{bmatrix}\vdots \\ 1081.719 \frac{kg}{m^3} \\ \vdots\end{bmatrix}, Temp\right)$ Dichte A

$\rho_B(Temp) := \text{linterp}\left(\begin{bmatrix}0\,°C \\ \vdots\end{bmatrix}, \begin{bmatrix}\vdots \\ 792.033 \frac{kg}{m^3} \\ \vdots\end{bmatrix}, Temp\right)$ Dichte B

$\rho_C(Temp) := \text{linterp}\left(\begin{bmatrix}0\,°C \\ \vdots\end{bmatrix}, \begin{bmatrix}968.454 \frac{kg}{m^3} \\ \vdots\end{bmatrix}, Temp\right)$ Dichte C

$\rho_D(Temp) := \text{linterp}\left(\begin{bmatrix}0\,°C \\ \vdots\end{bmatrix}, \begin{bmatrix}1059.282 \frac{kg}{m^3} \\ \vdots\end{bmatrix}, Temp\right)$ Dichte D

Verdampfungsenthalpie:

$$\Delta h_{V\_A}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}491852.490\ \frac{J}{kg}\\ \vdots\end{bmatrix}, Temp\right)$$ Verdampfungsenthalpie A

$$\Delta h_{V\_B}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}1205835.116\ \frac{J}{kg}\\ \vdots\end{bmatrix}, Temp\right)$$ Verdampfungsenthalpie B

$$\Delta h_{V\_C}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}457174.672\ \frac{J}{kg}\\ \vdots\end{bmatrix}, Temp\right)$$ Verdampfungsenthalpie C

$$\Delta h_{V\_D}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}393408.254\ \frac{J}{kg}\\ \vdots\end{bmatrix}, Temp\right)$$ Verdampfungsenthalpie D

Bildungsenthalpien:

$$\Delta H_{B\_A} := \frac{-624400}{M_A}\frac{J}{mol} = -6116172.005\ \frac{J}{kg}$$ Bildungsenthalpie A

$$\Delta H_{B\_B} := \frac{-201000}{M_B}\frac{J}{mol} = -6273408.24\ \frac{J}{kg}$$ Bildungsenthalpie B

$$\Delta H_{B\_C} := \frac{-445900}{M_C}\frac{J}{mol} = -6019168.467\ \frac{J}{kg}$$ Bildungsenthalpie C

$$\Delta H_{B\_D} := \frac{-433000}{M_D}\frac{J}{mol} = -7209457.209\ \frac{J}{kg}$$ Bildungsenthalpie D

$$\Delta H_{B\_N2} := 0\ \frac{J}{kg}$$ Bildungsenthalpie N2

Wärmekapazität Flüssigkeit:

$$c_{pl\_A}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}1.726\ \frac{J}{gm\ K}\\ \vdots\end{bmatrix}, Temp\right)$$ Wärmekapazität A

$$c_{pl\_B}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}2.403\ \frac{J}{gm\ K}\\ \vdots\end{bmatrix}, Temp\right)$$ Wärmekapazität B

$$c_{pl\_C}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}1.826\ \frac{J}{gm\ K}\\ \vdots\end{bmatrix}, Temp\right)$$ Wärmekapazität C

$$c_{pl\_D}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}1.931\ \frac{J}{gm\ K}\\ \vdots\end{bmatrix}, Temp\right)$$ Wärmekapazität D

Wärmekapazität Gas (isobar):

$$c_{pg\_A}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}0.908\ \frac{J}{gm\ K}\\ \vdots\end{bmatrix}, Temp\right)$$ Wärmekapazität A

$$c_{pg\_B}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}1.328\ \frac{J}{gm\ K}\\ \vdots\end{bmatrix}, Temp\right)$$ Wärmekapazität B

$$c_{pg\_C}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}1.084\ \frac{J}{gm\ K}\\ \vdots\end{bmatrix}, Temp\right)$$ Wärmekapazität C

$$c_{pg\_D}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}0.987\ \frac{J}{gm\ K}\\ \vdots\end{bmatrix}, Temp\right)$$ Wärmekapazität D

$c_{pg\_N2} := 1.040\ \frac{J}{gm \cdot K}$ Wärmekapazität N2

Wärmekapazität Gas (isochor):

$$c_{vg\_A}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}0.908\ \frac{J}{gm\ K}\\ \vdots\end{bmatrix}, Temp\right) - \frac{R}{M_A}$$ Wärmekapazität A

$$c_{vg\_B}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}1.328\ \frac{J}{gm\ K}\\ \vdots\end{bmatrix}, Temp\right) - \frac{R}{M_B}$$ Wärmekapazität B

$$c_{vg\_C}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}1.084\ \frac{J}{gm\ K}\\ \vdots\end{bmatrix}, Temp\right) - \frac{R}{M_C}$$ Wärmekapazität C

$$c_{vg\_D}(Temp) := \text{linterp}\left(\begin{bmatrix}0\ °C\\ \vdots\end{bmatrix}, \begin{bmatrix}0.987\ \frac{J}{gm\ K}\\ \vdots\end{bmatrix}, Temp\right) - \frac{R}{M_D}$$ Wärmekapazität D

$c_{vg\_N2}(Temp) := c_{pg\_N2} - \frac{R}{M_{N2}} = 0.743\ \frac{J}{gm \cdot K}$ Wärmekapazität N2

Dampfdruck:

Parameter A	Parameter B	Parameter C	Parameter D
$A_{ps\_A} := -8.15436$	$A_{ps\_B} := -8.72963$	$A_{ps\_C} := -8.57584$	$A_{ps\_D} := -9.34304$
$B_{ps\_A} := 1.80785$	$B_{ps\_B} := 1.4586$	$B_{ps\_C} := 4.22791$	$B_{ps\_D} := 3.77735$
$C_{ps\_A} := -3.76039$	$C_{ps\_B} := -2.78449$	$C_{ps\_C} := -5.37346$	$C_{ps\_D} := -3.59092$
$D_{ps\_A} := -3.04616$	$D_{ps\_B} := -0.70669$	$D_{ps\_C} := -0.82045$	$D_{ps\_D} := -1.57006$

$$p_{s\_A}(Temp) := p_{krit\_A} \cdot e^{\left(\frac{T_{krit\_A}}{Temp} \cdot \left(A_{ps\_A} \cdot \left(1 - \frac{Temp}{T_{krit\_A}}\right) + B_{ps\_A} \cdot \left(1 - \frac{Temp}{T_{krit\_A}}\right)^{1.5} + C_{ps\_A} \cdot \left(1 - \frac{Temp}{T_{krit\_A}}\right)^{2.5} + D_{ps\_A} \cdot \left(1 - \frac{Temp}{T_{krit\_A}}\right)^{5}\right)\right)}$$

$$p_{s\_B}(Temp) := p_{krit\_B} \cdot e^{\left(\frac{T_{krit\_B}}{Temp} \cdot \left(A_{ps\_B} \cdot \left(1 - \frac{Temp}{T_{krit\_B}}\right) + B_{ps\_B} \cdot \left(1 - \frac{Temp}{T_{krit\_B}}\right)^{1.5} + C_{ps\_B} \cdot \left(1 - \frac{Temp}{T_{krit\_B}}\right)^{2.5} + D_{ps\_B} \cdot \left(1 - \frac{Temp}{T_{krit\_B}}\right)^{5}\right)\right)}$$

$$p_{s\_C}(Temp) := p_{krit\_C} \cdot e^{\left(\frac{T_{krit\_C}}{Temp} \cdot \left(A_{ps\_C} \cdot \left(1 - \frac{Temp}{T_{krit\_C}}\right) + B_{ps\_C} \cdot \left(1 - \frac{Temp}{T_{krit\_C}}\right)^{1.5} + C_{ps\_C} \cdot \left(1 - \frac{Temp}{T_{krit\_C}}\right)^{2.5} + D_{ps\_C} \cdot \left(1 - \frac{Temp}{T_{krit\_C}}\right)^{5}\right)\right)}$$

$$p_{s\_D}(Temp) := p_{krit\_D} \cdot e^{\left(\frac{T_{krit\_D}}{Temp} \cdot \left(A_{ps\_D} \cdot \left(1 - \frac{Temp}{T_{krit\_D}}\right) + B_{ps\_D} \cdot \left(1 - \frac{Temp}{T_{krit\_D}}\right)^{1.5} + C_{ps\_D} \cdot \left(1 - \frac{Temp}{T_{krit\_D}}\right)^{2.5} + D_{ps\_D} \cdot \left(1 - \frac{Temp}{T_{krit\_D}}\right)^{5}\right)\right)}$$

Kinetik

Geschw.koeffizient:

$$k_{0\_1}(x) := -1.36 \cdot 10^8 \ \frac{L}{mol\ s} + 1.36 \cdot 10^8 \cdot \exp(2.2 \cdot x) \cdot \frac{L}{mol\ s}$$

$$k_{0\_2}(x) := 2 \cdot 10^7 \cdot \exp(-12.28 \cdot x) \cdot \frac{L^2}{mol^2\ s}$$

Aktivierungsenergie:

$$E_{A\_1}(x) := -15924 \cdot x^2 \ \frac{J}{mol} + 20568 \cdot x \ \frac{J}{mol} + 77337 \ \frac{J}{mol}$$

$$E_{A\_2}(x) := -40472 \cdot x \ \frac{J}{mol} + 80750 \ \frac{J}{mol}$$

Reaktionsenthalpie:

$$\Delta H_R := -66300 \ \frac{J}{mol} = -66300 \ \frac{J}{mol}$$

Prozessdaten

Referenztemperatur:

$$T_{ref} := 298.15 \ K$$

Referenzdruck:

$$p_{ref} := 1 \ bar$$

Dosierstrom:

$$m_{B\_F} := 0 \ \frac{kg}{s}$$

Dosiertemperatur:

$$T_{B\_F} := 80 \ °C$$

Berechnung des Anfangszustand im Reaktor pT-Flash

pT-Flash --> Druck und Temperatur sind bekannt und konstant. Gesucht ist die Zusammensetzung der Flüssigkeit und Gasphase bzw. ihre Massen je Komponente.

$$pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := \left\| \begin{array}{l} x_{spec\_A} \leftarrow \dfrac{\dfrac{m_{0\_A}}{M_A}}{\dfrac{m_{0\_A}}{M_A} + \dfrac{m_{0\_B}}{M_B} + \dfrac{m_{0\_C}}{M_C} + \dfrac{m_{0\_D}}{M_D}} \\ x_{spec\_B} \leftarrow \dfrac{\dfrac{m_{0\_B}}{M_B}}{\dfrac{m_{0\_A}}{M_A} + \dfrac{m_{0\_B}}{M_B} + \dfrac{m_{0\_C}}{M_C} + \dfrac{m_{0\_D}}{M_D}} \\ m_{0\_C} \end{array} \right.$$

$$x_{spec\_C} \leftarrow \frac{\frac{m_{0\_C}}{M_C}}{\frac{m_{0\_A}}{M_A}+\frac{m_{0\_B}}{M_B}+\frac{m_{0\_C}}{M_C}+\frac{m_{0\_D}}{M_D}}$$

$$x_{spec\_D} \leftarrow \frac{\frac{m_{0\_D}}{M_D}}{\frac{m_{0\_A}}{M_A}+\frac{m_{0\_B}}{M_B}+\frac{m_{0\_C}}{M_C}+\frac{m_{0\_D}}{M_D}}$$

$p_{sat\_A} \leftarrow p_{s\_A}(Temp)$

$p_{sat\_B} \leftarrow p_{s\_B}(Temp)$

$p_{sat\_C} \leftarrow p_{s\_C}(Temp)$

$p_{sat\_D} \leftarrow p_{s\_D}(Temp)$

$p_{spec} \leftarrow x_{spec\_A} \cdot p_{sat\_A} + x_{spec\_B} \cdot p_{sat\_B} + x_{spec\_C} \cdot p_{sat\_C} + x_{spec\_D} \cdot p_{sat\_D}$

for $i \in 0 .. 10$

$$m_l \leftarrow \frac{m_{0\_A}+m_{0\_B}+m_{0\_C}+m_{0\_D}-\frac{Vol}{R \cdot Temp}\left(x_{spec\_A} \cdot p_{sat\_A} \cdot M_A + x_{spec\_B} \cdot p_{sat\_B} \cdot M_B + x_{spec\_C} \cdot p_{sat\_C} \cdot M_C + x_{spec\_D} \cdot p_{sat\_D} \cdot M_D\right)}{1-\frac{1}{R \cdot Temp \cdot \left(x_{spec\_A} \cdot M_A + x_{spec\_B} \cdot M_B + x_{spec\_C} \cdot M_C + x_{spec\_D} \cdot M_D\right)} \cdot \left(\frac{x_{spec\_A} \cdot M_A}{\rho_A(Temp)}+\frac{x_{spec\_B} \cdot M_B}{\rho_B(Temp)}+\frac{x_{spec\_C} \cdot M_C}{\rho_C(Temp)}+\frac{x_{spec\_D} \cdot M_D}{\rho_D(Temp)}\right) \cdot \left(x_{spec\_A} \cdot p_{sat\_A} \cdot M_A + x_{spec\_B} \cdot p_{sat\_B} \cdot M_B + x_{spec\_C} \cdot p_{sat\_C} \cdot M_C + x_{spec\_D} \cdot p_{sat\_D} \cdot M_D\right)}$$

$$V_l \leftarrow \frac{m_l}{x_{spec\_A} \cdot M_A + x_{spec\_B} \cdot M_B + x_{spec\_C} \cdot M_C + x_{spec\_D} \cdot M_D} \cdot \left(\frac{x_{spec\_A} \cdot M_A}{\rho_A(Temp)}+\frac{x_{spec\_B} \cdot M_B}{\rho_B(Temp)}+\frac{x_{spec\_C} \cdot M_C}{\rho_C(Temp)}+\frac{x_{spec\_D} \cdot M_D}{\rho_D(Temp)}\right)$$

$V_g \leftarrow Vol - V_l$

$$m_{g\_A} \leftarrow \frac{x_{spec\_A} \cdot p_{sat\_A} \cdot V_g \cdot M_A}{R \cdot Temp}$$

$$m_{g\_B} \leftarrow \frac{x_{spec\_B} \cdot p_{sat\_B} \cdot V_g \cdot M_B}{R \cdot Temp}$$

$$m_{g\_C} \leftarrow \frac{x_{spec\_C} \cdot p_{sat\_C} \cdot V_g \cdot M_C}{R \cdot Temp}$$

$$m_{g\_D} \leftarrow \frac{x_{spec\_D} \cdot p_{sat\_D} \cdot V_g \cdot M_D}{R \cdot Temp}$$

$$m_{g\_N2} \leftarrow \frac{\left(p_{spec} - x_{spec\_A} \cdot p_{sat\_A} - x_{spec\_B} \cdot p_{sat\_B} - x_{spec\_C} \cdot p_{sat\_C} - x_{spec\_D} \cdot p_{sat\_D}\right) \cdot V_g \cdot M_{N2}}{R \cdot Temp}$$

$m_g \leftarrow m_{g\_N2} + m_{g\_A} + m_{g\_B} + m_{g\_C} + m_{g\_D}$

$m_{l\_A} \leftarrow m_{0\_A} - m_{g\_A}$

$m_{l\_B} \leftarrow m_{0\_B} - m_{g\_B}$

$m_{l\_C} \leftarrow m_{0\_C} - m_{g\_C}$

$m_{l\_D} \leftarrow m_{0\_D} - m_{g\_D}$

$$x_{spec\_A} \leftarrow \frac{\frac{m_{l\_A}}{M_A}}{\frac{m_{l\_A}}{M_A}+\frac{m_{l\_B}}{M_B}+\frac{m_{l\_C}}{M_C}+\frac{m_{l\_D}}{M_D}}$$

$$x_{spec\_B} \leftarrow \frac{\frac{m_{l\_B}}{M_B}}{\frac{m_{l\_A}}{M_A}+\frac{m_{l\_B}}{M_B}+\frac{m_{l\_C}}{M_C}+\frac{m_{l\_D}}{M_D}}$$

$$x_{spec\_C} \leftarrow \frac{\frac{m_{l\_C}}{M_C}}{\frac{m_{l\_A}}{M_A}+\frac{m_{l\_B}}{M_B}+\frac{m_{l\_C}}{M_C}+\frac{m_{l\_D}}{M_D}}$$

$$x_{spec\_D} \leftarrow \frac{\frac{m_{l\_D}}{M_D}}{\frac{m_{l\_A}}{M_A}+\frac{m_{l\_B}}{M_B}+\frac{m_{l\_C}}{M_C}+\frac{m_{l\_D}}{M_D}}$$

$$y_{spec\_A} \leftarrow \frac{\frac{m_{g\_A}}{M_A}}{\frac{m_{g\_A}}{M_A}+\frac{m_{g\_B}}{M_B}+\frac{m_{g\_C}}{M_C}+\frac{m_{g\_D}}{M_D}+\frac{m_{g\_N2}}{M_{N2}}}$$

$$y_{spec\_B} \leftarrow \frac{\frac{m_{g\_B}}{M_B}}{\frac{m_{g\_A}}{M_A}+\frac{m_{g\_B}}{M_B}+\frac{m_{g\_C}}{M_C}+\frac{m_{g\_D}}{M_D}+\frac{m_{g\_N2}}{M_{N2}}}$$

$$y_{spec\_C} \leftarrow \frac{\frac{m_{g\_C}}{M_C}}{\frac{m_{g\_A}}{M_A}+\frac{m_{g\_B}}{M_B}+\frac{m_{g\_C}}{M_C}+\frac{m_{g\_D}}{M_D}+\frac{m_{g\_N2}}{M_{N2}}}$$

$$y_{spec\_D} \leftarrow \frac{\frac{m_{g\_D}}{M_D}}{\frac{m_{g\_A}}{M_A}+\frac{m_{g\_B}}{M_B}+\frac{m_{g\_C}}{M_C}+\frac{m_{g\_D}}{M_D}+\frac{m_{g\_N2}}{M_{N2}}}$$

$$y_{spec\_N2} \leftarrow \frac{\frac{m_{g\_N2}}{M_{N2}}}{\frac{m_{g\_A}}{M_A}+\frac{m_{g\_B}}{M_B}+\frac{m_{g\_C}}{M_C}+\frac{m_{g\_D}}{M_D}+\frac{m_{g\_N2}}{M_{N2}}}$$

$$p_{spec} \leftarrow x_{spec\_A}\cdot p_{sat\_A}+x_{spec\_B}\cdot p_{sat\_B}+x_{spec\_C}\cdot p_{sat\_C}+x_{spec\_D}\cdot p_{sat\_D}+\frac{m_{g\_N2}\cdot R\cdot Temp}{V_g\cdot M_{N2}}$$

$$\begin{bmatrix} x_{spec\_A} & x_{spec\_B} & x_{spec\_C} & x_{spec\_D} & y_{spec\_A} & y_{spec\_B} & y_{spec\_C} & y_{spec\_D} & y_{spec\_N2} & m_l & m_g & V_l & V_g & p_{spec} \end{bmatrix}^{\mathrm{T}}$$

Startzusammensetzung Flüssigkeit:

$$x_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_0$$

$$x_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_1$$

$$x_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_2$$

$$x_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_3$$

Startzusammensetzung Gas:

$$y_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_4$$

$$y_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_5$$

$$y_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_6$$

$$y_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_7$$

$$y_{0\_N2}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_8$$

Startmassen und Startvolumen:

$$m_{0\_l}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_9$$

$$m_{0\_g}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{10}$$

$$m_0(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_l}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) + m_{0\_g}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$V_{0\_l}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{11}$$

$$V_{0\_g}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{12}$$

Startdruck:

$$p_0(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := pT\_Flash(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{13}$$

Startmassenanteile der Komponenten für Flüssigkeit und Gas:

$$\zeta_{0\_l\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := \frac{x_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_A}{x_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_A + x_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_B + x_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_C + x_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_D}$$

$$\zeta_{0\_l\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := \frac{x_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_B}{x_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_A + x_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_B + x_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_C + x_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_D}$$

$$\zeta_{0\_l\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := \frac{x_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_C}{x_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_A + x_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_B + x_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_C + x_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_D}$$

$$\zeta_{0\_l\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := \frac{x_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_D}{x_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_A + x_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_B + x_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_C + x_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_D}$$

$$\zeta_{0\_g\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := \frac{y_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_A}{y_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_A + y_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_B + y_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_C + y_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_D + y_{0\_N2}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_{N2}}$$

$$\zeta_{0\_g\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := \frac{y_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_B}{y_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_A + y_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_B + y_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_C + y_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_D + y_{0\_N2}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_{N2}}$$

$$\zeta_{0\_g\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := \frac{y_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_C}{y_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_A + y_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_B + y_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_C + y_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_D + y_{0\_N2}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_{N2}}$$

$$\zeta_{0\_g\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := \frac{y_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_D}{y_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_A + y_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_B + y_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_C + y_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_D + y_{0\_N2}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_{N2}}$$

$$\zeta_{0\_g\_N2}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := \frac{y_{0\_N2}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_{N2}}{y_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_A + y_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_B + y_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_C + y_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_D + y_{0\_N2}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot M_{N2}}$$

Startmassen der Komponenten für Flüssigkeit und Gas:

$$m_{0\_l\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_l}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot \zeta_{0\_l\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$m_{0\_l\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_l}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot \zeta_{0\_l\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$m_{0\_l\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_l}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot \zeta_{0\_l\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$m_{0\_l\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_l}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot \zeta_{0\_l\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$m_{0\_g\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_g}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot \zeta_{0\_g\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$m_{0\_g\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_g}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot \zeta_{0\_g\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$m_{0\_g\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_g}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot \zeta_{0\_g\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$m_{0\_g\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_g}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot \zeta_{0\_g\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$m_{0\_g\_N2}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_g}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot \zeta_{0\_g\_N2}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$m_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_l\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) + m_{0\_g\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$m_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_l\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) + m_{0\_g\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$m_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_l\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) + m_{0\_g\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$m_{0\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := m_{0\_l\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) + m_{0\_g\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})$$

$$x_0(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := \frac{\frac{m_{0\_l\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})}{M_A}}{\frac{m_{0\_l\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})}{M_A} + \frac{m_{0\_l\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})}{M_B}}$$

Innere Energien zum Startzeitpunkt:

$$\begin{aligned} h_{0\_l}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := {} & \zeta_{0\_l\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ & \cdot (\Delta H_{B\_A} + c_{pl\_A}(Temp) \cdot (Temp - T_{ref}) - \Delta h_{V\_A}(Temp)) \\ & + \zeta_{0\_l\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ & \cdot (\Delta H_{B\_B} + c_{pl\_B}(Temp) \cdot (Temp - T_{ref}) - \Delta h_{V\_B}(Temp)) \\ & + \zeta_{0\_l\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ & \cdot (\Delta H_{B\_C} + c_{pl\_C}(Temp) \cdot (Temp - T_{ref}) - \Delta h_{V\_C}(Temp)) \\ & + \zeta_{0\_l\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ & \cdot (\Delta H_{B\_D} + c_{pl\_D}(Temp) \cdot (Temp - T_{ref})) \end{aligned}$$

$$\begin{aligned} h_{0\_g}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := {} & \zeta_{0\_g\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ & \cdot (\Delta H_{B\_A} + c_{pg\_A}(Temp) \cdot (Temp - T_{ref})) \\ & + \zeta_{0\_g\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ & \cdot (\Delta H_{B\_B} + c_{pg\_B}(Temp) \cdot (Temp - T_{ref})) \\ & + \zeta_{0\_g\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ & \cdot (\Delta H_{B\_C} + c_{pg\_C}(Temp) \cdot (Temp - T_{ref})) \\ & + \zeta_{0\_g\_D}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ & \cdot (\Delta H_{B\_D} + c_{pg\_D}(Temp) \cdot (Temp - T_{ref})) \\ & + \zeta_{0\_g\_N2}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ & \cdot (\Delta H_{B\_N2} + c_{pg\_N2} \cdot (Temp - T_{ref})) \end{aligned}$$

$$\begin{aligned} H_0(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := {} & h_{0\_l}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot m_{0\_l}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ & + h_{0\_g}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot m_{0\_g}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \end{aligned}$$

$$\begin{aligned} U_0(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) := {} & H_0(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ & - p_0(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \cdot Vol \end{aligned}$$

$$\begin{bmatrix} Temp \\ p_0(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ Vol \\ V_{0\_l}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ V_{0\_g}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ x_{0\_A}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ x_{0\_B}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \\ x_{0\_C}(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}) \end{bmatrix}$$

$$Startbed\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) := \begin{bmatrix} x_{0\_D}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ y_{0\_A}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ y_{0\_B}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ y_{0\_C}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ y_{0\_D}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ y_{0\_N2}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_0\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_{0\_l}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_{0\_g}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ \zeta_{0\_l\_A}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ \zeta_{0\_l\_B}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ \zeta_{0\_l\_C}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ \zeta_{0\_l\_D}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ \zeta_{0\_g\_A}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ \zeta_{0\_g\_B}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ \zeta_{0\_g\_C}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ \zeta_{0\_g\_D}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ \zeta_{0\_g\_N2}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_{0\_l\_A}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_{0\_l\_B}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_{0\_l\_C}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_{0\_l\_D}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_{0\_g\_A}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_{0\_g\_B}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_{0\_g\_C}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_{0\_g\_D}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_{0\_g\_N2}\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ m_{0\_A} \\ m_{0\_B} \\ m_{0\_C} \\ m_{0\_D} \\ U_0\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \\ x_0\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right) \end{bmatrix}$$

UVm-Flash

UVm-Flash --> Innere Energie,Volumen und Gesamtmasse sind bekannt und konstant für einen Zeitpunk t. Gesucht ist die Zusammensetzung der Flüssigkeit und Gasphase bzw. ihre Massen je Komponente, sowie die intensiven Zustandsgrößen p und T.

$$UVm\_Flash\left(InnerEnergie, Vol, Mass, MasseA, MasseB, MasseC, MasseD, p_{spec}, T_{spec}, x_{spec\_A}, x_{spec\_B}, x_{spec\_C}, x_{spec\_D}\right) := \begin{bmatrix} K_{spec\_A} \leftarrow \dfrac{p_{s\_A}\left(T_{spec}\right)}{p_{spec}} \\ K_{spec\_B} \leftarrow \dfrac{p_{s\_B}\left(T_{spec}\right)}{p_{spec}} \\ K_{spec\_C} \leftarrow \dfrac{p_{s\_C}\left(T_{spec}\right)}{p_{spec}} \\ K_{spec\_D} \leftarrow \dfrac{p_{s\_D}\left(T_{spec}\right)}{p_{spec}} \\ j \leftarrow 0 \\ \varepsilon \leftarrow 10^{-3} \\ \text{for } i \in 0..15 \\ \quad \begin{bmatrix} p_{sat\_A} \leftarrow p_{s\_A}\left(T_{spec}\right) \\ p_{sat\_B} \leftarrow p_{s\_B}\left(T_{spec}\right) \\ p_{sat\_C} \leftarrow p_{s\_C}\left(T_{spec}\right) \\ p_{sat\_D} \leftarrow p_{s\_D}\left(T_{spec}\right) \end{bmatrix} \end{bmatrix}$$

$$\rho_{spec\_A} \leftarrow \rho_A(T_{spec})$$
$$\rho_{spec\_B} \leftarrow \rho_B(T_{spec})$$
$$\rho_{spec\_C} \leftarrow \rho_C(T_{spec})$$
$$\rho_{spec\_D} \leftarrow \rho_D(T_{spec})$$
$$m_l \leftarrow \frac{MasseA + MasseB + MasseC + MasseD - \frac{Vol}{R \cdot T_{spec}} \cdot (x_{spec\_A} \cdot p_{sat\_A} \cdot M_A + x_{spec\_B} \cdot p_{sat\_B} \cdot M_B + x_{spec\_C} \cdot p_{sat\_C} \cdot M_C + x_{spec\_D} \cdot p_{sat\_D} \cdot M_D}{1 - \frac{1}{R \cdot T_{spec} \cdot (x_{spec\_A} \cdot M_A + x_{spec\_B} \cdot M_B + x_{spec\_C} \cdot M_C + x_{spec\_D} \cdot M_D)} \cdot \left(\frac{x_{spec\_A} \cdot M_A}{\rho_{spec\_A}} + \frac{x_{spec\_B} \cdot M_B}{\rho_{spec\_B}} + \frac{x_{spec\_C} \cdot M_C}{\rho_{spec\_C}} + \frac{x_{spec\_D} \cdot M_D}{\rho_{spec\_D}}\right) \cdot (x_{spec\_A} \cdot p_{sat\_A} \cdot M_A + x_{spec\_B} \cdot p_{sat\_B} \cdot M_B +$$
$$m_g \leftarrow Mass - m_l$$
$$V_l \leftarrow \frac{m_l}{x_{spec\_A} \cdot M_A + x_{spec\_B} \cdot M_B + x_{spec\_C} \cdot M_C + x_{spec\_D} \cdot M_D} \cdot \left(\frac{x_{spec\_A} \cdot M_A}{\rho_{spec\_A}} + \frac{x_{spec\_B} \cdot M_B}{\rho_{spec\_B}} + \frac{x_{spec\_C} \cdot M_C}{\rho_{spec\_C}} + \frac{x_{spec\_D} \cdot M_D}{\rho_{spec\_D}}\right)$$
$$V_g \leftarrow Vol - V_l$$
$$m_{g\_A} \leftarrow \frac{x_{spec\_A} \cdot p_{sat\_A} \cdot V_g \cdot M_A}{R \cdot T_{spec}}$$
$$m_{g\_B} \leftarrow \frac{x_{spec\_B} \cdot p_{sat\_B} \cdot V_g \cdot M_B}{R \cdot T_{spec}}$$
$$m_{g\_C} \leftarrow \frac{x_{spec\_C} \cdot p_{sat\_C} \cdot V_g \cdot M_C}{R \cdot T_{spec}}$$
$$m_{g\_D} \leftarrow \frac{x_{spec\_D} \cdot p_{sat\_D} \cdot V_g \cdot M_D}{R \cdot T_{spec}}$$
$$m_{g\_N2} \leftarrow m_g - m_{g\_A} - m_{g\_B} - m_{g\_C} - m_{g\_D}$$
$$m_{l\_A} \leftarrow MasseA - m_{g\_A}$$
$$m_{l\_B} \leftarrow MasseB - m_{g\_B}$$
$$m_{l\_C} \leftarrow MasseC - m_{g\_C}$$
$$m_{l\_D} \leftarrow MasseD - m_{g\_D}$$
$$\zeta_{spec\_l\_A} \leftarrow \frac{m_{l\_A}}{m_{l\_A} + m_{l\_B} + m_{l\_C} + m_{l\_D}}$$
$$\zeta_{spec\_l\_B} \leftarrow \frac{m_{l\_B}}{m_{l\_A} + m_{l\_B} + m_{l\_C} + m_{l\_D}}$$
$$\zeta_{spec\_l\_C} \leftarrow \frac{m_{l\_C}}{m_{l\_A} + m_{l\_B} + m_{l\_C} + m_{l\_D}}$$
$$\zeta_{spec\_l\_D} \leftarrow \frac{m_{l\_D}}{m_{l\_A} + m_{l\_B} + m_{l\_C} + m_{l\_D}}$$
$$\zeta_{spec\_g\_A} \leftarrow \frac{m_{g\_A}}{m_{g\_A} + m_{g\_B} + m_{g\_C} + m_{g\_D} + m_{g\_N2}}$$
$$\zeta_{spec\_g\_B} \leftarrow \frac{m_{g\_B}}{m_{g\_A} + m_{g\_B} + m_{g\_C} + m_{g\_D} + m_{g\_N2}}$$
$$\zeta_{spec\_g\_C} \leftarrow \frac{m_{g\_C}}{m_{g\_A} + m_{g\_B} + m_{g\_C} + m_{g\_D} + m_{g\_N2}}$$
$$\zeta_{spec\_g\_D} \leftarrow \frac{m_{g\_D}}{m_{g\_A} + m_{g\_B} + m_{g\_C} + m_{g\_D} + m_{g\_N2}}$$
$$\zeta_{spec\_g\_N2} \leftarrow \frac{m_{g\_N2}}{m_{g\_A} + m_{g\_B} + m_{g\_C} + m_{g\_D} + m_{g\_N2}}$$
$$x_{spec\_A} \leftarrow \frac{\frac{m_{l\_A}}{M_A}}{\frac{m_{l\_A}}{M_A} + \frac{m_{l\_B}}{M_B} + \frac{m_{l\_C}}{M_C} + \frac{m_{l\_D}}{M_D}}$$
$$x_{spec\_B} \leftarrow \frac{\frac{m_{l\_B}}{M_B}}{\frac{m_{l\_A}}{M_A} + \frac{m_{l\_B}}{M_B} + \frac{m_{l\_C}}{M_C} + \frac{m_{l\_D}}{M_D}}$$
$$x_{spec\_C} \leftarrow \frac{\frac{m_{l\_C}}{M_C}}{\frac{m_{l\_A}}{M_A} + \frac{m_{l\_B}}{M_B} + \frac{m_{l\_C}}{M_C} + \frac{m_{l\_D}}{M_D}}$$

$x_{spec\_D} \leftarrow 1 - x_{spec\_A} - x_{spec\_B} - x_{spec\_C}$

$y_{spec\_A} \leftarrow \dfrac{\frac{m_{g\_A}}{M_A}}{\frac{m_{g\_A}}{M_A} + \frac{m_{g\_B}}{M_B} + \frac{m_{g\_C}}{M_C} + \frac{m_{g\_D}}{M_D} + \frac{m_{g\_N2}}{M_{N2}}}$

$y_{spec\_B} \leftarrow \dfrac{\frac{m_{g\_B}}{M_B}}{\frac{m_{g\_A}}{M_A} + \frac{m_{g\_B}}{M_B} + \frac{m_{g\_C}}{M_C} + \frac{m_{g\_D}}{M_D} + \frac{m_{g\_N2}}{M_{N2}}}$

$y_{spec\_C} \leftarrow \dfrac{\frac{m_{g\_C}}{M_C}}{\frac{m_{g\_A}}{M_A} + \frac{m_{g\_B}}{M_B} + \frac{m_{g\_C}}{M_C} + \frac{m_{g\_D}}{M_D} + \frac{m_{g\_N2}}{M_{N2}}}$

$y_{spec\_D} \leftarrow \dfrac{\frac{m_{g\_D}}{M_D}}{\frac{m_{g\_A}}{M_A} + \frac{m_{g\_B}}{M_B} + \frac{m_{g\_C}}{M_C} + \frac{m_{g\_D}}{M_D} + \frac{m_{g\_N2}}{M_{N2}}}$

$y_{spec\_N2} \leftarrow 1 - y_{spec\_A} - y_{spec\_B} - y_{spec\_C} - y_{spec\_D}$

$T_{spec} \leftarrow \dfrac{InnerEnergie + p_{spec} \cdot Vol - m_l \cdot \left(\zeta_{spec\_l\_A} \cdot \left(\Delta H_{B\_A} - \Delta h_{V\_A}\left(T_{spec}\right)\right) + \zeta_{spec\_l\_B} \cdot \left(\Delta H_{B\_B} - \Delta h_{V\_B}\left(T_{spec}\right)\right) + \zeta_{spec\_l\_C} \cdot \left(\Delta H_{B\_C} - \Delta h_{V\_C}\left(T_{spec}\right)\right) + \zeta_{spec\_l\_D} \cdot \left(\Delta H_{B\_D} - \Delta h_{V\_D}\left(T_{s}\right.\right.\right.\right.}{m_l \cdot \left(\zeta_{spec\_l\_A} \cdot c_{pl\_A}\left(T_{spec}\right) + \zeta_{spec\_l\_B} \cdot c_{pl\_B}\left(T_{spec}\right) + \zeta_{spec\_l\_C} \cdot c_{pl\_C}\left(T_{spec}\right) + \zeta_{spec\_l\_D} \cdot c_{pl\_D}\left(T_{spec}\right)\right) + m_g \cdot \left(\zeta_{spec\_g\_A} \cdot c_{pg\_A}\left(T_{spec}\right) + \zeta_{spec\_g\_B} \cdot c_{pg\_}\right.}$

$p_{spec} \leftarrow x_{spec\_A} \cdot p_{sat\_A} + x_{spec\_B} \cdot p_{sat\_B} + x_{spec\_C} \cdot p_{sat\_C} + x_{spec\_D} \cdot p_{sat\_D} + \dfrac{m_{g\_N2} \cdot R \cdot T_{spec}}{V_g \cdot M_{N2}}$

$K_{spec\_new\_A} \leftarrow \dfrac{p_{sat\_A}}{p_{spec}}$

$K_{spec\_new\_B} \leftarrow \dfrac{p_{sat\_B}}{p_{spec}}$

$K_{spec\_new\_C} \leftarrow \dfrac{p_{sat\_C}}{p_{spec}}$

$K_{spec\_new\_D} \leftarrow \dfrac{p_{sat\_D}}{p_{spec}}$

if $\dfrac{\left|K_{spec\_new\_A} - K_{spec\_A}\right|}{K_{spec\_A}} < \varepsilon \wedge \dfrac{\left|K_{spec\_new\_B} - K_{spec\_B}\right|}{K_{spec\_A}} < \varepsilon \wedge \dfrac{\left|K_{spec\_new\_C} - K_{spec\_C}\right|}{K_{spec\_A}} < \varepsilon \wedge \dfrac{\left|K_{spec\_new\_D} - K_{spec\_D}\right|}{K_{spec\_A}} < \varepsilon$

  break

else

  $j \leftarrow j + 1$

  $K_{spec\_A} \leftarrow K_{spec\_new\_A}$

  $K_{spec\_B} \leftarrow K_{spec\_new\_B}$

  $K_{spec\_C} \leftarrow K_{spec\_new\_C}$

  $K_{spec\_D} \leftarrow K_{spec\_new\_D}$

$\left[x_{spec\_A}\ \ x_{spec\_B}\ \ x_{spec\_C}\ \ x_{spec\_D}\ \ y_{spec\_A}\ \ y_{spec\_B}\ \ y_{spec\_C}\ \ y_{spec\_D}\ \ y_{spec\_N2}\ \ m_l\ \ m_g\ \ V_l\ \ V_g\ \ T_{spec}\ \ p_{spec}\ \ j\right]^{\mathrm{T}}$

DGL-System für Reaktor

Numerische Eingaben:

$\mathbf{TOL} := 10^{-7}$ $\mathbf{CTOL} := 10^{-7}$

Anfangsbedingungen:

$m_{l\_A}(0\ s) = Startbed\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right)_{26}$

$m_{l\_B}(0\ s) = Startbed\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right)$

$m_{l\_B}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{27}$

$m_{l\_C}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{28}$

$m_{l\_D}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{29}$

$m_{N2}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{34}$

$m(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{14}$

$xU(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{39}$

$T(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{0}$

$p(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{1}$

$x_A(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{5}$

$x_B(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{6}$

$x_C(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{7}$

$x_D(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{8}$

$y_A(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{9}$

$y_B(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{10}$

$y_C(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{11}$

$y_D(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{12}$

$y_{N2}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{13}$

$\zeta_{l\_A}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{17}$

$\zeta_{l\_B}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{18}$

$\zeta_{l\_C}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{19}$

$\zeta_{l\_D}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{20}$

$\zeta_{g\_A}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{21}$

$\zeta_{g\_B}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{22}$

$\zeta_{g\_C}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{23}$

$\zeta_{g\_D}(0\ s) = Startbed(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D})_{24}$

$$\zeta_{g\_N2}(0\ s) = Startbed\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right)_{25}$$

$$m_l(0\ s) = Startbed\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right)_{15}$$

$$m_g(0\ s) = Startbed\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right)_{16}$$

$$V_l(0\ s) = Startbed\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right)_{3}$$

$$V_g(0\ s) = Startbed\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}\right)_{4}$$

Massenbilanzen:

$$\frac{\mathrm{d}}{\mathrm{d}t} m_{l\_A}(t) = -k_{0\_1}(x_0)\cdot exp\left(-\frac{E_{A\_1}(x_0)}{R\cdot T(t)}\right)\cdot\frac{m_l(t)^2\cdot\zeta_{l\_A}(t)\cdot\zeta_{l\_B}(t)}{M_B\cdot V_l(t)} - k_{0\_2}(x_0)\cdot exp\left(-\frac{E_{A\_2}(x_0)}{R\cdot T(t)}\right)\cdot\frac{m_l(t)^3\cdot\zeta_{l\_A}(t)\cdot\zeta_{l\_B}(t)\cdot\zeta_{l\_D}(t)}{M_D\cdot M_B\cdot V_l(t)^2}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} m_{l\_B}(t) = m_{B\_F} - k_{0\_1}(x_0)\cdot exp\left(-\frac{E_{A\_1}(x_0)}{R\cdot T(t)}\right)\cdot\frac{m_l(t)^2\cdot\zeta_{l\_A}(t)\cdot\zeta_{l\_B}(t)}{M_A\cdot V_l(t)} - k_{0\_2}(x_0)\cdot exp\left(-\frac{E_{A\_2}(x_0)}{R\cdot T(t)}\right)\cdot\frac{m_l(t)^3\cdot\zeta_{l\_A}(t)\cdot\zeta_{l\_B}(t)\cdot\zeta_{l\_D}(t)}{M_A\cdot M_D\cdot V_l(t)^2}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} m_{l\_C}(t) = k_{0\_1}(x_0)\cdot exp\left(-\frac{E_{A\_1}(x_0)}{R\cdot T(t)}\right)\cdot\frac{m_l(t)^2\cdot\zeta_{l\_A}(t)\cdot\zeta_{l\_B}(t)}{M_A\cdot M_B\cdot V_l(t)}\cdot M_C + k_{0\_2}(x_0)\cdot exp\left(-\frac{E_{A\_2}(x_0)}{R\cdot T(t)}\right)\cdot\frac{m_l(t)^3\cdot\zeta_{l\_A}(t)\cdot\zeta_{l\_B}(t)\cdot\zeta_{l\_D}(t)}{M_A\cdot M_B\cdot M_D\cdot V_l(t)^2}\cdot M_C$$

$$\frac{\mathrm{d}}{\mathrm{d}t} m_{l\_D}(t) = k_{0\_1}(x_0)\cdot exp\left(-\frac{E_{A\_1}(x_0)}{R\cdot T(t)}\right)\cdot\frac{m_l(t)^2\cdot\zeta_{l\_A}(t)\cdot\zeta_{l\_B}(t)}{M_A\cdot M_B\cdot V_l(t)}\cdot M_D + k_{0\_2}(x_0)\cdot exp\left(-\frac{E_{A\_2}(x_0)}{R\cdot T(t)}\right)\cdot\frac{m_l(t)^3\cdot\zeta_{l\_A}(t)\cdot\zeta_{l\_B}(t)\cdot\zeta_{l\_D}(t)}{M_A\cdot M_B\cdot M_D\cdot V_l(t)^2}\cdot M_D$$

$$\frac{\mathrm{d}}{\mathrm{d}t} m_{N2}(t) = 0$$

$$m(t) = m_{l\_A}(t) + m_g(t)\cdot\zeta_{g\_A}(t) + m_{l\_B}(t) + m_g(t)\cdot\zeta_{g\_B}(t) + m_{l\_C}(t) + m_g(t)\cdot\zeta_{g\_C}(t) + m_{l\_D}(t) + m_g(t)\cdot\zeta_{g\_D}(t) + m_{N2}(t)$$

Energiebilanz:

$$\frac{\mathrm{d}}{\mathrm{d}t} xU(t) = m_{B\_F}\cdot\left(\Delta H_{B\_B} + c_{pg\_B}\langle T_{B\_F}\rangle\cdot\left(T_{B\_F} - T_{ref}\right) - \Delta h_{V\_B}\langle T_{B\_F}\rangle\right) - \Delta H_R\cdot\left(k_{0\_1}(x_0)\cdot exp\left(-\frac{E_{A\_1}(x_0)}{R\cdot T(t)}\right)\cdot\frac{m_l(t)^2\cdot\zeta_{l\_A}(t)\cdot\zeta_{l\_B}(t)}{M_A\cdot M_B\cdot V_l(t)} + k_{0\_2}(x_0)\cdot exp\left(-\frac{E_{A\_2}(x_0)}{R\cdot T(t)}\right)\cdot\frac{m_l(t)^3\cdot\zeta_{l\_A}(t)\cdot\zeta_{l\_B}(t)\cdot\zeta_{l\_D}(t)}{M_A\cdot M_B\cdot M_D\cdot V_l(t)^2}\right)$$

Flash Berechnung:

$$x_A(t) = UVm\_Flash\left(xU(t), Vol, m(t), m_{l\_A}(t) + m_g(t)\cdot\zeta_{g\_A}(t), m_{l\_B}(t) + m_g(t)\cdot\zeta_{g\_B}(t), m_{l\_C}(t) + m_g(t)\cdot\zeta_{g\_C}(t), m_{l\_D}(t) + m_g(t)\cdot\zeta_{g\_D}(t), p(t), T(t), x_A(t), x_B(t), x_C(t), x_D(t)\right)_0$$

$$x_B(t) = UVm\_Flash\left(xU(t), Vol, m(t), m_{l\_A}(t) + m_g(t)\cdot\zeta_{g\_A}(t), m_{l\_B}(t) + m_g(t)\cdot\zeta_{g\_B}(t), m_{l\_C}(t) + m_g(t)\cdot\zeta_{g\_C}(t), m_{l\_D}(t) + m_g(t)\cdot\zeta_{g\_D}(t), p(t), T(t), x_A(t), x_B(t), x_C(t), x_D(t)\right)_1$$

$$x_C(t) = UVm\_Flash\left(xU(t), Vol, m(t), m_{l\_A}(t) + m_g(t)\cdot\zeta_{g\_A}(t), m_{l\_B}(t) + m_g(t)\cdot\zeta_{g\_B}(t), m_{l\_C}(t) + m_g(t)\cdot\zeta_{g\_C}(t), m_{l\_D}(t) + m_g(t)\cdot\zeta_{g\_D}(t), p(t), T(t), x_A(t), x_B(t), x_C(t), x_D(t)\right)_2$$

$$x_D(t) = UVm\_Flash\left(xU(t), Vol, m(t), m_{l\_A}(t) + m_g(t)\cdot\zeta_{g\_A}(t), m_{l\_B}(t) + m_g(t)\cdot\zeta_{g\_B}(t), m_{l\_C}(t) + m_g(t)\cdot\zeta_{g\_C}(t), m_{l\_D}(t) + m_g(t)\cdot\zeta_{g\_D}(t), p(t), T(t), x_A(t), x_B(t), x_C(t), x_D(t)\right)_3$$

$$y_A(t) = \frac{x_A(t)\cdot p_{s\_A}(T(t))}{p(t)}$$

$$y_B(t) = \frac{x_B(t)\cdot p_{s\_B}(T(t))}{p(t)}$$

$$y_C(t) = \frac{x_C(t) \cdot p_{s\_C}(T(t))}{p(t)}$$

$$y_D(t) = \frac{x_D(t) \cdot p_{s\_D}(T(t))}{p(t)}$$

$$y_{N2}(t) = 1 - y_A(t) - y_B(t) - y_C(t) - y_D(t)$$

$$\zeta_{l\_A}(t) = \frac{x_A(t) \cdot M_A}{x_A(t) \cdot M_A + x_B(t) \cdot M_B + x_C(t) \cdot M_C + x_D(t) \cdot M_D}$$

$$\zeta_{l\_B}(t) = \frac{x_B(t) \cdot M_B}{x_A(t) \cdot M_A + x_B(t) \cdot M_B + x_C(t) \cdot M_C + x_D(t) \cdot M_D}$$

$$\zeta_{l\_C}(t) = \frac{x_C(t) \cdot M_C}{x_A(t) \cdot M_A + x_B(t) \cdot M_B + x_C(t) \cdot M_C + x_D(t) \cdot M_D}$$

$$\zeta_{l\_D}(t) = 1 - \zeta_{l\_A}(t) - \zeta_{l\_B}(t) - \zeta_{l\_C}(t)$$

$$\zeta_{g\_A}(t) = \frac{y_A(t) \cdot M_A}{y_A(t) \cdot M_A + y_B(t) \cdot M_B + y_C(t) \cdot M_C + y_D(t) \cdot M_D + y_{N2}(t) \cdot M_{N2}}$$

$$\zeta_{g\_B}(t) = \frac{y_B(t) \cdot M_B}{y_A(t) \cdot M_A + y_B(t) \cdot M_B + y_C(t) \cdot M_C + y_D(t) \cdot M_D + y_{N2}(t) \cdot M_{N2}}$$

$$\zeta_{g\_C}(t) = \frac{y_C(t) \cdot M_C}{y_A(t) \cdot M_A + y_B(t) \cdot M_B + y_C(t) \cdot M_C + y_D(t) \cdot M_D + y_{N2}(t) \cdot M_{N2}}$$

$$\zeta_{g\_D}(t) = \frac{y_D(t) \cdot M_D}{y_A(t) \cdot M_A + y_B(t) \cdot M_B + y_C(t) \cdot M_C + y_D(t) \cdot M_D + y_{N2}(t) \cdot M_{N2}}$$

$$\zeta_{g\_N2}(t) = 1 - \zeta_{g\_A}(t) - \zeta_{g\_B}(t) - \zeta_{g\_C}(t) - \zeta_{g\_D}(t)$$

$$m_l(t) = UVm\_Flash\left(xU(t), Vol, m(t), m_{l\_A}(t) + m_g(t) \cdot \zeta_{g\_A}(t), m_{l\_B}(t) + m_g(t) \cdot \zeta_{g\_B}(t), m_{l\_C}(t) + m_g(t) \cdot \zeta_{g\_C}(t), m_{l\_D}(t) + m_g(t) \cdot \zeta_{g\_D}(t), p(t), T(t), x_A(t), x_B(t), x_C(t), x_D(t)\right)_9$$

$$m_g(t) = UVm\_Flash\left(xU(t), Vol, m(t), m_{l\_A}(t) + m_g(t) \cdot \zeta_{g\_A}(t), m_{l\_B}(t) + m_g(t) \cdot \zeta_{g\_B}(t), m_{l\_C}(t) + m_g(t) \cdot \zeta_{g\_C}(t), m_{l\_D}(t) + m_g(t) \cdot \zeta_{g\_D}(t), p(t), T(t), x_A(t), x_B(t), x_C(t), x_D(t)\right)_{10}$$

$$V_l(t) = UVm\_Flash\left(xU(t), Vol, m(t), m_{l\_A}(t) + m_g(t) \cdot \zeta_{g\_A}(t), m_{l\_B}(t) + m_g(t) \cdot \zeta_{g\_B}(t), m_{l\_C}(t) + m_g(t) \cdot \zeta_{g\_C}(t), m_{l\_D}(t) + m_g(t) \cdot \zeta_{g\_D}(t), p(t), T(t), x_A(t), x_B(t), x_C(t), x_D(t)\right)_{11}$$

$$V_g(t) = UVm\_Flash\left(xU(t), Vol, m(t), m_{l\_A}(t) + m_g(t) \cdot \zeta_{g\_A}(t), m_{l\_B}(t) + m_g(t) \cdot \zeta_{g\_B}(t), m_{l\_C}(t) + m_g(t) \cdot \zeta_{g\_C}(t), m_{l\_D}(t) + m_g(t) \cdot \zeta_{g\_D}(t), p(t), T(t), x_A(t), x_B(t), x_C(t), x_D(t)\right)_{12}$$

$$T(t) = UVm\_Flash\left(xU(t), Vol, m(t), m_{l\_A}(t) + m_g(t) \cdot \zeta_{g\_A}(t), m_{l\_B}(t) + m_g(t) \cdot \zeta_{g\_B}(t), m_{l\_C}(t) + m_g(t) \cdot \zeta_{g\_C}(t), m_{l\_D}(t) + m_g(t) \cdot \zeta_{g\_D}(t), p(t), T(t), x_A(t), x_B(t), x_C(t), x_D(t)\right)_{13}$$

$$p(t) = UVm\_Flash\left(xU(t), Vol, m(t), m_{l\_A}(t) + m_g(t) \cdot \zeta_{g\_A}(t), m_{l\_B}(t) + m_g(t) \cdot \zeta_{g\_B}(t), m_{l\_C}(t) + m_g(t) \cdot \zeta_{g\_C}(t), m_{l\_D}(t) + m_g(t) \cdot \zeta_{g\_D}(t), p(t), T(t), x_A(t), x_B(t), x_C(t), x_D(t)\right)_{14}$$

DAE-System lösen

$$Lsg\left(Vol, Temp, m_{0\_A}, m_{0\_B}, m_{0\_C}, m_{0\_D}, x_0, t_{end}, n\right) := \mathbf{odesolve}\left(\begin{bmatrix} m_{l\_A}(t) \\ m_{l\_B}(t) \\ m_{l\_C}(t) \\ m_{l\_D}(t) \\ m_{N2}(t) \\ m(t) \\ xU(t) \\ T(t) \\ p(t) \\ x_A(t) \\ x_B(t) \\ x_C(t) \\ x_D(t) \\ y_A(t) \\ y_B(t) \\ y_C(t) \\ y_D(t) \\ y_{N2}(t) \\ \zeta_{l\_A}(t) \\ \zeta_{l\_B}(t) \\ \zeta_{l\_C}(t) \\ \zeta_{l\_D}(t) \\ \zeta_{g\_A}(t) \\ \zeta_{g\_B}(t) \\ \zeta_{g\_C}(t) \\ \zeta_{g\_D}(t) \\ \zeta_{g\_N2}(t) \\ m_l(t) \\ m_g(t) \\ V_l(t) \\ V_g(t) \end{bmatrix}, t_{end}, n\right)$$

Startmasse im Reaktor Komponente:

$m_{1\_A} := 0.051\ kg$ $m_{1\_B} := 0.006408\ kg$ $m_{1\_C} := 0\ kg$ $m_{1\_D} := 0\ kg$

Starttemperatur:

$T_1 := 66\ °C$

Reaktorvolumen:

$V_1 := 0.07\ L$

Startzeit, Endzeit, Schrittänge, Schrittanzahl, Kinetikparameter:

$t_{start\_1} := 0\ s$ $t_{end\_1} := 15\ min$ $\Delta t_1 := 0.01\ min$ $n_1 := \frac{t_{end\_1} - t_{start\_1}}{\Delta t_1} = 1500$

$x_1 := Startbed\left(V_1, T_1, m_{1\_A}, m_{1\_B}, m_{1\_C}, m_{1\_D}\right)_{40} = 0.714$

Startmasse im Reaktor Komponente:

$m_{2\_A} := 0.04915\ kg$ $m_{2\_B} := 0.03085\ kg$ $m_{2\_C} := 0\ kg$ $m_{2\_D} := 0\ kg$

Starttemperatur:

$T_2 := 24.5\ °C$

Reaktorvolumen:

$V_2 := 0.11\ L$

Startzeit, Endzeit, Schrittänge, Schrittanzahl, Kinetikparameter:

$t_{start\_2} := 0\ s$ $t_{end\_2} := 166\ min$ $\Delta t_2 := 0.01\ min$ $n_2 := \frac{t_{end\_2} - t_{start\_2}}{\Delta t_2} = 16600$

$x_2 := Startbed\left(V_2, T_2, m_{2\_A}, m_{2\_B}, m_{2\_C}, m_{2\_D}\right)_{40} = 0.333$

Startmasse im Reaktor Komponente:

$m_{3\_A} := 0.03656\ kg$ $m_{3\_B} := 0.02302\ kg$ m_3

Starttemperatur:

$T_3 := 24.75\ °C$

Reaktorvolumen:

$V_3 := 0.082\ L$

Startzeit, Endzeit, Schrittänge, Schrittan

$t_{start\_3} := 0\ s$ $t_{end\_3} := 166\ min$ $\Delta t_3 := 0.01\ min$

$x_3 := Startbed\left(V_3, T_3, m_{3\_A}, m_{3\_B}, m_{3\_C}, m_{3\_D}\right)_{40}$

$$\begin{bmatrix} m_{l\_A1} \\ \vdots \end{bmatrix} := Lsg\left(V_1, T_1, m_{1\_A}, m_{1\_B}, m_{1\_C}, m_{1\_D}, x_1, t_{end\_1}, n_1\right)$$

Startmasse im Reaktor Komponente:

$m_{4\_A} := 6.0586\ kg$ $m_{4\_B} := 1.9014\ kg$ $m_{4\_C} := 0\ kg$ $m_{4\_D} := 0\ kg$

Starttemperatur:

$T_4 := 29.5\ °C$

Reaktorvolumen:

$V_4 := 10\ L$

Startzeit, Endzeit, Schrittänge, Schrittanzahl, Kinetikparameter:

$t_{start\_4} := 0\ s$ $t_{end\_4} := 93\ min$ $\Delta t_4 := 0.001\ min$ $n_4 := \frac{t_{end\_4} - t_{start\_4}}{\Delta t_4} = 93000$

$x_4 := Startbed\left(V_4, T_4, m_{4\_A}, m_{4\_B}, m_{4\_C}, m_{4\_D}\right)_{40} = 0.5$

$$\begin{bmatrix} m_{l\_A4} \\ \vdots \end{bmatrix} := Lsg\left(V_4, T_4, m_{4\_A}, m_{4\_B}, m_{4\_C}, m_{4\_D}, x_4, t_{end\_4}, n_4\right)$$

$$\begin{bmatrix} m_{l\_A2} \\ \vdots \end{bmatrix} := Lsg\left(V_2, T_2, m_{2\_A}, m_{2\_B}, m_{2\_C}, m_{2\_D}, x_2, t_{end\_2}, n_2\right)$$

Startmasse im Reaktor Komponente:

$m_{5\_A} := 0.4918\ kg$ $m_{5\_B} := 0.3078\ kg$ $m_{5\_C} := 0\ kg$ $m_{5\_D} := 0\ kg$

Starttemperatur:

$T_5 := 15.5\ °C$

Reaktorvolumen:

$V_5 := 1\ L$

Startzeit, Endzeit, Schrittänge, Schrittanzahl, Kinetikparameter:

$t_{start\_5} := 0\ s$ $t_{end\_5} := 316\ min$ $\Delta t_5 := 0.001\ min$ $n_5 := \frac{t_{end\_5} - t_{start\_5}}{\Delta t_5} = 316000$

$x_5 := Startbed\left(V_5, T_5, m_{5\_A}, m_{5\_B}, m_{5\_C}, m_{5\_D}\right)_{40} = 0.334$

$$\begin{bmatrix} m_{l\_A5} \\ \vdots \end{bmatrix} := Lsg\left(V_5, T_5, m_{5\_A}, m_{5\_B}, m_{5\_C}, m_{5\_D}, x_5, t_{end\_5}, n_5\right)$$

$$\begin{bmatrix} m_{l\_A3} \\ \vdots \end{bmatrix} := Lsg\left(V_3, T_3, m_{3\_A}, m_{3\_B}\right.$$