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From molecules to dollars:
Integrating molecular design into thermo-economic process design using consistent thermodynamic modeling

J. Schilling[a], D. Tillmanns[a], M. Lampe[a], M. Hopp[b], J. Gross[b] and A. Bardow[a]*

S 1. Non-conventional properties

S 1.1 Flammability

The flammability of the molecules is regarded using the so-called F-Number Γ defined as:

$$\Gamma = 1 - \sqrt{\frac{L}{U}}\,, \tag{S.1}$$

where L denotes the lower flammability limit and U the upper flammability limit. The risk to obtain a flammable mixture of fuel and oxygen decreases if the lower flammability limit is closer to the upper flammability limit and, thus, if the F-number is small. Kondo *et al.*[1] propose a classification of molecules based on the F-number (Table 1).

Table 1: Classification of the F-number Γ based on Kondo *et al.*[1].

Classification	Range
vaguely flammable	$0.0 \leq \Gamma < 0.2$
weakly flammable	$0.2 \leq \Gamma < 0.4$
normally flammable	$0.4 \leq \Gamma < 0.6$

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[a] *Chair of Technical Thermodynamics, RWTH Aachen University, Germany*
[b] *Institute of Thermodynamics and Thermal Process Engineering, Stuttgart University, Germany*
**Corresponding author: andre.bardow@ltt.rwth-aachen.de*

strongly flammable	$0.6 \leq \Gamma < 0.8$
super flammable	$0.8 \leq \Gamma < 1.0$

A GC approach is used to predict the F-number from the molecular structure of the molecules as:[1]

$$\Gamma = p_1\left(1 + p_2 C + \sum_{i\in I} n_{\mathrm{i}} \cdot \Delta R_{\mathrm{A,i}}\right)\left(1 + \sum_{i\in I} n_{\mathrm{i}} \cdot \Delta R_{\mathrm{B,i}}\right), \tag{S.2}$$

where p_1, p_2 and C are constants of the model. $\Delta R_{\mathrm{A,i}}$ and $\Delta R_{\mathrm{B,i}}$ are the group contributions of group *i*. For many processes, highly flammable molecules show a good performance. However, the investment costs increase for flammable molecules as additional equipment might be necessary to ensure safety.[2,3] Thus, the F-number is limited to 0.8 in our analysis so that super flammable molecules are excluded from the design space. Thereby, the trade-off between investment in safety and better molecule performance can be considered in the results.

S 1.2 Auto-ignition temperature

The design space of the optimization is limited to molecules, whose auto-ignition temperature (AIT) is higher than the maximal process temperature. Using a GC approach of Albahri and George[4], the AIT is predicted as:

$$AIT = 729.7 + 24.9 \cdot \widehat{AIT} - 1.57 \cdot \widehat{AIT}^2 - 0.0773 \cdot \widehat{AIT}^3 + 0.0032 \cdot \widehat{AIT}^4 \tag{S.3}$$

with

$$\widehat{AIT} = \sum_{i\in I} n_{\mathrm{i}} \cdot AIT_i, \tag{S.4}$$

where AIT_i is the group contribution of group i. The AIT is limited to $T_{\mathrm{max,process}} + 30\ K \leq AIT$ considering a safety reserve of $30\ K$ to the maximal process temperature $T_{\mathrm{max,process}}$.

S 1.3 Toxicity

Another non-conventional property of the molecules is toxicity, which has to be considered during the design. The United Nations Globally Harmonized System of classification and labelling of chemicals (GHS)[5] is used to classify the molecules. Here, we consider the 96-h LC50 toxicity to the fathead minnow (Pimephales promelas), in the following abbreviated with LC50 (Table 2). In this approach, the highly toxic categories 1 and 2 are excluded from the design space by an additional constraint. Martin and Young[6] present a GC approach to calculate the LC50 from the molecular structure of the molecules as:

$$-\log(LC50) = \sum_{i \in I} n_{\mathrm{i}} \cdot \alpha_i, \tag{S.5}$$

where α_i is the group contribution of group *i*. In this GC approach, benzenes are defined using second order groups, which cannot be captured by the first order groups of the presented optimization approach. Therefore, we describe benzenes by one group, which underestimate the contribution of the groups for benzenes proposed by Martin and Young[6]. The detailed prediction of the toxicity of benzenes can be performed in a subsequent assessment, if benzenes are identified by the approach.

Table 2: Classification of the 96-h LC50 toxicity based on GHS[5]

Classification	Range
Category Acute 1	$\mathrm{LC50} \leq 1\ \frac{\mathrm{mg}}{l}$
Category Acute 2	$1\ \frac{\mathrm{mg}}{l} \leq \mathrm{LC50} < 10\ \frac{\mathrm{mg}}{l}$
Category Acute 3	$10\ \frac{\mathrm{mg}}{l} \leq \mathrm{LC50} < 100\ \frac{\mathrm{mg}}{l}$
Category Acute 4	$100\ \frac{\mathrm{mg}}{l} \leq \mathrm{LC50}$

S 1.4 Environmental impact

The environmental impact can be considered by additional constraints on the global warming potential (GWP) and ozone depletion potential (ODP) of the molecules. For this purpose, first-order GC approaches of Hukkerikar *et al.*[7] can be used to predict both environmental properties by:

$$\log(GWP) = \sum_{i \in I} n_i \cdot GWP_i \tag{S.6}$$

and

$$\log(ODP) = \sum_{i \in I} n_i \cdot ODP_i, \tag{S.7}$$

where GWP_i and ODP_i are the group contributions of group i. The GWP is limited to $GWP < 150$ based on the decision of the European union to phase down the utilization of high GWP refrigerants in vehicles[8] and the ODP is limited to $ODP = 0$.

S 2. Thermodynamic process model

In this work, an ORC process is considered to demonstrate the applicability of the integrated thermo-economic design using 1-stage CoMT-CAMD. The degrees of freedom of the process are the mass flow rate of the working fluid $\dot{m}_{\mathrm{wf}}$, the reduced operating pressure levels of the condenser $p_{\mathrm{cond}}^{\mathrm{red}}$ and the evaporator $p_{\mathrm{evap}}^{\mathrm{red}}$ and the degree of superheating at turbine inlet ΔT_{sh}. The molecule is described by its pure component parameters of PC-SAFT z and the molecular structure y^{S}.

The net power output of the process is calculated as (indices corresponding to Figure 5):

$$P_{\mathrm{net}} = \eta_{\mathrm{G}} \cdot (P_{\mathrm{T}} - P_{\mathrm{P}}) = \eta_{\mathrm{G}} \cdot \dot{m}_{\mathrm{wf}} \cdot ((h_3 - h_4) - (h_2 - h_1)). \qquad (\mathrm{S.8})$$

The enthalpy drop in the turbine $(h_3 - h_4)$ is calculated based on an isotropic expansion (3 → 4s) and the constant isentropic efficiency of the turbine $\eta_{\mathrm{T,is}}$:

$$h_3 - h_4 = \eta_{\mathrm{T,is}} \cdot (h_3 - h_{4\mathrm{s}}), \qquad (\mathrm{S.9})$$

and the enthalpy increase in the pump $(h_2 - h_1)$ based on an isentropic compression (1 → 2s) and the constant isentropic efficiency of the pump $\eta_{\mathrm{P,is}}$:

$$h_2 - h_1 = \eta_{\mathrm{P,is}}^{-1} \cdot (h_{2\mathrm{s}} - h_1). \qquad (\mathrm{S.10})$$

The enthalpies at the states 1, 2s, 3 and 4s are calculated using the PC-SAFT equation of state as

$$h_1 = \mathrm{h}'(p_{\mathrm{cond}}, z, y^S), \qquad (\mathrm{S.11})$$

$$h_{2\mathrm{s}} = \mathrm{h}\left(p_{\mathrm{evap}}, s_1, z, y^S\right), \qquad (\mathrm{S.12})$$

$$h_3 = \mathrm{h}\left(p_{\mathrm{evap}}, T_3, z, y^S\right), \qquad (\mathrm{S.13})$$

$$h_{4\mathrm{s}} = \mathrm{h}(p_{\mathrm{cond}}, s_3, z, y^S), \qquad (\mathrm{S.14})$$

and

$$s_1 = \mathrm{s}'(p_{\mathrm{cond}}, z, y^S), \qquad (\mathrm{S.15})$$

$$s_3 = \mathrm{s}\left(p_{\mathrm{evap}}, T_3, z, y^S\right), \tag{S.16}$$

$$T_3 = \mathrm{T}^{\mathrm{sat}}\left(p_{\mathrm{evap}}, z\right) + \Delta T_{\mathrm{sh}}. \tag{S.17}$$

Here, upright letters are used for PC-SAFT functions for vapor/liquid enthalpies $\mathrm{h}(p, T, z, y^S)$ and $\mathrm{h}(p, s, z, y^S)$, saturation temperature $\mathrm{T}^{\mathrm{sat}}(p, z)$ and entropy $\mathrm{s}(p, T, z, y^S)$, whereas italic letters denote properties in the process. The functions $\mathrm{h}'(p, z, y^S)/\mathrm{s}'(p, z, y^S)$ calculate properties at the boiling point. In general, the residual PC-SAFT model calculates molar properties and depends on the pure component parameters z which are here computed from the molecular structure y^{S} by a group-contribution model. The molecular structure y^{S} is also used directly to calculate absolute, specific properties based on the molar mass and Joback's GC approach for the heat capacity of the ideal gas.

The heat flows in the preheater $\dot{Q}_{\mathrm{pre}}$, evaporator $\dot{Q}_{\mathrm{evap}}$ and condenser $\dot{Q}_{\mathrm{cond}}$ are calculated based on energy balances around the heat exchangers as:

$$\dot{Q}_{\mathrm{pre}} = \dot{m}_{\mathrm{wf}} \cdot (h_{2'} - h_2), \tag{S.18}$$

$$\dot{Q}_{\mathrm{evap}} = \dot{m}_{\mathrm{wf}} \cdot (h_3 - h_{2'}), \tag{S.19}$$

$$\dot{Q}_{\mathrm{cond}} = \dot{m}_{\mathrm{wf}} \cdot (h_4 - h_1), \tag{S.20}$$

with

$$h_{2'} = \mathrm{h}'\left(p_{\mathrm{evap}}, z, y^S\right). \tag{S.21}$$

The temperatures of the heat source (HS) and cooling water (CW) are calculated based on the corresponding mass flowrates $\dot{m}_{\mathrm{HS}}/\dot{m}_{\mathrm{CW}}$ and heat capacities $c_{\mathrm{p,HS}}/c_{\mathrm{p,CW}}$ as:

$$T_{\mathrm{HS}}^{\mathrm{out}} = T_{\mathrm{HS}}^{\mathrm{in}} - \frac{\dot{Q}_{\mathrm{pre}} + \dot{Q}_{\mathrm{evap}}}{\dot{m}_{\mathrm{HS}} \cdot c_{\mathrm{p,HS}}}, \tag{S.22}$$

$$T_{\mathrm{HS}}' = T_{\mathrm{HS}}^{\mathrm{in}} - \frac{\dot{Q}_{\mathrm{evap}}}{\dot{m}_{\mathrm{HS}} \cdot c_{\mathrm{p,HS}}}, \tag{S.23}$$

$$T_{\mathrm{CW}}^{\mathrm{out}} = T_{\mathrm{CW}}^{\mathrm{in}} + \frac{\dot{Q}_{\mathrm{cond}}}{\dot{m}_{\mathrm{CW}} \cdot c_{\mathrm{p,CW}}} \tag{S.24}$$

$$T_{\mathrm{CW}}'' = T_{\mathrm{CW}}^{\mathrm{in}} + \frac{\dot{m}_{\mathrm{wf}} \cdot (h_{4''} - h_1)}{\dot{m}_{\mathrm{CW}} \cdot c_{\mathrm{p,CW}}} \tag{S.25}$$

with

$$h_{4''} = \mathrm{h}''(p_{\mathrm{cond}}, z, y^S). \tag{S.26}$$

Here, the function h'' calculates the enthalpy at the dew point. The remaining temperatures of the process are calculated with PC-SAFT functions for vapor/liquid temperatures $\mathrm{T}(p, h, z, y^S)$ and saturation temperatures $\mathrm{T}^{\mathrm{sat}}(p, z)$ as:

$$T_1 = \mathrm{T}^{\mathrm{sat}}(p_{\mathrm{cond}}, z) \tag{S.27}$$

$$T_2 = \mathrm{T}(p_{\mathrm{evap}}, h_2, z, y^S), \tag{S.28}$$

$$T_{2'} = \mathrm{T}^{\mathrm{sat}}(p_{\mathrm{evap}}, z), \tag{S.29}$$

$$T_4 = \mathrm{T}(p_{\mathrm{cond}}, h_4, z, y^S), \tag{S.30}$$

$$T_{4''} = \mathrm{T}^{\mathrm{sat}}(p_{\mathrm{cond}}, z) \tag{S.31}$$

S 3. Modelling heat transfer

To ensure feasible heat transfer, the minimal approach temperature in the different heat exchangers is constrained to be positive (indices corresponding to Figure 5):

$$\begin{gathered} T_2 - T_{\mathrm{HS}}^{\mathrm{out}} \leq 0 \\ T_{2'} - T'_{\mathrm{HS}} \leq 0 \\ T_3 - T_{\mathrm{HS}}^{\mathrm{in}} \leq 0 \\ T_{\mathrm{CW}}^{\mathrm{out}} - T_4 \leq 0 \\ T''_{\mathrm{CW}} - T_{4''} \leq 0 \end{gathered} \tag{S.32}$$

S 3.1 Heat transfer by single-phase, forced convection

For heat transfer of single-phase, forced convection is assumed. This heat transfer type occurs for the heating and cooling medium as well as for the working fluid in the preheater and during the superheating. In this case, the heat transfer coefficient α is calculated using the general Nusselt-correlation[9]:

$$\alpha = \frac{\mathrm{Nu} \cdot \lambda}{\mathcal{L}}, \tag{S.33}$$

where Nu denotes the Nusselt-Number, λ the thermal conductivity of the fluid and $\mathcal{L}$ the characteristic length. In general, the heat transfer in ORCs proceeds in turbulent flow conditions, since turbulent flow improves the heat transfer significantly. Thus, the Nusselt-correlation of Gnielinski[10] is used:

$$\mathrm{Nu_{sp}} = \frac{\mathrm{Re}\cdot\mathrm{Pr}\cdot\frac{\zeta}{8}}{1+12.7\cdot\sqrt{\frac{\zeta}{8}}\cdot\left(Pr^{\frac{2}{3}}-1\right)}\cdot\left(1+\left(\frac{\mathcal{L}}{L_{\mathrm{HE}}}\right)^{\frac{2}{3}}\right), \tag{S.34}$$

with

$$\zeta = (1.8\cdot log_{10}(\mathrm{Re})-1.5)^{-2}, \tag{S.35}$$

$$\mathrm{Re} = \frac{\rho\cdot c\cdot\mathcal{L}}{\eta} \tag{S.36}$$

and

$$\mathrm{Pr} = \frac{\eta\cdot c_{\mathrm{p}}}{\lambda}, \tag{S.37}$$

where L_{HE} denotes the length of the heat exchanger, ρ the density, c the velocity and c_{p} the heat capacity of the fluid. All fluid properties are calculated at arithmetical mean temperatures. The characteristic length $\mathcal{L}$ is defined as: [9]

$$\mathcal{L} = \begin{cases} d_{\mathrm{i}} & \text{on tube side} \\ d_{\mathrm{h}} & \text{on shell side} \end{cases} \tag{S.38}$$

with

$$d_{\mathrm{h}} = \frac{4\cdot A_{\mathrm{shell}}}{U_{\mathrm{R}}} \tag{S.39}$$

where A_{shell} denotes the passed through area of the shell and U_{R} the overall pipe circumference. Since the length of the heat exchanger is not known initially, it is assumed that $L_{\mathrm{HE}} \gg \mathcal{L}$ to prevent an iterative calculation of the heat exchanger area.

S 3.2 Heat transfer by evaporation

On the shell side of the evaporator, flow boiling heat transfer occurs. Gungor and Winterton[11] give the heat transfer coefficient for flow boiling α_{fb} as a superposition of forced convection and bulk boiling defined by:

$$\alpha_{\mathrm{fb}} = E \cdot \alpha_{\mathrm{fc}} + S \cdot \alpha_{\mathrm{bb}} \tag{S.40}$$

In the work of Gungor and Winterton[11], the heat coefficient for forced convection α_{fc} is calculated based on Dittus and Boelter[12] as:

$$\alpha_{\mathrm{fc}} = 0.023 \cdot \mathrm{Re}_{\mathrm{l}}^{0.8} \cdot \mathrm{Pr}_{\mathrm{l}}^{0.4} \cdot \frac{\lambda_{\mathrm{l}}}{d_{\mathrm{h}}} \tag{S.41}$$

with

$$\mathrm{Re}_{\mathrm{l}} = \frac{\dot{m}_{\mathrm{wf}} \cdot (1-\varphi) \cdot d_{\mathrm{h}}}{A_{\mathrm{shell}} \cdot \eta_{\mathrm{l}}} \tag{S.42}$$

where φ denotes the steam quality and the index l the liquid phase. The heat transfer coefficient for bulk boiling α_{bb} is calculated based on Cooper[13] as:

$$\alpha_{\mathrm{bb}} = 55 \cdot \left(p^{\mathrm{red}}\right)^{0.12} \cdot \left(-log_{10}\left(p^{\mathrm{red}}\right)\right)^{-0.55} \cdot M^{-0.5} \cdot \left(\frac{\dot{Q}}{A_{\mathrm{HE}}}\right)^{0.67}, \tag{S.43}$$

where $\dot{Q}$ denotes the transferred heat flow. Since the heat transfer coefficient for bulk boiling depends on the heat exchanger area A_{HE}, an iterative calculation of the heat exchanger area of the evaporator is required.

In Equation (S.40), the forced convection term is multiplied by an enhancement factor E defined by:

$$E = 1 + 24{,}000 \cdot \mathrm{Bo}^{1.16} + 1.37 \cdot \frac{1}{X_{\mathrm{tt}}^{0.86}} \tag{S.44}$$

and the bulk boiling term by a suppression factor S defined by:

$$S = \frac{1}{1 + 1.15 \cdot 10^{-6} \cdot E^{2} \cdot \mathrm{Re}_{\mathrm{l}}^{1.17}}, \tag{S.45}$$

which consider the influence of the steam quality φ on the heat transfer. Herein, the Boiling number Bo is calculated as:

$$\mathrm{Bo} = \frac{\dot{Q}}{\dot{m}_{\mathrm{wf}} \cdot \Delta h_{\mathrm{evap}}\left(p_{\mathrm{evap}}\right)} \tag{S.46}$$

and the Martinelli parameter X_{tt} as:

$$X_{\mathrm{tt}} = \left(\frac{1-\varphi}{\varphi}\right)^{0.9} \cdot \left(\frac{\rho_{\mathrm{v}}}{\rho_{\mathrm{l}}}\right)^{0.5} \cdot \left(\frac{\eta_{\mathrm{l}}}{\eta_{\mathrm{v}}}\right)^{0.1}, \tag{S.47}$$

where $\Delta h_{\mathrm{evap}}(p_{\mathrm{evap}})$ denotes the enthalpy of evaporation at p_{evap} and the index v the vapor phase. The heat transfer coefficient for flow boiling α_{fb} thus represents the local heat transfer for a given steam quality φ. Therefore, the evaporation is divided into 10 equal intervals of steam quality $\Delta\varphi$. For each interval j, the needed heat exchanger area A_{j} is individually calculated for a constant mean steam quality $\bar{\varphi}_{\mathrm{j}}$. To obtain the whole evaporation surface, the individual heat exchanger areas A_{j} are summarized. The division into 10 intervals serves as a compromise between accuracy and computational effort.

S 3.3 Heat transfer by condensation

On the shell side of the condenser, filmwise condensation of pure vapors occurs with a concurrent flow of gaseous and liquid phases. Here, the condensation film shows a laminar sublayer near the tube and turbulences in the boundary layer near the vapor.[9] The heat transfer coefficient α of the condensation can be calculated using Equation (S.33) and the Nusselt-number for filmwise condensation $\mathrm{Nu}_{\mathrm{fc}}$ calculated as:

$$\mathrm{Nu}_{fc} = \sqrt{\left(K_{\mathrm{ph,l}} \cdot K_{\mathrm{W}} \cdot \mathrm{Nu}_{\mathrm{F,\varphi,l}}\right)^2 + \left(K_{\mathrm{ph,t}} \cdot K_{\mathrm{W}} \cdot \mathrm{Nu}_{\mathrm{F,\varphi,t}}\right)^2}, \tag{S.48}$$

combining the laminar Nusselt-number $\mathrm{Nu}_{\mathrm{F,\varphi,l}}$ and the turbulent Nusselt-number $\mathrm{Nu}_{\mathrm{F,\varphi,t}}$ of the condensation film without vapour flow.[9] The following assumptions are made:[9]

- The correction for temperature-depending properties is neglected.
- The density of the liquid phase is much higher than the density of the vapor phase and thus $1 - \frac{\rho_{\mathrm{v}}}{\rho_{\mathrm{l}}} \approx 1$.
- The condensation film thickness δ_{F}^{+} is much smaller than the outer diameter of the tubes d_{o}.
- The relative velocity between the condensation film and the vapor corresponds to the absolute velocity of the vapor.
- Wall normal mass flows are neglected.

Thereby, the laminar Nusselt-number $\mathrm{Nu}_{\mathrm{F,\varphi,l}}$ of the condensation film is calculated by:

$$\mathrm{Nu}_{\mathrm{F,\varphi,l}} = 0.693 \cdot \mathrm{Re}_{\mathrm{CF}}^{-0.29} \tag{S.49}$$

with

$$\mathrm{Re}_{\mathrm{CF}} = \frac{(1-\varphi)\cdot \dot{m}_{\mathrm{wf}}}{n_{\mathrm{tubes}}\cdot \pi \cdot d_{\mathrm{o}} \cdot \eta_{\mathrm{l}}}. \qquad (\mathrm{S.50})$$

The turbulent Nusselt-number $\mathrm{Nu}_{\mathrm{F},\varphi,\mathrm{t}}$ of the condensation film is calculated by:

$$\mathrm{Nu}_{\mathrm{F},\varphi,\mathrm{t}} = \frac{0.0283\cdot \mathrm{Re}_{\mathrm{CF}}^{0.292}\cdot \mathrm{Pr}_{\mathrm{l}}^{0.333}}{1+9.66\cdot \mathrm{Re}_{\mathrm{CF}}^{-0.375}\cdot \mathrm{Pr}_{\mathrm{l}}^{-0.167}}. \qquad (\mathrm{S.51})$$

Since high vapor velocities can occur, the interaction between the condensation film and the vapor is considered in a correction factor K_{W}:

$$K_{\mathrm{W}} = (1+\tau_{\mathrm{v}}^{*})^{\frac{1}{3}} \qquad (\mathrm{S.52})$$

This correction factor considers the shear stress acting on the condensate film. The correction factor $K_{\mathrm{ph,l}}$ and $K_{\mathrm{ph,t}}$ regards the difference between the influence of the shear stress for laminar and turbulent conditions respectively and are calculated as:

$$K_{\mathrm{ph,l}} = 1 + (\mathrm{Pr}_{\mathrm{l}}^{0.56}-1)\cdot \tanh(\tau_{\mathrm{v}}^{*}) \qquad (\mathrm{S.53})$$

and

$$K_{\mathrm{ph,t}} = 1 + (\mathrm{Pr}_{\mathrm{l}}^{0.08}-1)\cdot \tanh(\tau_{\mathrm{v}}^{*}). \qquad (\mathrm{S.54})$$

The dimensionless shear stress τ_{v}^{*} is iteratively calculated depending on the dimensionless shear stress of a hydraulically smooth tube $\tau_{\mathrm{v,g}}^{*}$ and the flow parameter F by:

$$\begin{aligned} \tau_{\mathrm{v}}^{*} &= \tau_{\mathrm{v,g}}^{*}\cdot\left(1+550\cdot F\cdot {\tau_{\mathrm{v}}^{*}}^{0.3}\right) &&\text{for}\quad \tau_{\mathrm{v}}^{*}>1 \\ \tau_{\mathrm{v}}^{*} &= \tau_{\mathrm{v,g}}^{*}\cdot\left(1+550\cdot F\cdot {\tau_{\mathrm{v}}^{*}}^{0.85}\right) &&\text{for}\quad \tau_{\mathrm{v}}^{*}\le 1 \end{aligned} \qquad (\mathrm{S.55})$$

with

$$\tau_{\mathrm{v,g}}^{*} = \frac{\tau_{\mathrm{v,g}}}{\rho_{\mathrm{l}}\cdot g\cdot \delta_{\mathrm{F}}^{+}}, \qquad (\mathrm{S.56})$$

$$\delta_{\mathrm{F}}^{+} = \frac{6.59\cdot F\cdot d_{\mathrm{o}}}{\sqrt{1+1400\cdot F}}, \qquad (\mathrm{S.57})$$

$$F = \frac{max\left[(2\cdot \mathrm{Re}_{\mathrm{CF}})^{0.5}; 0.132\cdot \mathrm{Re}_{\mathrm{CF}}^{0.9}\right]}{\mathrm{Re}_{\mathrm{v}}^{0.9}}\cdot\frac{\eta_{\mathrm{l}}}{\eta_{\mathrm{v}}}\cdot\sqrt{\frac{\rho_{\mathrm{v}}}{\rho_{\mathrm{l}}}}, \qquad (\mathrm{S.58})$$

$$\tau_{\mathrm{v,g}} = \frac{\xi_{\mathrm{g}}}{8}\cdot \rho_{\mathrm{v}}\cdot \bar{c}_{\mathrm{v}}^{2}, \qquad (\mathrm{S.59})$$

$$\xi_{\mathrm{g}} = 0.184 \cdot \mathrm{Re}_{\mathrm{v}}^{2}, \tag{S.60}$$

$$\bar{c}_{\mathrm{v}} = \frac{\dot{m}_{\mathrm{wf}} \cdot \varphi}{A_{\mathrm{shell}} \cdot \rho_{\mathrm{v}}}, \tag{S.61}$$

$$\mathrm{Re}_{\mathrm{v}} = \frac{\dot{m}_{\mathrm{wf}} \cdot \varphi \cdot d_{\mathrm{h}}}{A_{\mathrm{shell}} \cdot \eta_{\mathrm{v}}}, \tag{S.62}$$

where g denotes the gravity. The characteristic length in Equation (S.33) is defined as:

$$\mathcal{L} = \left(\frac{\eta_{\mathrm{l}}^{2}}{\rho_{\mathrm{l}}^{2} \cdot g}\right)^{\frac{1}{3}}. \tag{S.63}$$

The Nusselt-numbers and correction factors depend on the steam quality φ and, thus, describe the local behavior of the condensation heat transfer. Therefore, the condensation is also divided into 10 intervals of equal steam quality $\Delta\varphi$ and the needed heat exchanger area A_{j} of interval j is calculated individually for a constant mean steam quality $\bar{\varphi}_{\mathrm{j}}$. The heat exchanger area of the condensation A_{cond} is obtained by a summarization of all individual heat exchanger area A_{j}. If the vapor is superheated after the turbine, the whole heat exchanger area of the condenser $A_{\mathrm{cond,sup}}$ is extrapolated from the heat exchanger area of the sole condensation A_{cond} by:

$$A_{\mathrm{cond,sup}} = A_{\mathrm{cond}} \cdot \frac{h_4 - h_1}{\Delta h_{\mathrm{evap}}(p_{\mathrm{cond}})}, \tag{S.64}$$

where $\Delta h_{\mathrm{evap}}(p_{\mathrm{cond}})$ denotes the enthalpy of evaporation at p_{cond}.[9]

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