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FACULTY OF ENGINEERING AND ARCHITECTURE

Development of a 1D simulation model for a steam cracker convection section

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Steam cracking

Crude oil

Natural gas

Bio-based feeds

Naphtha

Light gasoil

crude oil

Natural gas liquids

Gas-condensates

Hydrode-oxygenated FAME

Steam cracking

Ethene

Propene

Butadiene

Aromatics

Consumer goods from chemical industry

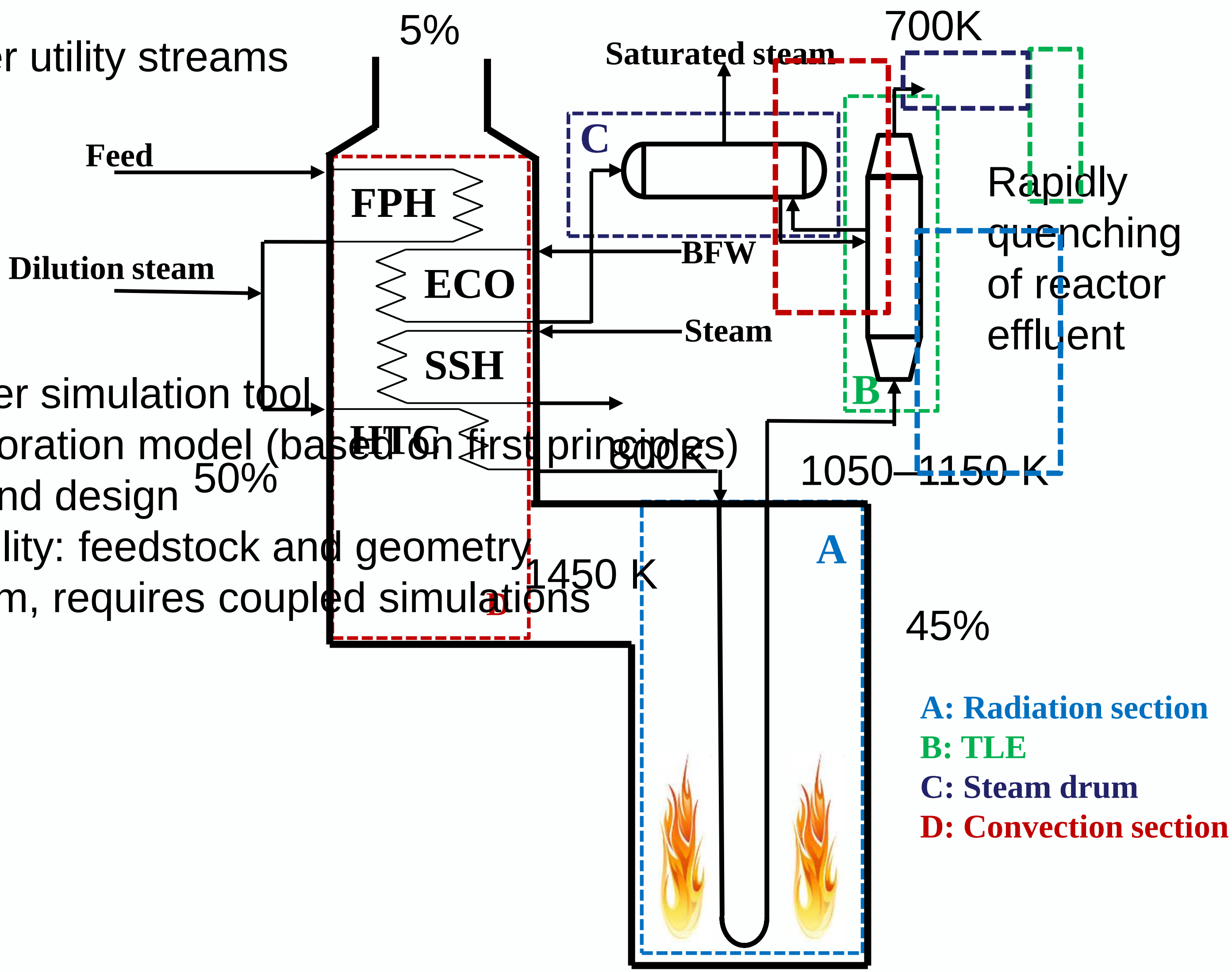
atozforex.com; pnnl.org; districtenergy.org; scade.fr; schmidt-clemens.de; Linde Group

Steam cracking

Preheat feed and other utility streams

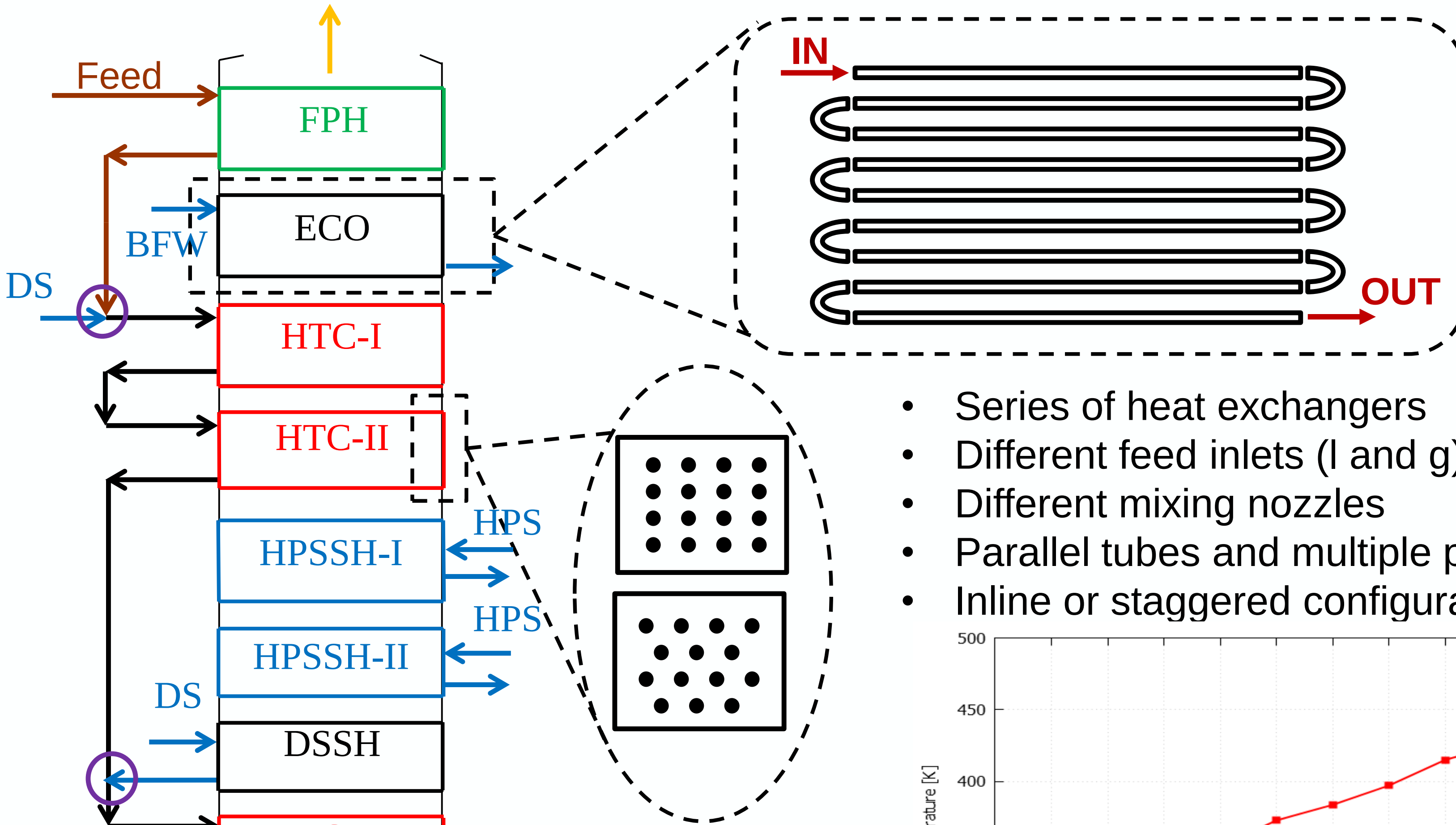
CONVEC-1D

- 1D heat transfer simulation tool
- Accurate evaporation model (based on first principles)
- Optimization and design
- Extreme flexibility: feedstock and geometry
- Coupled system, requires coupled simulations

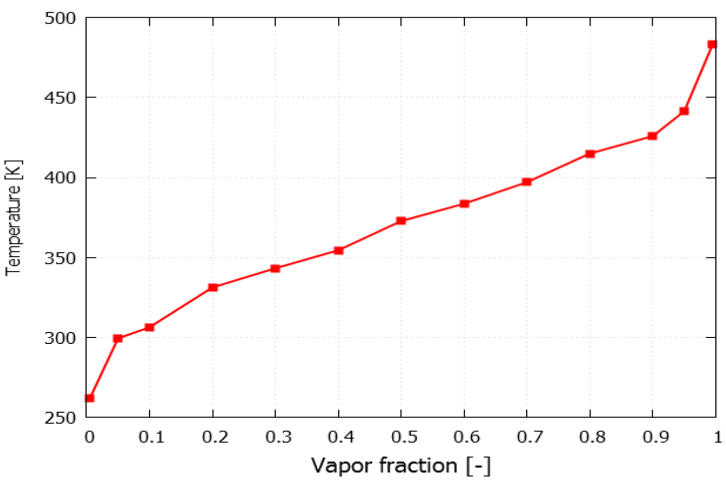


Endothermic process 1050–1150 K

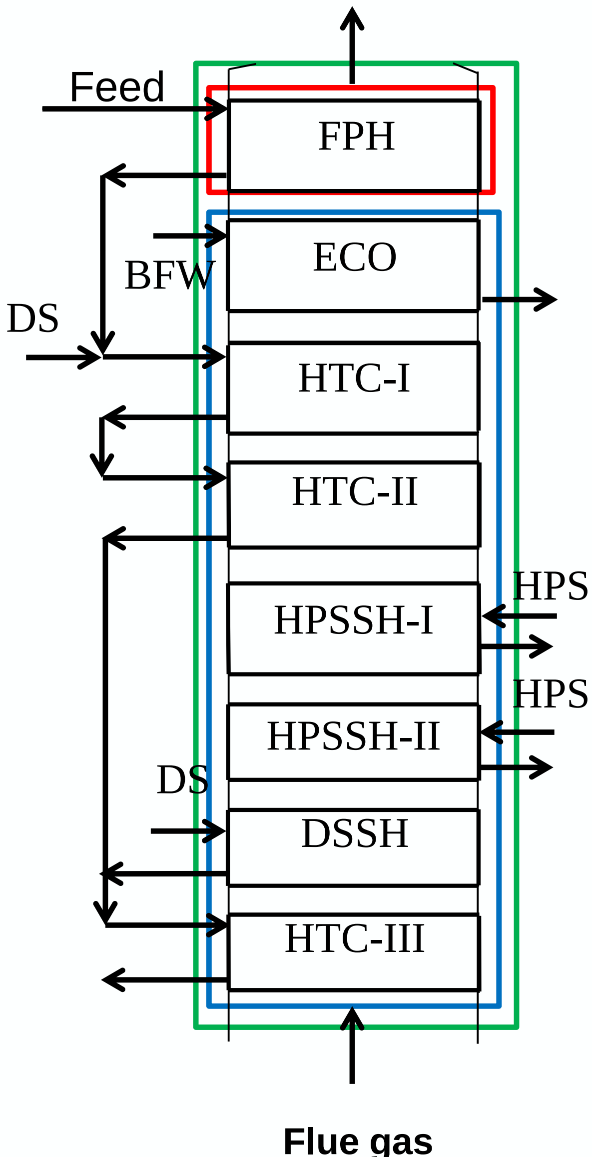
Convection section



- Series of heat exchangers
- Different feed inlets (l and g)
- Different mixing nozzles
- Parallel tubes and multiple passes
- Inline or staggered configuration



Convection section



Heat transfer mechanisms

Single phase

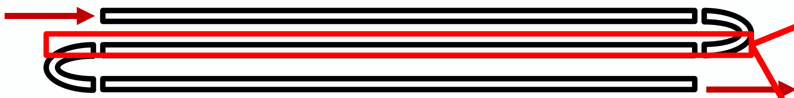
- Convective flow over horizontal tube bank (Flue gas)
- Forced convection (all banks except FPH)

Two phase

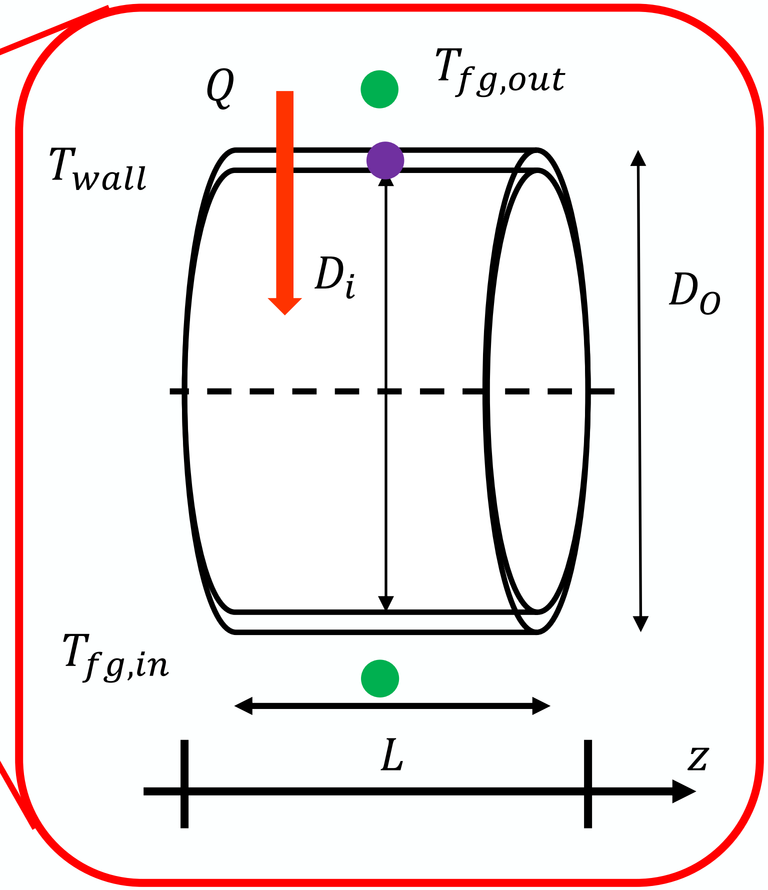
- Flow boiling (FPH)
  - Empirical model
  - Mechanistic model

Numerical model: Flue gas side

Valid for all banks



One tube row



$$Q = h_{fg}\, \omega \frac{(T_{fg,out} - T_{fg,in})}{ln\left(\frac{T_{wall} - T_{fg,in}}{T_{wall} - T_{fg,out}}\right)}$$

Convective flow over horizontal tube bank

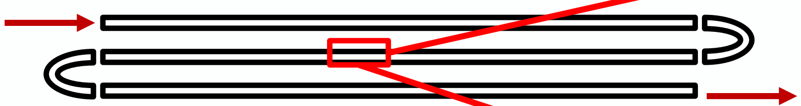
Energy balance for the flue gas side

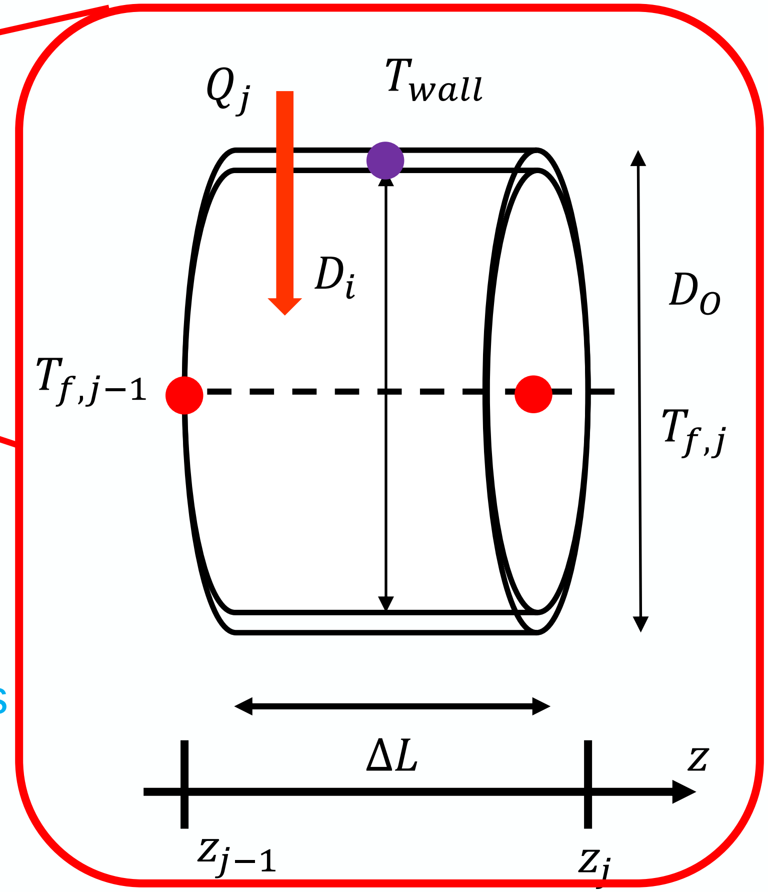
$$Q = \dot{m}_{fg}\, c_p\, (T_{fg,out} - T_{fg,in})$$

Numerical model: Process side

Infinitesimal small increment

Valid for all tube rows





$$Q_j = \alpha\, \omega\, \Delta L\, (T_{wall} - T_{f,j})$$

$$\frac{1}{\alpha} = \left(\frac{1}{h} + \frac{D_i \ln(\frac{D_O}{D_i})}{2\kappa}\right)$$

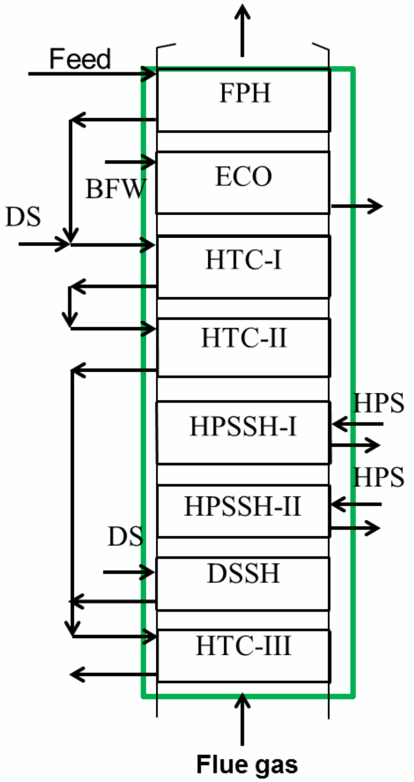
Correlations for different heat transfer mechanisms

Energy balance at process side

$$Q_j = \begin{cases} \dot{m}_{total}\, c_{p,mix}(T_{f,j} - T_{f,j-1}) \\ \Delta\dot{m}_l\, \Delta H_{latent} \end{cases}$$

Important to be computed accurately !

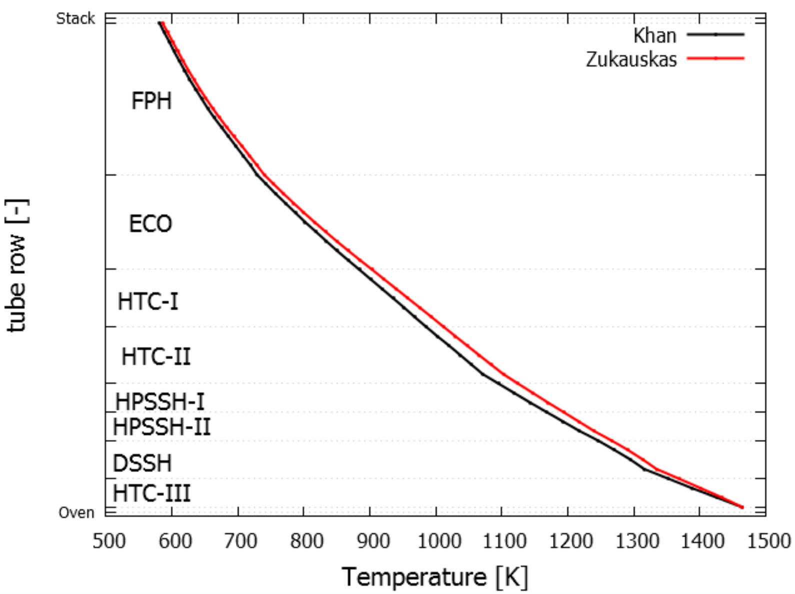
Convective flow over horizontal tube bank



Convective flow over horizontal tube bank

- Empirical model: Zukauskas[1]
- Analytical model: Khan et al.[2]

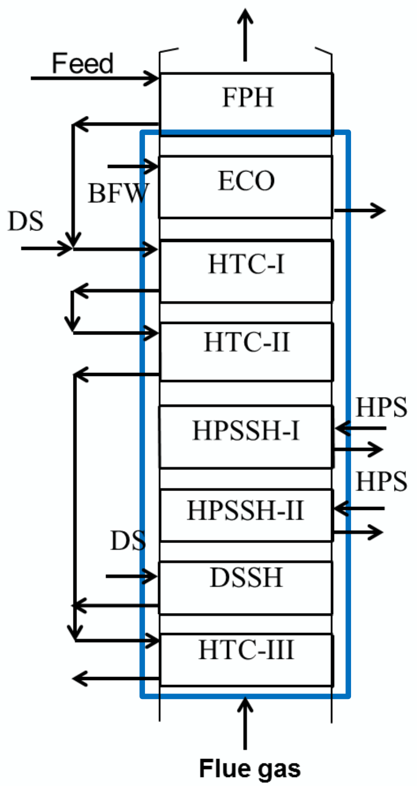
Imposed fixed T_{wall} profile



Both models performs equally well

1. A. Zukauskas, in *Adv. Heat Transfer*, **1972**.
2. W. A. Khan, J. R. Culham, M. M. Yovanovich, *International Journal of Heat and Mass Transfer* **2006,** *49 (25–26)*, 4831-4838. DOI: 10.1016/j.ijheatmasstransfer.2006.05.042.

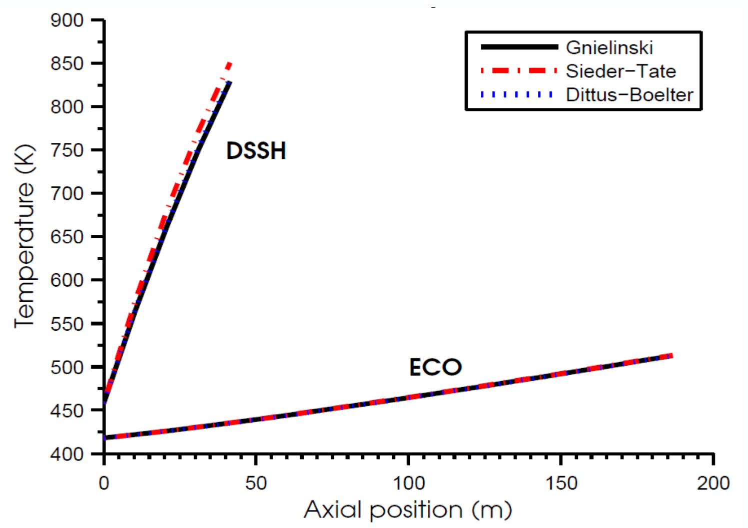
Single phase forced convection



Single phase forced convection

- Dittus-Boelter[1]
- Sieder-Tate[2]
- Gnielinski[3]

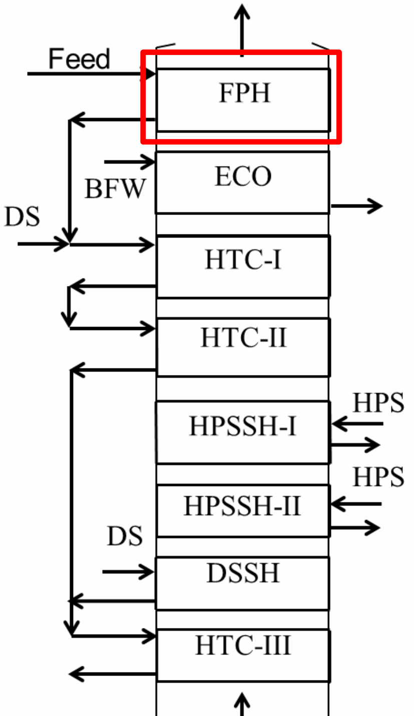
Imposed fixed T_{wall} profile



Simulation results hardly differ when applied correlation changes

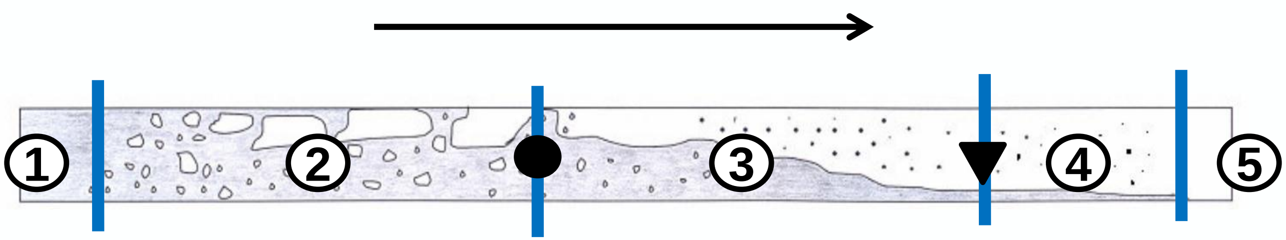
1. F. W. Dittus, L. M. K. Boelter, *University of California Publications in Engineering* **1930,** *2*, 443.
2. E. N. Sieder, G. E. Tate, *Industrial & Engineering Chemistry* **1936,** *28 (12)*, 1429-1435. DOI: 10.1021/ie50324a027.
3. V. Gnielinski, *International Journal of Chemical Engineering* **1976,** *16 (2)*, 359-368.

Two phase flow boiling: Empirical model



Two phase flow boiling

- **Empirical model**
- Mechanistic model

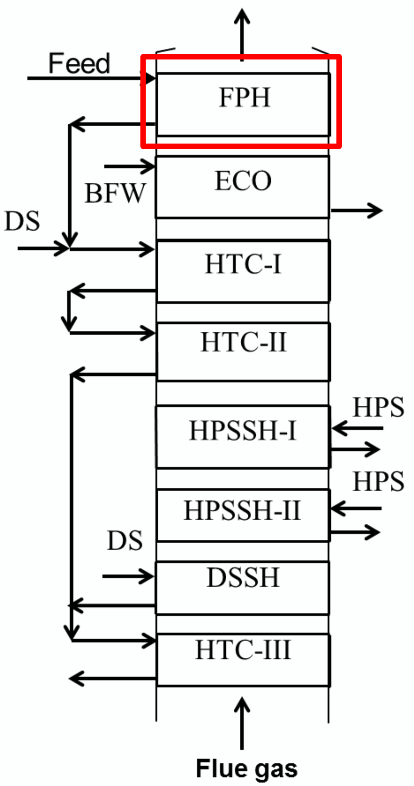


5 different flow regimes:

1. Single-phase liquid — Gnielinski[1]
2. Saturated flow boiling — Gungor-Winterton[2]
3. Partial dry-out — Interpolation between ● and ▼
4. Mist flow — Adapted Groeneveld[3]
5. Single-phase vapor — Gnielinski[1]

1. V. Gnielinski, *International Journal of Chemical Engineering* **1976,** *16 (2)*, 359-368.
2. K. E. Gungor, R. H. S. Winterton, *Chemical Engineering Research and Design* **1987,** *65 (2)*, 148-156.
3. L. Wojtan, T. Ursenbacher, J. R. Thome, *International Journal of Heat and Mass Transfer* **2005,** *48 (14)*, 2970-2985. DOI: 10.1016/j.ijheatmasstransfer.2004.12.013.
4. L. Wojtan, T. Ursenbacher, J. R. Thome, *International Journal of Heat and Mass Transfer* **2005,** *48 (14)*, 2955-2969. DOI: 10.1016/j.ijheatmasstransfer.2004.12.012.

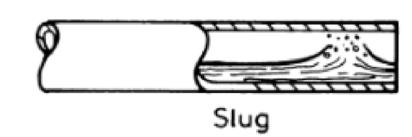
Two phase flow boiling: Mechanistic model

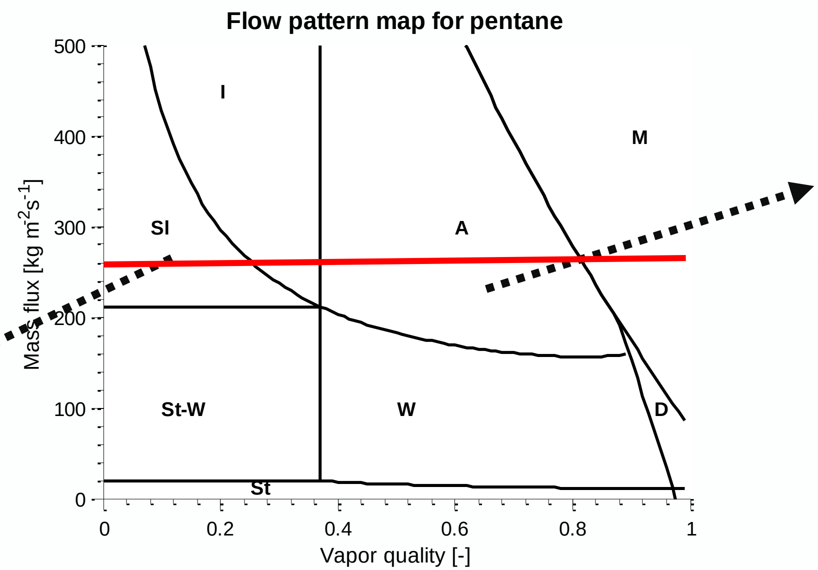


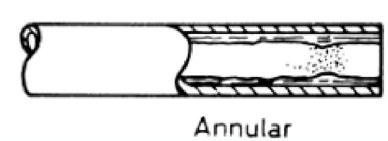
Two phase flow boiling

- Empirical model
- **Mechanistic model**

- Diabatic two-phase flow pattern map using WUT[1]
- Component specific

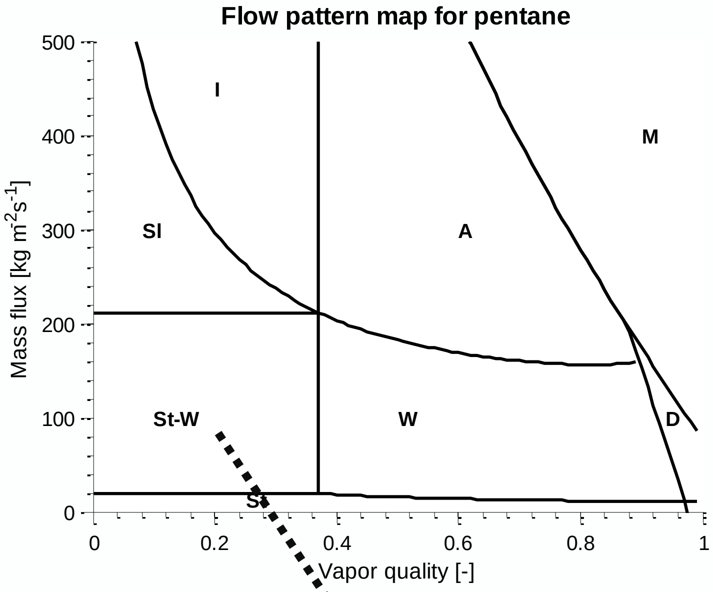




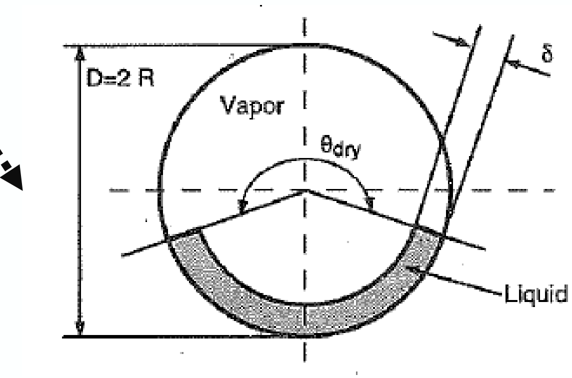


1. L. Wojtan, T. Ursenbacher, J. R. Thome, *International Journal of Heat and Mass Transfer* **2005,** *48 (14)*, 2955-2969. DOI: 10.1016/j.ijheatmasstransfer.2004.12.012.
2. N. Kattan, J. R. Thome, D. Favrat, *Journal of Heat Transfer* **1998,** *120 (1)*, 156-165. DOI: 10.1115/1.2830039.
3. S. C. De Schepper, G. J. Heynderickx, G. B. Marin, *Chemical Engineering Journal* **2008,** *138 (1)*, 349-357

Two phase flow boiling: Mechanistic model



- Stratified flow (St)
- Stratified-wavy flow (St-W)
- Slug flow (Sl)
- Intermittent flow (I)
- Annular flow (A)
- Wavy flow (W)
- Mist flow (M)
- Dryout flow (D)



Heat transfer coefficient is calculated as a function of the parameters D, δ, θ_{dry} and $\theta_{stratified}$

1. L. Wojtan, T. Ursenbacher, J. R. Thome, *International Journal of Heat and Mass Transfer* **2005,** *48 (14)*, 2955-2969. DOI: 10.1016/j.ijheatmasstransfer.2004.12.012.
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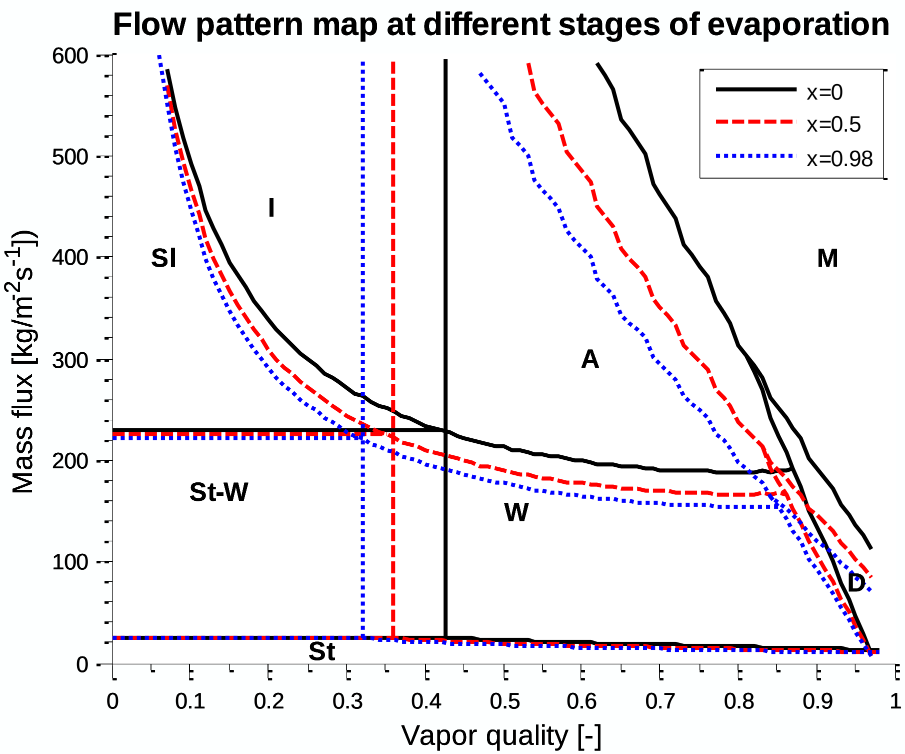
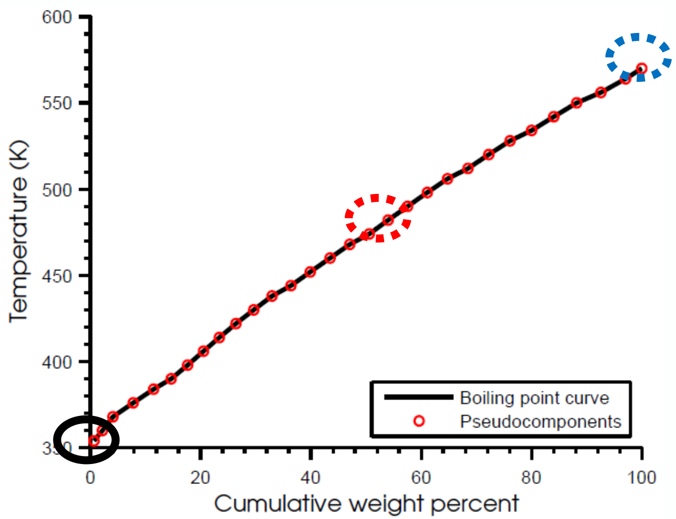
Two phase flow boiling: Mechanistic model

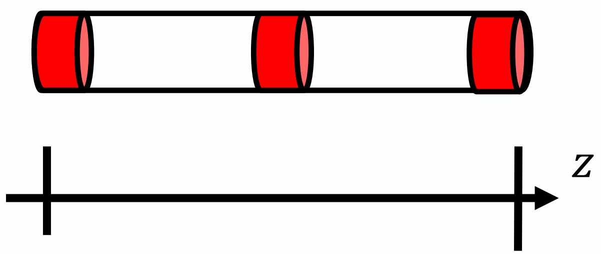
Extension to multicomponent feeds

Composition of vapor and liquid changes through the evaporation process and hence properties change affecting the flow pattern map

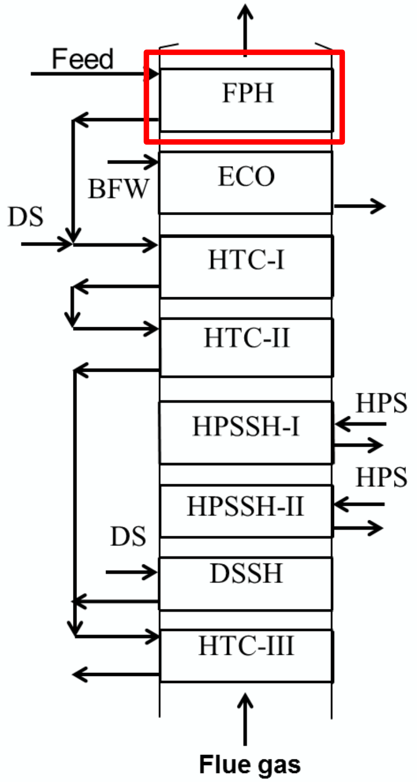
Naphtha represented by 30 pseudo components







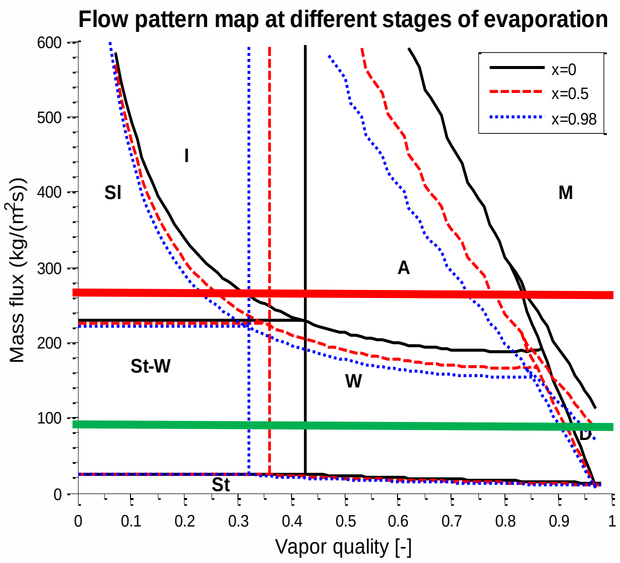
Two phase flow boiling: Model evaluation



Two phase flow boiling

- Empirical model
- Mechanistic model

Imposed fixed T_{wall} profile



Case	Naphtha G kg/(m² s)
1	250
2	100

Two different trajectories in flow pattern map

1. L. Wojtan, T. Ursenbacher, J. R. Thome, *International Journal of Heat and Mass Transfer* **2005,** *48 (14)*, 2955-2969. DOI: 10.1016/j.ijheatmasstransfer.2004.12.012.
2. N. Kattan, J. R. Thome, D. Favrat, *Journal of Heat Transfer* **1998,** *120 (1)*, 156-165. DOI: 10.1115/1.2830039.
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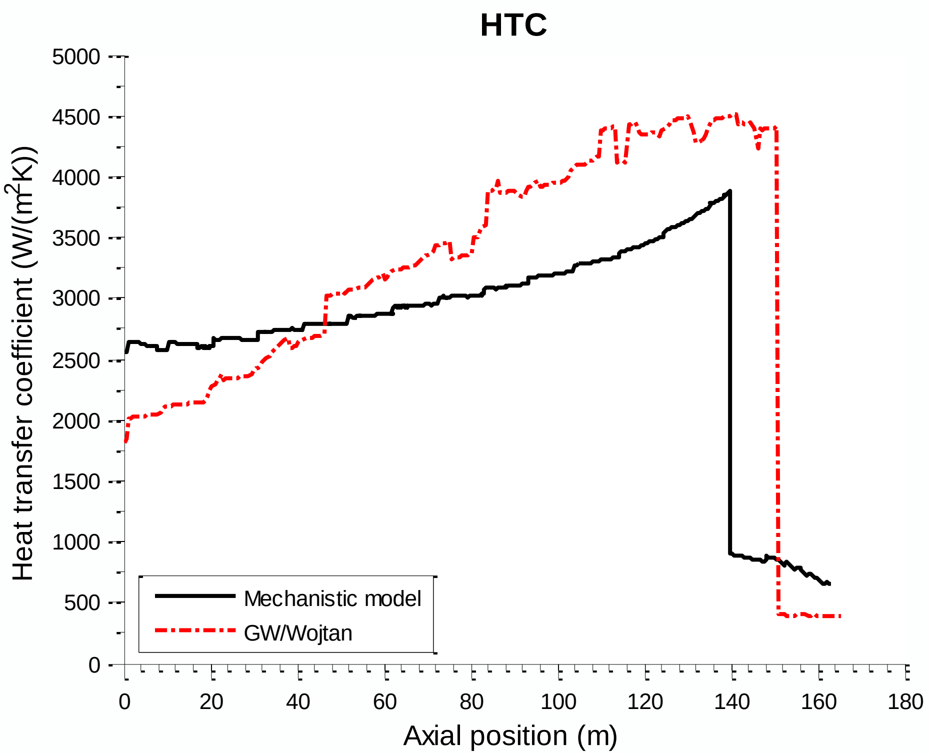
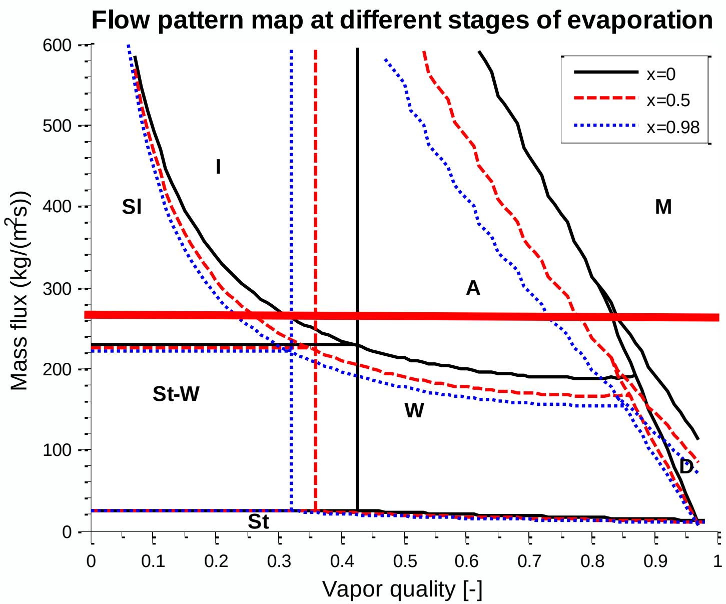
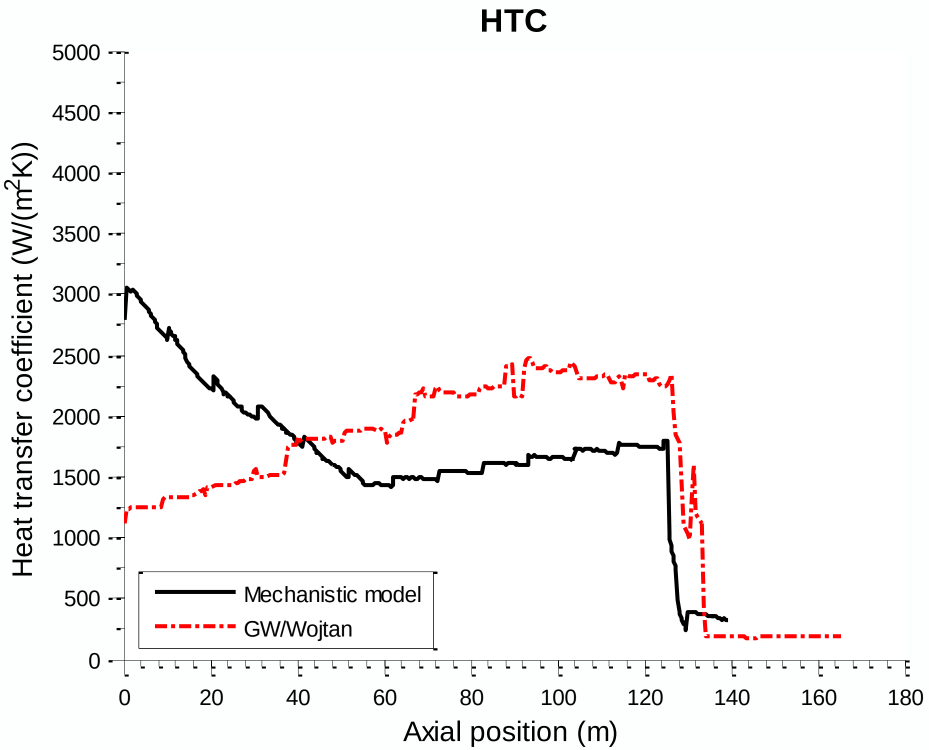
Case 1

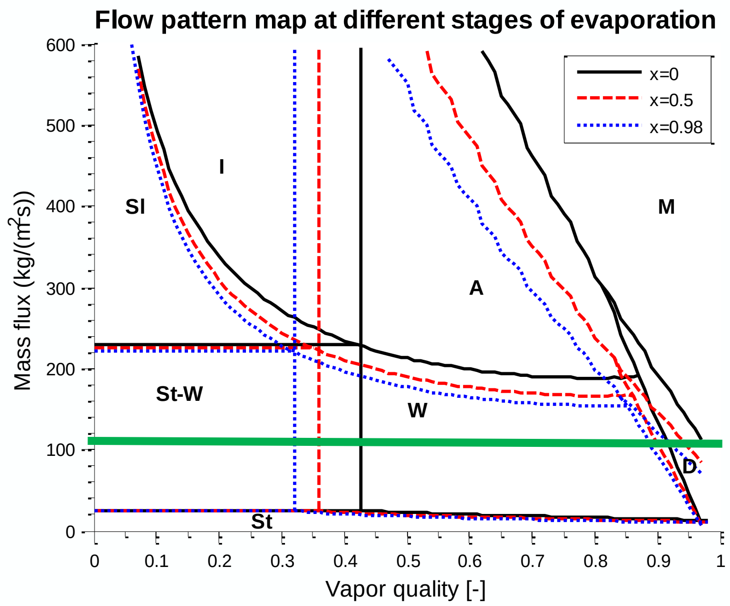




- Results correspond qualitatively
- Increasing trend until mist flow is encountered
- Shift from angular to mist at vapor quality of approximately 0.77

Case 2





- Other flow regimes are encountered compared to previous case
- Results do not correspond qualitatively
- Empirical model can not capture these flow regimes correctly
- Incomplete evaporation can lead to fouling in lower banks

Conclusions

- CONVEC-1D has been developed for complete steam cracker convection section simulation
- Flexible tool in terms of feedstock and geometry
- Accurate estimation of heat transfer coefficient is important for accurate simulations (fouling)
- Flow boiling is challenging to model and hence urging for more detailed models
  - Empirical model captures the trends for sufficient high mass fluxes for lower mass fluxes simulation results shows important discrepancies
  - Mechanistic model describes well the evaporation of HC-mixtures for broad range of conditions
  - Current commercial well-know heat transfer simulation software packages use empirical models for evaporating flow in tubes and hence urging caution when used

Acknowledgements

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