Model description

Supercritical Extraction: A process model and a sensitivity analysis

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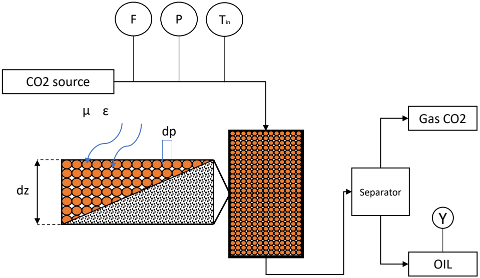

- One-dimensional model
- Plug flow
- No pressure drop
- Negligible external diffusion
- Single component
- Pseudo-homogeneous thermal properties
- Uniformly distribution of the particles

Differential model of the extractor[1]

State variables, control variables, parameters, other variables (state vars, parameters)

Fluid phase mass balance

$$\frac{\partial c(t,z)}{\partial t} = \underbrace{-\frac{1}{\epsilon A}\frac{F(t)}{\rho(T(t,z)P(t))}\frac{\partial c(t,z)}{\partial z}}_{\text{Convection}} + \underbrace{D_e^M(T(t,z)P(t))\frac{\partial^2 c(t,z)}{\partial z^2}}_{\text{Diffusion}} + \underbrace{\frac{1-\epsilon}{\epsilon} r_e(t,z)}_{\text{Kinetics}}$$

Solid phase mass balance

$$\frac{\partial q(t,z)}{\partial t} = \underbrace{r_e(t,z)}_{\text{Kinetics}}$$

Heat balance

$$\frac{\partial T(t,z)}{\partial t} = \underbrace{-\frac{F(t)}{A}\frac{C_p(T(t,z)P(t))}{[(1-\epsilon)\rho(T(t,z)P(t))C_p(T(t,z)P(t)) + \epsilon\rho_s C_{ps}]}\frac{\partial T(t,z)}{\partial z}}_{\text{Convection}} + \underbrace{D_e^T(T(t,z)P(t))\frac{\partial^2 T(t,z)}{\partial z^2}}_{\text{Diffusion}}$$

Extraction kinetics

$$r_e(t,z) = -\frac{D_i(T(t,z))}{\mu l^2}\left(q(t,z) - c(t,z)\frac{\rho_s}{k_m(T(t,z))\rho(T(t,z)P(t))}\right)$$

Measurment - Yield

$$y(t) = \frac{\sum_{i=1}^{N_z}\left(\frac{1}{N_z}(m_0 - m_i(q_i(t,z)))\right)}{m_0} = \underbrace{\frac{\sum_{i=1}^{N_z}\left(\frac{V}{N_z}(q_0 - q_i(t,z))\right)}{q_0 V}}_{g(x(t))}$$

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[1] E. Reverchon, Mathematical modeling of supercritical extraction of sage oil, AIChE J 42 (6), 1996

PDE to ODE and sensitivity analysis

Sensitivity analysis[2] measures the susceptibility of the model to changes in its parameters

$$\frac{dx(t)}{dt} = \begin{bmatrix} \frac{dc_1(t)}{dt} \\ \vdots \\ \frac{dc_{N_z}(t)}{dt} \\ \hline \frac{dq_1(t)}{dt} \\ \vdots \\ \frac{dq_{N_z}(t)}{dt} \\ \hline \frac{dT_1(t)}{dt} \\ \vdots \\ \frac{dT_{N_z}(t)}{dt} \end{bmatrix} = \underbrace{\begin{bmatrix} F_1\left(c(t), q(t), T(t); p\right) \\ \vdots \\ F_{N_z}\left(c(t), q(t), T(t); p\right) \\ \hline F_{N_z+1}\left(c(t), q(t), T(t); p\right) \\ \vdots \\ F_{2N_z}\left(c(t), q(t), T(t); p\right) \\ \hline F_{2N_z+1}\left(c(t), q(t), T(t); p\right) \\ \vdots \\ F_{3N_z}\left(c(t), q(t), T(t); p\right) \end{bmatrix}}_{F(t;p)}$$

State sensitivity

$$\begin{aligned} \dot{Z} &= \partial_t Z(t,p) = \partial_t\left(\partial_p x(t,p)\right) = \\ &= \partial_p\left(\partial_t x(t,p)\right) = \partial_p F(x(t);p) \end{aligned}$$

$$\partial_p F(x(t);p) = \underbrace{\partial_{x(t)} F(x(t);p)}_{J_x(x(t);p)} \underbrace{\partial_p x(t)}_{S(x(t);p)} + \underbrace{\partial_p F(x(t);p)}_{J_p(x(t);p)}$$

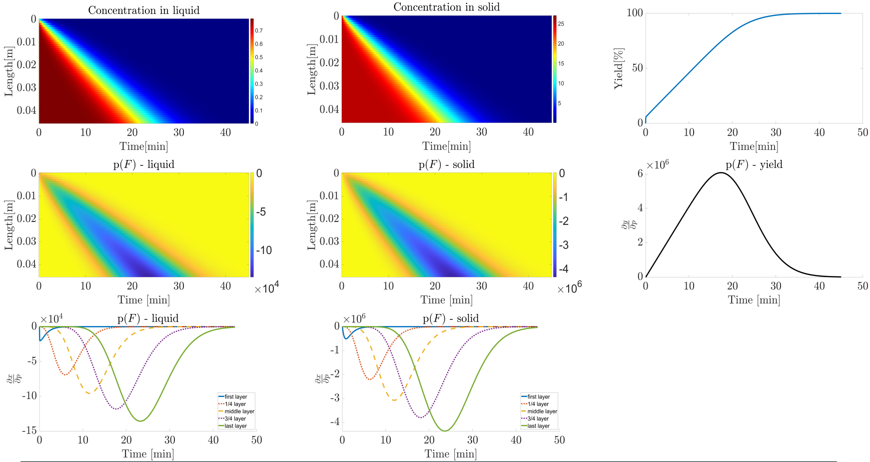
Output sensitivity

$$\frac{dy(t)}{dp} = \frac{dg(x(t))}{dp} = \partial_{x(t)} g(x(t))\ S(x(t);p)$$

[2] T. Maly, L. R. Petzold, Numerical methods and software for sensitivity analysis of differential-algebraic systems, Applied Numerical Mathematics 20 (1-2), 1996

Sensitivity analysis - flow rate

Ref	$F[kg/hr]$	$T_{Inlet}[C]$	$T_{extractor}[C]$	$P[bar]$	$c[kg/m^3]$	$q[kg/m^3]$
Vargas[3]	0.035	50	50	90	0	27



[3] R.Vargas, Supercritical extraction of carqueja essential oil: experiments and modeling, Brazilian Journal of Chemical Engineering (2006)