Aplicação de Volumes Finitos a Modelo de Vaso de Adsorção

COQ-862 - Métodos Numéricos para Sistemas Distribuídos

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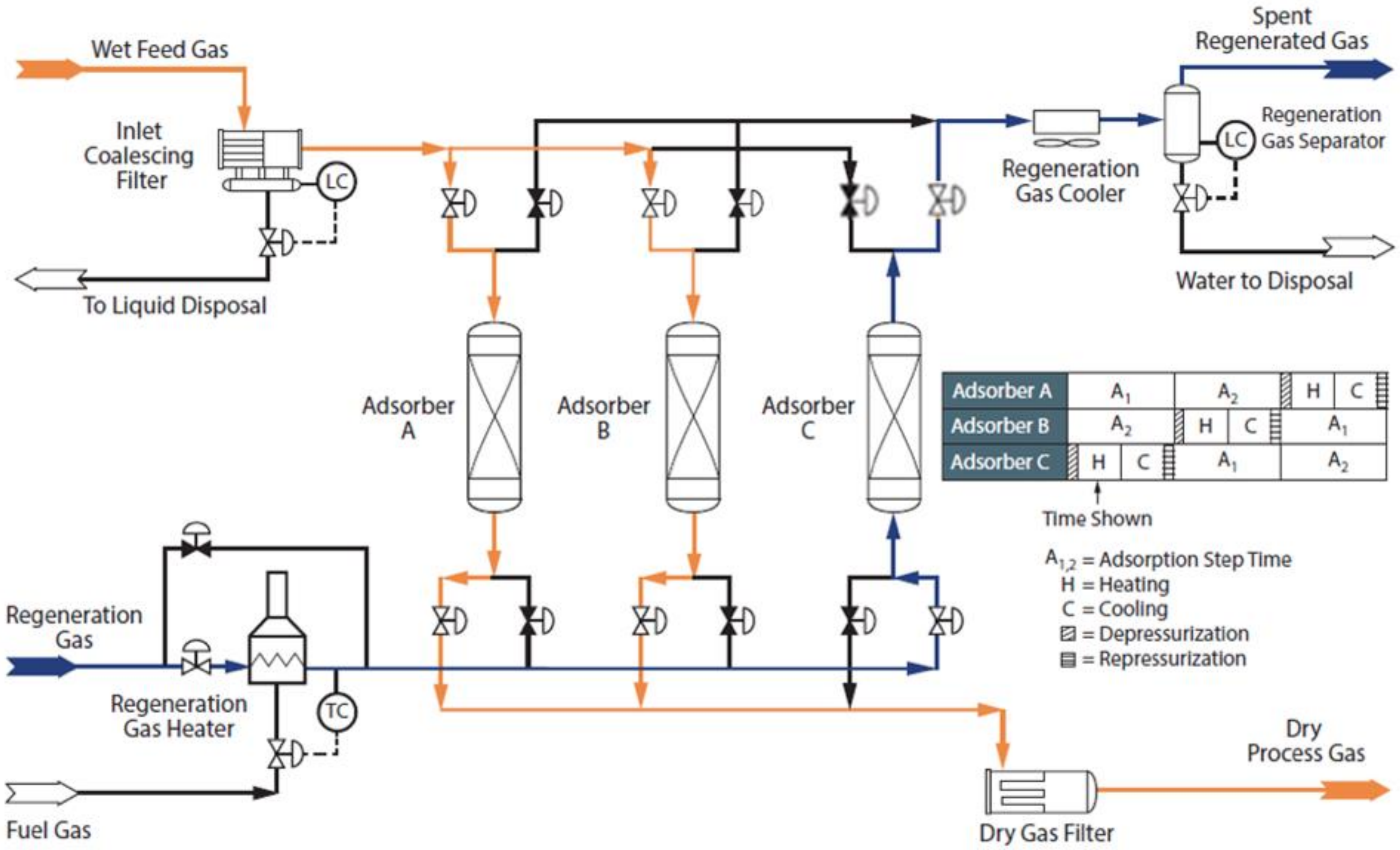
Desidratação de Gás Natural *(PPP offshore)*



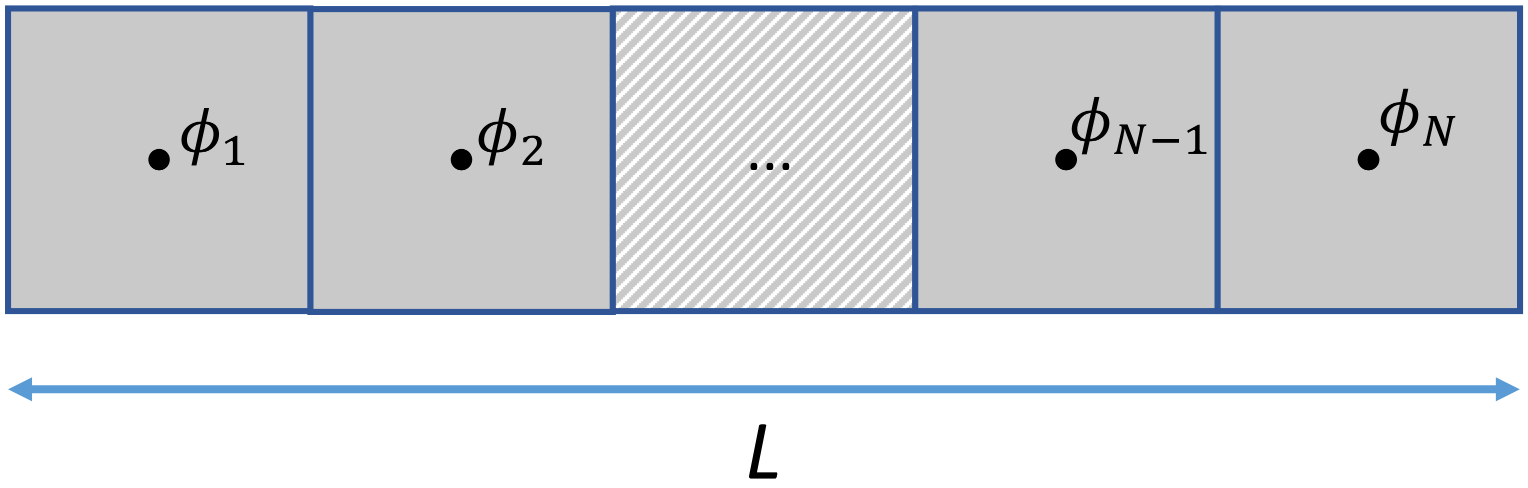
Campbell, J.M., Gas Conditioning and Processing, Volume 2: The Equipment Modules, 9th Edition, 2nd Printing, Editors Hubbard, R. and Snow–McGregor, K., Campbell Petroleum Series, Norman, Oklahoma, 2014.

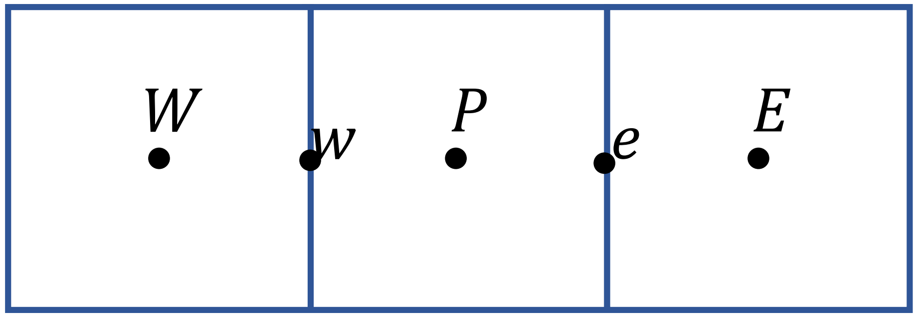
Hipóteses Simplificadoras

$H1$	Somente dois componentes no gás: água e etanol. Considera-se que o etanol não é adsorvido pelas peneiras moleculares.
$H2$	Gás ideal
$H3$	Velocidade constante
$H4$	Sistema adiabático
$H5$	A resistência à transferência de massa segue um modelo linear (LDF)
$H6$	Isoterma de Langmuir
⋮	⋮

Volumes Finitos

Volumes Discretos de Mesmo Tamanho





Conservação de Massa da Fase Fluida

Modelo

$\frac{\partial c_a}{\partial t} = \frac{\partial^2 (D_{ax} \cdot c_a)}{\partial z^2} - \frac{\partial \left(\frac{u}{\epsilon} \cdot c_a\right)}{\partial z} - \left(\frac{1-\epsilon}{\epsilon}\right) \rho_s \cdot \frac{\partial q_a}{\partial t}$	Concentração molar de água
$D_{ax} \cdot \frac{\partial c_a}{\partial z}\Big\|_{w=0} - \left(\frac{u}{\epsilon} \cdot c_a\right)\Big\|_{w=0} = -u_f \cdot c_{a\,f}$	Condição de contorno em $z\ =\ 0$
$\frac{\partial c_a}{\partial z}\Big\|_{e=L} = 0$	Condição de contorno em $z = L$

Concentração em um volume interno P

$\int_w^e \frac{\partial c_a}{\partial t} dz = \int_w^e \frac{\partial^2 (D_{ax} \cdot c_a)}{\partial z^2} dz - \int_w^e \frac{\partial \left(\frac{u}{\epsilon} \cdot c_a\right)}{\partial z} dz - \int_w^e S_c(Y,T,P)\, dz$	
$\frac{\partial c_{a_P}}{\partial t} \cdot \Delta z = D_{ax} \cdot \left(\frac{\partial c_a}{\partial z}\Big\vert_e - \frac{\partial c_a}{\partial z}\Big\vert_w\right) - \frac{1}{\epsilon} \cdot \left((u \cdot c_a)\Big\vert_e - (u \cdot c_a)\Big\vert_w\right) - \bar{S}_c \cdot \Delta z$	
$\frac{\partial c_{a_P}}{\partial t} = \frac{D_{ax}}{\Delta z} \cdot \left(\frac{\partial c_a}{\partial z}\Big\vert_e - \frac{\partial c_a}{\partial z}\Big\vert_w\right) - \frac{1}{\epsilon \Delta z} \cdot \left((u \cdot c_a)\Big\vert_e - (u \cdot c_a)\Big\vert_w\right) - \bar{S}_c$	
$\frac{\partial c_{a_P}}{\partial t} = \frac{D_{ax}}{\Delta z} \cdot \left(\frac{\partial c_a}{\partial z}\Big\vert_e - \frac{\partial c_a}{\partial z}\Big\vert_w\right) - \frac{1}{\epsilon \Delta z} \cdot \left((u \cdot c_a)\Big\vert_e - (u \cdot c_a)\Big\vert_w\right) - \bar{S}_c$	
$\frac{\partial c_{a_P}}{\partial t} = \frac{D_{ax}}{\Delta z^2} \cdot \left(c_{a_{P+1}} - 2c_{a_P} + c_{a_{P-1}}\right) - \frac{1}{\epsilon \Delta z} \cdot \left(u_P c_{a_P} - u_{P-1} c_{a_{P-1}}\right) - \bar{S}_c$	Aproximação de primeira ordem para os termos advectivo e dispersivo.

Concentração no primeiro volume

$\frac{\partial c_{a_1}}{\partial t} = \frac{D_{ax}}{\Delta z} \cdot \left(\frac{\partial c_a}{\partial z}\Big\|_e - \frac{\partial c_a}{\partial z}\Big\|_0 \right) - \frac{1}{\epsilon \Delta z} \cdot \left((u \cdot c_a)\Big\|_e - (u \cdot c_a)\Big\|_0 \right) - \bar{S}_c$	$P = 1$
$\frac{\partial c_{a_1}}{\partial t} = \frac{D_{ax}}{\Delta z} \cdot \frac{\partial c_a}{\partial z}\Big\|_e - \frac{D_{ax}}{\Delta z} \cdot \frac{\partial c_a}{\partial z}\Big\|_0 - \frac{1}{\epsilon \Delta z} \cdot (u \cdot c_a)\Big\|_e + \frac{1}{\epsilon \Delta z} \cdot (u \cdot c_a)\Big\|_0 - \bar{S}_c$	
$\frac{\partial c_{a_1}}{\partial t} = \frac{D_{ax}}{\Delta z} \cdot \frac{\partial c_a}{\partial z}\Big\|_e - \left(\frac{D_{ax}}{\Delta z} \cdot \frac{\partial c_a}{\partial z}\Big\|_0 - \frac{1}{\epsilon \Delta z} \cdot (u \cdot c_a)\Big\|_0 \right) - \frac{1}{\epsilon \Delta z} \cdot (u \cdot c_a)\Big\|_e - \bar{S}_c$	
$D_{ax} \cdot \frac{\partial c_a}{\partial z}\Big\|_0 - \frac{u}{\epsilon} \cdot c_a\Big\|_0 = -\left(\frac{F_f \cdot W_a}{MM_a} \right) = -u_f \cdot c_{a_f}$	Condição de contorno em z = 0
$\frac{\partial c_{a_1}}{\partial t} = \frac{D_{ax}}{\Delta z} \cdot \frac{\partial c_a}{\partial z}\Big\|_e + (u_f \cdot c_{a_f}) - \frac{1}{\epsilon \Delta z} \cdot (u \cdot c_a)\Big\|_1 - \bar{S}_c$	Aproximação de primeira ordem para o termo advectivo
$\frac{\partial c_{a_1}}{\partial t} = \frac{D_{ax}}{\Delta z^2} \cdot (c_{a_2} - c_{a_1}) + (u_f \cdot c_{a_f}) - \frac{1}{\epsilon \Delta z} \cdot (u \cdot c_a)\Big\|_1 - \bar{S}_c$	Aproximação de primeira ordem para o termo dispersivo

Concentração no último volume

$\frac{\partial c_{a_N}}{\partial t} = \frac{D_{ax}}{\Delta z} \cdot \left(\frac{\partial c_a}{\partial z}\Big\rvert_e - \frac{\partial c_a}{\partial z}\Big\rvert_w \right) - \frac{1}{\epsilon \Delta z} \cdot \left[(u \cdot c_a)\Big\rvert_e - (u \cdot c_a)\Big\rvert_w \right] - \bar{S}_c$	$P = N$
$\frac{\partial c_a}{\partial z}\Big\rvert_e = 0$	Condição de contorno em z = L
$\frac{\partial c_{a_N}}{\partial t} = \frac{D_{ax}}{\Delta z} \cdot \left(0 - \frac{\partial c_a}{\partial z}\Big\rvert_w \right) - \frac{1}{\epsilon \Delta z} \cdot \left[(u \cdot c_a)\Big\rvert_e - (u \cdot c_a)\Big\rvert_w \right] - \bar{S}_c$	
$\frac{\partial c_{a_N}}{\partial t} = -\frac{D_{ax}}{\Delta z} \cdot \frac{\partial c_a}{\partial z}\Big\rvert_w - \frac{1}{\epsilon \Delta z} \cdot \left[(u \cdot c_a)\Big\rvert_e - (u \cdot c_a)\Big\rvert_w \right] - \bar{S}_c$	
$\frac{\partial c_{a_N}}{\partial t} = -\frac{D_{ax}}{\Delta z} \cdot \frac{\partial c_a}{\partial z}\Big\rvert_w - \frac{1}{\epsilon \Delta z} \cdot \left[(u \cdot c_a)\Big\rvert_N - (u \cdot c_a)\Big\rvert_{N-1} \right] - \bar{S}_c$	Aproximação de primeira ordem pra trás nos termos advectivos
$\frac{\partial c_{a_N}}{\partial t} = -\frac{D_{ax}}{\Delta z^2} \cdot \left(c_{a_N} - c_{a_{N-1}} \right) - \frac{1}{\epsilon \Delta z} \cdot \left[(u \cdot c_a)\Big\rvert_N - (u \cdot c_a)\Big\rvert_{N-1} \right] - \bar{S}_c$	Aproximação de primeira ordem centrais nos termos dispersivos

Conservação de Massa no Sólido

$$\frac{\partial q}{\partial t} = K_{LDF} \cdot [q_{eq}(z) - q]$$

$$\int_w^e \frac{\partial q}{\partial t} dz = K_{LDF} \int_w^e q_{eq}(z)\, dz - K_{LDF} \int_w^e q\, dz$$

$$\frac{\partial q_P}{\partial t} \Delta z = K_{LDF} \cdot q_{eq_P} \cdot \Delta z - K_{LDF} \cdot q_P \cdot \Delta z$$

$$\frac{\partial q_P}{\partial t} = K_{LDF} \cdot \left(q_{eq_P} - q_P\right)$$

Conservação da Massa Global

$\frac{\partial C}{\partial t} = -\frac{1}{\epsilon} \cdot \frac{\partial (u \cdot C)}{\partial z} - \left(\frac{1-e}{e}\right) \cdot \rho_s \cdot \frac{\partial q}{\partial t}$	
$(u \cdot C)\Big\|_{w=0} = \frac{F_f}{A \cdot MM_{tot}}$	Condição de contorno em $z = 0$.
$\frac{\partial C}{\partial t} = -\frac{1}{\epsilon \Delta z}\left[(u \cdot C)\Big\|_e - (u \cdot C)\Big\|_w\right] - \bar{S}_C(Y, T, P)$	Equação em termos de fluxo
$\frac{\partial C_P}{\partial t} = -\frac{1}{\epsilon}\left[(u \cdot C)\Big\|_P - (u \cdot C)\Big\|_{P-1}\right] - \bar{S}_{C_P}(Y, T, P)$	Aproximação de primeira ordem para os termos advectivos
$\frac{\partial C_1}{\partial t} = -\frac{1}{\epsilon}\left[(u \cdot C)\Big\|_1 - (u \cdot C)\Big\|_0\right] - \bar{S}_{C_P}(Y, T, P)$	
$\frac{\partial C_1}{\partial t} = -\frac{1}{\epsilon}\left[(u \cdot C)\Big\|_1 - \left(\frac{F_f}{A \cdot MM_{tot}}\right)\right] - \bar{S}_{C_P}(Y, T, P)$	

Conservação de Energia

Conservação de Energia

$$\left[\rho_g c_{\rho_g} + \left(\frac{1-\epsilon}{\epsilon}\right)\rho_s c_{\rho_s}\right]\frac{\partial T}{\partial t} = \frac{\partial^2 (k_{ef} \cdot T)}{\partial z^2} - \frac{\partial \left(\frac{u\rho_g c_{\rho_g}}{\epsilon} \cdot T\right)}{\partial z} - Q \cdot \left(\frac{1-\epsilon}{\epsilon}\right)\rho_s \cdot \frac{\partial q}{\partial t}$$

$$\frac{k_{ef}}{\left[\rho_g c_{\rho_g} + \left(\frac{1-\epsilon}{\epsilon}\right)\rho_s c_{\rho_s}\right]} = \alpha$$

$$\frac{u\rho_g c_{\rho_g}}{\epsilon\left[\rho_g c_{\rho_g} + \left(\frac{1-\epsilon}{\epsilon}\right)\rho_s c_{\rho_s}\right]} = \beta$$

$$\frac{Q \cdot \left(\frac{1-\epsilon}{\epsilon}\right)\rho_s}{\left[\rho_g c_{\rho_g} + \left(\frac{1-\epsilon}{\epsilon}\right)\rho_s c_{\rho_s}\right]} = \gamma$$

$$\frac{\partial T}{\partial t} = \frac{\partial^2 (\alpha \cdot T)}{\partial z^2} - \frac{\partial (\beta \cdot T)}{\partial z} - \gamma \cdot \frac{\partial q}{\partial t}$$

Temperatura em um volume interno (P = 2:N-1)

$\frac{\partial T}{\partial t} = \frac{\partial^2(\alpha \cdot T)}{\partial z^2} - \frac{\partial(\beta \cdot T)}{\partial z} - \gamma \cdot \frac{\partial q}{\partial t}$	Assumindo que a densidade varia pouco com o tempo e com z.
$\frac{\partial T_P}{\partial t} \Delta z = \alpha \left(\frac{\partial T}{\partial z}\Big\rvert_e - \frac{\partial T}{\partial z}\Big\rvert_w \right) - \beta \left(T\Big\rvert_e - T\Big\rvert_w \right) - \gamma \cdot \frac{\partial q_P}{\partial t} \Delta z$	
$\frac{\partial T_P}{\partial t} = \frac{\alpha}{\Delta z} \left(\frac{\partial T}{\partial z}\Big\rvert_e - \frac{\partial T}{\partial z}\Big\rvert_w \right) - \frac{\beta}{\Delta z} \left(T\Big\rvert_e - T\Big\rvert_w \right) - \gamma \cdot \frac{\partial q_P}{\partial t}$	
$\frac{\partial T_P}{\partial t} = \frac{\alpha}{\Delta z^2} (T_{P+1} - 2T_P + T_{P-1}) - \frac{\beta}{\Delta z} (T_P - T_{P-1}) - \gamma \cdot \frac{\partial q_P}{\partial t}$	Aproximação de primeira ordem para os termos advectivo e dispersivo.

Temperatura no primeiro volume (P = 1)

$\alpha \cdot \frac{\partial T}{\partial z}\Big\|_0 - \beta \cdot T\Big\|_0 = -\beta \cdot \epsilon \cdot T_f$	Assumindo que a densidade varia pouco com o tempo e com z.
$\frac{\partial T_1}{\partial t} = \frac{\alpha}{\Delta z}\left(\frac{\partial T}{\partial z}\Big\|_e - \frac{\partial T}{\partial z}\Big\|_0\right) - \frac{\beta}{\Delta z}\left(T\Big\|_e - T\Big\|_0\right) - \gamma \cdot \frac{\partial q_1}{\partial t}$	P = 1
$\frac{\partial T_1}{\partial t} = \frac{1}{\Delta z} \cdot \left(\alpha \cdot \frac{\partial T}{\partial z}\Big\|_e - \beta \cdot T\Big\|_e\right) - \frac{1}{\Delta z}\left(\alpha \cdot \frac{\partial T}{\partial z}\Big\|_0 - \beta \cdot T\Big\|_0\right) - \gamma \cdot \frac{\partial q_1}{\partial t}$	
$\frac{\partial T_1}{\partial t} = \frac{1}{\Delta z} \cdot \left(\alpha \cdot \frac{\partial T}{\partial z}\Big\|_e - \beta \cdot T\Big\|_e\right) + \frac{1}{\Delta z}(\beta \cdot \epsilon \cdot T_f) - \gamma \cdot \frac{\partial q_1}{\partial t}$	
$\frac{\partial T_1}{\partial t} = \frac{1}{\Delta z^2} \cdot [\alpha \cdot (T_{P+1} - T_P) - \beta \cdot T_P] + \frac{1}{\Delta z}(\beta \cdot \epsilon \cdot T_f) - \gamma \cdot \frac{\partial q_1}{\partial t}$	

Temperatura no primeiro volume (P = 1)

$\alpha \cdot \frac{\partial T}{\partial z}\Big\|_0 - \beta \cdot T\Big\|_0 = -\beta \cdot \epsilon \cdot T_f$	Assumindo que a densidade varia pouco com o tempo e com z.
$\frac{\partial T_1}{\partial t} = \frac{\alpha}{\Delta z}\left(\frac{\partial T}{\partial z}\Big\|_e - \frac{\partial T}{\partial z}\Big\|_0\right) - \frac{\beta}{\Delta z}\left(T\Big\|_e - T\Big\|_0\right) - \gamma \cdot \frac{\partial q_1}{\partial t}$	P = 1
$\frac{\partial T_1}{\partial t} = \frac{1}{\Delta z} \cdot \left(\alpha \cdot \frac{\partial T}{\partial z}\Big\|_e - \beta \cdot T\Big\|_e\right) - \frac{1}{\Delta z}\left(\alpha \cdot \frac{\partial T}{\partial z}\Big\|_0 - \beta \cdot T\Big\|_0\right) - \gamma \cdot \frac{\partial q_1}{\partial t}$	
$\frac{\partial T_1}{\partial t} = \frac{1}{\Delta z} \cdot \left(\alpha \cdot \frac{\partial T}{\partial z}\Big\|_e - \beta \cdot T\Big\|_e\right) + \frac{1}{\Delta z}(\beta \cdot \epsilon \cdot T_f) - \gamma \cdot \frac{\partial q_1}{\partial t}$	
$\frac{\partial T_1}{\partial t} = \frac{1}{\Delta z^2} \cdot [\alpha \cdot (T_{P+1} - T_P) - \beta \cdot T_P] + \frac{1}{\Delta z}(\beta \cdot \epsilon \cdot T_f) - \gamma \cdot \frac{\partial q_1}{\partial t}$	

Temperatura no último volume (P = N)

$\left.\frac{\partial T}{\partial z}\right\|_e = 0$	P = N
$\frac{\partial T_N}{\partial t} = \frac{\alpha}{\Delta z}\left(\left.\frac{\partial T}{\partial z}\right\|_e - \left.\frac{\partial T}{\partial z}\right\|_w\right) - \frac{\beta}{\Delta z}\left(T\big\|_N - T\big\|_{N-1}\right) - \gamma \cdot \frac{\partial q_N}{\partial t}$	
$\frac{\partial T_N}{\partial t} = \frac{\alpha}{\Delta z}\left(0 - \left.\frac{\partial T}{\partial z}\right\|_w\right) - \frac{\beta}{\Delta z}\left(T\big\|_N - T\big\|_{N-1}\right) - \gamma \cdot \frac{\partial q_N}{\partial t}$	
$\frac{\partial T_N}{\partial t} = -\frac{\alpha}{\Delta z^2}(T_N - T_{N-1}) - \frac{\beta}{\Delta z}\left(T\big\|_N - T\big\|_{N-1}\right) - \gamma \cdot \frac{\partial q_N}{\partial t}$	

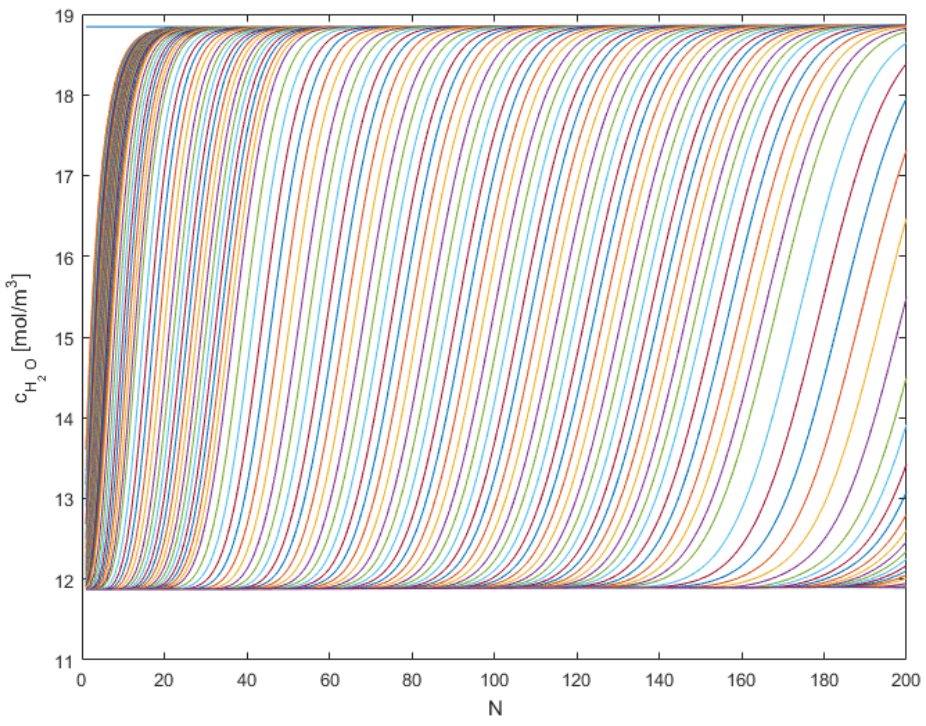
Simulação

Desidratação de Etanol

Parâmetro e Constantes	*Valor*	*Unidade*	*Parâmetro e Constantes*	*Valor*	*Unidade*
MM_{H_2O}	18	g	T_b	450	K
$MM_{C_2H_6O}$	46	g	N	300	pontos
R	8.314598	$J(K\ mol)^{-1}$	dL	0.0244	m
MF_w	0.182	%	ρ_s	729	kg/m3
c_{ps}	1260	$J\ (kg\ K)^{-1}$	r_p	0.0015875	m
F_f	5.6694 X 100	kg/s	q_s	10.6656	mol/kg
T_f	440	K	T_0	323	K
P_f	379.2120	kPa	K_0	0.0441765	Pa^{-1}
L	7.3	m	K_{LDF}	0.5E-4	
D	2.4	m	μ	1e-6	
A	4.5239	m2	RelTol	2e-4	
ϵ	0.63	[ ]	AbsTol	3e-3	
ϵ_b	0.4	[ ]	D_{ax}	0.00113	m^2s^{-1}
Q	51900	J	k_{ef}	41.26	$W\ (m\ K)^{-1}$
c_{pg}	1000	$J\ (kg\ K)^{-1}$			

M. Simo, C. J. Brown, and V. Hlavacek, “Simulation of pressure swing adsorption in fuel ethanol production process,” *Comput. Chem. Eng.*, vol. 32, no. 7, pp. 1635–1649, 2008.

Concentração de Água no Gás



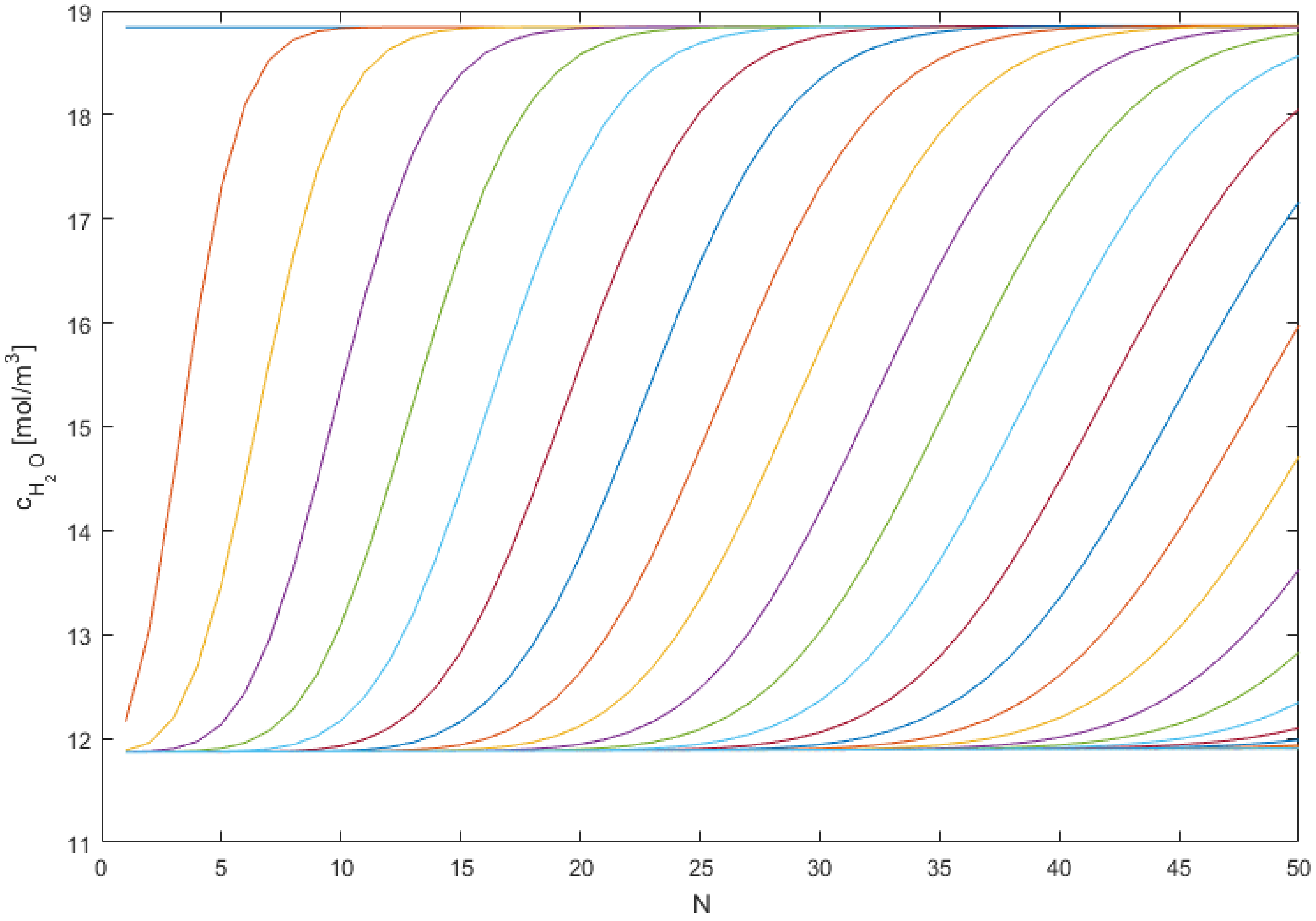
N = 200

0 < t < 20

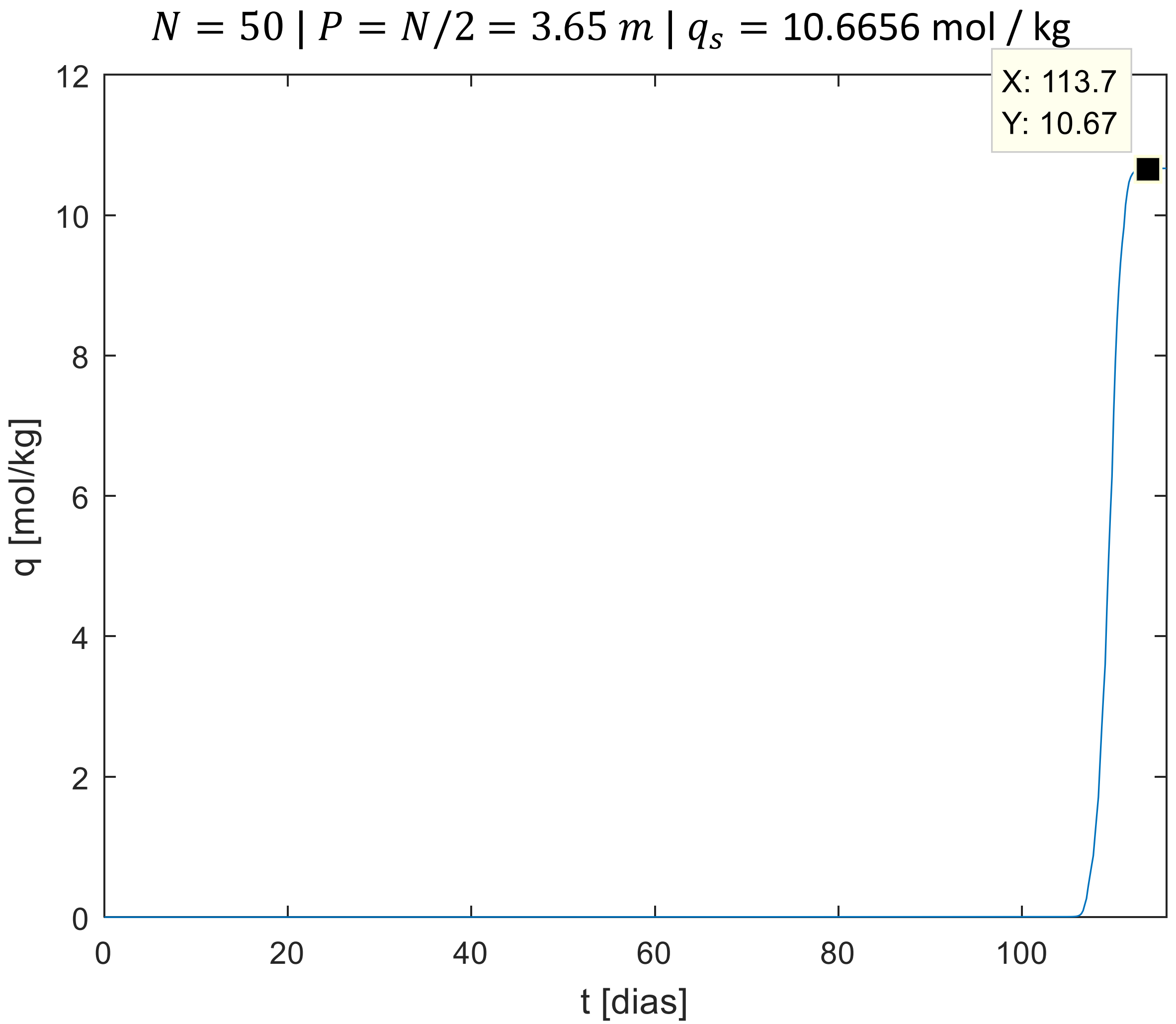
$C_0 = 18.8\, mol/m^3$

Concentração de Água no Gás

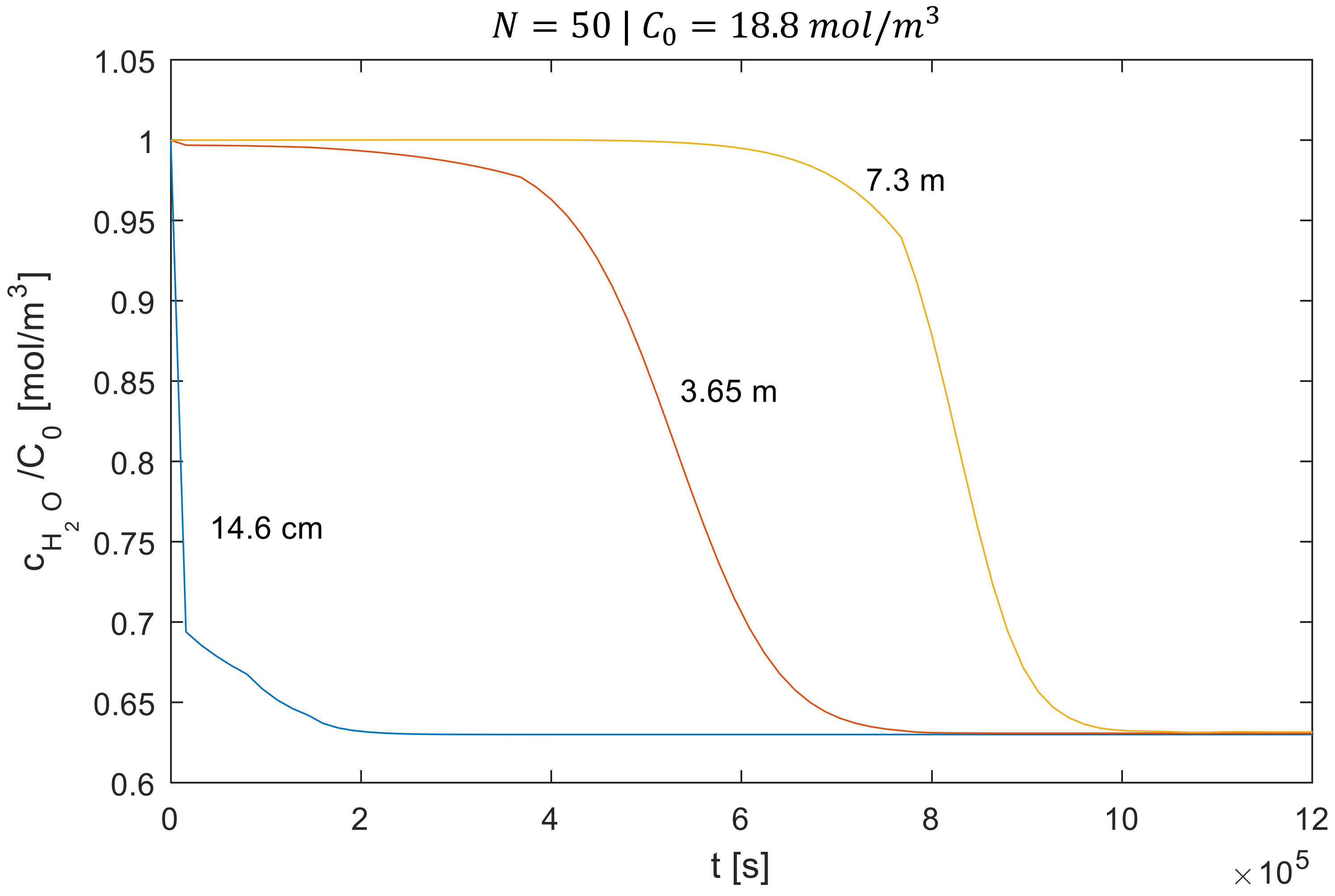
$$N = 50 \mid T = 1:0.01:20 \mid C_0 = 18.8\ mol/m^3$$



Água adsorvida por kg de material adsorvente

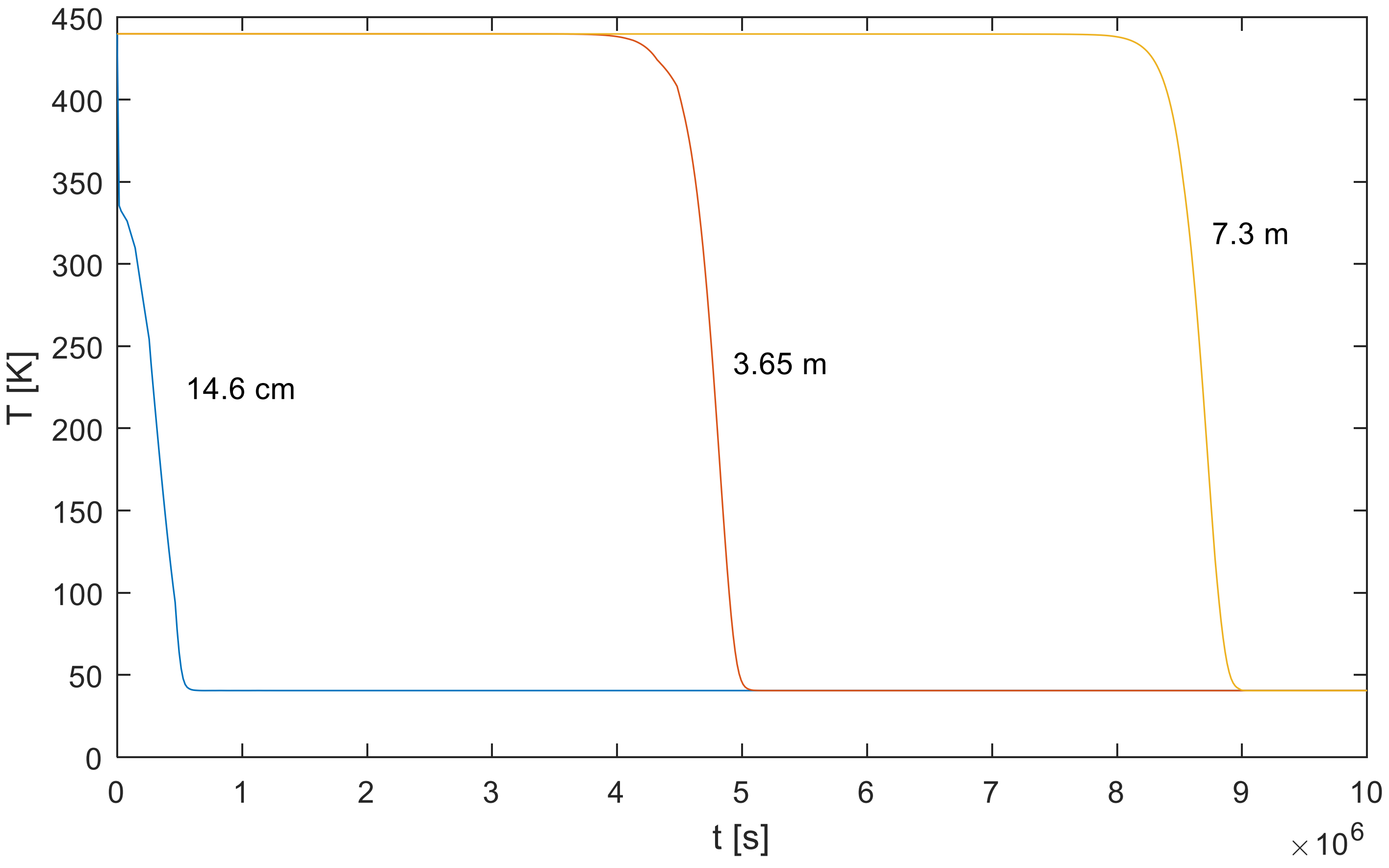


Curva de Ruptura



Variação de Temperatura

$N = 50 \mid T_0 = 440K$



Obrigada