**%Data From:**

**%M.A.S.D. Barros, E.A. Silva, P.A. Arroyo, C.R.G. Tavares, R.M. Schneider, M. Suszek, E.F. Sousa-Aguiar, Removal of Cr(III) in the fixed bed column and batch reactors using as adsorbent zeolite NaX, Chem Eng Sci. 59 (2004) 5959–5966. https://doi.org/10.1016/j.ces.2004.07.040.**

**%Cr(III) Cl on zeolite, fixed flux, 3 inlet concentrations**

**%Isotherm values for c\_eq, q\_eq**

**Barros works in meq/L to convert multiply by (52/3) e-3kg/eq**

ce=[0.3,0.95,1.45,1.89,2.89]\*(52/3)e-3; %Adsorbate inlet concentration [kg/m^3]

qe=[1.54,2.34,2.75,3.15,3.27]\*(52/3)e-3; %Adsorbed fraction at equilibrium [kg/kg]

**%Langmuir isotherm parameters**

qm=3.61\*(52/3)e-3; %[kg adsorbate/kg adsorbent]

kL=2.39\*1e3; %[m^3solution/kgadsorbent]

qeexp=[2.34,3.15,3.27]\*(52/3)e-3; %qe experimental

**%3 inlet concentrations and half times**

ci=[0.95,1.89,2.89]\*(52/3)e-3; %Adsorbate initial concentration [kg/m^3]

t12=[83.31,73.2,51.706]\*60; %Time at which the c/c\_in=1/2 [s]

**%3 sets of times for breakthrough data with 3 inlet concentrations**

texp={[0 10 15 20 27 30 36 40 46 50 55 61 76 93 107 122 135 150 166 200 231 261 290 321 351 381 434]\*60,

[0 5 12 16 21 31 41 51 61 71 81 91 101 111 121 136 150 167 189 215 276 306 335]\*60,

[0 5 12 16 21 26 31 36 41 51 61 71 81 91 124 136 150 177 209 256]\*60};

**%Corresponding breakthrough concentration**

cexpci={[0 0.001305483 0.002610966 0.002610966 0.01305483 0.031331593 0.07310705 0.130548303 0.203655352 0.255874674 0.2845953 0.328981723 0.44386423 0.574412533 0.634464752 0.699738903 0.759791123 0.798955614 0.804177546 0.866840731 0.895561358 0.929503916 0.958224543 0.979112272 1 1 1],

[0 0 0 0.003257329 0.016286645 0.127035831 0.241042345 0.345276873 0.442996743 0.482084691 0.563517915 0.61237785 0.661237785 0.713355049 0.736156352 0.781758958 0.843648208 0.895765472 0.928338762 0.960912052 0.980456026 1.003257329 1.003257329],

[0 0.003937008 0.023622047 0.05511811 0.11023622 0.181102362 0.244094488 0.295275591 0.37007874 0.503937008 0.582677165 0.665354331 0.771653543 0.791338583 0.921259843 0.948818898 0.984251969 1 1 1]};

**%Various operating parameters**

Lb=1.6e-2; %Column height [m]

Db=0.9e-2; %Column diameter [m]

Sb=pi\*(Db^2)/4; %Bed section area [m^2]

Vb=Sb\*Lb; %Bed volume [m^3]

Pa=101325; %Atmospheric pressure [Pa]

T=30+273.15; %Column temperature 25 ºC [K]

rhoCr=7.19e3; %Adsorbate density at 26 ºC and 1.12 bar [kg/m^3]

MCr=52/1000; %Adsorbate Molecular Mass [kg/mol]

Rg=8.314; %Ideal gas constant [J/(K·mol)]

MH2O=0.018; %Water Molecular Mass [kg/mol]

muH2O=0.0008891; %Water dynamic viscosity [Pa·s]

rhoH2O=1000; %Water density [kg/m^3]

d=0.18e-3; %Particle diameter (2.00-2.38 mm) [m]

Q=9/(60\*1000000); %Flow rate [m^3/s]

us=Q/Sb; %Initial superficial velocity [m/s]

rhob=440; %Bulk density [kg/m^3]

e=0.5; %Porosity of the bed [m^3void/m^3bed]

u=us/e; %Interstitial velocity [m/s]

Re=d\*e\*u\*rhoH2O/muH2O;

D1=1.6\*u\*d;

D2=2\*u\*d;