**%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) on zeolite, fixed inlet concentration, 3 fluxes**

Q=[7,9,11]/(60\*1000000); %Flow rate [m^3/s]

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

ce=[0.3,0.95,1.45,1.89,2.89]\*(52/3)e-3; %Adsorbate initial 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=0.0036\*(52/3)e-3; %[kg adsorbate/kg adsorbent]

kL=2443.1; %[m^3solution/kgadsorbent]

qeexp=3.27\*(52/3)e-3; %qe experimental

**%Inlet concentration and t1/2 values for 3 fluxes**

ci=0.018\*(52/3)e-3; %Adsorbate initial concentration [kg/m^3]

t12=[1555.042017 1206.422018 976.9767442]\*60; %Time at which the c/c\_in=1/2 [s]

**%3 sets of times for breakthrough data with 3 fluxes**

texp={[1240 1300 1370 1435 1510 1670 1725 1765 1825 1880 1945 2005]\*60,

[440 500 570 620 680 780 830 900 960 1030 1090 1140 1220 1290 1335 1465 1555 1945]\*60,

[410 475 525 600 650 745 795 840 890 955 1025 1070 1160 1310]\*60};

cexpci={[0 0 0 0.086642599 0.379061372 0.80866426 0.895306859 1 1 1 1 1],

[0.003610108 0.003610108 0.003610108 0.003610108 0.003610108 0.003610108 0.003610108 0.003610108 0.003610108 0.003610108 0.02166065 0.173285199 0.566787004 0.783393502 0.797833935 1.003610108 0.989169675 0.992779783],

[0.007220217 0.007220217 0.007220217 0.007220217 0.007220217 0.007220217 0.050541516 0.14801444 0.314079422 0.451263538 0.606498195 0.667870036 0.805054152 0.953068592]};

**%Various operating parameters**

Lb=8.8e-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 [m]

rhoac=880; %Adsorbent aparent density [kg/m^3] Calculated using rhoac=rhob/(1-e) with data from appfitCrLSQ

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

mcoal=3e-3; %Mass of initial adsorbent [kg]

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

e=1-(rhob/rhoac); %Porosity of the bed [m^3void/m^3bed]

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

kp=((d^2)/150)\*(e^2)/((1-e)^2); %Permeability [m^2]