**Supplementary information**

The overall and component mass balances are presented in Eq. 1-2.

 (Eq. 1)

 (Eq. 2)

The axial dispersion coefficient Ez is estimated according to Eq. 3

 (Eq. 3)

The rate of sorption is presented in Eq. 4-5. Factors of sorption frequency Ak and sorption activation energy Eak were considered as model fitting parameters which equal 1.208 × 10-6 m2/s and 1622.33 kJ/kmol for oxygen, and 8.186 × 10-5 m2/s and 25098.55 kJ/kmol for nitrogen, respectively.

 (Eq. 4)

 (Eq. 5)

The energy balances of gas and solid phases are presented in Eq. 6-7, respectively.

 (Eq. 6)

 (Eq. 7)

The explicit data of oxygen and nitrogen adsorption isotherms are presented in Tab. 1-2, respectively.

**Tab. 1** Oxygen adsorption isotherms on MSC CT-350

|  |  |  |
| --- | --- | --- |
| 20 °C | 40 °C | 60 °C |
| p [bar] | w\* [mol/g] | p [bar] | w\* [mol/g] | p [bar] | w\* [mol/g] |
| 0.00942 | 4.209E-06 | 0.00962 | 3.390E-06 | 0.00916 | 2.679E-06 |
| 0.0146 | 6.723E-06 | 0.01424 | 4.682E-06 | 0.01426 | 3.848E-06 |
| 0.0205 | 9.653E-06 | 0.01944 | 6.385E-06 | 0.01968 | 5.382E-06 |
| 0.0291 | 1.384E-05 | 0.02932 | 8.982E-06 | 0.03034 | 7.729E-06 |
| 0.03956 | 1.887E-05 | 0.04216 | 1.284E-05 | 0.0456 | 1.088E-05 |
| 0.0797 | 3.736E-05 | 0.0791 | 2.357E-05 | 0.0939 | 2.001E-05 |
| 0.1511 | 6.895E-05 | 0.1535 | 4.465E-05 | 0.1545 | 3.188E-05 |
| 0.2045 | 9.253E-05 | 0.2031 | 5.884E-05 | 0.1937 | 3.905E-05 |
| 0.354 | 1.455E-04 | 0.345 | 9.447E-05 | 0.349 | 6.483E-05 |
| 0.554 | 2.223E-04 | 0.55 | 1.458E-04 | 0.549 | 9.969E-05 |
| 0.964 | 3.564E-04 | 0.955 | 2.395E-04 | 0.954 | 1.652E-04 |
| 1.469 | 4.994E-04 | 1.46 | 3.456E-04 | 1.464 | 2.405E-04 |
| 1.969 | 6.219E-04 | 1.96 | 4.397E-04 | 1.964 | 3.095E-04 |
| 2.979 | 8.285E-04 | 2.97 | 6.025E-04 | 2.974 | 4.348E-04 |
| 3.989 | 9.977E-04 | 3.98 | 7.414E-04 | 3.979 | 5.446E-04 |
| 5.004 | 1.141E-03 | 4.985 | 8.627E-04 | 4.994 | 6.430E-04 |
| 7.529 | 1.424E-03 | 7.51 | 1.109E-03 | 7.514 | 8.489E-04 |
| 10.049 | 1.638E-03 | 10.03 | 1.302E-03 | 10.039 | 1.017E-03 |
| 12.569 | 1.808E-03 | 12.54 | 1.459E-03 | 12.549 | 1.159E-03 |
| 15.079 | 1.948E-03 | 15.055 | 1.591E-03 | 15.059 | 1.280E-03 |
| 17.594 | 2.066E-03 | 17.565 | 1.704E-03 | 17.569 | 1.385E-03 |
| 18.599 | 2.108E-03 | 18.565 | 1.745E-03 | 18.569 | 1.425E-03 |
| 19.609 | 2.149E-03 | 19.565 | 1.784E-03 | 19.564 | 1.463E-03 |
| 19.809 | 2.157E-03 | 20.035 | 1.803E-03 | 20.034 | 1.482E-03 |

**Tab. 2** Nitrogen adsorption isotherms on MSC CT-350

|  |  |  |
| --- | --- | --- |
| 20 °C | 40 °C | 60 °C |
| p [bar] | w\* [mol/g] | p [bar] | w\* [mol/g] | p [bar] | w\* [mol/g] |
| 0.00908 | 4.844E-06 | 0.00888 | 3.425E-06 | 0.00914 | 2.480E-06 |
| 0.01718 | 1.106E-05 | 0.01184 | 5.339E-06 | 0.01634 | 4.925E-06 |
| 0.03284 | 2.022E-05 | 0.01842 | 8.254E-06 | 0.01934 | 6.832E-06 |
| 0.05982 | 3.799E-05 | 0.0332 | 1.365E-05 | 0.03062 | 1.028E-05 |
| 0.1015 | 6.074E-05 | 0.06 | 2.254E-05 | 0.0596 | 1.728E-05 |
| 0.1847 | 1.034E-04 | 0.0947 | 3.484E-05 | 0.1003 | 2.913E-05 |
| 0.25 | 1.314E-04 | 0.1387 | 4.964E-05 | 0.1469 | 3.738E-05 |
| 0.545 | 2.471E-04 | 0.1681 | 6.136E-05 | 0.2069 | 4.819E-05 |
| 0.95 | 3.779E-04 | 0.1969 | 7.353E-05 | 0.29 | 6.126E-05 |
| 1.46 | 5.125E-04 | 0.3575 | 1.232E-04 | 0.35 | 8.503E-05 |
| 1.97 | 6.253E-04 | 0.415 | 1.392E-04 | 0.55 | 1.257E-04 |
| 2.975 | 8.053E-04 | 0.545 | 1.710E-04 | 0.955 | 1.955E-04 |
| 3.99 | 9.461E-04 | 0.945 | 2.654E-04 | 1.46 | 2.727E-04 |
| 5 | 1.064E-03 | 1.45 | 3.670E-04 | 1.965 | 3.420E-04 |
| 7.52 | 1.287E-03 | 1.95 | 4.551E-04 | 2.97 | 4.606E-04 |
| 10.04 | 1.452E-03 | 2.965 | 6.038E-04 | 3.98 | 5.571E-04 |
| 12.555 | 1.580E-03 | 3.965 | 7.253E-04 | 4.99 | 6.401E-04 |
| 15.06 | 1.683E-03 | 4.975 | 8.290E-04 | 7.52 | 8.140E-04 |
| 17.56 | 1.767E-03 | 7.495 | 1.032E-03 | 10.04 | 9.507E-04 |
| 18.555 | 1.796E-03 | 10.015 | 1.189E-03 | 12.55 | 1.062E-03 |
| 20.025 | 1.837E-03 | 12.52 | 1.313E-03 | 15.065 | 1.156E-03 |
|  |  | 15.02 | 1.414E-03 | 17.57 | 1.235E-03 |
|  |  | 17.515 | 1.497E-03 | 18.57 | 1.265E-03 |
|  |  | 18.52 | 1.527E-03 | 19.56 | 1.294E-03 |
|  |  | 19.515 | 1.555E-03 | 20.03 | 1.308E-03 |
|  |  | 19.97 | 1.568E-03 |  |  |

The temperature-dependent Sips isotherm model is presented in Eq. 8-11.

 (Eq. 8)

; ;  (Eq. 9-11)

Parameters of isotherms are listed in Tab. 3.

**Tab. 3** Sips isotherm parameters of oxygen and nitrogen adsorption on CMS

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |  |
| O2 | 3.384 × 10-3 | 1.104 | 9.436 × 10-2 | 1.222 × 104 | 1.120 | 3.341 × 10-1 |
| N2 | 2.707 × 10-3 | 1.146 | 1.205 × 10-1 | 1.187 × 104 | 1.185 | 2.263 × 10-1 |

The isosteric heat of adsorption is displayed in Eq. 12.

 (Eq. 12)

The pressure drop along the packed bed is presented in Eq. 13

 (Eq. 13)

Other parameters of the dynamic model are listed in Tab. 4.

**Tab. 4** Parameters of the PSA dynamic model

|  |  |  |
| --- | --- | --- |
| Inter-particle voidage | εi [m3 void/m3 bed] | 0.404 |
| Intra-particle voidage | εp [m3 void/m3 pellet] | 0.234 |
| Adsorbent particle radius | rp [mm] | 0.830 |
| Adsorbent shape factor | ψ [-] | 1.959 |
| Adsorbent thermal conductivity | ksz [W/m/K]  | 0.675 |
| Adsorbent specific heat capacity | Cps [J/kg/K] | 880 |
| Heat transfer coefficient between gas and wall | hw [W/m2/K] | 50 |

**Notation**

Ak sorption frequency factor of component k [m2/s]

ap specific particle surface area per unit volume of bed [m2(particle area)/m3(bed)]

cg gas phase molar density [kmol/m3]

ck molar concentration of component k [kmol/m3]

Cpak specific adsorbed phase heat capacity at constant pressure of component k [MJ/kmol/K]

Cpg specific gas phase heat capacity at constant pressure [MJ/kmol/K]

Cps specific solid phase heat capacity at constant pressure [MJ/kg/K]

Cvg specific gas phase heat capacity at constant volume [MJ/kmol/K]

D0k corrected diffusion coefficient of component k [m2/s]

Dek effective diffusion coefficient of component k [m2/s]

Eak sorption activation energy of component k [kJ/kmol]

Ezk axial dispersion coefficient of component k [m2/s]

h gas-solid heat transfer coefficient [MW/m2/K]

hw gas-wall heat transfer coefficient [MW/m2/K]

kg gas phase thermal conductivity [MW/m/K]

kgz effective axial gas phase thermal conductivity [MW/m/K]

ksz effective axial solid phase thermal conductivity [MW/m/K]

M molecular weight [kg/kmol]

MTCk mass transfer coefficient of component k [1/s]

P pressure [bar]

pk partial pressure of component k [bar]

rp adsorbent particle radius [m]

Ta ambient temperature [K]

Tg gas phase temperature [K]

Ts solid phase temperature [K]

vg gas phase superficial velocity [m/s]

wk loading of component k [kmol/kg]

wk\* equilibrium loading of component k [kmol/kg]

wsk\* saturation equilibrium loading of component k [kmol/kg]

ΔHk heat of adsorption of component k [MJ/kmol]

εB total bed voidage [m3(void+pore)/m3(bed)]

εi interparticle voidage [m3(void)/m3(bed)]

μ dynamic viscosity [Ns/m2]

θ adsorbent surface coverage [-]

ρs solid phase bulk density [kg/m3]