

Volatile Fatty Acids Adsorption: Equilibrium Characterization and Breakthrough Dynamics

Cristiana Gomes^{a,*}, Ana M. Ribeiro^a, Alírio E. Rodrigues^a, Alexandre F.P. Ferreira^a

^a LSRE-LCM, ALiCE, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

* Corresponding authors: Cristiana Gomes (email: up201403931@edu.fe.up.pt)

Supporting Information

- Tracer breakthrough experiment, as well as the adjustment of Equation 5 (dashed line)

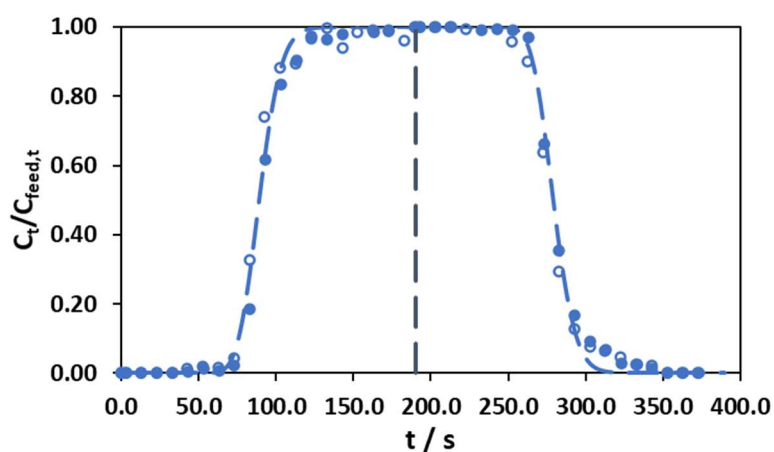


Figure S1. Blue Dextran 2000 breakthrough curve. The points represent experimental data (open and closed symbols correspond to duplicate assays), and the dashed line is the respective model fitting.

- Single-component breakthrough curves of isobutyric, valeric, isovaleric, and hexanoic acids

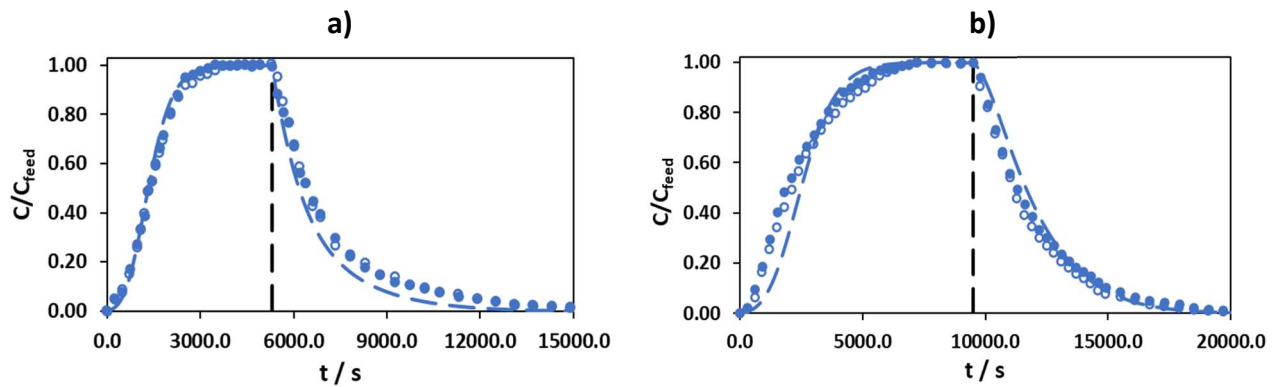


Figure S2. Breakthrough curve of isobutyric acid on the Amberlite XAD-4 resin, with a feed concentration of a) 50 mM and b) 10 mM. The points represent experimental data (open and closed symbols correspond to duplicate assays), and the dashed line is the respective model simulation with a $k_{LC} = 2.0 \times 10^{-3} \text{ s}^{-1}$ and a $k_{HC} = 3.8 \times 10^{-3} \text{ s}^{-1}$. The vertical dark dashed line represents the start of the desorption step.

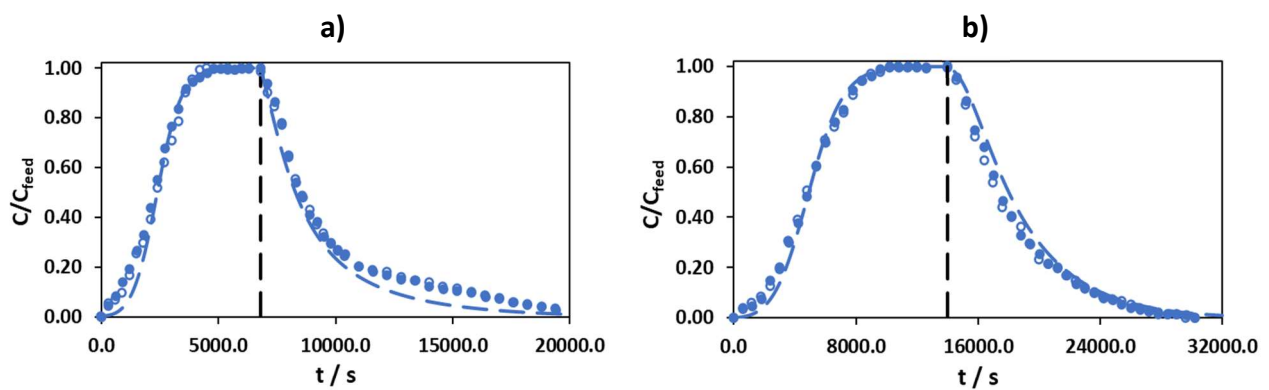


Figure S3. Breakthrough curve of valeric acid on the Amberlite XAD-4 resin, with a feed concentration of a) 50 mM and b) 10 mM. The points represent experimental data (open and closed symbols correspond to duplicate assays), and the dashed line is the respective model simulation with a $k_{LC} = 1.0 \times 10^{-3} \text{ s}^{-1}$ and a $k_{HC} = 3.2 \times 10^{-3} \text{ s}^{-1}$. The vertical dark dashed line represents the start of the desorption step.

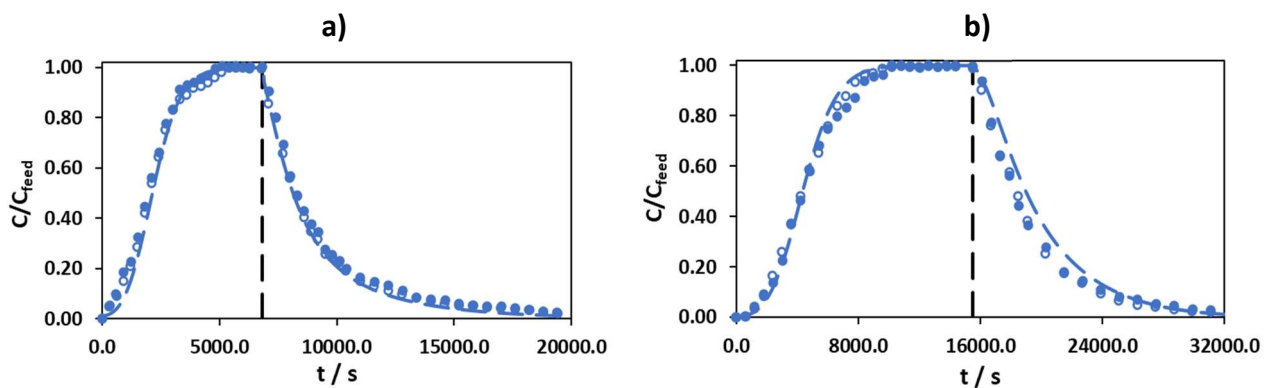


Figure S4. Breakthrough curve of isovaleric acid on the Amberlite XAD-4 resin, with a feed concentration of a) 50 mM and b) 10 mM. The points represent experimental data (open and closed symbols correspond to duplicate assays), and the dashed line is the respective model simulation with a $k_{LC} = 1.0 \times 10^{-3} \text{ s}^{-1}$ and a $k_{HC} = 2.8 \times 10^{-3} \text{ s}^{-1}$. The vertical dark dashed line represents the start of the desorption step.

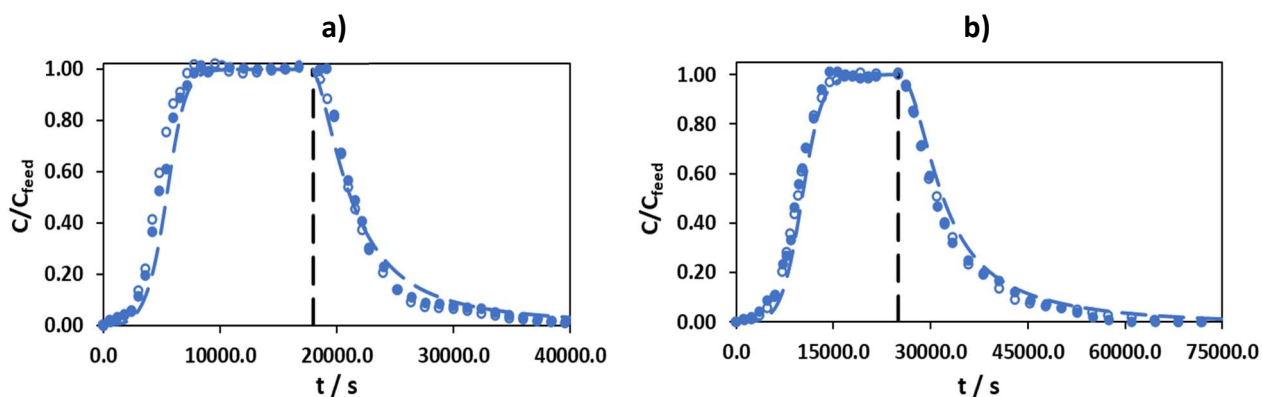


Figure S5. Breakthrough curve of hexanoic acid on the Amberlite XAD-4 resin, with a feed concentration of a) 50 mM and b) 10 mM. The points represent experimental data (open and closed symbols correspond to duplicate assays), and the dashed line is the respective model simulation with a $k_{LC} = 0.3 \times 10^{-3} \text{ s}^{-1}$ and a $k_{HC} = 2.2 \times 10^{-3} \text{ s}^{-1}$. The vertical dark dashed line represents the start of the desorption step.

Table S1. Stoichiometric time and adsorption capacity of isobutyric, valeric, isovaleric, and hexanoic acids for the single-component breakthrough curves.

Acid		t_{st} / s	$q_{col} / \text{mmol} \cdot \text{g}_{\text{ads}}^{-1}$	$q^* / \text{mmol} \cdot \text{g}_{\text{ads}}^{-1}$
Isobutyric 50 mM	Adsorption	1443.8	1.627	1.547
	Desorption	1874.9	2.145	
Isobutyric 10 mM	Adsorption	2403.8	0.590	0.641
	Desorption	2373.9	0.582	
Valeric 50 mM	Adsorption	2275.3	2.472	2.614
	Desorption	3063.2	3.362	
Valeric 10 mM	Adsorption	4905.1	1.125	1.150
	Desorption	4366.6	1.000	
Isovaleric 50 mM	Adsorption	2058.8	2.173	2.324
	Desorption	2485.4	2.640	
Isovaleric 10 mM	Adsorption	4627.5	1.038	1.001
	Desorption	3840.5	0.858	
Hexanoic 35 mM	Adsorption	4607.6	3.248	3.775
	Desorption	4613.7	3.252	
Hexanoic 10 mM	Adsorption	9312.8	2.020	2.208
	Desorption	8411.1	1.823	

- Binary breakthrough curves of acetic acid with isobutyric, valeric, isovaleric, and hexanoic acids

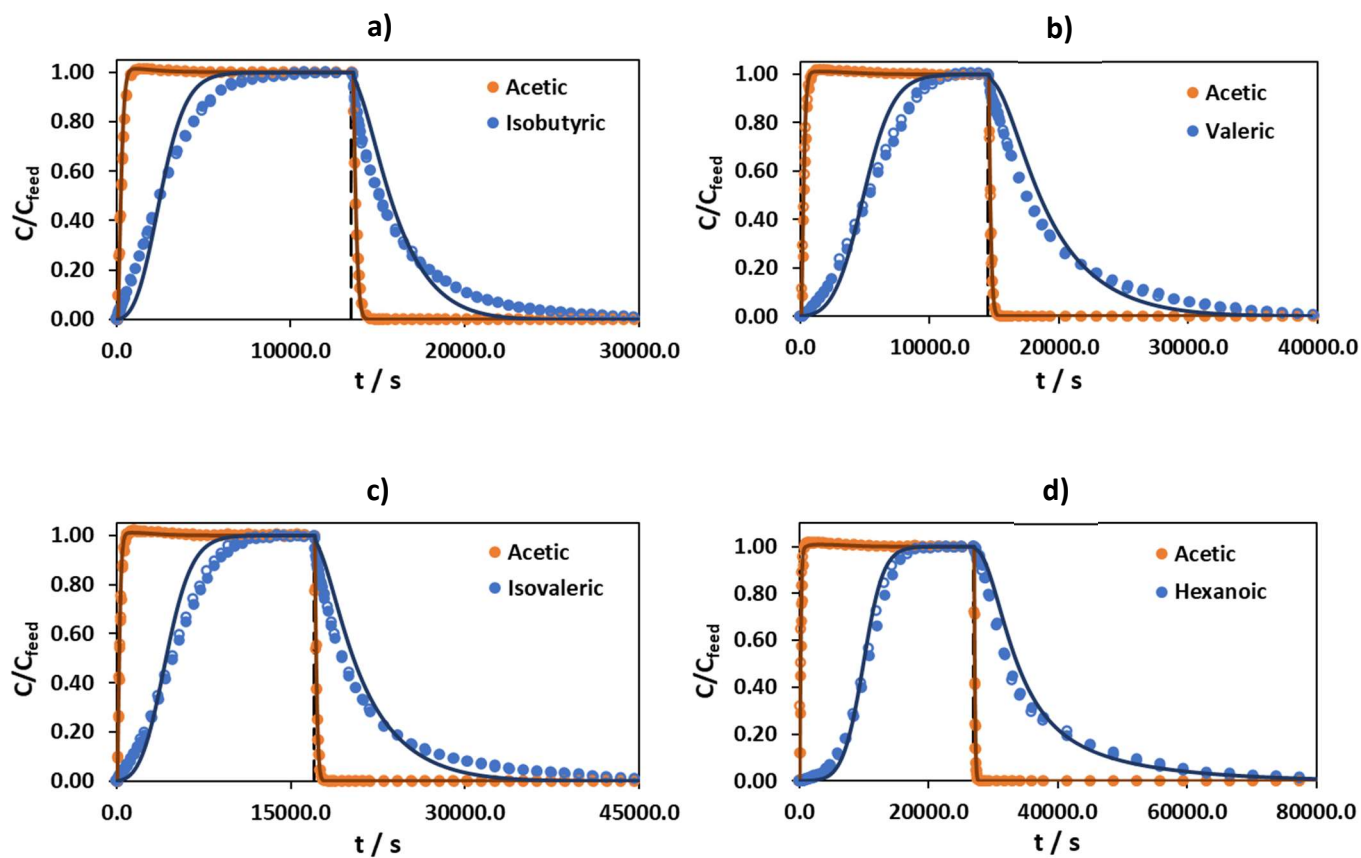


Figure S6. Breakthrough curve of a) acetic/isobutyric acids, b) acetic/valeric acids, c) acetic/isovaleric acids, and d) acetic/hexanoic acids on the Amberlite XAD-4 resin, with a feed concentration of 50/10 mM. The points represent experimental data (open and closed symbols correspond to duplicate assays), and the full lines are the respective model simulation. The vertical dark dashed line represents the start of the desorption step.

Table S2. Stoichiometric time and adsorption capacity of volatile fatty acids for the binary solutions breakthrough curves (acetic/isobutyric acids, acetic/valeric acids, acetic/isovaleric acids, acetic/hexanoic acids).

Acid		t_{st} / s	$q_{col} / \text{mmol} \cdot \text{g}_{\text{ads}}^{-1}$	$q^* / \text{mmol} \cdot \text{g}_{\text{ads}}^{-1}$
		VFA1 / VFA2	VFA1 / VFA2	VFA1 / VFA2
VFA1 -Acetic / VFA2 -Isobutyric	Adsorption	309.2 / 2879.1	0.255 / 0.670	0.172 / 0.605
	Desorption	279.2 / 2741.7	0.220 / 0.637	
VFA1 -Acetic / VFA2 -Valeric	Adsorption	254.2 / 5314.6	0.192 / 1.216	0.150 / 1.136
	Desorption	223.1 / 4821.4	0.156 / 1.101	
VFA1 -Acetic / VFA2 -Isovaleric	Adsorption	259.3 / 4970.0	0.196 / 1.137	0.155 / 1.002
	Desorption	235.2 / 4480.5	0.168 / 1.023	
VFA1 -Acetic / VFA2 -Hexanoic	Adsorption	190.5 / 10222.4	0.116 / 2.315	0.115 / 2.247
	Desorption	191.7 / 9562.2	0.118 / 2.164	

- Binary breakthrough curves of propanoic acid with isobutyric, valeric, isovaleric, and hexanoic acids

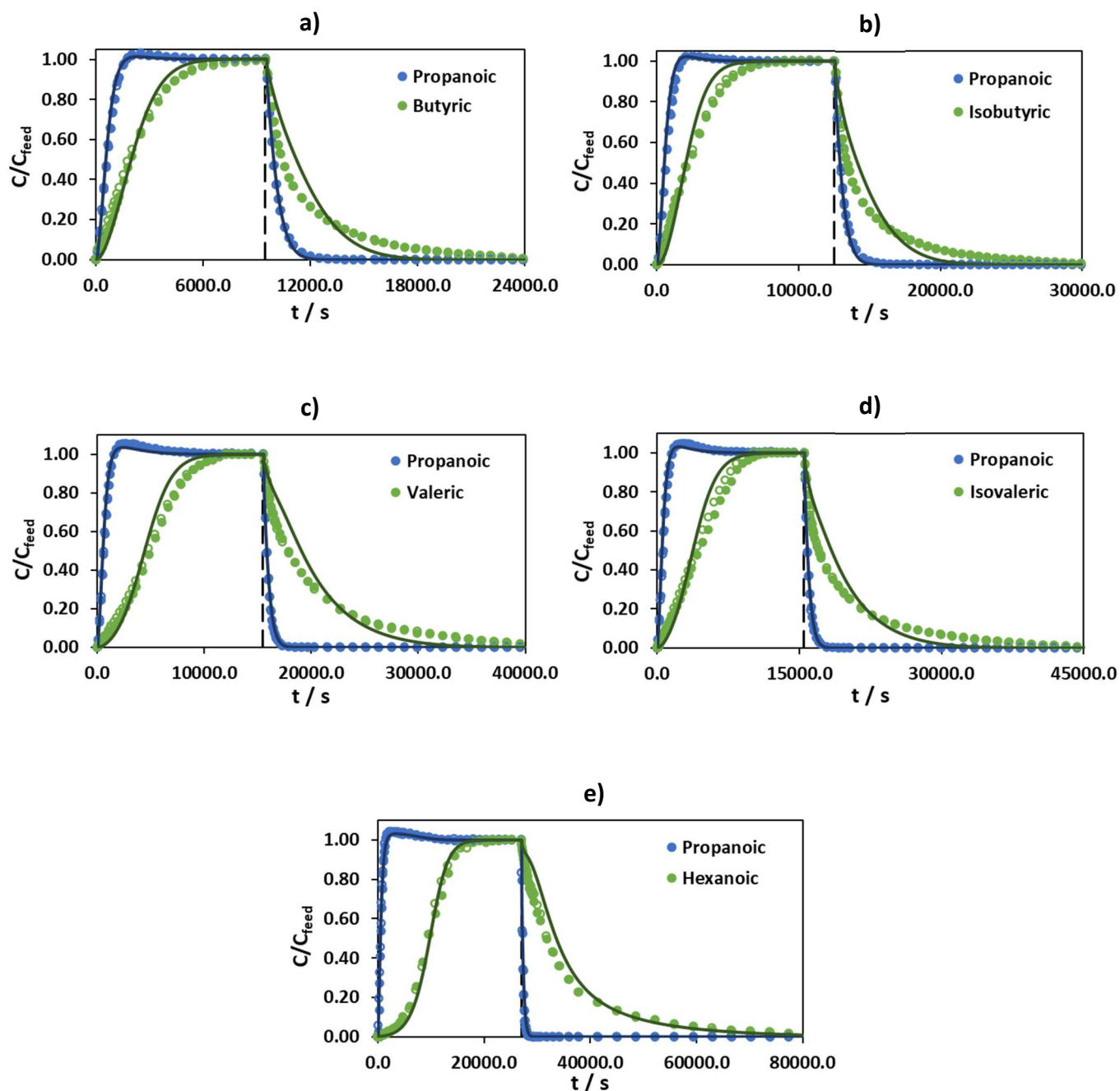


Figure S7. Breakthrough curve of a) propanoic/isobutyric acids, b) propanoic/isobutyric acids, c) propanoic/valeric acids, d) propanoic/isovaleric acids, and e) propanoic/hexanoic acids on the Amberlite XAD-4 resin, with a feed concentration of 50/10 mM. The points represent experimental data (open and closed symbols correspond to duplicate assays), and the full lines are the respective model simulation. The vertical dark dashed line represents the start of the desorption step.

Table S3. Stoichiometric time and adsorption capacity of volatile fatty acids for the binary solutions breakthrough curves (propanoic/butyric acids, propanoic/isobutyric acids, propanoic/valeric acids, propanoic/isovaleric acids, propanoic/hexanoic acids).

Acid		t_{st} / s	$q_{col} / \text{mmol} \cdot \text{g}_{\text{ads}}^{-1}$	$q^* / \text{mmol} \cdot \text{g}_{\text{ads}}^{-1}$
		VFA1 / VFA2	VFA1 / VFA2	VFA1 / VFA2
VFA1 -Propanoic / VFA2 -Butyric	Adsorption	643.4 / 2284.9	0.667 / 0.512	0.608 / 0.483
	Desorption	631.5 / 2160.2	0.653 / 0.483	
VFA1 -Propanoic / VFA2 -Isobutyric	Adsorption	655.6 / 2546.9	0.678 / 0.592	0.560 / 0.510
	Desorption	629.5 / 2237.3	0.647 / 0.517	
VFA1 -Propanoic / VFA2 -Valeric	Adsorption	442.8 / 4987.0	0.425 / 1.149	0.473 / 1.043
	Desorption	464.6 / 4525.4	0.451 / 1.041	
VFA1 -Propanoic / VFA2 -Isovaleric	Adsorption	493.1 / 4421.1	0.484 / 1.003	0.488 / 0.894
	Desorption	483.3 / 3934.1	0.472 / 0.890	
VFA1 -Propanoic / VFA2 -Hexanoic	Adsorption	339.6 / 9518.7	0.298 / 2.150	0.313 / 2.184
	Desorption	328.4 / 8803.4	0.284 / 1.987	
VFA1 -Butyric / VFA2 - Isobutyric	Adsorption	2282.1 / 2198.6	0.515 / 0.509	0.453 / 0.523
	Desorption	2111.9 / 2162.6	0.475 / 0.501	
VFA1 -Valeric / VFA2 -Isovaleric	Adsorption	4242.2 / 3380.9	0.956 / 0.770	0.880 / 0.741
	Desorption	3915.7 / 3026.3	0.881 / 0.686	