# Supplementary material

**for**

**Prediction of breakthrough curves for multicomponent adsorption in a fixed-bed column using logistic and Gompertz functions**

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Prior to establishment of the empirical multicomponent breakthrough models, it is necessary to introduce the basic information of the logistic and Gompertz functions. The logistic function is given as:

|  |  |
| --- | --- |
|  | (1) |

The first and second derivatives of Eq. (1) with respect to *x* are given as:

|  |  |
| --- | --- |
|  | (2) |
|  | (3) |

The second derivative is equal to zero at the inflection point *x* = *xi*.

|  |  |
| --- | --- |
|  | (4) |

The slope of the curve can be obtained by calculating the first derivative at *x* = *xi*.

|  |  |
| --- | --- |
|  | (5) |

The description of the tangent line through the inflection point is:

|  |  |
| --- | --- |
|  | (6) |

The Gompertz function is given as:

|  |  |
| --- | --- |
|  | (7) |

The first and second derivatives of Eq. (7) with respect to *x* are given as:

|  |  |
| --- | --- |
|  | (8) |
|  | (9) |

The second derivative is equal to zero at the inflection point *x* = *xi*.

|  |  |
| --- | --- |
|  | (10) |

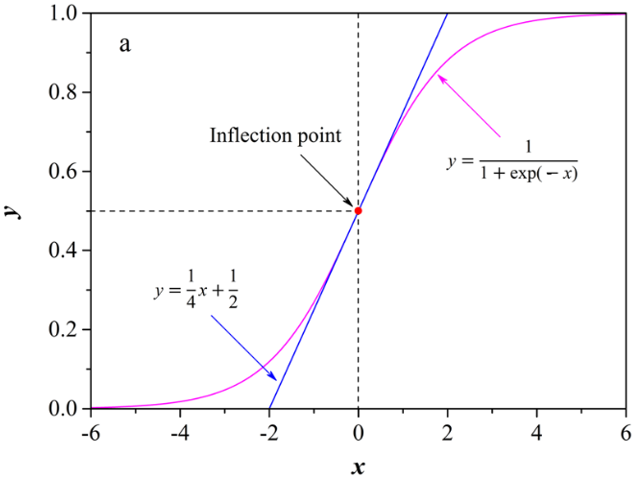
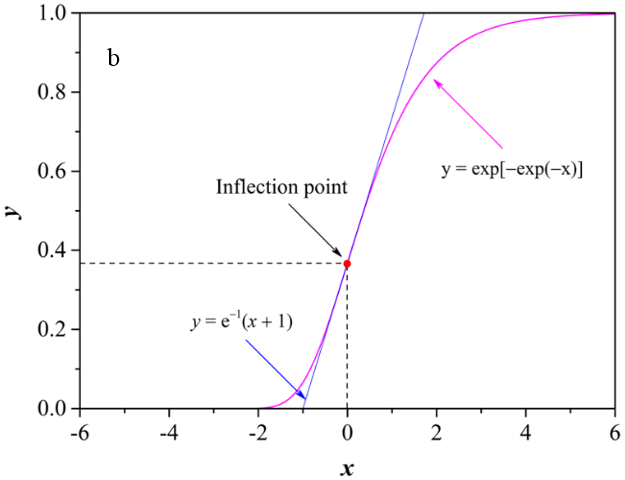
The slope of the curve can be obtained by calculating the first derivative at *x* = *xi*.

|  |  |
| --- | --- |
|  | (11) |

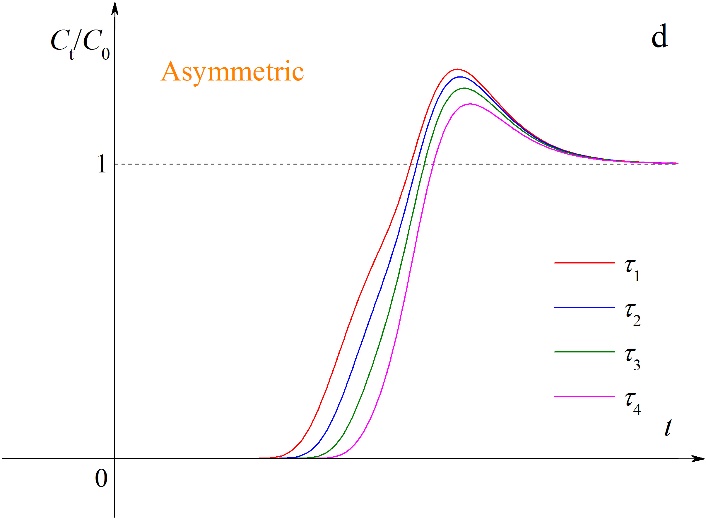
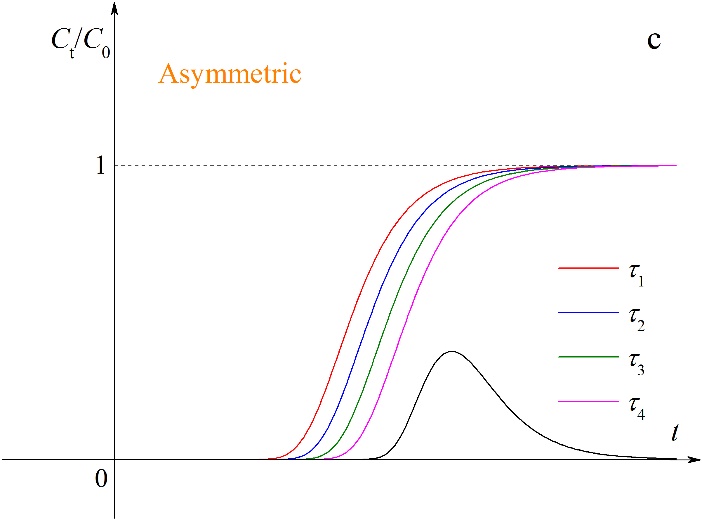
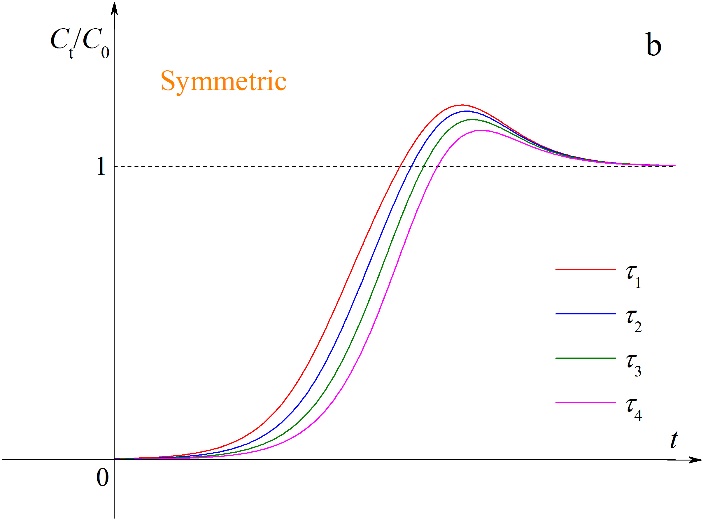
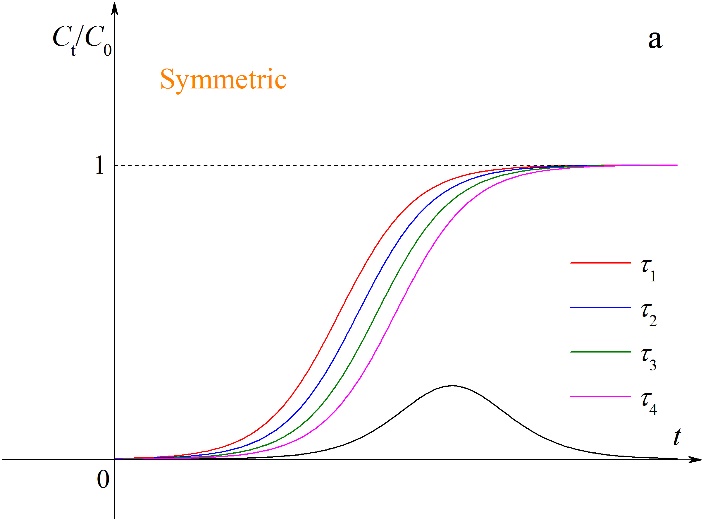
The description of the tangent line through the inflection point is:

|  |  |
| --- | --- |
|  | (12) |

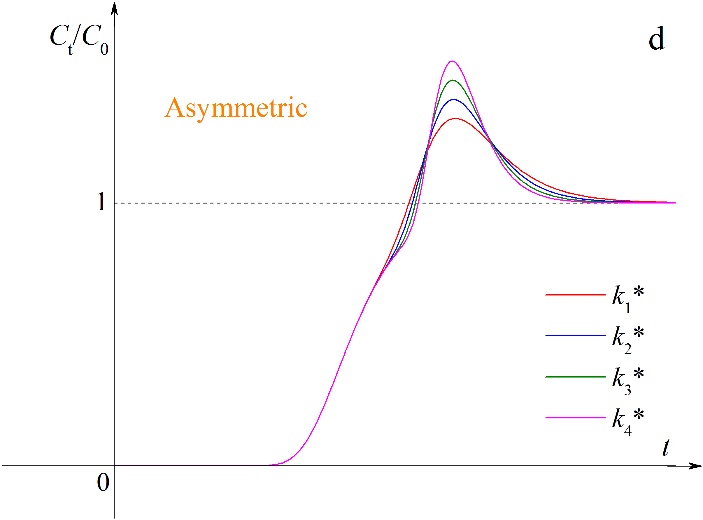
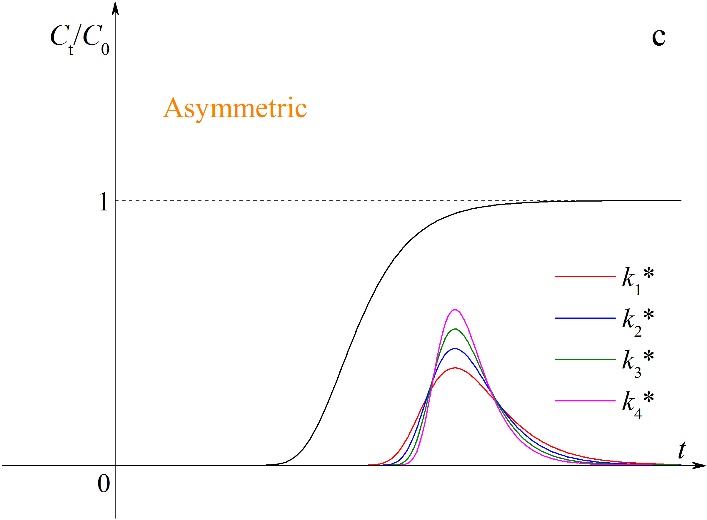
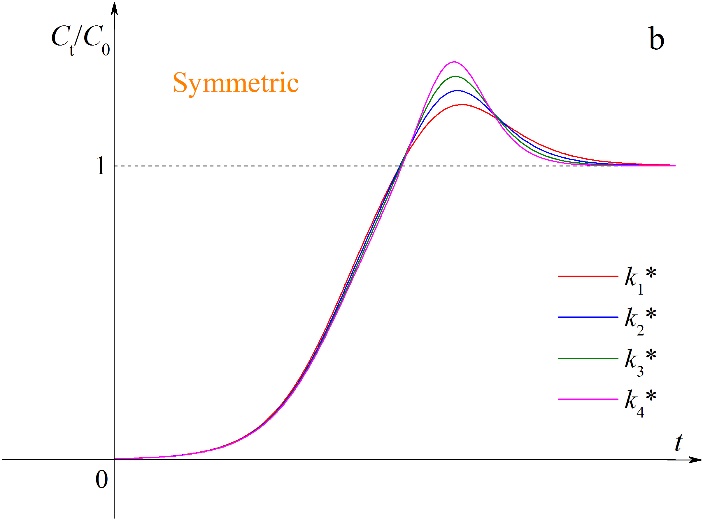
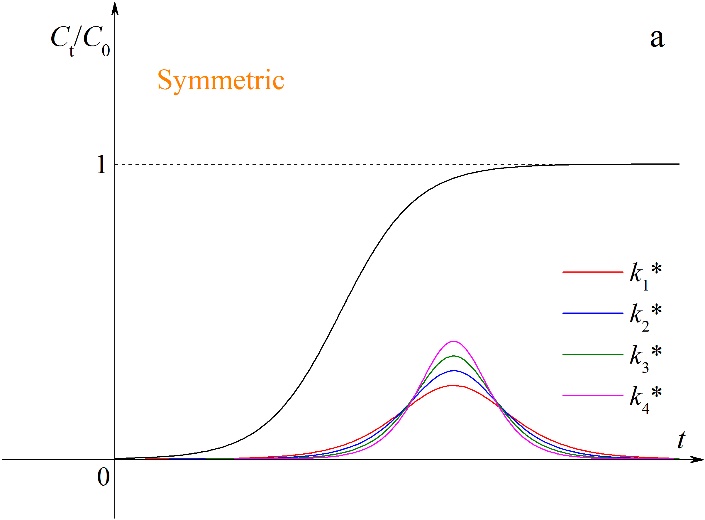
The mathematical characteristics of the logistic and Gompertz functions are depicted in Fig. S1. One can readily see that the logistic and Gompertz functions represent asymptotic and asymptotic S-shaped curves, respectively. The two function curves are well consistent with the breakthrough curve. Thus, the logistic and Gompertz functions can be appropriately transformed to describe the breakthrough curves.

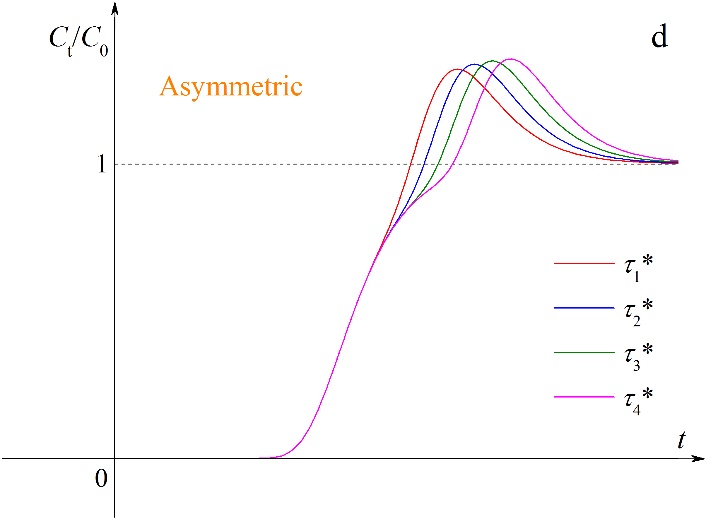
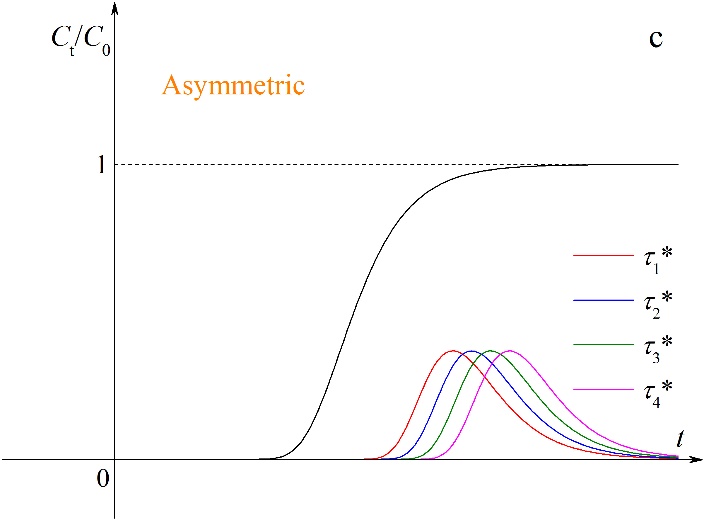
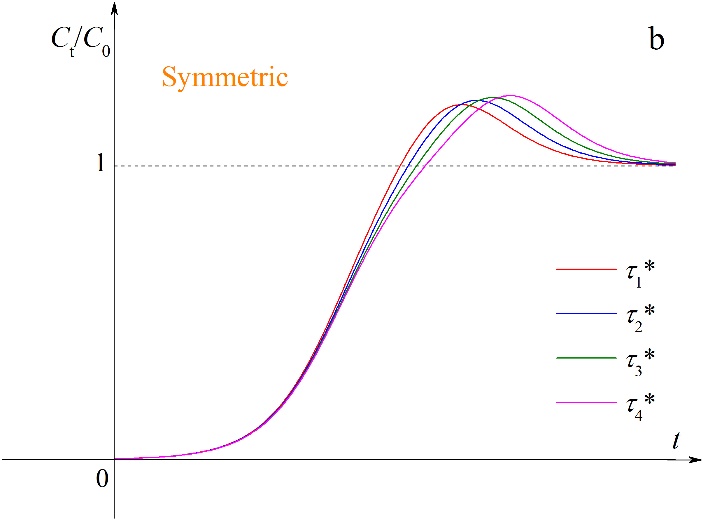
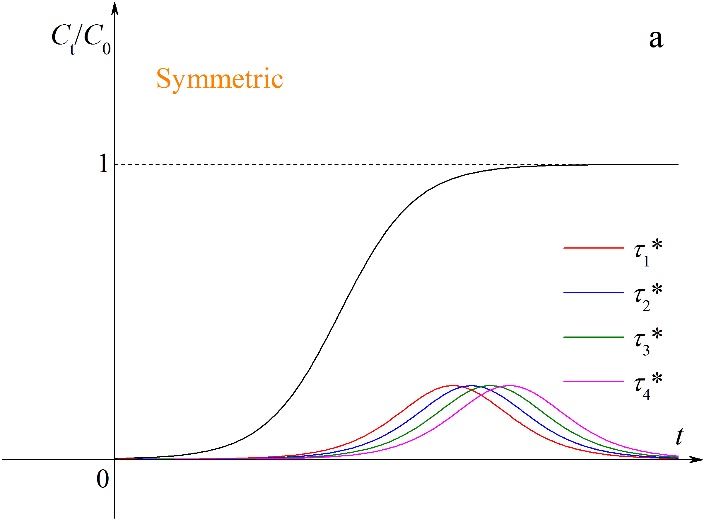
**Fig. S1.** Mathematical characteristics of (a) logistic and (b) Gompertz functions.



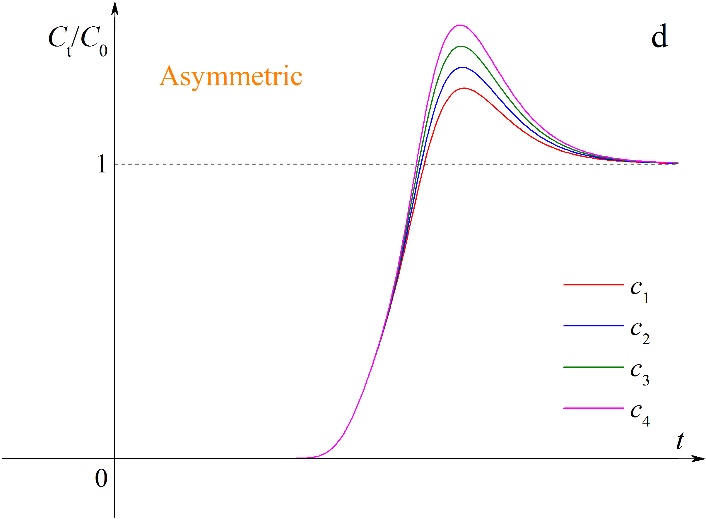
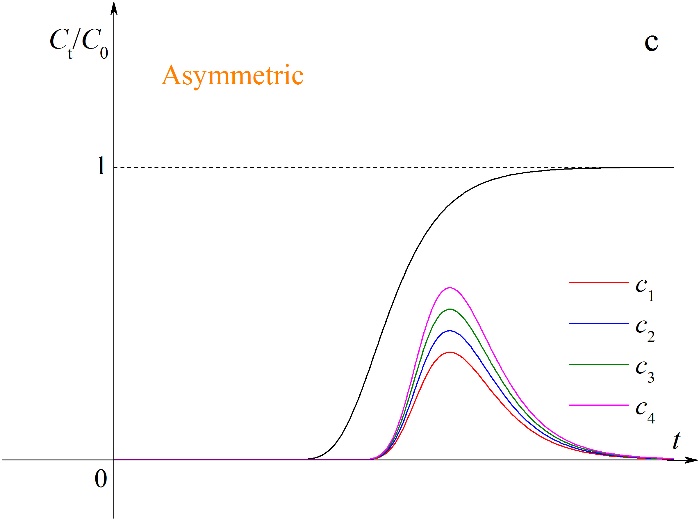
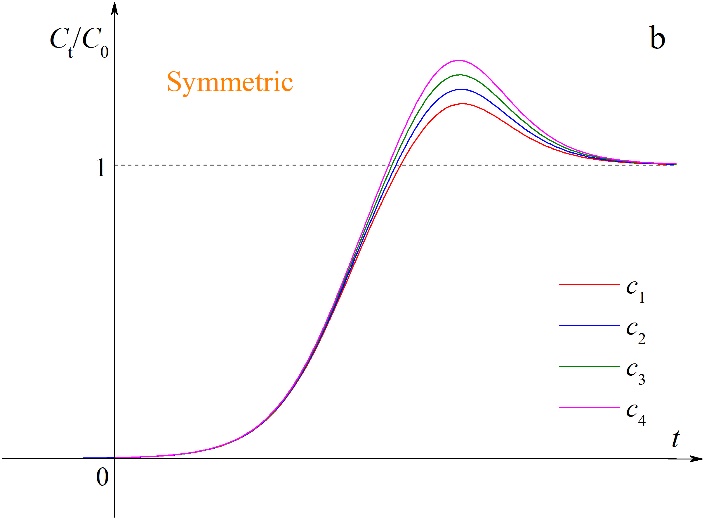
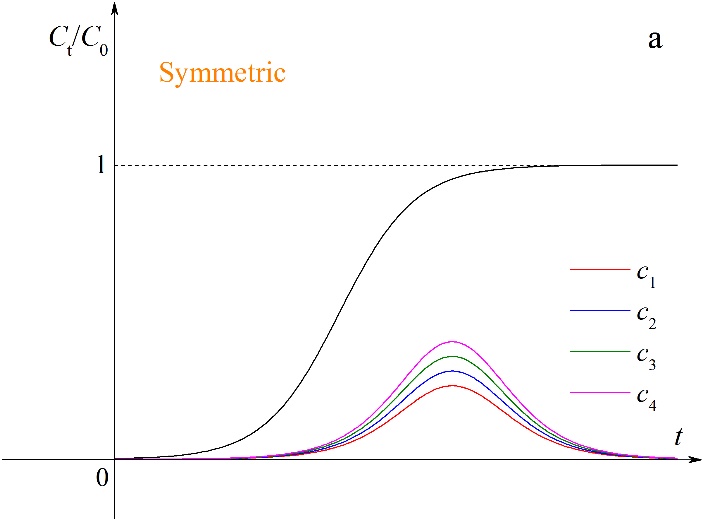
**Fig. S2.** Effects of the parameter *τ* on breakthrough curves before and after superposition (*τ*1 < *τ*2 < *τ*3 < *τ*4).



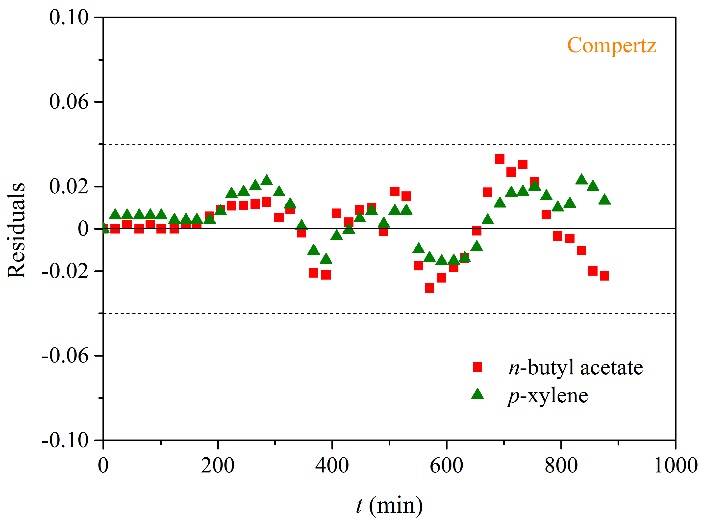
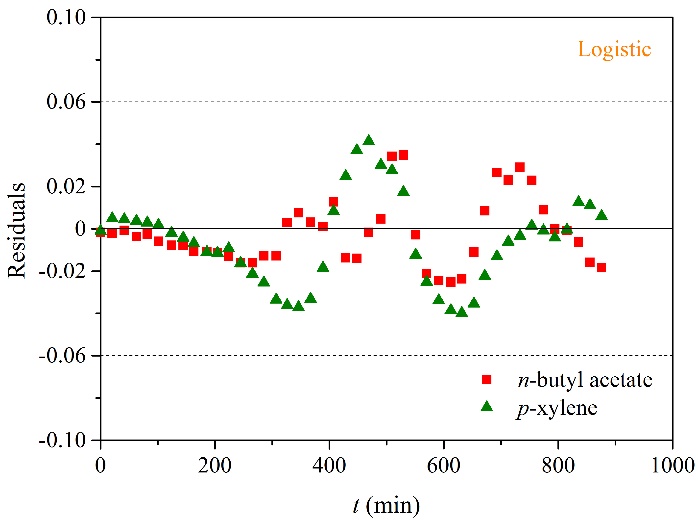
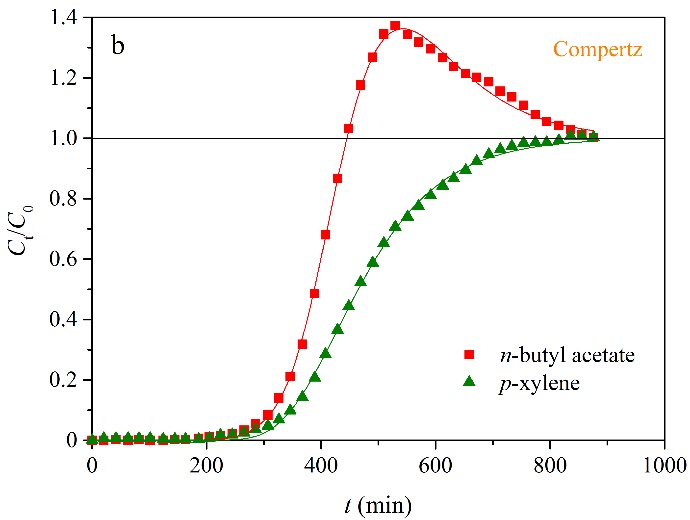
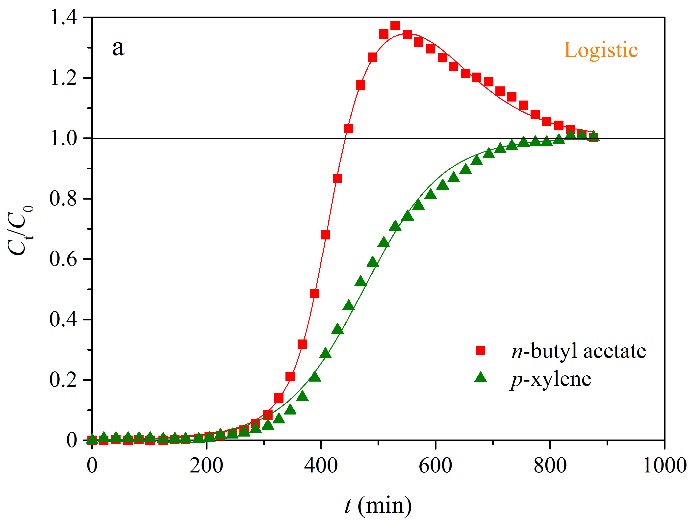
**Fig. S3.** Effects of the parameter *k*\* on breakthrough curves before and after superposition (*k*1\* < *k*2\* < *k*3\* < *k*4\*).



**Fig. S4.** Effects of the parameter *τ*\* on breakthrough curves before and after superposition (*τ*1\* < *τ*2\* < *τ*3\* < *τ*4\*).



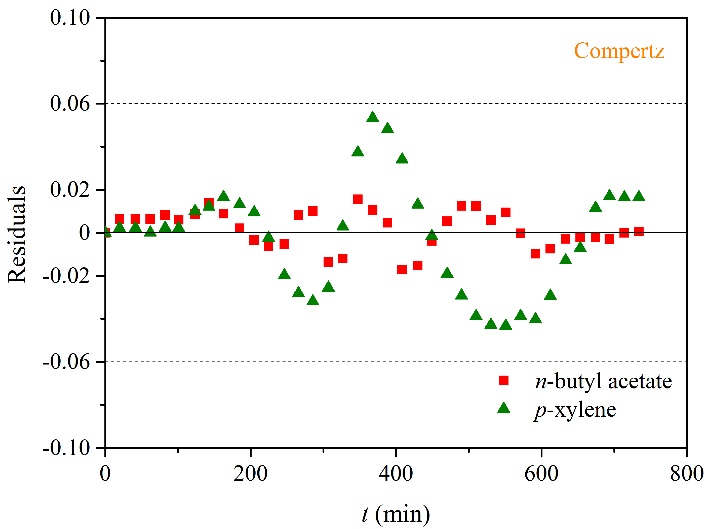
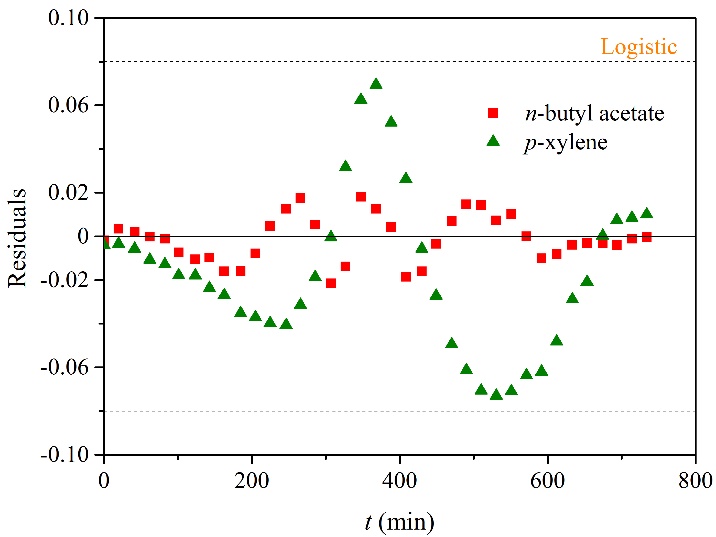
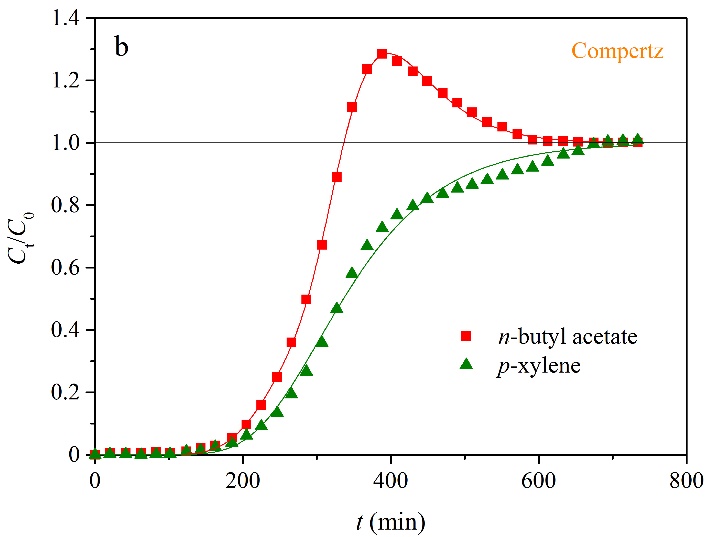
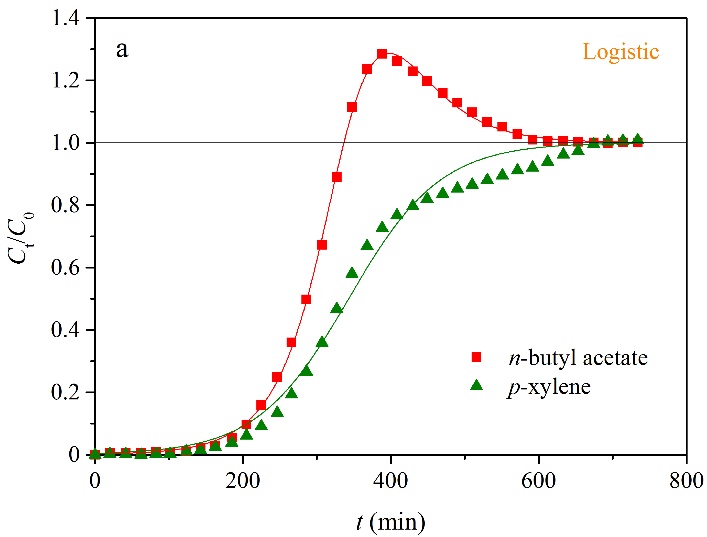
**Fig. S5.** Effects of the parameter *c* on breakthrough curves before and after superposition (*c*1 < *c*2 < *c*3 < *c*4).



**Fig. S6.** Breakthrough curves and residual plots of *n*-butyl acetate and *p*-xylene binary system (0.45 Ndm3 min−1): (a) Eq. (7) and (b) Eq. (8).

**Table S1** Fitting results of *n*-butyl acetate and *p*-xylene binary system (0.45 Ndm3 min−1).

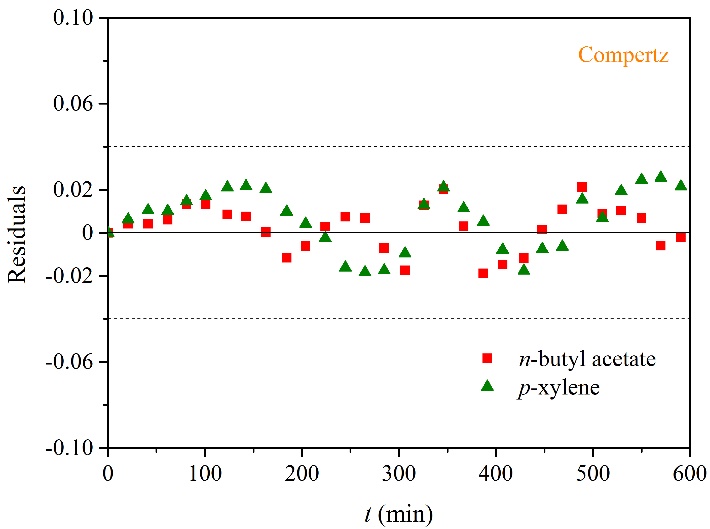
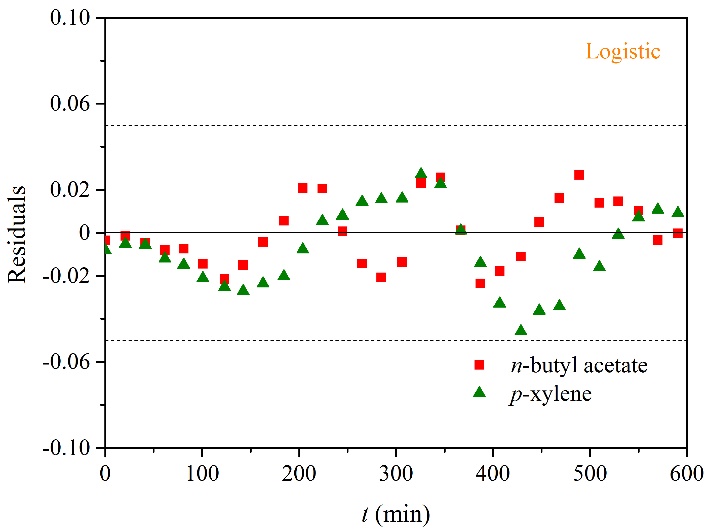
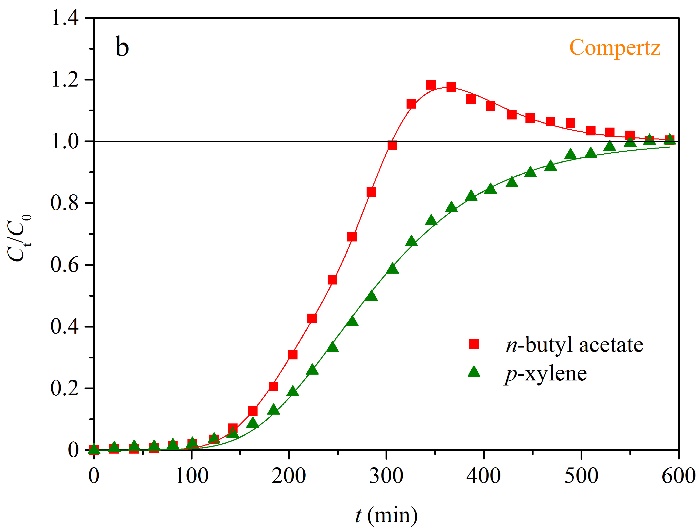
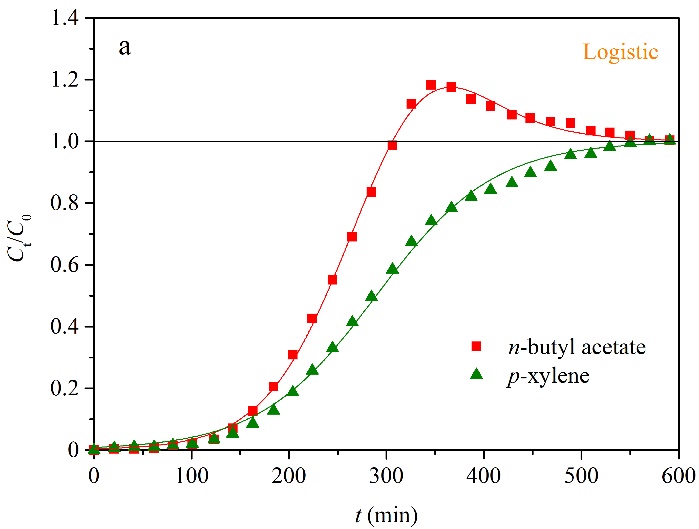
|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Models | Adsorbate | *k* (min−1) | *τ* (min) | *k*\* (min−1) | *τ*\* (min−1) | *c* | *R*2 |
| Logistic | *n*-butyl acetate | 3.47 × 10−2 | 410 | 1.25 × 10−2 | 540 | 114 | 0.9992 |
|  | *p*-xylene | 1.45 × 10−2 | 474 | 0 | 0 | 0 | 0.9973 |
| Gompertz | *n*-butyl acetate | 9.02 × 10−3 | 414 | 1.03 × 10−2 | 505 | 179 | 0.9993 |
|  | *p*-xylene | 1.02 × 10−2 | 429 | 0 | 0 | 0 | 0.9991 |



**Fig. S7.** Breakthrough curves and residual plots of *n*-butyl acetate and *p*-xylene binary system (0.75 Ndm3 min−1): (a) Eq. (7) and (b) Eq. (8).

**Table S2** Fitting results of *n*-butyl acetate and *p*-xylene binary system (0.75 Ndm3 min−1).

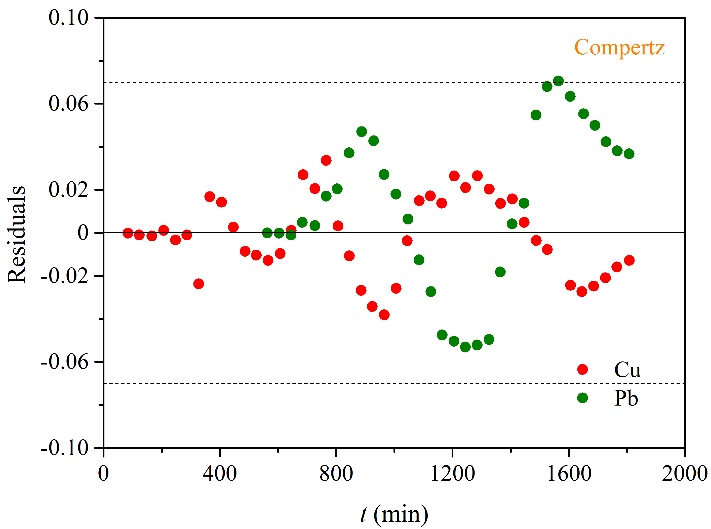
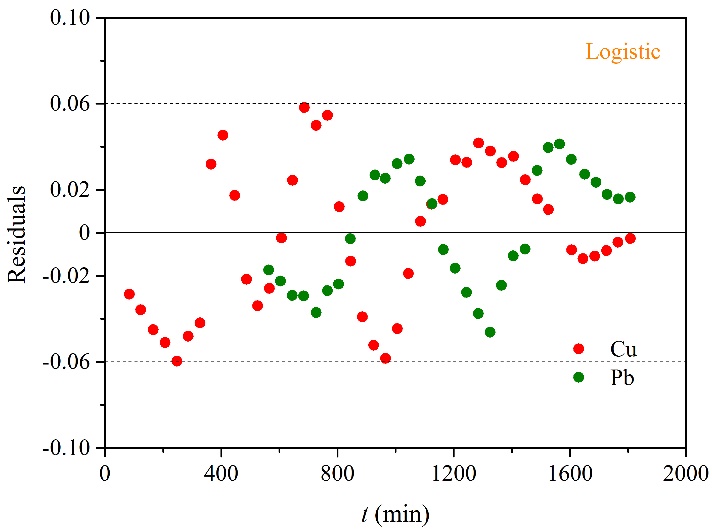
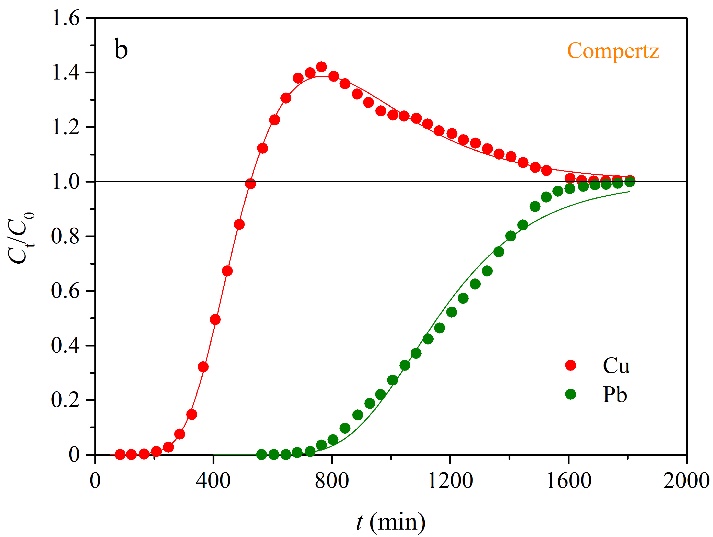
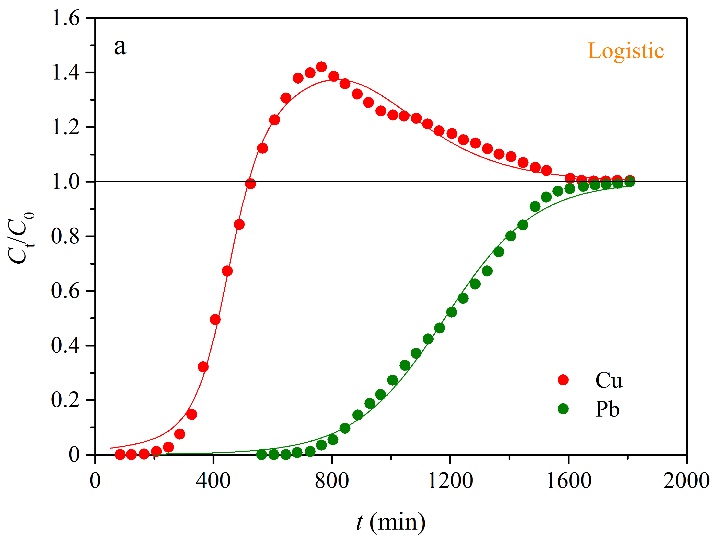
|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Models | Adsorbate | *k* (min−1) | *τ* (min) | *k*\* (min−1) | *τ*\* (min−1) | *c* | *R*2 |
| Logistic | *n*-butyl acetate | 3.26 × 10−2 | 326 | 1.90 × 10−2 | 357 | 90.8 | 1.000 |
|  | *p*-xylene | 1.61 × 10−2 | 343 | 0 | 0 | 0 | 0.991 |
| Gompertz | *n*-butyl acetate | 1.24 × 10−2 | 272 | 1.66 × 10−2 | 378 | 81.3 | 1.000 |
|  | *p*-xylene | 1.11 × 10−2 | 303 | 0 | 0 | 0 | 0.996 |



**Fig. S8.** Breakthrough curves and residual plots of *n*-butyl acetate and *p*-xylene binary system (0.90 Ndm3 min−1): (a) Eq. (7) and (b) Eq. (8).

**Table S3** Fitting results of *n*-butyl acetate and *p*-xylene binary system (0.90 Ndm3 min−1).

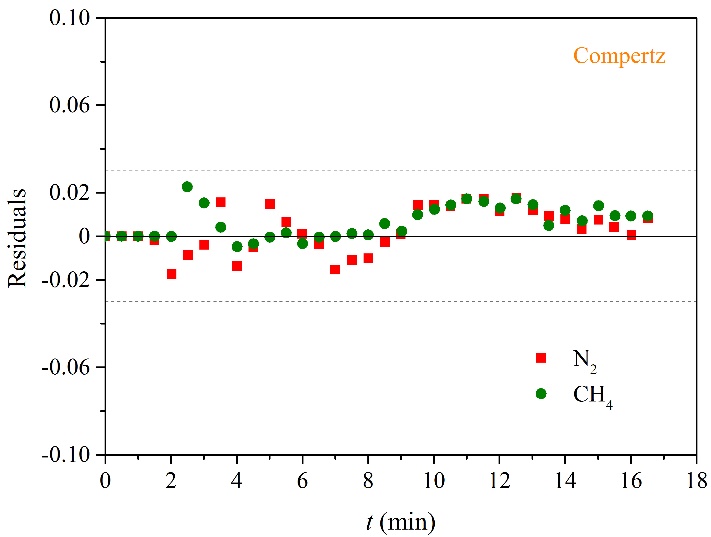
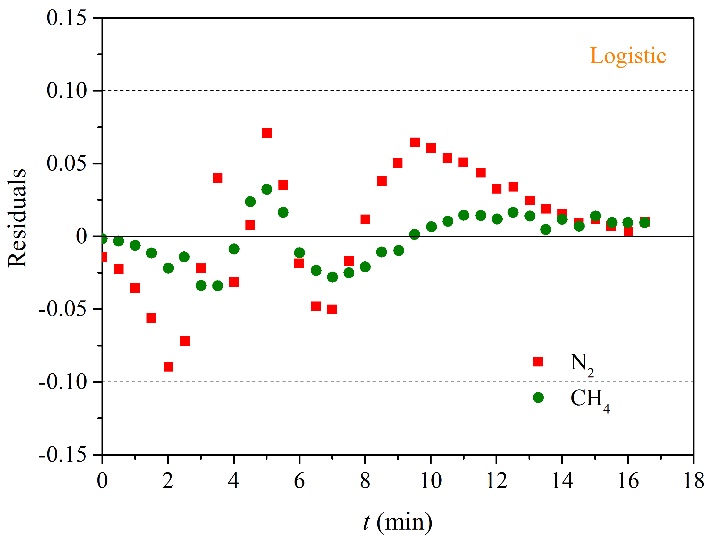
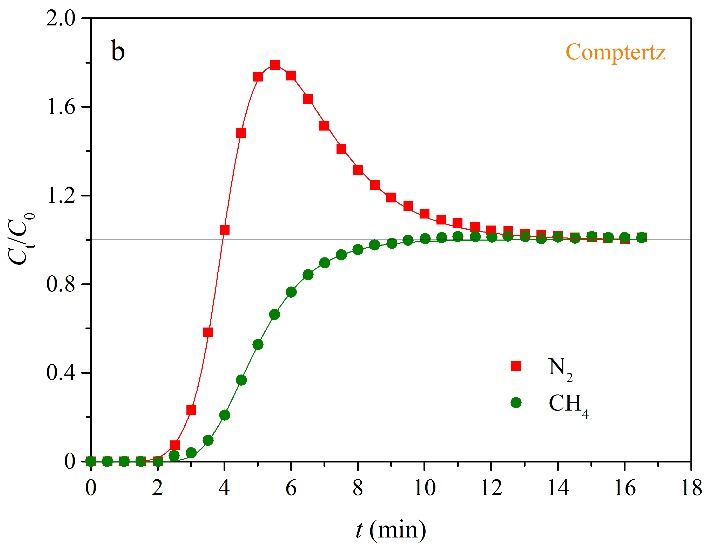
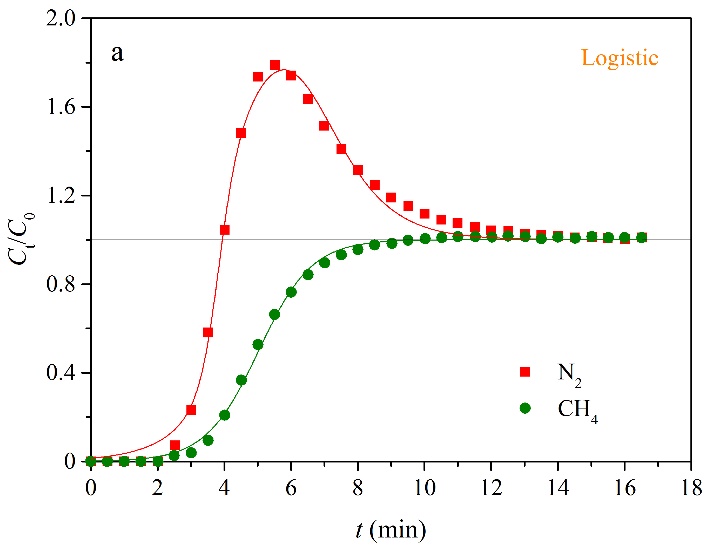
|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Models | Adsorbate | *k* (min−1) | *τ* (min) | *k*\* (min−1) | *τ*\* (min−1) | *c* | *R*2 |
| Logistic | *n*-butyl acetate | 2.30 × 10−2 | 253 | 2.23 × 10−2 | 340 | 47.6 | 0.999 |
|  | *p*-xylene | 1.66 × 10−2 | 290 | 0 | 0 | 0 | 0.997 |
| Gompertz | *n*-butyl acetate | 1.43 × 10−2 | 214 | 1.77 × 10−2 | 342 | 46.8 | 0.999 |
|  | *p*-xylene | 1.16 × 10−2 | 250 | 0 | 0 | 0 | 0.999 |



**Fig. S9.** Breakthrough curves and residual plots of Cu and Pb binary system: (a) Eq. (7) and (b) Eq. (8).

**Table S4** Fitting results of Cu and Pb binary system.

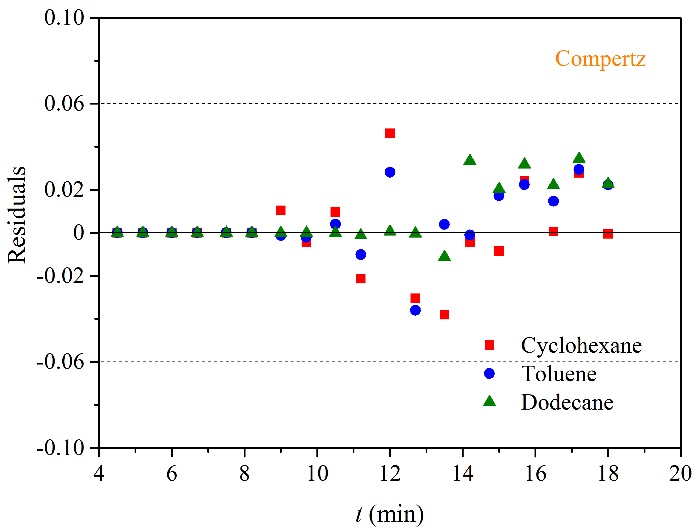
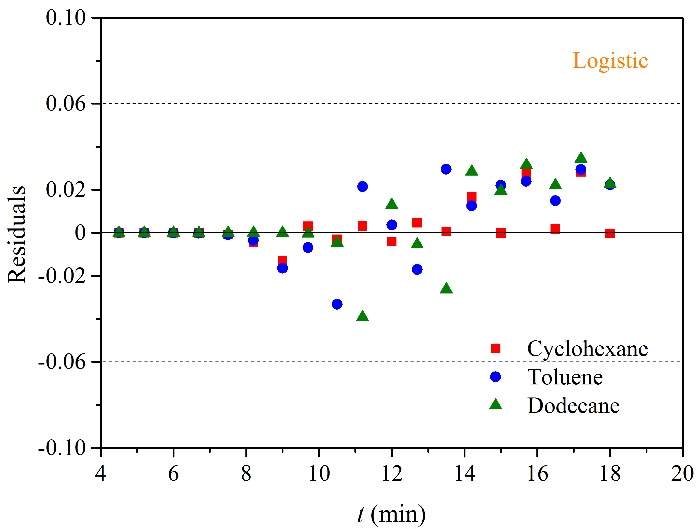
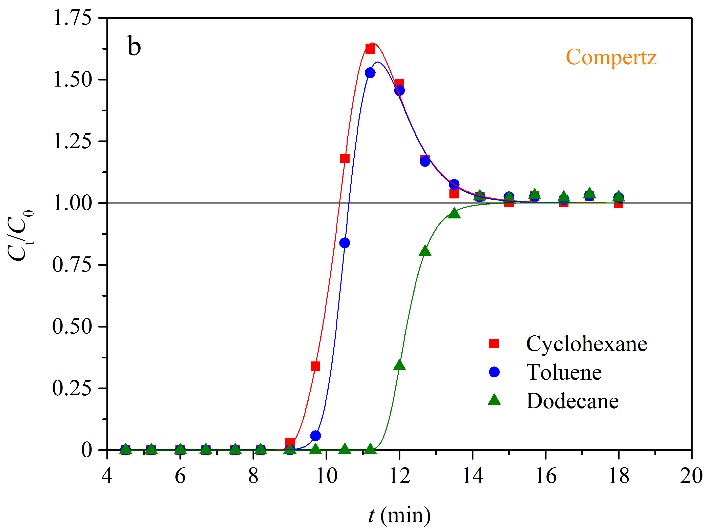
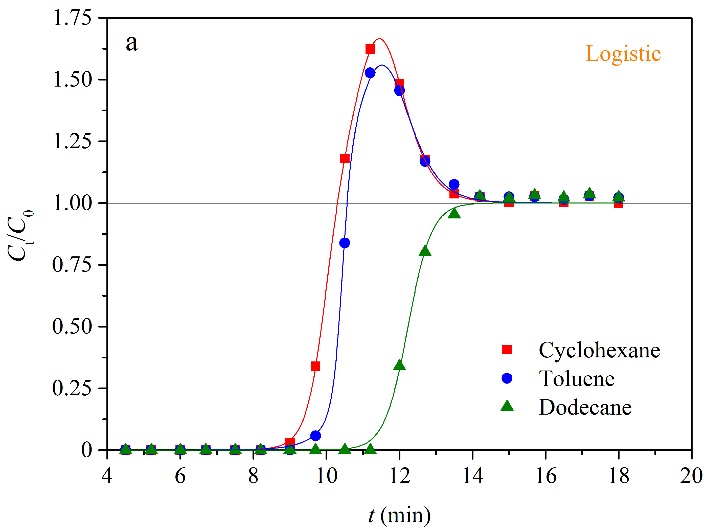
|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Models | Adsorbate | *k* (min−1) | *τ* (min) | *k*\* (min−1) | *τ*\* (min−1) | *c* | *R*2 |
| Logistic | Cu | 1.87 × 10−2 | 447 | 5.43 × 10−3 | 814 | 276 | 0.994 |
|  | Pb | 6.53 × 10−3 | 1182 | 0 | 0 | 0 | 0.995 |
| Gompertz | Cu | 8.94 × 10−3 | 421 | 3.85 × 10−3 | 704 | 313 | 0.998 |
|  | Pb | 4.49 × 10−3 | 1076 | 0 | 0 | 0 | 0.989 |



**Fig. S10.** Breakthrough curves and residual plots of N2 and CH4 binary system: (a) Eq. (7) and (b) Eq. (8).

**Table S5** Fitting results of N2 and CH4 binary system.

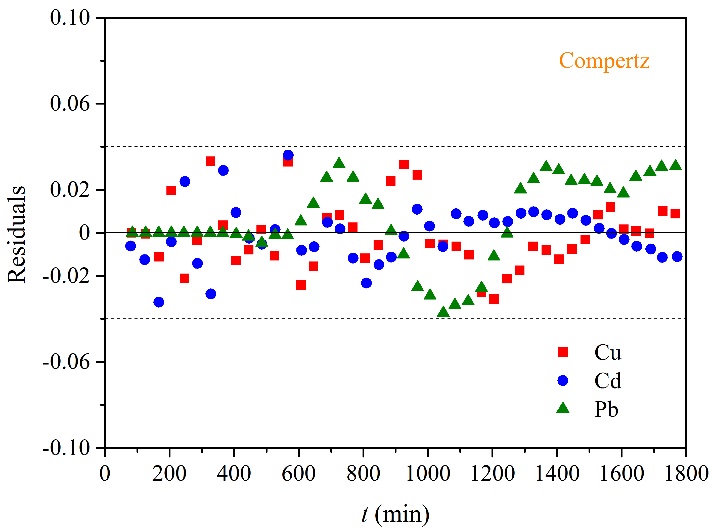
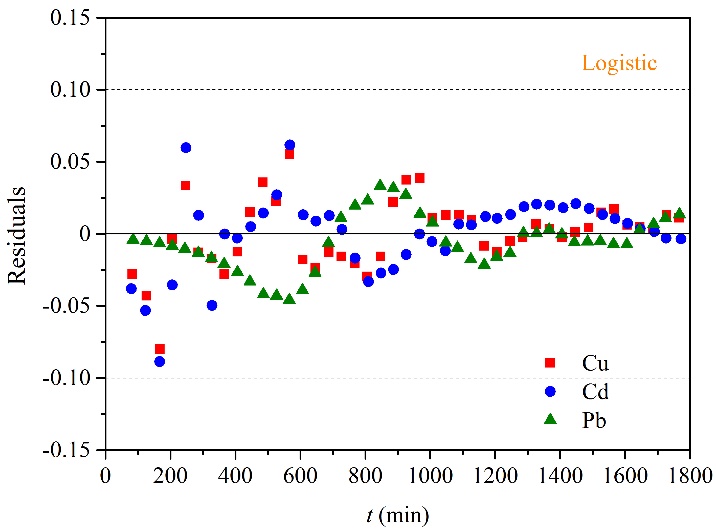
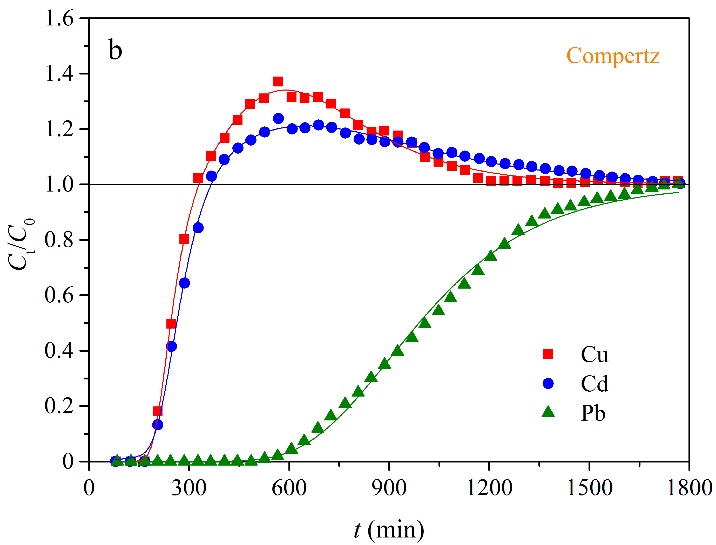
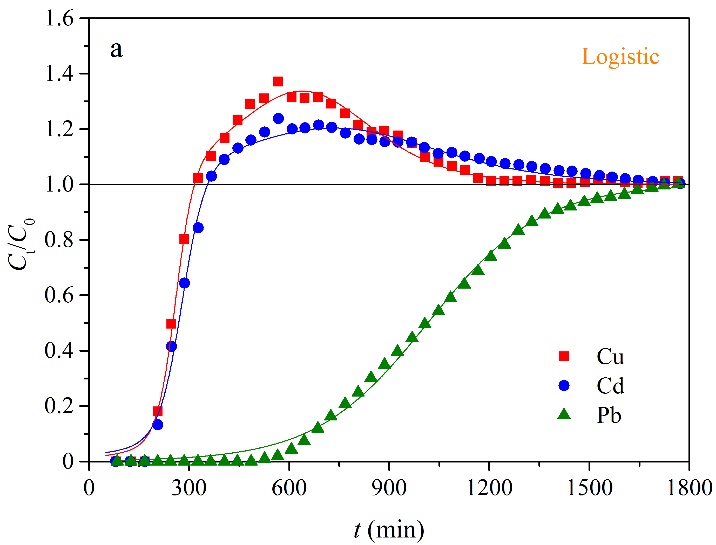
|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Models | Adsorbate | *k* (min−1) | *τ* (min) | *k*\* (min−1) | *τ*\* (min−1) | *c* | *R*2 |
| Logistic | Cu | 3.59 | 3.83 | 0.93 | 5.77 | 3.31 | 0.994 |
|  | Pb | 1.26 | 5.03 | 0 | 0 | 0 | 0.998 |
| Gompertz | Cu | 1.62 | 3.98 | 0.63 | 5.08 | 3.86 | 1.000 |
|  | Pb | 0.88 | 4.51 | 0 | 0 | 0 | 0.999 |



**Fig. S11.** Breakthrough curves and residual plots of cyclohexane, toluene and dodecane ternary adsorption system: (a) Eq. (7) and (b) Eq. (8).

**Table S6** Fitting results of cyclohexane, toluene and dodecane ternary adsorption systems.

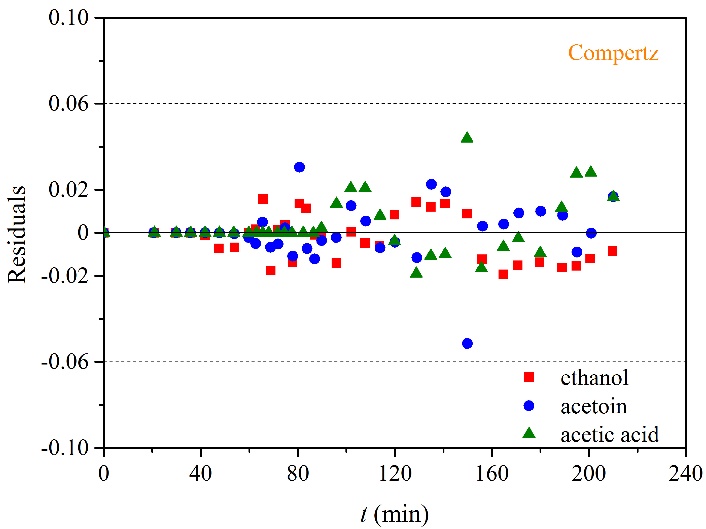
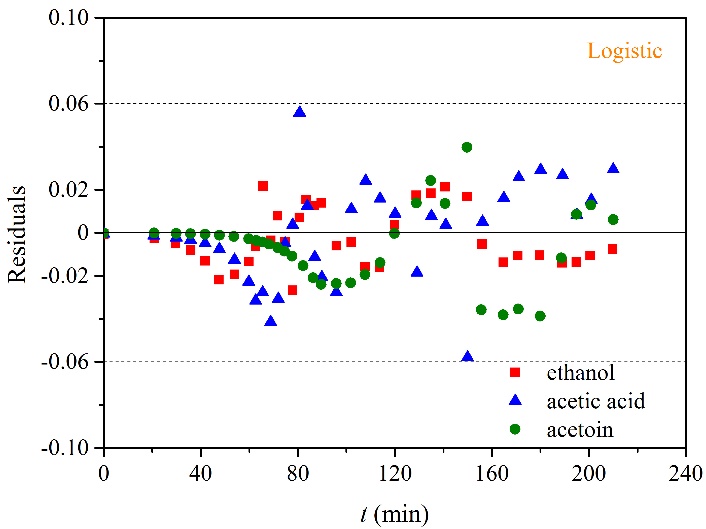
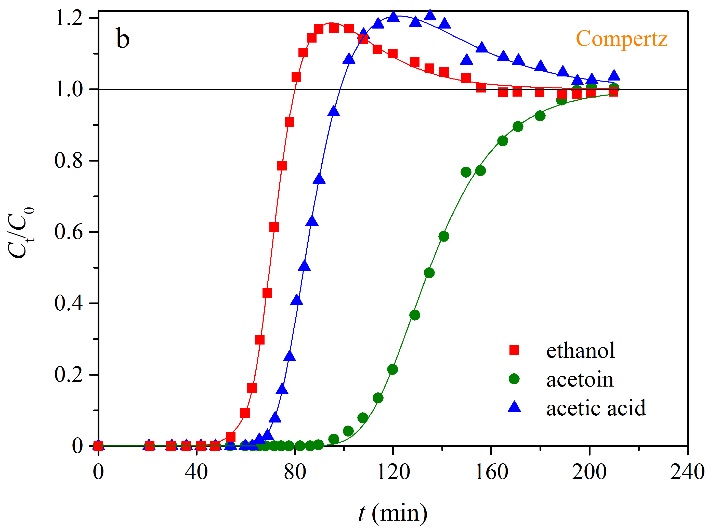
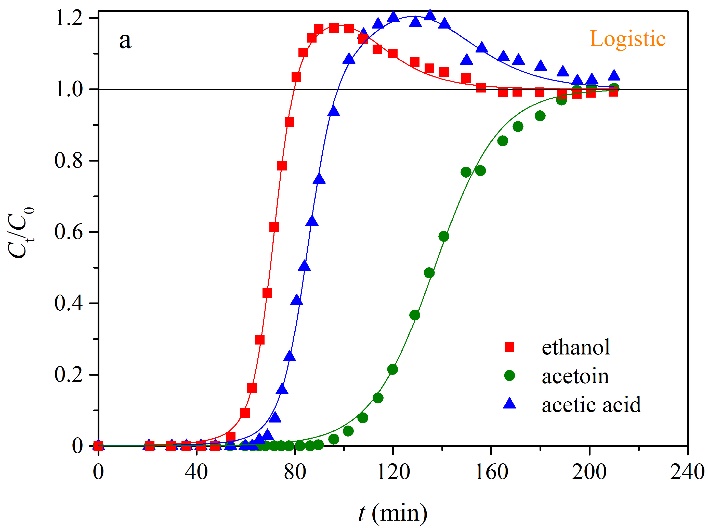
|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Models | Adsorbate | *k* (min−1) | *τ* (min) | *k*\* (min−1) | *τ*\* (min−1) | *c* | *R*2 |
| Logistic | Cyclohexane | 3.90 | 9.96 | 2.07 | 11.4 | 1.29 | 1.000 |
|  | Toluene | 7.96 | 10.4 | 1.94 | 11.5 | 591 | 0.999 |
|  | Dodecane | 3.09 | 12.2 | 0 | 0 | 0 | 0.998 |
| Gompertz | Cyclohexane | 1.89 | 9.75 | 1.37 | 11.2 | 1.40 | 0.999 |
|  | Toluene | 1.09 | 10.7 | 1.33 | 11.2 | 2.04 | 0.999 |
|  | Dodecane | 2.28 | 12.0 | 0 | 0 | 0 | 0.999 |



**Fig. S12.** Breakthrough curves and residual plots of Cu, Cd and Pb ternary system: (a) Eq. (7) and (b) Eq. (8).

**Table S7** Fitting results of Cu, Cd and Pb ternary systems.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Models | Adsorbate | *k* (min−1) | *τ* (min) | *k*\* (min−1) | *τ*\* (min−1) | *c* | *R*2 |
| Logistic | Cu | 3.61 × 10−2 | 259 | 7.02 × 10−3 | 639 | 192 | 0.995 |
|  | Cd | 2.86 × 10−2 | 279 | 4.69 × 10−3 | 732 | 173 | 0.994 |
|  | Pb | 5.91 × 10−3 | 1015 | 0 | 0 | 0 | 0.997 |
| Gompertz | Cu | 2.40 × 10−2 | 232 | 4.92 × 10−3 | 589 | 188 | 0.998 |
|  | Cd | 1.81 × 10−2 | 252 | 3.29 × 10−3 | 645 | 175 | 0.998 |
|  | Pb | 4.06 × 10−3 | 899 | 0 | 0 | 0 | 0.997 |



**Fig. S13.** Breakthrough curves and residual plots of ethanol, acetoin and acetic acid ternary adsorption system: (a) Eq. (7) and (b) Eq. (8).

**Table S8** Fitting results of ethanol, acetoin and acetic acid ternary adsorption systems.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Models | Adsorbate | *k* (min−1) | *τ* (min) | *k*\* (min−1) | *τ*\* (min−1) | *c* | *R*2 |
| Logistic | Ethanol | 0.23 | 71.3 | 7.36 × 10−2 | 97.1 | 9.85 | 0.999 |
|  | Acetoin | 0.18 | 85.2 | 6.00 × 10−2 | 128 | 13.7 | 0.998 |
|  | Acetic acid | 7.62 × 10−2 | 137 | 0 | 0 | 0 | 0.998 |
| Gompertz | Ethanol | 0.13 | 70.9 | 5.17 × 10−2 | 80.5 | 13.7 | 0.999 |
|  | Acetoin | 9.99 × 10−2 | 82.3 | 3.68 × 10−2 | 115 | 17.0 | 0.999 |
|  | Acetic acid | 5.18 × 10−2 | 128 | 0 | 0 | 0 | 0.999 |

**References**

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