**Simulation and risk assessment of typical antibiotics in the multi-media environment of the Yangtze River Estuary under tidal effect**

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**Table S1 Environmental parameters of the study area**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| symbol | definition | Study area values | Reference | symbol | definition | Study area values | Reference |
| A2 | Freshwater area(m2) | 2.84E+09 | \* | X23 | Solid volume fraction in Freshwater | 1.67E-04 | (Zhang et al., 2014) |
| A3 | Seawater area(m2) | 2.34E+09 | \* | X33 | Solid volume fraction in seawater | 1.67E-04 | (Zhang et al., 2014) |
| A4 | Soil area(m2) | 5.77E+09 | \* | O53 | Proportion of solid organic carbon in sediments | 1.98E-02 | (Zhang et al., 2015a) |
| A5 | Sediment area(m2) | 2.84E+09 | \* | O63 | Proportion of solid organic carbon in groundwater | 3.72E-02 | (Zhang et al., 2015a) |
| A6 | Groundwater area(m2) | 5.99E+09 | \* | Qt | advection velocity(m3/h) | 2.47E+06 | (Zhang et al., 2014) |
| h2 | depth of Freshwater(m) | 8.32 | (Zhang et al., 2015a) | T | Temperature(K) | 2.89E+02 | (Zhang et al., 2014) |
| h3 | depth of seawater(m) | 7 | (Zhang et al., 2015a) | Kw | Rainfall rate(m/h) | 1.20E-04 | (Zhang et al., 2015a) |

\*Access to remote sensing image data

**Table S2 Toxicological data of six antibiotics on algae in freshwater**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | CAS | *EC50*(mg/L) | *AF* | *PNEC* (ng/L) |
| OTC | 79-57-2 | 0.110 | 1000 | 110.0 |
| TC | 60-54-8 | 0.090 | 1000 | 90.0 |
| NOR | 70458-96-7 | 0.038 | 1000 | 38.0 |
| OFX | 82419-36-1 | 0.018 | 1000 | 18.0 |
| ETM | 114-07-8 | 0.020 | 1000 | 20.0 |
| AMOX | 26787-78-0 | 0.0037 | 1000 | 3.7 |

**Table S3 Toxicological data of six antibiotics on algae in soil**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | CAS | *EC50*(mg/kg) | *AF* | *PNEC*/(ng/g) |
| OTC | 79-57-2 | 415.00 | 1000 | 743.00 |
| TC | 60-54-8 | 170.00 | 1000 | 305.00 |
| NOR | 70458-96-7 | 1.23 | 1000 | 2.20 |
| OFX | 82419-36-1 | 1.11 | 1000 | 2.00 |
| ETM | 114-07-8 | 0.015 | 1000 | 0.034 |
| AMOX | 26787-78-0 | - | - | - |

**Table S4 DWI and BW of different age groups**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Age | *BW*/kg | *DWI*/(L/d) | Age | *BW*/kg | *DWI*/(L/d) |
| 0-3 M | 5.6 | 1.15 | 3-6 Y | 19 | 1.16 |
| 3-6 M | 7.2 | 1.14 | 6-11 Y | 36 | 1.55 |
| 6-12 M | 9.4 | 1.18 | 11-16 Y | 56 | 1.90 |
| 1-2 Y | 12.0 | 0.85 | 16-18 Y | 57 | 1.77 |
| 2-3 Y | 13.8 | 0.83 | Adult | 60 | 2.04 |

**Table S5 ADI and HQ of different age groups**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | *ADI*  [μg/(kg·d)] | *HQ* | | | |  | |  |
| 0-3 M | 3-6 M | 6-12 M | 1-2 Y | | 2-3 Y | | |
| OTC | 30 | 1.38E-06 | 1.06E-06 | 8.44E-07 | 4.76E-07 | | 4.04E-07 | | |
| TC | 30 | 1.18E-05 | 9.12E-06 | 7.23E-06 | 4.08E-06 | | 3.46E-06 | | |
| NOR | 2 | 9.46E-05 | 7.3E-05 | 5.78E-05 | 3.26E-05 | | 2.77E-05 | | |
| OFX | 150 | 1.71E-08 | 1.32E-08 | 1.04E-08 | 5.89E-09 | | 5E-09 | | |
| ETM | 40 | 4.09E-08 | 3.15E-08 | 2.5E-08 | 1.41E-08 | | 1.2E-08 | | |
|  | *ADI*  [μg/(kg·d)] | 3-6 Y | 6-11 Y | 11-16 Y | 16-18 Y | | Adult | | |
| OTC | 30 | 4.1E-07 | 2.89E-07 | 2.28E-07 | 2.09E-07 | | 2.28E-07 | | |
| TC | 30 | 3.52E-06 | 2.48E-06 | 1.95E-06 | 1.79E-06 | | 1.96E-06 | | |
| NOR | 2 | 2.81E-05 | 1.98E-05 | 1.56E-05 | 1.43E-05 | | 1.57E-05 | | |
| OFX | 150 | 5.08E-09 | 3.58E-09 | 2.82E-09 | 2.58E-09 | | 2.83E-09 | | |
| ETM | 40 | 1.22E-08 | 8.58E-09 | 6.76E-09 | 6.19E-09 | | 6.77E-09 | | |

**6Table S5 Number of resident population and scale of animal farming in the study area**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Year | Pig  （104） | Poultry（104） | Permanent population（104） | Rural population（104） | Urban population（104） |
| 2011 | 267.00 | 4300.00 | 2135.77 | 311.18 | 1824.59 |
| 2012 | 241.64 | 3650.00 | 2165.80 | 289.70 | 1876.10 |
| 2013 | 241.84 | 2642.00 | 2197.65 | 283.50 | 1914.15 |
| 2014 | 243.13 | 2166.00 | 2206.75 | 271.56 | 1935.19 |
| 2015 | 201.37 | 1944.00 | 2197.65 | 260.09 | 1937.56 |
| 2016 | 171.11 | 1713.00 | 2201.29 | 256.67 | 1944.62 |
| 2017 | 111.72 | 1252.00 | 2200.38 | 253.58 | 1946.80 |
| 2018 | 148.86 | 984.00 | 2204.93 | 241.56 | 1963.37 |
| 2019 | 117.00 | 844.00 | 2209.48 | 230.00 | 1979.48 |

**7 Table S2 Calculation expression of Z value**

|  |  |  |
| --- | --- | --- |
| Main phase | Sub phase | Z values |
| Air | Gas phase | *ZA=1/RT* |
|  | Suspended particulate | *ZAP=ZA×6×106/PLS* |
|  | Total phase | *ZAB=ZAP×γAP* |
| Surface water | Water body | *ZW=1/H* |
|  | Suspended particulate | *ZPW=ZW×ρPW×KOC×foc,pw* |
|  | Total phase | *ZBw=ZPw×γPw* |
| Soil | Solid phase | *ZS=ZW×ρS×0.14KOW×foc,S* |
| Sediment | Solid phase | *ZSed=ZW×ρsed×0.14KOW×foc,sed* |
|  | Total phase | *Zbsed=Zw×γw+Zsed×γsed* |
| Groundwater | Total phase | *ZGW=ZW×KGW-W* |

symbolic meaning as shown in Table S9

**Table S8 Calculation expression of D value**

|  |  |  |
| --- | --- | --- |
| Process | Phase | D values |
| Advection | Air-Outside | *D0-a=Q0-a(t)×Za* |
|  | Water-Outside | *D0-w=Q0-w(t)×Zsw* |
| Diffusion | Air-Freshwater | *D12=A2/(1/(K21×Z11)+1/(K21×Z22))* |
|  | Freshwater-Air | *D21=A2/(1/(K12×Z11)+1/(K21×Z22))* |
|  | Air-Seawater | *D13=A3/(1/(K13×Z11)+1/(K31×Z33))* |
|  | Seawater-Air | *D31=A3/(1/(K13×Z11)+1/(K31×Z33))* |
|  | Air-Soil | *D14=A4/(1/(K14×Z11)+L3/(B1×Z11+B2×Z22))* |
|  | Soil-Air | *D41=A4/(1/(K14×Z11)+L3/(B1×Z11+B2×Z22))* |
|  | Water-Sediment | *D25=A5/(1/(K25×Z22)+L5/(B5×Z22))* |
| Degradation | Air | *Dr1=Km1×A1×h1×Z1* |
|  | Freshwater | *Dr2=Km2×A2×h2×(Z2-X2f×Z2f)* |
|  | Seawater | *Dr3=Km3×A3×h3×Z3* |
|  | Soil | *Dr4=Km4×A4×h4×Z4* |
|  | Sediment | *Dr5=Km5×A5×h5×Z5* |
|  | Groundwater | *Dr6=Km6×A6×h6×Z6* |
| Others | Sediment resuspension | *D52=A5/(1/(K25×Z22)+L5/(B5×Z22))* |
|  | Air-Water dry deposition | *D12=A2×Kp×X13×Z13* |
|  | Air-Water wet deposition | *D12=A2×Kw×Sc×X13×Z13* |
|  | Air-Soil dry deposition | *D14=A4×Kp×X13×Z13* |
|  | Air-Soil wet deposition | *D14=A4×Kw×Sc×X13×Z13* |
|  | Water-Sediment deposition | *D25=A5×Ks×Z23* |
|  | Sediment-Water resuspension | *D52=A5×Kr×Z53* |
|  | Particle erosion | *D42=A4×Ke×Z33* |
|  | Normal erosion | *D42=A4×Kl×Z22* |
|  | Biological concentration | *D2f=Yf×Z2f/f* |

symbolic meaning as shown in **Table S2** and **Table S4**

**Table S9 Symbolic notes used in the paper**

|  |  |
| --- | --- |
| Symbol | Means |
| *D* | Transport parameters |
| *Dri* | Degradation coefficient of phase i |
| *D10t* | Transport parameters of Air-Outside |
| *D20t* | Transport parameters of Freshwater-Outside |
| *D30t* | Transport parameters of Seawater-Outside |
| *Dij* | Transport parameters of phase *i* to phase *j* |
| *f* | Fugacity (Pa) |
| *fi,j* | Fugacity of phase *i* to phase *j* (Pa) |
| *Z* | Fugacity capacity [mol/(m3**·**Pa)] |
| *ZA* | Fugacity capacity of air [mol/(m3**·**Pa)] |
| *R* | Gas constant 8.314[(m3·Pa)/(K·mol)] |
| *T* | Temperature (K) |
| *ZAP* | Fugacity capacity of suspended particulate in air phase [mol**/(**m3**·**Pa)] |
| *PLS* | Vapor pressure of liquid (Pa) |
| *ZAB* | Fugacity capacity of air phase [mol/(m3**·**Pa)] |
| *ZW* | Fugacity capacity of water phase [mol/(m3**·**Pa)] |
| *ZPW* | Fugacity capacity of suspended particulate in water phase [mol/(m3·Pa)] [mol/(m3**·**Pa)] |
| *Zij* | Fugacity capacity of substance i in phase j [mol/(m3**·**Pa)], i = 1, 2, 3, 4, 5 and 6 represent air phase, fresh water phase, seawater phase, soil phase, sediment phase and groundwater phase, respectively, j = 1, 2 and 3 respectively represent air, water and particulate matter |
| *γPW* | Proportion of suspended particles in water phase |
| *γAP* | Proportion of suspended particles in air phase |
| *γsed* | The proportion of sediments in sediment phase |
| *γW* | The proportion of water in sediment phase |
| *H* | Henry's constant [(m3·Pa )/mol] |
| *ρ* | Density (kg/L) |
| *ρpw* | Particle density in water (kg/L) |
| *ρsed* | Density of sediments (kg/L) |
| *ρs* | Density of soils (kg/L) |
| *KOW* | Distribution coefficient of octanol and water |
| *KOC* | Distribution coefficient of organic carbon and water |
| *KGW-W* | Distribution coefficient of surface and groundwater |
| *foc,pw* | The fugacity of particulate matter in water (Pa) |
| *foc,s* | The fugacity of soil (Pa) |
| *foc,sed* | The fugacity of sediment (Pa) |
| *D0-a* | Transport parameters of Outside-Air |
| *Q0-a(t)* | Flux of Outside-Air |
| *D0-w* | Transport parameters of Outside-Freshwater |
| *Q0-w(t)* | Flux of Outside-Freshwater |
| *Za* | Fugacity capacity of adjacent air phase |
| *Zsw* | Fugacity capacity of adjacent freshwater phase |
| *T02* | Rate of pollutant emission into freshwater(mol/h) |
| *T04* | Rate of pollutant emission into soil(mol/h) |

**Table S10 Proportion of antibiotic excretion in humans and animals**(Zhang et al., 2015b)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Antibiotics | Excretion ratio (%) | | | |
| Human | Pig | | Poultry |
| Urine | Feces |
| OTC | 66.70 | 59.00 | 28.10 | 52.50 |
| TC | 57.90 | 52.50 | 25.00 | 52.50 |
| NOR | 0.00 | 21.00 | 19.20 | 53.00 |
| OFX | 75.80 | 27.80 | 25.50 | 53.00 |
| ETM | 35.00 | 12.60 | 18.20 | 67.00 |
| AMOX | 70.00 | 65.00 | 10.00 | 70.00 |

**Table S11 Consumption rate of human and animal antibiotics**(Zhang et al., 2015b)

|  |  |  |  |
| --- | --- | --- | --- |
| Antibiotics | Pig | Poultry | Human |
|  | (mol/h） | (mol/h) | (mol/h) |
| OTC | 1.12E-07 | 0 | 2.05E-10 |
| TC | 3.85E-06 | 7.71E-08 | 4.36E-07 |
| NOR | 2.14E-07 | 7.15E-09 | 2.97E-09 |
| OFX | 6.48E-07 | 1.49E-07 | 1.75E-09 |
| ETM | 0 | 6.53E-08 | 1.43E-07 |
| AMOX | 1.95E-06 | 1.12E-07 | 2.50E-09 |

**Table S12 Measurement data of antibiotic content in Yangtze River Estuary**

|  |  |  |
| --- | --- | --- |
| Antibiotics | Concentration (ng/L) | Reference |
| OTC in freshwater | 0.02 | (Zhang et al., 2014) |
| TC in freshwater | 7.14 | (Zhang et al., 2014) |
| NOR in freshwater | 4.69 | (Zhang et al., 2014) |
| OFX in freshwater | 5.79 | (Zhang et al., 2014) |
| ETM in freshwater | 6.4 | (Zhang et al., 2014) |
| AMOX in freshwater | 10.34 | (Zhang et al., 2014) |
| OTC in seawater | 0.01 | (Guo et al., 2018) |
| TC in seawater | 3.57 | (Guo et al., 2018) |
| NOR in seawater | 2.09 | (Guo et al., 2018) |
| OFX in seawater | 3.19 | (Guo et al., 2018) |
| ETM in seawater | 3.2 | (Guo et al., 2018) |
| AMOX in seawater | 2.2 | (Guo et al., 2018) |
| OTC in soil | 42 | (Ji et al., 2012) |
| TC in soil | 15 | (Ji et al., 2012) |
| NOR in soil | 4.8 | (Ji et al., 2012) |
| OFX in soil | 4.8 | (Ji et al., 2012) |
| ETM in soil | 4.4 | (Ji et al., 2012) |
| AMOX in soil | 6.7 | (Ji et al., 2012) |
| OTC in sediment | 0.28 | (Jiang et al., 2011) |
| TC in sediment | 1.18 | (Jiang et al., 2011) |
| NOR in sediment | 2.54 | (Jiang et al., 2011) |
| OFX in sediment | 12.7 | (Jiang et al., 2011) |
| ETM in sediment | 44 | (Jiang et al., 2011) |
| AMOX in sediment | 3 | (Jiang et al., 2011) |
| OTC in groundwater | 1 | (Ma et al., 2015) |
| TC in groundwater | 1 | (Ma et al., 2015) |
| NOR in groundwater | 0.5 | (Ma et al., 2015) |
| OFX in groundwater | 0.5 | (Ma et al., 2015) |
| ETM in groundwater | 14.3 | (Ma et al., 2015) |
| AMOX in groundwater | 0.9 | (Ma et al., 2015) |

**Table S13 Environmental parameter table for tidal stage**

|  |  |  |  |
| --- | --- | --- | --- |
| symbol | definition | Study area values | Reference |
| *A3* | Seawater area (m2) | 5.18E+09 | \* |
| *A4* | Soil area (m2) | 5.77E+09 | \* |
| *A6* | Groundwater area (m2) | 5.99E+09 | \* |
| *h3* | depth of Seawater (m) | 7.00-8.32 | (Bintein and Devillers, 1996) |
| *h6* | depth of Groundwater (m) | 10 | (Bintein and Devillers, 1996) |

\*Access to remote sensing image data (https://earthexplorer.usgs.gov)

**Reference**

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