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## Simulating the Fungicide Chlorothalonil in East Tiaoxi River Using the RICEWQ-EXAMS Model

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# Outline

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- **STUDY OBJECTIVES**
- **STUDY METHODS**
- **RESULTS**
- **SUMMARY**
- **ACKNOWLEDGEMENT**





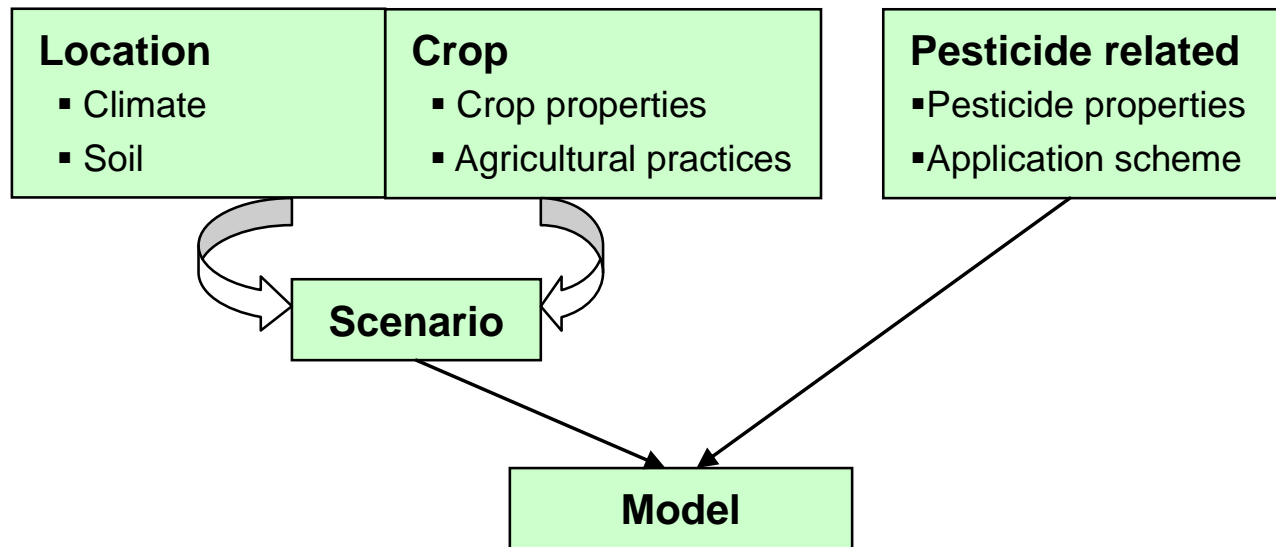
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# BACKGROUND

- ◆ In China, rice is one of the most important food crops. And currently, one third of pesticide active ingredients are registered on rice. Therefore, rice planting has become one of the major nonpoint pollution source of pesticide.

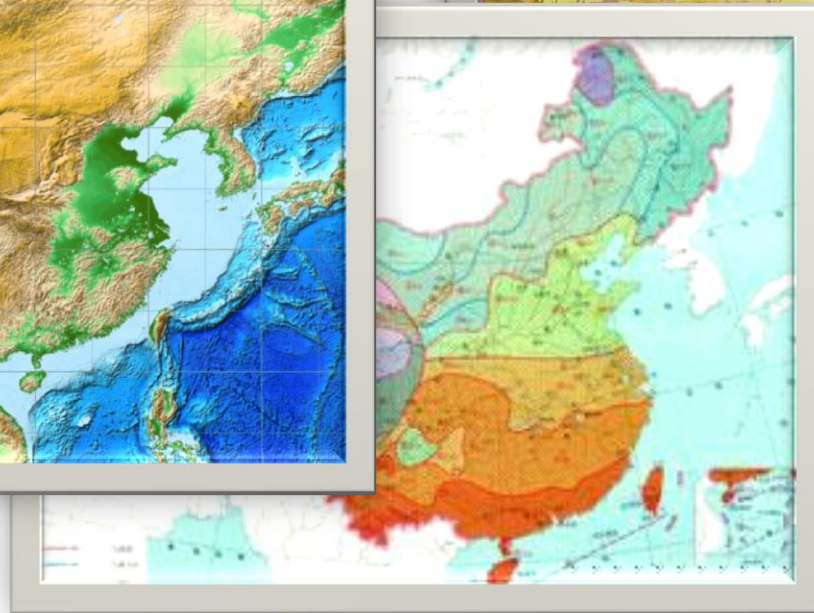
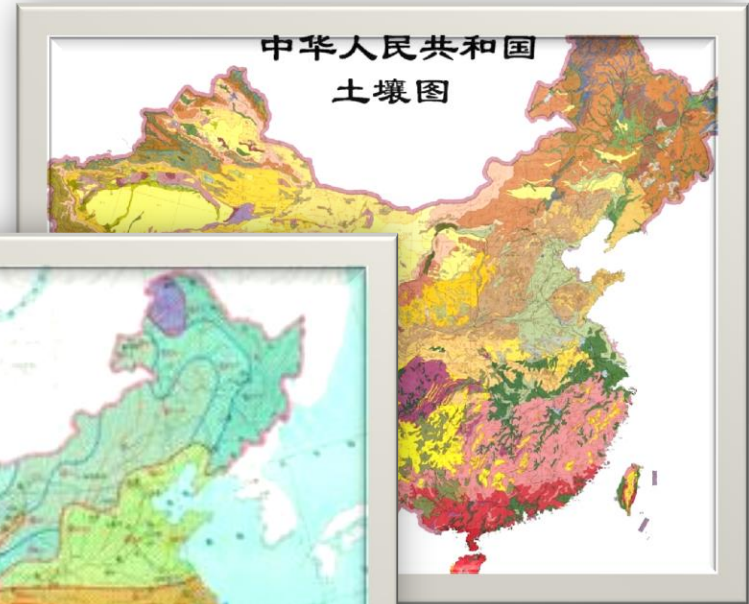
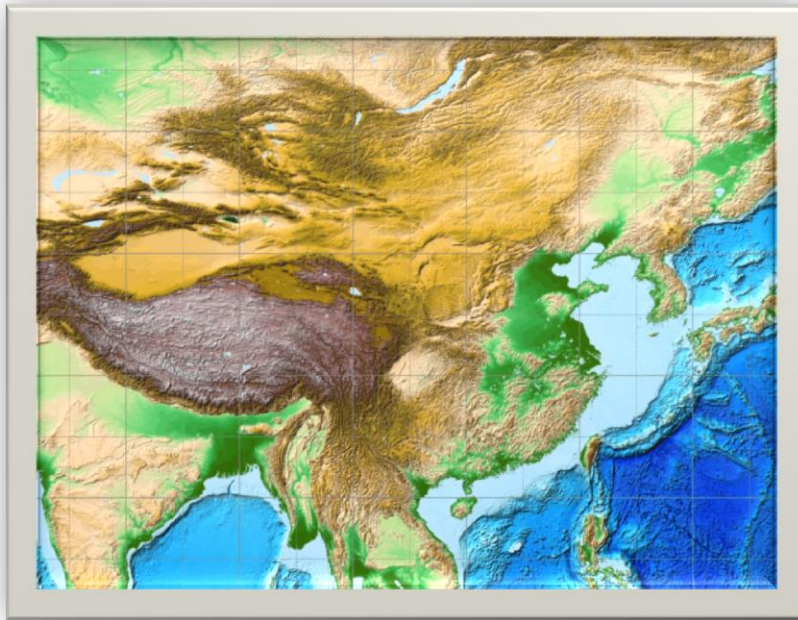


- ◆ Models and scenarios have been regarded as important tools for evaluating the exposure concentrations of pesticide in different environmental medias.



**Scenario:** A set of fixed input parameters in a pesticide fate model i.e. soil parameters, climate parameters, and etc. (FOCUS).

- ◆As a large agricultural country, China exhibits significant differences in climate, soil, terrain conditions and water management practices among the various rice-cultivation regions. The existence of such differences suggests that it would be more appropriate to develop various region-specific scenarios.





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# STUDY OBJECTIVES

- To develop a representative scenario for estimating predicted environmental concentrations (PECs) of pesticides in river water associated with the discharge from neighboring paddy fields.
- To do an exercise modelling using RICEWQ and EXAMS and to validate their suitability in China.



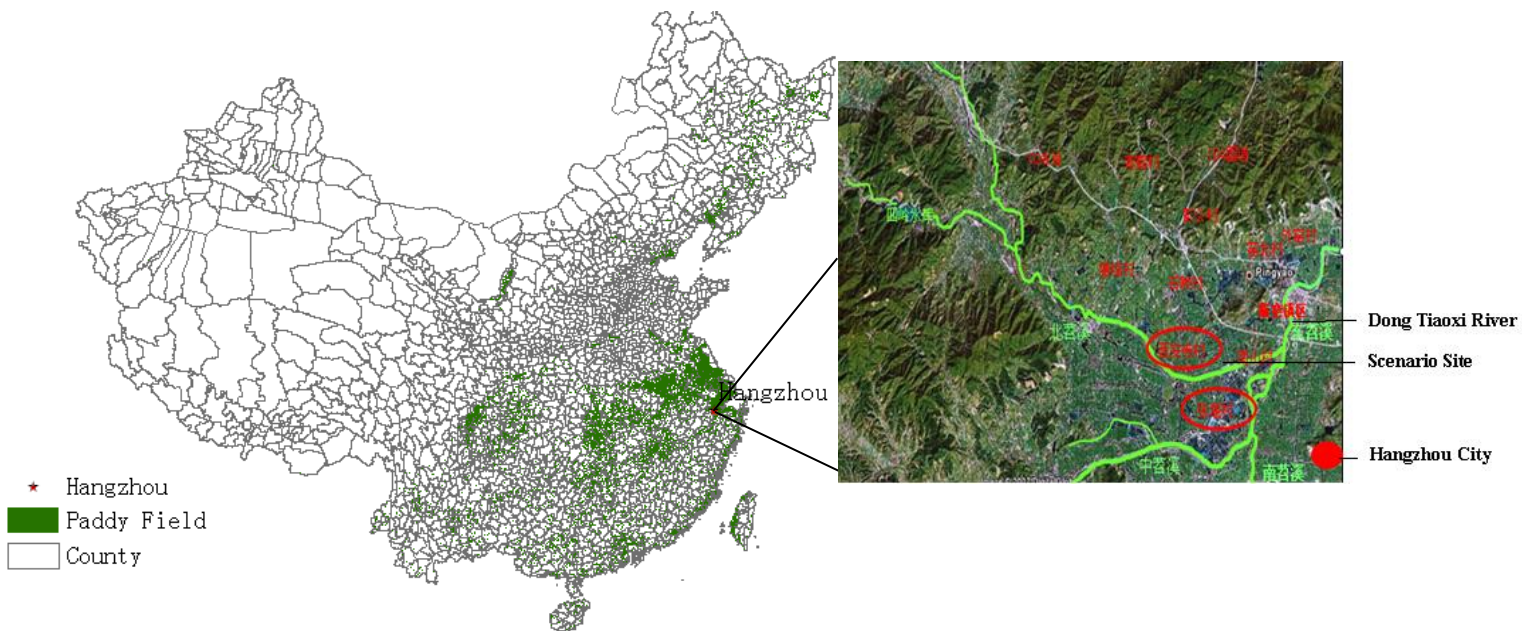


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# STUDY METHODS

## Study Area:

Located in Zhejiang Hangzhou, East Tiaoxi River basin is one of the main rice cultivation regions in China. A scenario was developed to represent the agricultural, water management and pesticide application in the East Tiaoxi River basin.



## Scenario Parameterization:

### ■ Weather data (1971-2000)

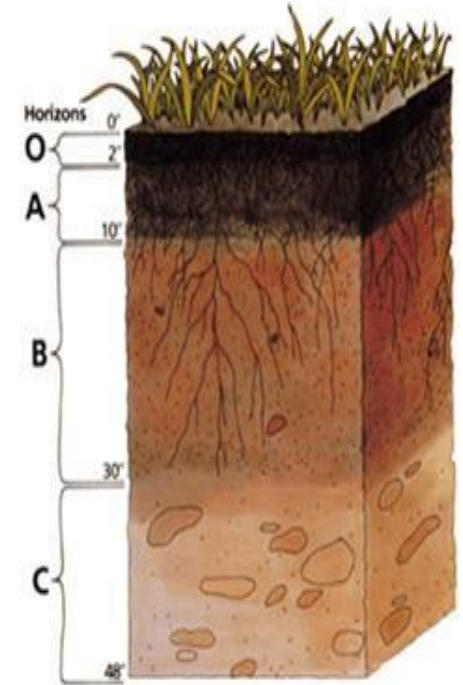
- Daily precipitation
- Average daily temperature
- Average daily wind speed at 10m
- Cloud cover
- Daily pan-evaporation

Data source: National Meteorological Information center

## Scenario Parameterization:

### ■ Soil data

- Soil profile depth
- Texture
- Percent sand
- Percent clay
- pH-H<sub>2</sub>O
- Percent OM
- Bulk density
- Field capacity
- Wilting point



Data source: China Soil Scientific Database

## Scenario Parameterization:

### ■ Crop data

- Maximum rooting depth
- Maximum canopy height at maturation date
- Typical date of crop planting, emergence, maturity and harvest
- Deposition of plant matter after harvest
- Date to irrigate and drain paddy
- Maximum drainage rate

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**Data source: Field trip**



## Scenario Parameterization:

### ■ Water body and watershed data

- Size field
- Percent crop area
- Default % Area treated
- Size Water
- pH
- Bulk density of sediment
- Organic carbon content of sediment
- Suspended sediment concentration
- Average flow rate of water body
- .....

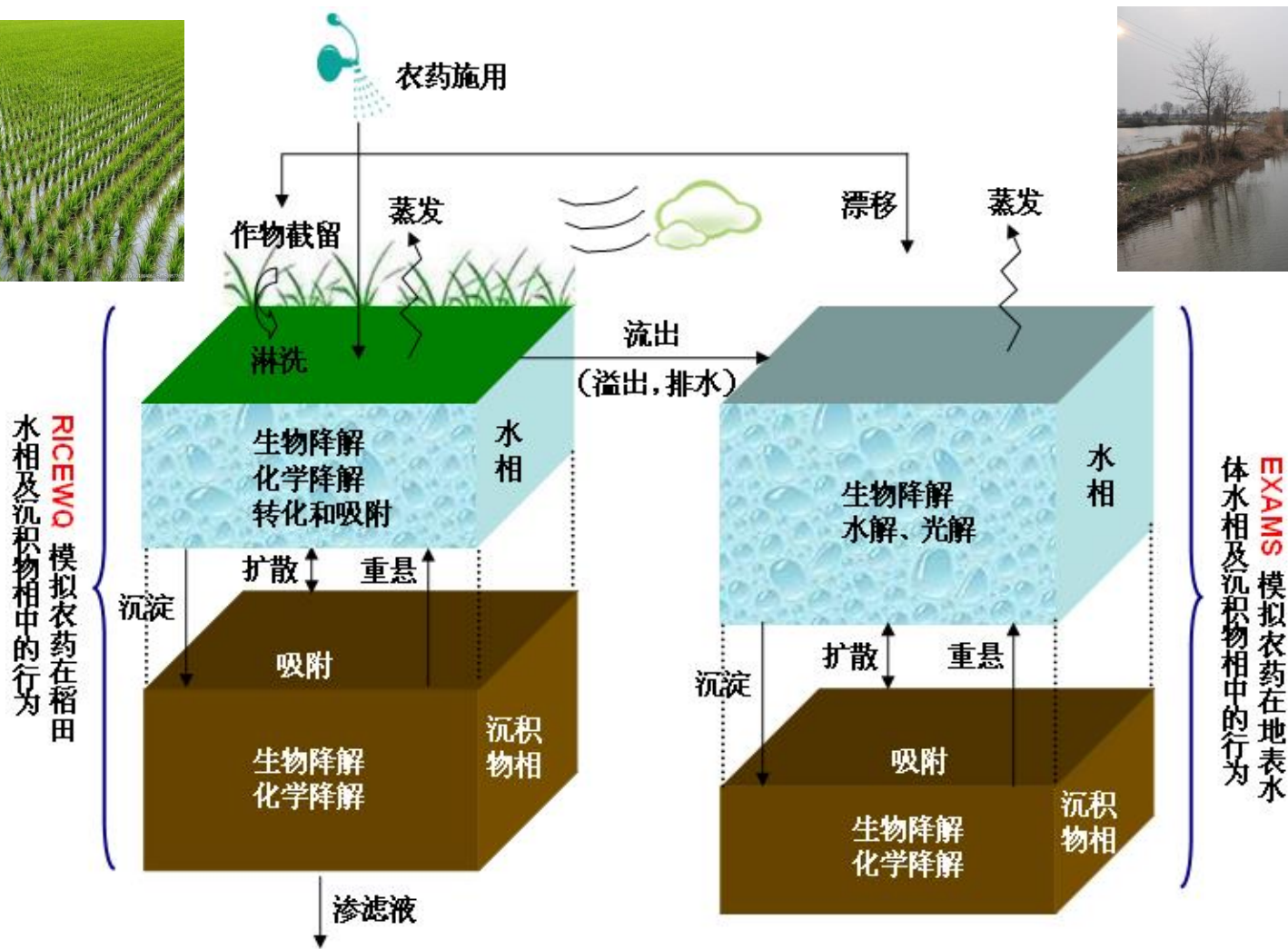
Data source:  
Field trip, lab  
test



## Model Description:

- ◆ RICEWQ, developed by Waterborne Environmental, Inc. (WEI), is a water quality simulation model that can be used to simulate water and chemical mass balance associated with the unique flooding conditions, overflows, and controlled water releases that are typical in a rice cropping system (Williams et al., 2012).
- ◆ The Exposure Analysis Modeling System (EXAMS), developed by U.S. Environmental Protection Agency (USEPA), is a tool for readily deriving and evaluating the behavior of synthetic chemicals in the water body (Burns, 2004).
- ◆ In this study, the RICEWQ model and the EXAMS model were coupled together to calculate PECs for paddy fields and the related surface water system.

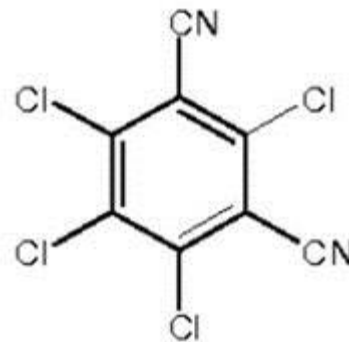
# Model Description:





## Chemical Properties:

- Chlorothalonil [ 2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile; CAS No. 1897-45-6] ;
- Commonly applied in rice paddies in China to control rice blast and rice sheath blight;
- The maximum recommended dose for the rice fungicide was used for model parameterization.



# Chemical Properties:

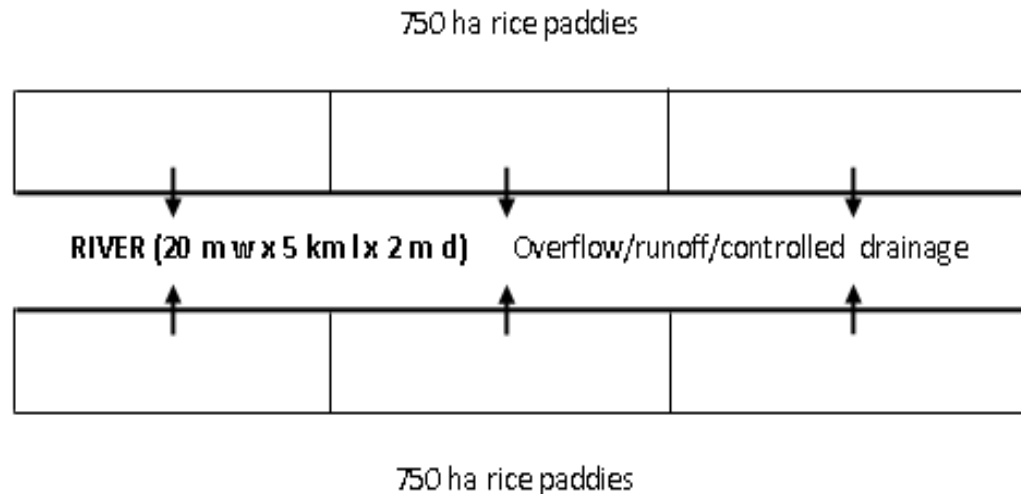
Parameters	Values	Comments
<b>Physi-chemical properties</b>		
Molecular weight	265.91	PPDB*
Solubility (mg·L <sup>-1</sup> )	0.81 (20°C)	PPDB
Koc (mL·g <sup>-1</sup> )	2632	PPDB
Vapor pressure (mPa)	0.076 (25°C)	PPDB
<b>Degradation properties</b>		
Hydrolysis DT <sub>50</sub> under different pHs (day)	29.6 (pH7)	PPDB
Direct photolysis DT <sub>50</sub> (day)	0.72	PPDB
EXAMS aerobic metabolism DT <sub>50</sub> (day)	1.51	PPDB
EXAMS anaerobic metabolism DT <sub>50</sub> (day)	1.87	PPDB
RICEWQ aerobic metabolism DT <sub>50</sub> (day)	1.51	PPDB
RICEWQ anaerobic metabolism DT <sub>50</sub> (day)	1.87	PPDB
<b>Application properties in rice paddy</b>		
Application rate (kg·ha <sup>-1</sup> )	1.428	Typical practice for the region
Application time	20 days after planting	Typical practice for the region
Application method	Ground spray	Typical practice for the region
Number of application	3	Typical practice for the region
Application interval (d)	10	Typical practice for the region



# STUDY RESULTS

## Basic information and concept model of the scenario:

- The annual precipitation of East Tiaoxi River basin is greater than 800 mm and the average temperature is between 8-20 °C;
- The scenario representative of the basin consists of a 1500 ha rice-cultivated area and a segment of a large river system of East Tiaoxi river, with the rice paddies locating on the side-banks of the river system.



## Soil properties of the scenario:

Horizon	Depth (cm)	Classification	pH-H <sub>2</sub> O	Percent sand (>20µm)	Percent clay (<2µm)	Om (%)	Bulk density (g cm <sup>-3</sup> )
Aa	0-15	CL	6.0	48.43	16.39	1.56	1.38
Ap	15-23	L	6.8	47.24	14.57	1.39	1.38
P	23-60	CL	7.7	34.03	21.47	0.64	1.38
C	60-100	LS	8.0	86.5	3.0	0.17	1.38

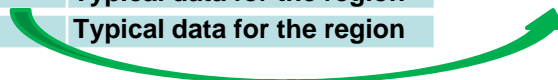
## Crop data of the scenario:

Parameters	Value
Crop emergence date	10 <sup>th</sup> -June
Crop maturity date	28 <sup>th</sup> - Oct
Crop harvest date	18 <sup>th</sup> -Nov
Maximum crop coverage (fraction)	0.8
Date to irrigate paddy (initial flood)	1 <sup>st</sup> -June
Date to drain paddy (first drain)	10 <sup>th</sup> -Sep
Date to irrigate paddy (second flood)	20 <sup>th</sup> -Sep
Date to drain paddy (final)	28 <sup>th</sup> - Oct
Maximum drainage rate (cm/day)	5
Irrigation rate (cm/day)	2
Depth of paddy outlet (cm)	15
Initial depth of paddy (cm)	0
Depth at which irrigation will begin (cm)	3
Depth at which irrigation will cease (cm)	5

# Water body and watershed data of the scenario:

Parameters	Values	Comments
<b>Geometry parameters</b>		
Segment area (m <sup>2</sup> )	100,000	Typical data for the region
Mixing length (m)	1.025	Typical data for the region
Segment thickness (m)	2.0	Typical data for the region
Bed sediment segment thickness (m)	0.05	USEPA guidelines
Number of segments	2	USEPA guidelines
Segment width (m)	20	Typical data for the region
Segment length (m)	5000	Typical data for the region
Segment volume (m <sup>3</sup> ) - water	200,000	Typical data for the region
Segment volume (m <sup>3</sup> ) - sediment	5,000	Typical data for the region
<b>Flow and loading parameters</b>		
Part flow advected	1.0	USEPA standard
Stream flow (m <sup>3</sup> ·hr <sup>-1</sup> )	12286.8	Typical data for the region
<b>Environmental parameters</b>		
Anion exchange capacity (meq·100 g <sup>-1</sup> )	0.01	USEPA standard
Atmospheric turbidity (km)	2.0	USEPA standard
Plankton population (cfu·ml <sup>-1</sup> )	1.0	USEPA standard
Benthic bacteria (cfu·100 g <sup>-1</sup> )	37	USEPA standard
Benthic biomass (g·m <sup>2</sup> )	6.00E-03	USEPA standard
Bulk density (g·cm <sup>3</sup> )	1.34	Typical data for the region
Cation exchange capacity (meq·100 g <sup>-1</sup> )	0.01	USEPA standard
Distribution Factor (dimensionless)	1.19	USEPA standard
Dissolved oxygen (mg·L <sup>-1</sup> )	5.0	USEPA standard
Dissolved organic carbon (mg·L <sup>-1</sup> )	5.0	USEPA standard
Vertical dispersion coefficient (m <sup>2</sup> ·hr <sup>-1</sup> )	3E-05	USEPA standard
Fraction of organic carbon (dimensionless)	0.0368	Typical data for the region
Mean monthly ozone (cm NTP)	0.3	USEPA standard
Percent water benthic (%)	137.00	USEPA standard
PH	7.0	USEPA standard
POH	7.0	USEPA standard
Suspended sediment (mg·L <sup>-1</sup> )	30.00	Typical data for the region
Water temperature (° C)	See table	Typical data for the region

Month	Temperature (°C)
1	5.3
2	4.1
3	9.9
4	18.6
5	22.0
6	24.6
7	27.5
8	26.2
9	25.0
10	23.1
11	17.6
12	5.0



# Scenario files:

Crop and soil file: .prn

Waterbody file: .exv

Climate file: .dvh

File (F)	Edit (E)	Format (O)	View (V)	Help (H)	
010151	0.000	0.190	5.000	100.000	0.000
010251	0.000	0.200	4.900	130.000	7.500
010351	0.000	0.380	6.500	230.000	0.200
010451	0.000	0.410	0.000	480.000	0.000

PARAMETER	VALUE USED	SOURCE/RATIONALE
SCNTYPE: 2		
Date simulation begins (/M/ID)	01/01	

Environment name:	China River		
Count of segments:	2		
Layers (Littoral, Benthic, Epilimnion, Hypolimnion):	L	B	
Lat, decimal degrees/Long, decimal degrees/Elev, m:	30.00	120.00	200.0
Volume, m3 (1,2):	2.0000E+05 5000.		
Surface area, m2 (1,2):	1.0000E+05 1.0000E+05		
Depth, m (1,2):	2.000 5.000E-02		
Cross sectional area, m2 (1,2):	0.000 0.000		
Length, m (1,2):	5000.0 5000.0		
Width, m (1,2):	20.0 20.0		
Count of advection paths:	2		
J from advection (path):	1	2	
I to advection (path):	0	1	
Advection Fraction (path):	1.000	1.000	
Count of dispersion paths:	1		
J from dispersion (path):	1		
I to dispersion (path):	2		
Cross sectional area of dispersion, m2 (path):	1.0000E+05		
Mixing length (path):	1.025		
Dispersion coefficient, m3/hr (path, month):	3.0000E-05		
Windspeed, m/s (segment, month):	1.000	0.000	
Stream flow, m3/h (segment, month):	12286.8 0.000		
Stream sediment, kg/h (segment, month):	0.000 0.000		
Non-point source flow, m3/h (segment, month):	0.000 0.000		
Non-point source sediment, kg/h (segment, month):	0.000 0.000		
Seepage flow, m3/h (segment, month):	0.000 0.000		
Rainfall, mm (month):	0.000		
Cloudiness, 0 - 10 (month):	0.000		
Ozone, cm NTP (month):	0.2965		

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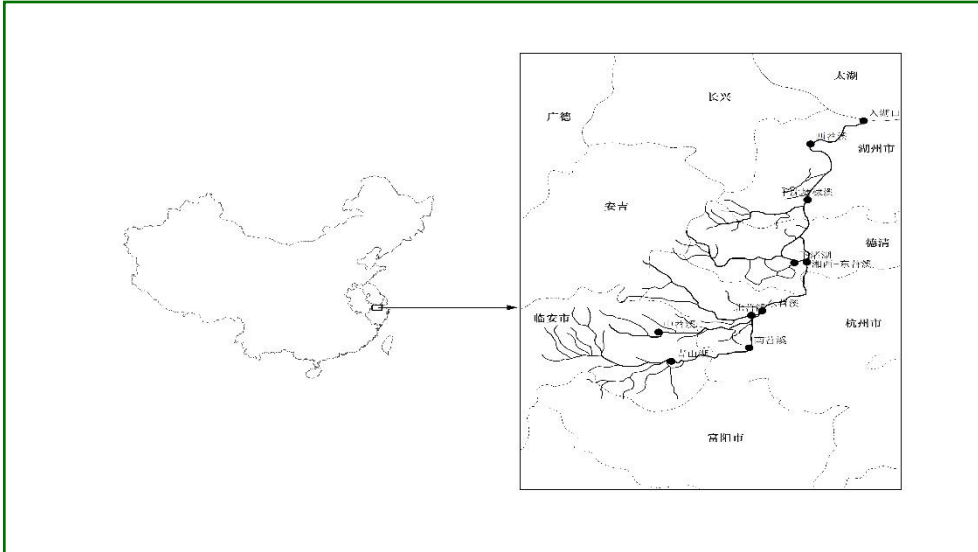




## Predicted Concentrations of Chlorothalonil in East Tiaoxi River:

Time	Concentration ( $\mu\text{g/L}$ )
Peak	2.48
96h	1.31
21d	0.309
60d	0.155
90d	0.0767
Annual average	0.0189

## Validation of the modelling with measured pesticide concentrations:



The maximum measured concentration of chlorothalonil in the East Tiao-xi river in 2008, 2009 and 2010 was  $0.236 \mu\text{g L}^{-1}$  and the 90th percentile of the predicting yearly maximum daily EECs for chlorothalonil was  $2.48 \mu\text{g L}^{-1}$ .

Comparison of the 90th percentile of maximum daily river PECs with the maximum measured concentrations of chlorothalonil in the East Tiaoxi river revealed acceptable agreement.





# SUMMARY

- ◆ This study derived a well-defined scenario representative of rice cultivation in Hangzhou Zhejiang Province, China.
- ◆ In general, surface water PECs obtained by the combination of RICEWQ and EXAMS models were in acceptable agreement with the monitoring results, suggesting that the model and scenario developed could be potentially used in the assessment for rice paddy pesticides used in such regions in China.
- ◆ This study could be considered as a first step towards the development of a standard watershed scale risk assessment approach for the registration of pesticides used in rice paddies. Further studies should focus on the development of similar representative scenarios for other rice-cultivated basins in China.

# Acknowledgement

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**The study received a lot of support, thanks...**

- ◆ **Waterborne Environmental Inc.**
- ◆ **Project group**



***Thank you for your attention!***