

Metabolism, transport, and distribution of typical herbicide in a bay of the northwest Pacific Ocean

Yu Zhang et al.

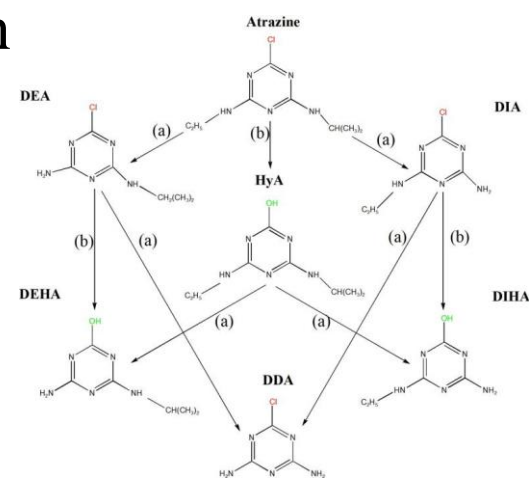
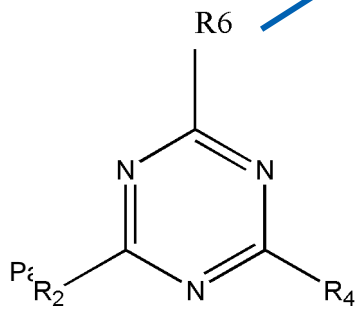
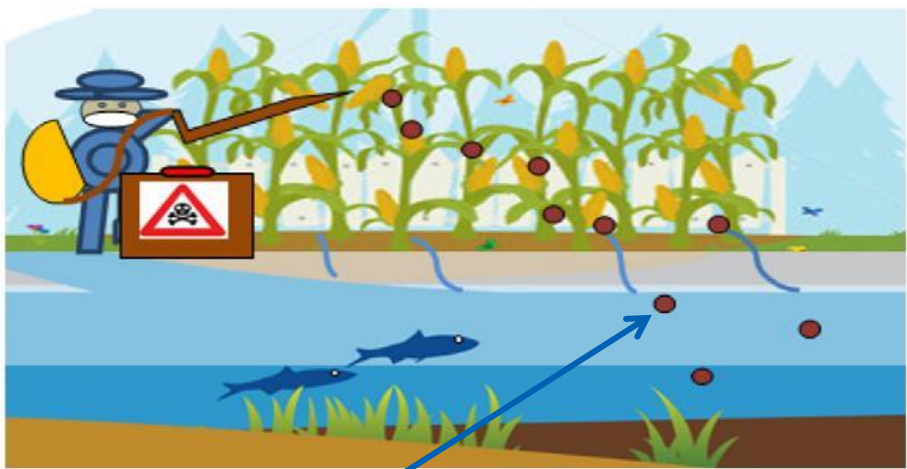
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Contents

- **Research Background**
- **Occurrence, transportation and distribution difference of typical herbicides from estuary to bay**
- **Next step: simulation experiments for migration and transformation of herbicides**

Research Background

- ✓ Source: agricultural use of atrazine
- ✓ Property: low solubility, long half-life, strong leaching, difficult degrading
- ✓ Toxicity: endocrine disrupter, potential cancerogen

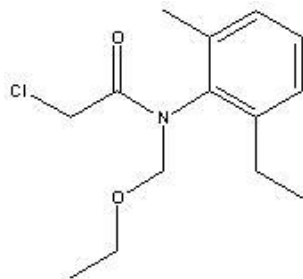


$R_2 = \text{NHCH}(\text{CH}_3)_2, \text{NH}_2$ $R_4 = \text{NH}_2, \text{NHC}_2\text{H}_5$ $R_6 = \text{Cl}, \text{OH}$

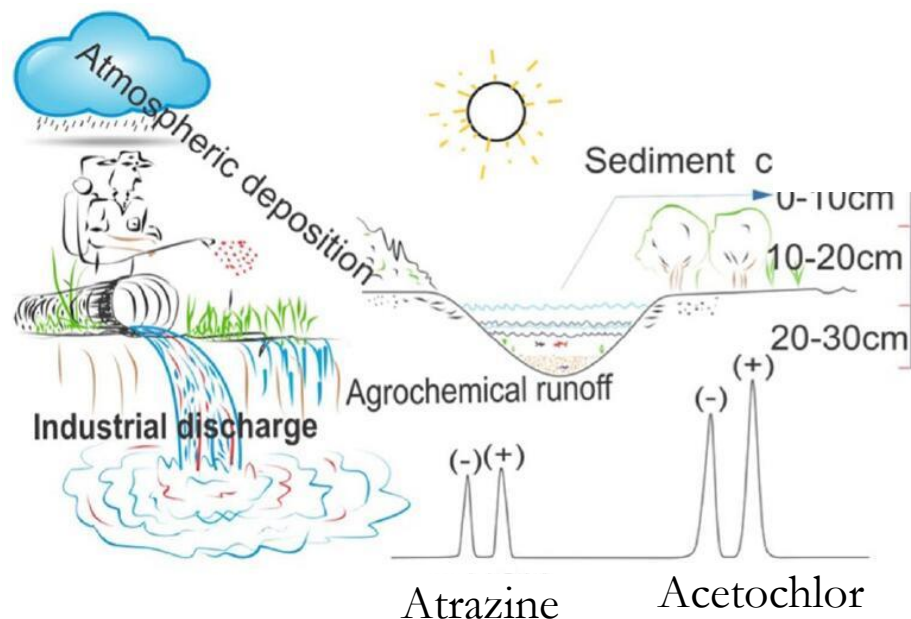
compound	abbr	substituent group			LogK _{oc}	LogK _{ow}	pKa
		R2-	R4-	R6-			
Atrazine	ATR	NHCH(CH ₃) ₂	NHC ₂ H ₅	Cl	2.7	2.75	1.7
Deethylatrazine	DEA	NHCH(CH ₃) ₂	NH ₂	Cl	1.6	1.24	1.3
Hydroxyatrazine	HyA	NHCH(CH ₃) ₂	NHC ₂ H ₅	OH	1.4	1.94	4.9
Deisopropylatrazine	DIA	NH ₂	NHC ₂ H ₅	Cl	1.2	1.15	1.3
Hydroxydeethylatrazine	DEHA	NHCH(CH ₃) ₂	NH ₂	OH	0.2	-0.08	4.5
Hydroxydeisopropylatrazine	DIHA	NH ₂	NHC ₂ H ₅	OH	-0.1	-0.3	4.6
Deethyldeisopropylatrazine	DDA	NH ₂	NH ₂	Cl	0	0.32	1.5

Research Background

- ✓ Source: agricultural use of **acetochlor**
- ✓ Property: high solubility, non-photolysis, non-volatile
- ✓ Usage: top three herbicides worldwide

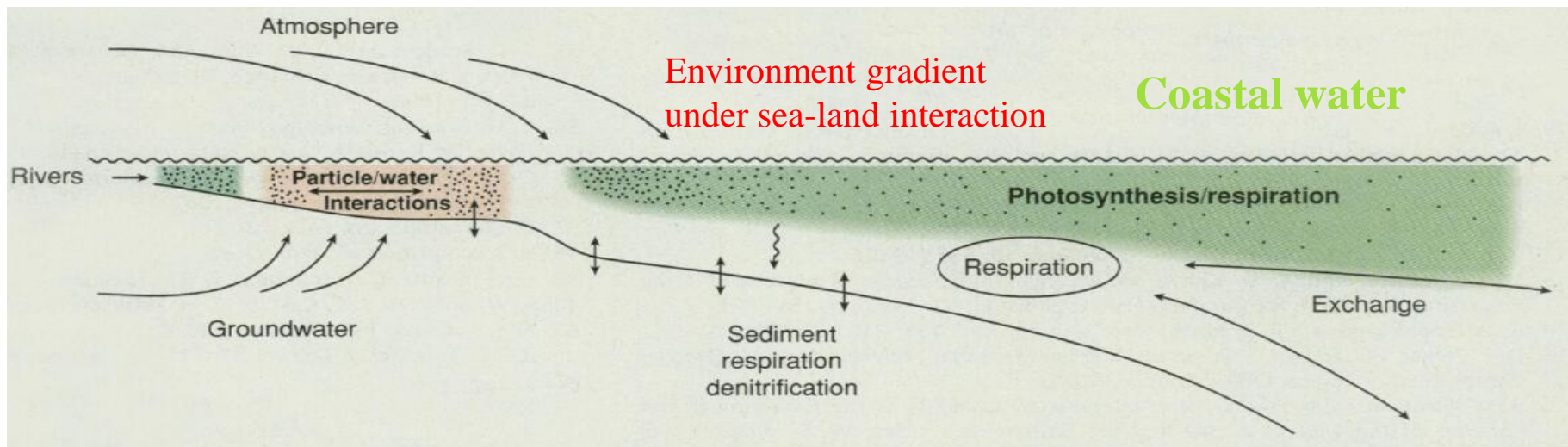


Acetochlor



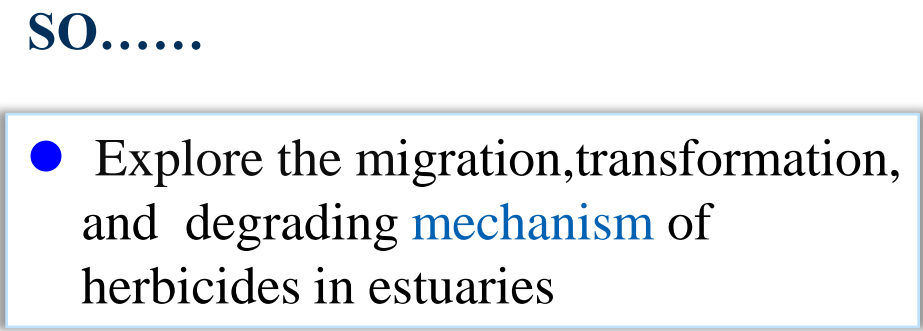
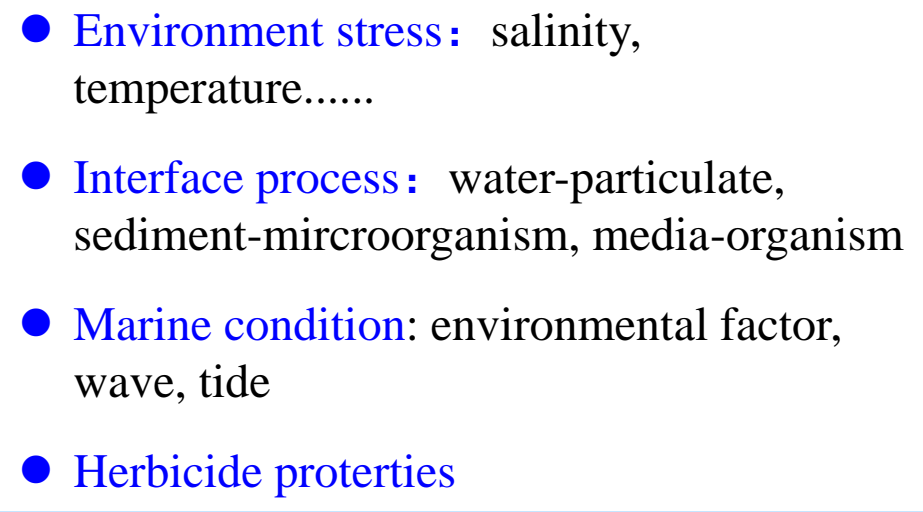
Research Background

- Special habitat patterns under salinity gradient influenced by Multi-scale hydrodynamic process in the estuary.
- Bays are the ultimate recipients of agricultural nonpoint source pollution from continental watersheds
- Provide ecosystem services of Supporting, Provisioning, Regulating and Cultural: Biodiversity + Fishery Production + Economic Supports.
- Presently about 40% of the world's population lives within 100 km of the coast.



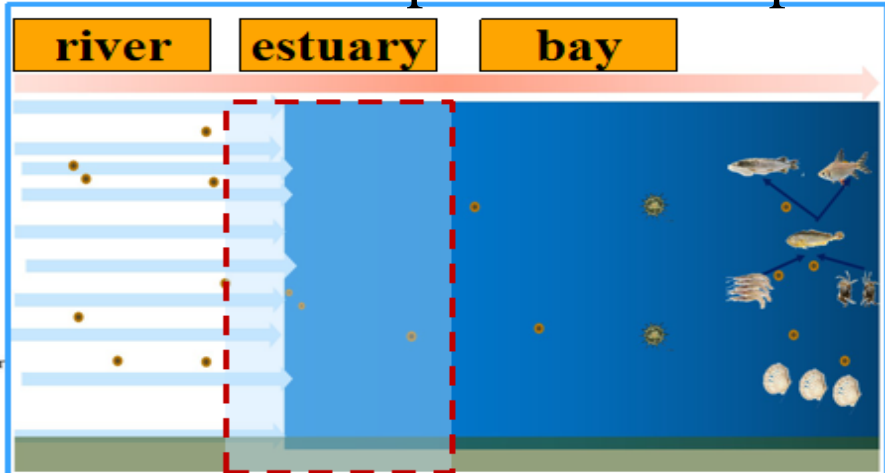
- What is distribution of herbicides during transport from river to bay? What are the mechanisms involved? Technology of pollution control?

■ Transportation mechanism of herbicides



Hot topics in coastal zone and bay

Herbicide response and adaption to marine conditions



- **Finding:** spatial-temporal and vertical variation of typical herbicides are large



Review

The Challenge of Micropollutants in Aquatic Systems

Rein P. Schwarzenbach,* Beate I. Escher, Kathrin F. Fent, Thomas B. Hofmeister, C. Annette Johnson, Urs von Gunten, Bernhard Wehr

...with thousands of industrial and natural chemical compounds is one of the key environmental problems facing humanity. Although most of these compounds are present at low concentrations, many of them raise considerable toxicological concerns, particularly when present as components of complex mixtures. Here we review three scientific challenges in addressing water-quality problems caused by such micropollutants. First, tools to assess the impact of these pollutants on aquatic life and human health must be further developed and refined. Second, cost-effective and appropriate remediation and water-treatment technologies must be explored and implemented. Third, usage and disposal strategies, coupled with the search for environmentally more benign products and processes, should aim to minimize introduction of critical pollutants into the aquatic environment.

About one-fifth of the world's population does not have access to safe water, and two-fifths suffer the consequences of unacceptable sanitary conditions (1). Pathogens in water cause more than 7 million deaths annually; most are children under the age of 5. The increasing chemical pollution of surface and groundwater, with largely unknown long-term effects on aquatic life and on human health, could easily lead to a problem of similar or even greater magnitude. More than one-third of the Earth's accessible renewable freshwater is used for agricultural, industrial, and domestic purposes, and most of these activities lead to water contamination with numerous synthetic and geogenic compounds (Table 1). It therefore comes as no surprise that chemical pollution of natural waters has already become a major public concern in almost all parts of the world.

Industry and municipalities use about 10% of the globally accessible runoff and generate a stream of wastewater, which flows or seeps into rivers, lakes, groundwater, or the coastal zone (2). These wastewaters contain numerous chemical compounds in varying concentrations. About 340 million tons of synthetic compounds are used in industrial and consumer products annually. In addition, about 1.5 million tons of pesticides are applied each year (2). In the European Union, for instance, there are more than 100,000 registered chemicals, of which 30,000 to 70,000 are in daily use (ENES, European Inventory of Existing Chemical Substances). The type of 6.4 million tons of oil and plastic components through accidental spills represents yet another important source of water pollution. Other notable sources of contamination are the situation of salty water intrusion due to overexploitation of aquifers, the hazardous mobilization of naturally occurring geogenic toxic chemicals, including heavy metal and metalloids (Table 1), and the biological production of toxins and malodorous compounds.

To date, an effective and sustainable global strategy against this massive and mostly unseen contamination of aquatic environments has yet to emerge. Some controls and technical solutions, such as wastewater treatment plants, function as barriers, particularly in highly industrialized countries, but major challenges remain. The source, behavior, and treatment of the relatively small number of micropollutants (3–5), such as pharmaceuticals, pesticides, and natural organic compounds, are relatively well understood. High interest in the development of new pharmaceuticals, pesticides, and natural organic compounds is also evident.

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How to.....

- Understand the distribution of typical herbicides in marine conditions

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Occurrence, transportation and distribution difference of typical herbicides from estuary to bay

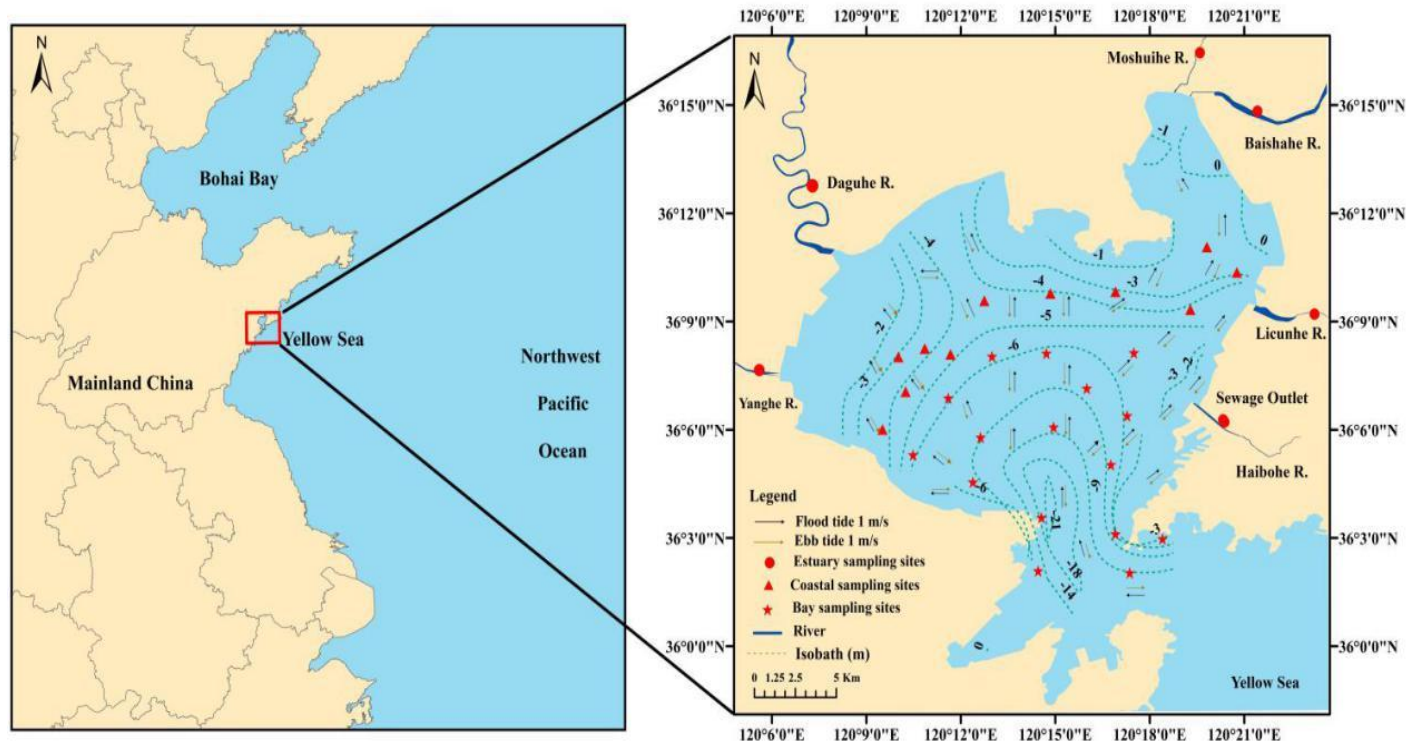


Fig. 1 Location of the study area, bathymetry, sampling locations, and tidal currents in the Jiaozhou Bay

- A total of 37 sampling sites, including 7 sites in the estuary, 11 sites in coastal areas and 16 sites in the bay, were investigated to express the transportation dynamics.

(1) Spatial transport of atrazine and acetochlor from the estuary to the bay

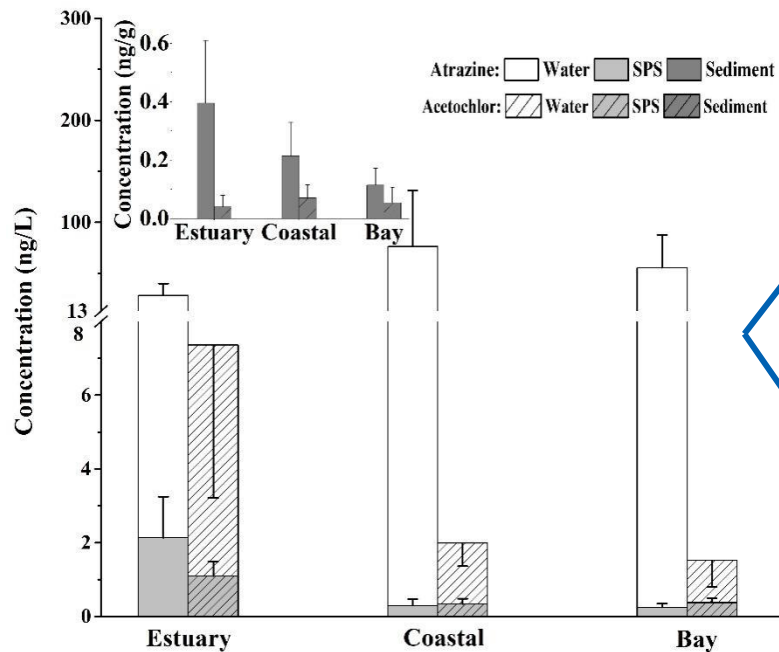
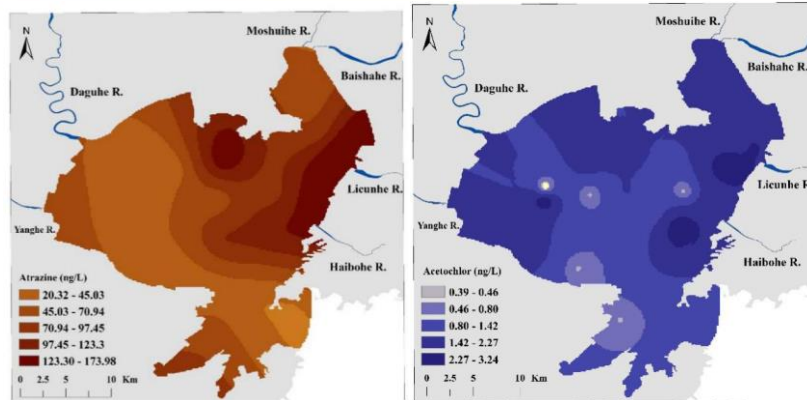


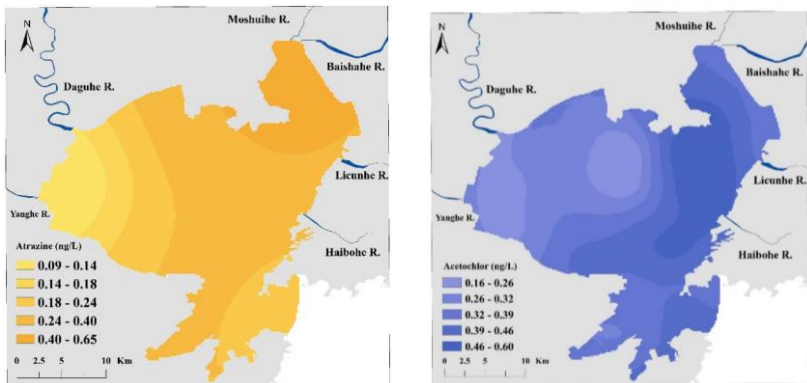
Fig. 2 Distribution of atrazine and acetochlor concentrations in water (ng/L), SPS (suspended particulate matter, ng/L), and sediment (ng/g dw) of three zones (estuary, costal and bay)

- **Finding:** The total concentration of atrazine was higher in coastal areas and in the bay than in the estuary, which indicate that it accumulates and has a bigger resistance rate in marine water.
- **Finding:** The concentration decreased significantly in coastal areas and the bay, showing that the acetochlor existence was sensitive to the marine environment and that its solubility may decrease in marine environments.

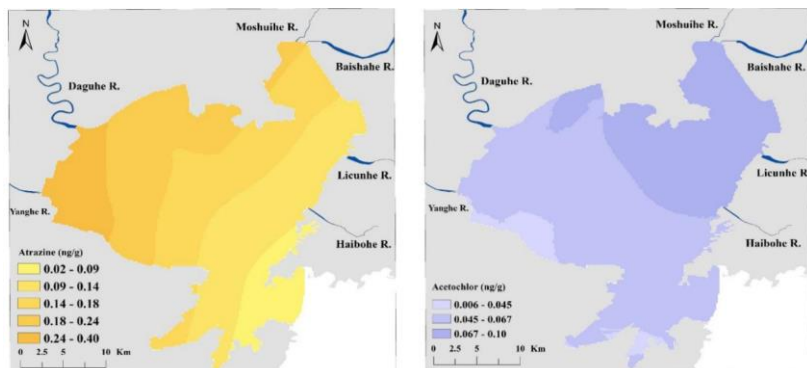
(2) Spatial distribution of atrazine and acetochlor



Water: Although their molecular structures, saturated solubility and concentrations in estuary water were different, the spatial patterns were similar.

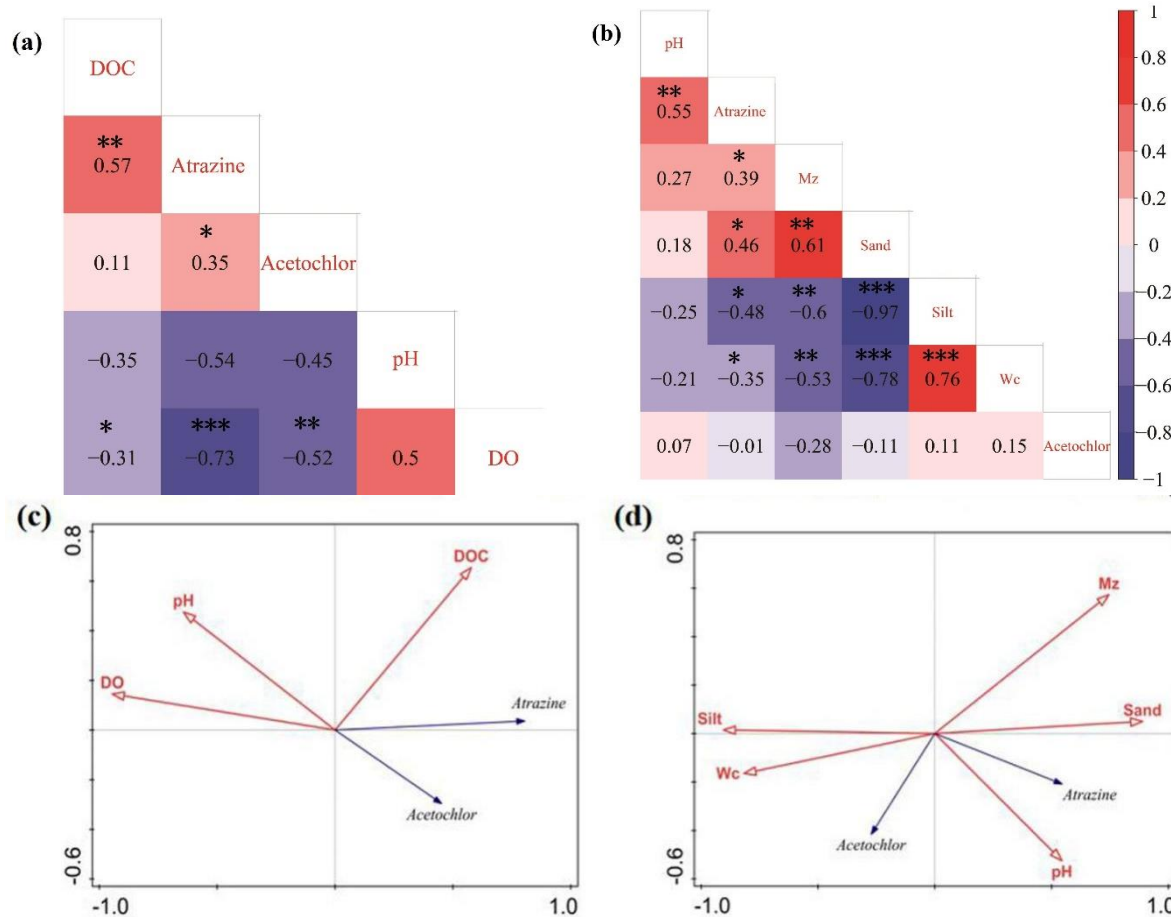


SPM: The trends of the two herbicides were reversed

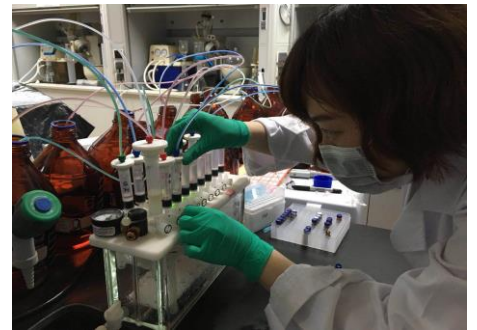
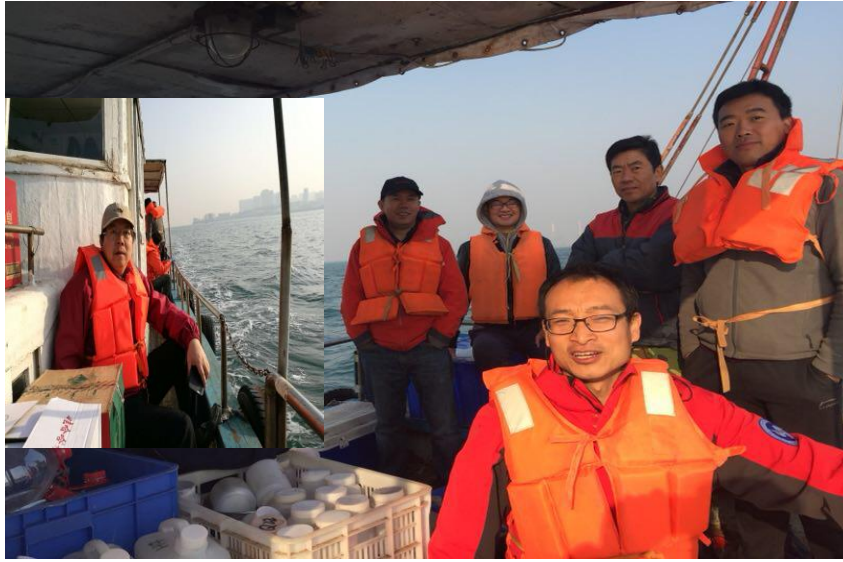


Sediment: The higher atrazine concentration in the sediment near the river mouth proved that it quickly sinks during the transport process. The highest concentration of acetochlor occurred in the northeast, which was the same result as the previous two patterns

(3) Differences in transport factors for the two herbicide



- The atrazine and acetochlor shared more impacts related to water DO and DOC, but the DOC had a more direct influence on atrazine.
- The particle size and sand percentage were the positive factors related to atrazine sorption.



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Thank you for your attention!

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