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Biotic Ligand Model 的简化模型及预测性能评价

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摘要: 通过检索 4 物种 (Fathead minnow、*D. magna*、*D. pulex*、Rainbow trout) 在地表水中实测的铜半致死浓度 (Observed_{LC50}) 及 Biotic Ligand Model (BLM) 预测其半致死浓度 (Predicted_{LC50}), 得到 4 物种的预测精度依次为 0.075、0.52、0.96、0.29, 模型对 Fathead minnow 与 Rainbow trout 的预测性能较差. 在此基础上, 分析显示预测误差值与 LA₅₀ 呈指数关系, 表明 LA₅₀ 值并非常数. 通过对 BLM 的 LA₅₀ 的校正, Fathead minnow 与 Rainbow trout 的预测精度升为 0.59、0.42. 通过分析 LA₅₀ 与硬度的关系, 发现 BLM 在软水环境中预测效果较差. 另外, 随机均匀生成 500 组水质参数组, 通过 BLM 预测, 筛选出 4 项敏感参数为 DOC、pH、HCO₃⁻ 浓度及温度, 并建立相应物种的 LC₅₀ 与其的多元线性关系, 大大简化了生物配位模型.

关键词: BLM; 4 物种; 预测性能; 模型简化; LA₅₀

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Simplification of Biotic Ligand Model and Evaluation of Predicted Results

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Abstract: The prediction accuracy of LC₅₀ on four species (Fathead minnow, *D. magna*, *D. pulex*, Rainbow trout) was 0.075, 0.52, 0.96 and 0.29 respectively as determined by their observed values of LC₅₀ in surface water. Predicted results indicated that the correlation between forecast error and LA₅₀ was exponential. The accuracy of Fathead minnow and Rainbow trout became 0.59 and 0.42 after adjusting LA₅₀. The correlation between hardness and LA₅₀ showed that the prediction effectiveness of BLM was poor in soft water. In addition, four important parameters (DOC, pH values, the concentration of HCO₃⁻, temperature) were selected to build the multiple linear relationship with LC₅₀ by applying 500 groups of random uniform water quality parameter in BLM. Biotic ligand model was effectively simplified.

Key words: BLM; four species; predicted results; model simplification; LA₅₀

水环境中重金属的形态与其生物有效性(毒性)有直接的关系,并不是所有形态的重金属都具有毒性.因此在金属水质标准制定或金属生态风险评估中,考虑生物有效性问题至关重要.然而重金属的生物有效性与环境介质中水质参数密切相关,并且物种的生理特性也影响其敏感程度.生物配位模型(Biotic Ligand Model)用于解释及预测水化学环境中重金属对有机体的急性毒性影响,毒性定义为生物体内的重金属积累超过一个重要阈值(LA₅₀)而对生物体产生的负面影响^[1].生物配位模型已被广泛用于各类水体中的重金属对生物体毒性的预测^[2~5],其预测精度较高,机制解释清晰.但大量文献报道^[6~9],生物配位模型也存在明显的缺陷,即对较高或较低 pH、硬度水体、较多 POM 水体等预测性能较差.生物配位模型应用需要考虑众多水环境参数^[10](温度、pH、DOC、Ca、Mg、Na、K、SO₄²⁻、碱度等),制约了模型更广泛的推广应用.本研究在 Biotic Ligand Model Windows Interface, Version 2.2.3 平台下,通过对分布广泛的 4 物种

(Fathead minnow、*D. magna*、*D. pulex*、Rainbow trout)文献检索其具体水体应用中的铜 LC₅₀数据,评价生物配位模型的预测精度.在此基础上得出预测效果差的关键因子及影响该因子的水质参数,然后通过因子校正,预测性能明显提高.另外,本研究通过随机生成水质参数组,利用 BLM 预测其 LC₅₀,然后通过统计分析评价模型各水质参数的相对灵敏度,并在此基础上对 BLM 加以简化.模型的预测性能评价将为生物配位模型的进一步完善及新物种的生物配位模型建立提供参考.

1 材料与方法

1.1 毒性数据的获取及水质参数组的随机生成

本研究的 LC₅₀ 数据检索涵盖了不同水体(湖泊、河流)和较广泛的水质参数范围,具有较好代表性.

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指标除了模型本身所需的输入参数外,还包括硬度, 随机均匀生成 500 组水质参数,各水质参数的范围
 LC_{50} ^[11-22]. 水质参数范围及毒性数据数量见表 1. 为中国地表水体的主要含量范围,见表 2.

表 1 铜对 4 物种的毒性数据汇总¹⁾

Table 1 Statistics of cupreous toxicity data about the four species

物种	pH	温度	DOC	Ca	Mg	Na	K	SO ₄ ²⁻	碱度	硬度	Cl ⁻	数量
Fathead minnow	5.4~8.5	22~25	0.2~16	0.204~403	0.024~111	0.16~370	0.039~32.5	0.096~1090	0.3~228	6.6~1210	0.32~530	93
<i>D. pulex</i>	7~8.62	20~22	0.07~9.8	1.34~403	0.56~111	2.07~370	0.28~29.4	1.2~1090	8~288	8~1210	0.3~530	45
<i>D. magna</i>	5.5~8.7	20~25	0.07~22.8	0.9~174	0.48~38	2.07~149	0.039~21.06	1.4~185	0.013~577	7.1~211	0.3~386.95	161
Rainbow trout	5~8.5	7.7~16.3	0.05~2.2	0.204~51	20.024~25.5	0.16~51	0.039~4.5	0.096~188	7.2~198	20~220	0.32~15.98	24

1) 温度单位为℃,碱度(以 CaCO₃ 计)及硬度单位为 mg·L⁻¹,其余为 mg·L⁻¹

表 2 水质参数范围表

Table 2 Range of water quality parameters

项目	含量范围 /mg·L ⁻¹	项目	含量范围
Ca	2~120	T/℃	10~25
Cl	1~35	pH	6~9
K	0.5~10	HA/%	10~60
Mg	0.4~6		
Na	0.7~25		
SO ₄ ²⁻	0.2~40		
HCO ₃ ⁻	6~19		
DOC	1~10		

1.2 BLM 应用简介

本研究应用软件平台为 Biotic Ligand Model Windows Interface, Version 2.2.3 (HydroQual, Inc.). 该软件为模型应用平台的最新版本,已被广泛采用. 该软件只需注重模型的输入输出,并且方便修改模型参数,所以使用较为简便. 利用 4 物种的 Observed_{LC50} 相对应的水质参数,输入软件中可预测其 Predicted_{LC50}. 比较 Observed_{LC50} 及 Predicted_{LC50}, 可得到模型对 4 物种的预测精度. 在软件形态分布平台下,利用 4 物种的 Observed_{LC50} 及其相对应的水质参数,输入软件中可得到其 LA₅₀. 软件主要默认参数见表 3.

表 3 BLM 关键参数表

Table 3 Key parameters of BLM

物种	Fathead minnow	<i>D. magna</i>	<i>D. pulex</i>	Rainbow trout
LA ₅₀ (wet)/nmol·g ⁻¹	5.48	0.12	0.0447	3.7
P _{Cu-HA}	1.5	1.5	1.5	1.5
lgK _{BL-Cu}	7.4	7.4	7.4	7.4
lgK _{BL-CuOH}	-1.3	-1.3	-1.3	-1.3

1.3 模型简化及精度评价方法

采用多元线性统计中的逐步回归法进行模型简化,筛选出灵敏度较高且所占影响比重较大的因子组. 预测误差设定为 Predicted/Observed Value (P/O), 0.5 < P/O < 2 为可接受范围内. 预测精度定义为 $N(0.5 < P/O < 2)/N(\text{total})$, 其中 N 代表数量.

2 结果与讨论

2.1 BLM 预测值与实测值比较

从图 1 可计算出,4 物种 (Fathead minnow、*D. magna*、Rainbow trout、*D. pulex*) 的预测精度值分别为 0.075、0.52、0.29、0.96. *D. magna*、*D. pulex* 的预测效果较好,而 Fathead minnow、Rainbow trout 的预测值普遍高于实测值,这说明 BLM 中存在某个参数的值与实际不相符合.

2.2 半致死累积量 (LA₅₀) 与预测精度的关系

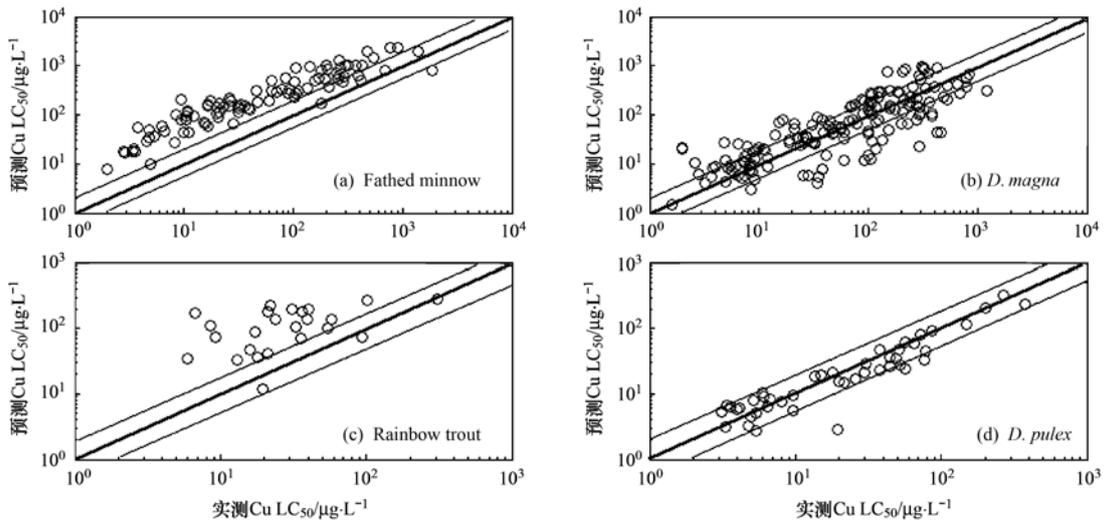
利用毒性数据,通过 BLM 软件铜的形态分布分

析获取 4 物种的半致死体内积累量 (LA₅₀). LA₅₀ 并非模型描述的为一个常量,其随着水环境参数的变化会相应变化. 图 2 利用预测误差与 LA₅₀ 作图,发现预测误差的好坏与 LA₅₀ 值密切相关,其统计分析见表 4.

由表 4 分析可知,LA₅₀ 与 P/O 之间呈指数关系,拟合效果较好. LA₅₀ 值是否合理直接关系到预测精度的好坏,所以找到一个合理的 LA₅₀ 值或者建立其与影响因子之间的关系式显得较为重要. 物种的本身生理特征 (年龄,大小等) 对 LA₅₀ 值有所影响,水环境化学参数 (如 pH、硬度等) 对 LA₅₀ 值的影响更不容忽视. 目前水质参数对 LA₅₀ 的影响机制研究较少,在 BLM 里已把 LA₅₀ 假设为一个常数.

2.3 BLM 的 LA₅₀ 的校正

由上述叙述可知,提高预测精度的重要方法为修正模型中的 LA₅₀ 值. 4 物种的 Cu 形态分布 LA₅₀ 统计显示如表 5.



细线代表 0.5 < P/O < 2 的范围

图 1 4 物种的预测值与实测值比较图

Fig. 1 Log-log plots of predicted versus observed copper concentration associated with the 50% of mortality (LC_{50}) for the four species

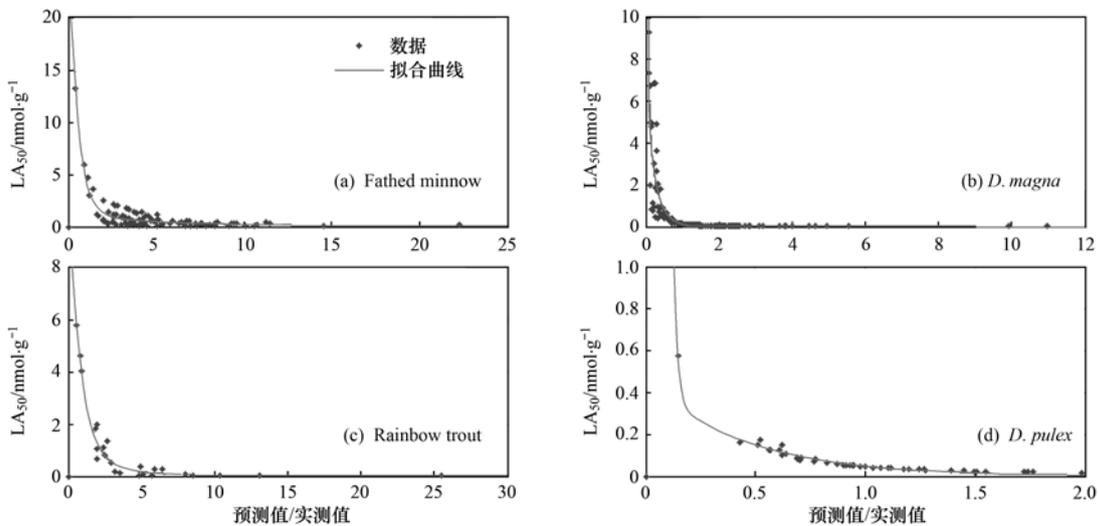


图 2 4 物种的预测误差与 LA_{50} 的关系

Fig. 2 plots of P/O versus LA_{50} for the four species

表 4 预测误差与 LA_{50} 的拟合关系式¹⁾

物种	指数关系式	R^2_{Adj}
Fathead minnow	$LA_{50} = 28.55e^{(-2.00Ac)} + 1.20e^{(-0.18Ac)}$	0.90
<i>D. magna</i>	$LA_{50} = 46.77e^{(-31.39Ac)} + 6.40e^{(-4.05Ac)}$	0.73
Rainbow trout	$LA_{50} = 10.64e^{(-1.2Ac)} + 0.70e^{(-0.31Ac)}$	0.97
<i>D. pulex</i>	$LA_{50} = 1353e^{(-58.34Ac)} + 0.46e^{(-2.26Ac)}$	0.99

1) Ac 为预测误差, 即 P/O

表 5 分析可知, 物种 Fathead minnow 和 Rainbow trout 的均值远远小于模型默认值, 即该两种物种模型的 LA_{50} 值明显偏高. 利用均值对物种 Fathead minnow 和 Rainbow trout 的 LA_{50} 进行校正, 校正后结

表 5 4 物种 LA_{50} 统计

物种	[mean, std]
Fathead minnow	[0.89, 1.61]
<i>D. magna</i>	[0.15, 0.19]
Rainbow trout	[1.05, 1.58]
<i>D. pulex</i>	[0.07, 0.08]

果见图 3.

物种 Fathead minnow 和 Rainbow trout 校正前预测精度分别为 0.075 和 0.29, 而校正后依次为 0.59 和 0.42, 预测性能明显提高. 因此, 在生物配位模型应用中, 选择一个合理的 LA_{50} 值较为重要.

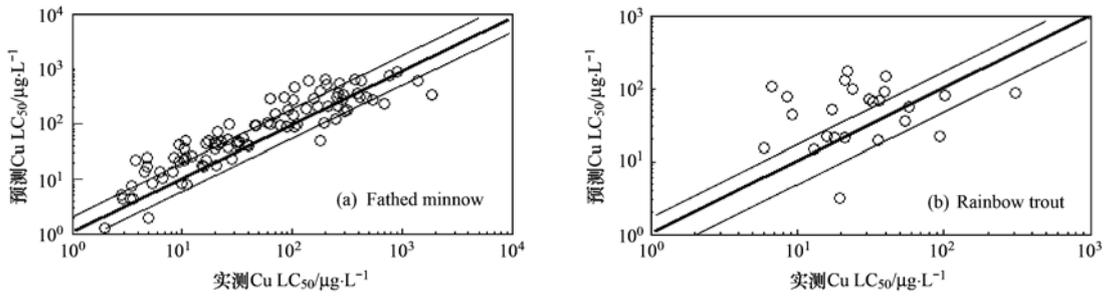


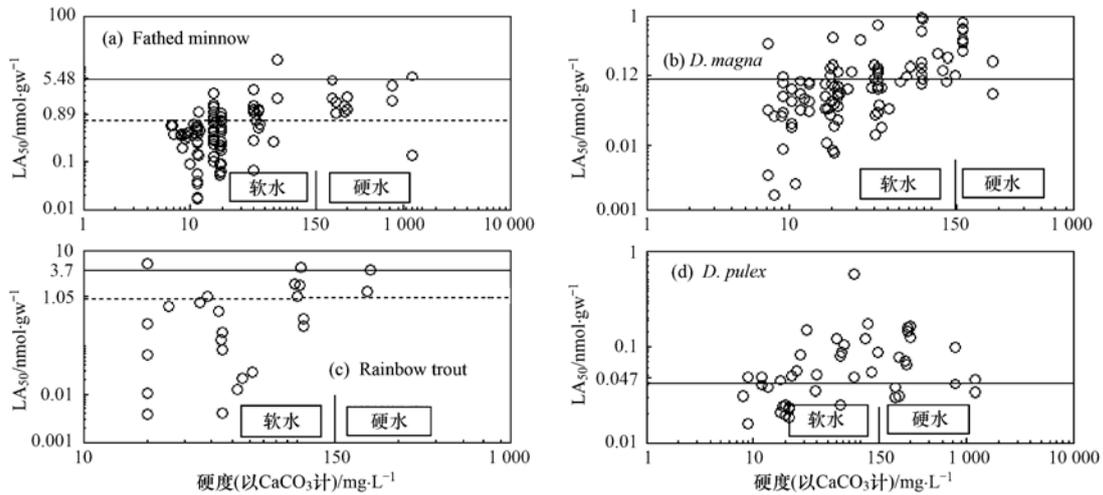
图 3 2 物种的预测值与实测值比较

Fig. 3 Log-log plots of predicted versus observed copper concentration associated with the 50% of mortality (LC_{50}) for two species

2.4 半致死累积量 (LA_{50}) 与水体硬度的关系

由于 LA_{50} 会随水质参数的变化而变化, LA_{50} 与水体硬度的关系见图 4. 从中可见, 随着硬度的增加, LA_{50} 值呈现上升的趋势, 并逐渐接近于模型默认

值. 图 4 也显示, 在软水环境^[23]中, 3 物种 (Fathead minnow、*D. magna*、Rainbow trout) 的 LA_{50} 值远小于模型默认值, 即生物配位模型不适合于软水环境中铜对物种的毒性预测.



实线代表模型默认 LA_{50} 值, 虚线代表校正 LA_{50} 值

图 4 4 物种的 LA_{50} 与硬度关系

Fig. 4 Plots of hardness versus LA_{50} for the four species

2.5 BLM 的简化

生物配位模型能较好诠释水环境参数对重金属生物有效性的影响, 但其需较多水质参数, 而很多水质参数较难检测或者代价昂贵, 这制约着 BLM 在经济科技不发达地区的推广应用. 本研究基于该模型, 筛选出 4 个重要参数 (pH、DOC、碱度、温度),

建立了其与 LC_{50} 之间的多元线性关系, 见表 6.

在实际应用中, DOC、pH、碱度、温度这 4 个参数对毒性的影响非常敏感, 其解释了生物有效性的很大一部分. 对于特定水环境, 温度在不同季节会有较大差异, 所以在生态风险评价或者基准建立中, 温度指标应给与足够重视.

表 6 4 物种的模型简化线性式

Table 6 Simplified linear expression of the four species

物种	多元线性关系	R^2_{Adj}
Fathead minnow	$LC_{50} = 75.44 \times DOC + pH \times 66.74 - 15.11 \times HCO_3^- - 11.39 \times T$	0.919
<i>D. magna</i>	$LC_{50} = 25.32 \times DOC + pH \times 37.14 - 9.43 \times HCO_3^- - 6.71 \times T$	0.811
<i>D. pulex</i>	$LC_{50} = 15.51 \times DOC + pH \times 26.84 - 7.04 \times HCO_3^- - 4.59 \times T$	0.768
Rainbow trout	$LC_{50} = 69.02 \times DOC + pH \times 60.60 - 14.14 \times HCO_3^- - 0.67 \times T$	0.916

3 结论

(1) 生物配位模型能较好预测 *D. magna*、*D. pulex*, 而对 Fathead minnow、Rainbow trout 的预测效果较差。

(2) 半致死累积量 (LA_{50}) 并非一个常数值, 其直接影响模型预测的好坏。建立新物种的 BLM 时, 应重视 LA_{50} 的修改或计算。

(3) 软水环境中, BLM 预测结果较差, 其原因为硬度对 LA_{50} 值的影响。模型应该考虑水体的总硬度, 而不只是单纯的 Ca、Mg 的影响。

(4) 4 物种简化的线性模型较好, 能为相对不发达地区提供生态风险评价依据。

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