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中文题名	重金属随泥沙迁移的数学模型及应用
英文题名	Mathematical Model for Heavy Metal Transport with Sediment in Water and Its Applications
中文关键词	重金属迁移,数学泥沙,分配系数,表面络合模型
英文关键词	heavy metal transport, mathematical sediment, distribution coefficient, surface complexation model, numerical modeling
中文文摘	水环境中的重金属污染已经成为了威胁现代文明最严重的环境问题之一。而我国现行的行业规范在模拟重金属的迁移过程时并没有考虑泥沙颗粒对重金属的吸附，即使有一些模型已经考虑了吸附作用，但也没有涉及到吸附的机理，从而使得模拟结果与实际污染情况偏差较大。因此，研究泥沙颗粒吸附重金属的机理并将其应用到重金属迁移模拟的工程计算中具有较高的理论价值和现实意义。从热力学的尺度来看，泥沙颗粒对于重金属的吸附是一种物理的非弹性碰撞现象在宏观上的表现，因此除了传统河流动力学中的粒径和级配两个参数以外，泥沙颗粒的表面形貌和孔隙将对重金属的吸附结果产生至关重要的影响。论文基于对泥沙颗粒表面形貌研究的结果，结合热力学分子扩散的相关知识，从理论上推导出了天然泥沙颗粒吸附重金属的分配系数 Kd，并提出了一套适用于天然泥沙颗粒不规则多孔隙表面的吸附等温式。从化学的尺度来看，泥沙颗粒吸附重金属的化学机理可以表述为泥沙颗粒表面的化学基团（主要为羟基）与水体中不同化学形态的重金属化合物（离子）之间发生的化学反应。因此，论文研究了常见重金属与海水中的一些离子发生化学反应后生成的重金属化合物（离子）的存在形态，以及泥沙颗粒表面羟基的形式、密度等特性。然后通过修正传统的表面络合模型来揭示天然泥沙颗粒与重金属之间的化学吸附机理。当重金属进入到水体中以后，一部分重金属将随水流输移扩散，而另一部分重金属将被泥沙颗粒所吸附并跟随其发生输移、沉降、再悬浮等运动。因此，在建立数学模型的时候，除了要考虑泥沙颗粒与重金属之间的热力学或者化学吸附机理外，还必须考虑水体流动、悬移质泥沙输移扩散、床面地形的演变等自然过程对于重金属迁移的影响。论文基于上述的动水动床条件，然后分别从热力学吸附和化学吸附两个角度建立了两类不同尺度的重金属迁移数学模型。将上面建立的基于热力学吸附理论和基于化学吸附理论的两类重金属迁移模型分别应用到我国大亚湾海域和杭州湾海域重金属污染物的迁移模拟中。计算结果表明水体中大量的重金属污染物在迁移过程中将被泥沙颗粒所吸附，并随着泥沙颗粒的运动不断地在空间上进行重金属浓度的重新分布。因此，在理论研究和工程应用中都有必要考虑泥沙颗粒对于重金属等污染物的吸附作用。
外文文摘	Heavy metal pollution, including radionuclide contamination, has posed a major environmental challenge to the modern world and threatens its environmental safety. However, the current standards and traditional models have usually avoided addressing the adsorption process or have adopted a simple adsorption isotherm to describe the adsorption process. As a result, the simulation results will usually be inconsistent with the actual situation of contamination. Therefore, the research on the adsorption mechanism between sediments and heavy metal contaminants has a high theoretical and practical significance.From the thermodynamic point of view, the adsorption of heavy metal contaminants on sediments is essentially an inelastic collision. Therefore, in addition to the two parameters of particle size and gradation in the field of traditional river dynamics, the sediment surface micromorphology will have a crucial impact on the adsorption process. Thus, Based on the mechanisms of adsorption/desorption at solid/liquid interfaces and a surface micromorphology model of sediments, a theoretical expression of the distribution coefficient Kd is derived and a new adsorption isotherm for irregular surface is proposed in this thesis.From the chemical point of view, heavy metal contaminants have different chemical forms in water and aquatic sediment surfaces have various types of surface groups. The primary adsorption mechanisms between heavy metal contaminants and sediments involve different types of chemical reactions. Therefore, the chemical reactions between heavy metal contaminants and ions in water are studied in this thesis. Furthermore, the surface characteristics, such as the density of surface hydroxyl groups are also studied. Then, the chemical adsorption mechanism can be revealed by a revised surface complexation model, which is suitable for natural

	sediments. After the heavy metal contaminants being discharged by factories into the water, some of them will transport with water, and the other will be adsorpted on sediment particles and transport with sediments. As a result, the mathematical model of heavy metal transport will not only include the thermodynamic or chemical adsorption mechanism, but also should include the process of convection-diffusion, sediment deposition/resuspension, seafloor topography evolution, etc. Therfore, two kinds of models, that couples hydrodynamics, sediment transport and heavy metal transport are developed respectively based on thermodynamic and chemical adsorption theory.Finally, the model based on thermodynamic adsorption theory is applied to simulate the 90Sr transport in the sea near the Daya Bay Nuclear Power Plant, and the chemical adsorption theory is applied to simulate the transport of Cu, Cd, Zn, Pb, Ni, 90Sr and 137Cs in Hangzhou Bay. Both results show that a large amount of the heavy metal contaminants will be adsorpted by sediments after discharging into the water. The heavy metal contaminants which were adsorpted by sediments will keep redistributed in space, so that the concentration distribution of heavy metal contaminants will be great affected by the process of adsorption. Therefore, it is necessary to include the function of sediments adsorption both in theoretical researches and engineering applications.
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