

KP16

Development of a model for predicting bioconcentration by using the test data of chemical substances control law

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A simple model for the bioconcentration mechanism of the chemical substance is formulated and proposed. The model consists of two processes, in which chemical substances permeate thorough biomembrane and permeated substances disappear from fish cells by metabolism and excretion of a fish. Consequently, the bioconcentration factor (BCF) can be expressed by a following equation:

$$\log \text{BCF} = \log P + \log D + \log(1 - \alpha_a) + \log(1 - \alpha_b) + \log(1 - \beta) + \text{constant}$$

where

P: Partition coefficient,

D: diffusion coefficient,

α_a : degree of dissociation of acid,

α_b : degree of dissociation of base,

and β ; the rate of disappearance by the metabolism and by excretion of a fish.