

GDCh-Advisory Committee  
on Existing Chemicals (BUA)

**Model-Based Exposure  
Assessment in Terrestrial  
and Near-Shore Marine  
Environments**

O. Fränzle and I. Jensen

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(Version: August 1998)



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Committee on Existing Chemicals

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# **Model-Based Exposure Assessment in Terrestrial and Near-Shore Marine Environments**

**O. Fränze and I. Jensen**

## **Abstract**

In compliance with national and international legal regulations, the ecotoxicological hazard assessment of substances is generally based on the comparison of their predicted environmental concentration (PEC) with the predicted no-effect concentration (PNEC), which is normally calculated from single-species acute or chronic laboratory tests. Introducing plausible safety factors, it is assumed that, where the PEC exceeds the PNEC, there could be a potential for adverse environmental effects, and the corresponding risk then is the ecosystem-specific probability of such a hazard.

As regards PEC value determination, which is the scope of the present paper, comprehensive and geostatistically valid monitoring data in the compartments water, sediment, soil, biota and air would be the best basis for environmental exposure assessment purposes. Such data are rarely available, however, and usually only for parts of the environment, such as main rivers, some lakes, marine estuaries or the atmosphere in towns and industrial areas. In addition, the environmental exposure may undergo rapid change, due to changes in production rates and techniques, treatment of waste water or exhaust gases. Therefore, the quantities of a chemical released into the environment are estimated by using all available data on production, use pattern, disposal, its physical-chemical properties, environmental fate and behavior.

In order to facilitate a coherent interpretation of such data sets, the Technical Guidance Documents (TGDs) suggest predictive models for local and regional PEC estimates. These general models may be replaced or complemented by more specific ones, if this is deemed appropriate in terms of higher precision or for other scientifically or practically relevant reasons. Clearly, the use of a model other than those recommended in the TGDs would need to be justified and the full details of the parameters used recorded, which is an issue for the assessor to resolve.

It is the purpose of the present paper to provide an overview of available models for such more detailed exposure assessment approaches in terrestrial, estuarine and near-shore marine environments. It starts with a description of water flow in porous media and related balance models, followed by models on chemical transport and distribution (FRÄNZLE), then marine circulation models suited for incorporating chemical flux and deposition modules (JENSEN), and finally a review of chemicals/sediment interactions (JENSEN, FRÄNZLE).