Summary

For the evaluation of environmental contamination organic pollutants are most important next to heavy metals. The aim of this thesis was to gain an insight into the load of organic pollutants in different aquatic compartments. Sediments bind organic material with high adsorption capacity, and in particular lipophilic substances reach considerable accumulation rates. A highly complex mixture of biogenic, geogenic and anthropogenic substances is formed and a separation into several fractions is necessary prior to gaschromatographic analysis. In surface water as well as in ground water the organic fraction is less complex, and solvent-extracts can be analysed directly without further separation.

The work was thematically influenced by three BMBF funded projects (International Odra Project – IOP, Mulde "ad-hoc" project, bioassay–directed fractionation of sediments – ISIS).

In the International Odra Project, evaluation of screening analyses of 44 sediment samples and quantitative determinations showed a pool of biogenic substances and a high, omnipresent load of polycyclic aromatic hydrocarbons in the Odra system. Among these, most prominent were the so-called EPA-PAHs, although methyl- and ethyl substituted homologues and heterocyclic PAHs were frequently observed. Certain distribution patterns and concentration ratios of specific compounds (e.g., phenanthrene/anthracene) indicated that pyrogenic entries contributed considerably resulting from atmospheric deposition and surface run-off into the Odra system. In addition, at some sampling locations the influence of mineral oil contamination was observed. The PAH load in the Odra system requires an ecological-toxicological classification, were damages are possible or expected in the ecological system.
The most problematic situation in the Odra system was observed in the tributary Strzegomka and at the downstream Odra probing site, Brzeg Dolny. In the Strzegomka river benzothiazoles were found which point towards entry from a local industrial source. The spreading of benzothiazole derivatives was limited to the Strzegomka river and to Brzeg Dolny. Only 2-methylthiobenzothiazole was observed throughout the Odra system, probably not from a point source, but resulting from atmospheric deposition and surface run-off (e.g. automobile tyre abrasion on the streets, washed by rain and carried into the Odra river).
The number of chlorinated compounds, often with relevant toxicological properties, was low and included primarily PCB and pesticides. Both groups showed no extreme loads, PCB were detected at a little higher values in the Warta river and in the area of the Szezecin lagoon while increased levels of pesticides were observed in regions with intensive agriculture and at sampling locations with dry flood sediments which were probably mixed with terrestrial material. An up to now unknown metabolite of endosulfan (1,2,3,4,7,7-hexachloro-5,6-bis(methylene)-bicyclo[2.2.1]hept-2-ene) was identified in the dry sediment of a sample from Frankfurt/Slubice.

During the Mulde "ad-hoc" Project 6 sediment samples, 7 surface water samples and 12 ground water samples from the Lower Mulde river area and the Elbe river were analysed. Apart from the ubiquitous distribution patterns of biogenic compounds, aliphatic hydrocarbons, phenylalkanes, alkylbenzenes, PAH and hetero-PAH, the samples of the Mulde river contained a large number of substances that have been neglected or not analysed before or were entirely new pollutants.

A sediment sample close to the Mulde reservoir (most upstream in this work) was least contaminated. In the next downstream sampling locations and in the Spittelwasser river extreme entries of mono and poly-chlorinated compounds (benzenes, naphthalenes, styrenes, anilines, butadienes, HCH etc.), isomeric alkylsulfonic acid arylesters, tetrabutyl stannane and DDT with all known metabolites were detected. The DDT contamination did not indicate a typical ubiquitous background contamination caused by the formerly worldwide application of DDT but pointed towards a massive entry of the technical product from former productionsites of the Bitterfeld chemical plants or from close-by refuse dumps. Especially 1,3-dichloro-1-phenyl-2-methoxymethylpropane is mentioned here as a contaminant rarely observed so far.
The influence of the Mulde river on the Elbe river contamination was shown with a considerable dilution effect which lowered the load in comparison to the Mulde river.
The samples of the surface water showed a similar picture of the contamination profile. The Spittelwasser is dominated by chlorinated anilines and nitrobenzenes, as well as the herbicide prometrin. From the group of the triazines, simetrin and propazin were detected while the pesticides included DDT and HCH. Compared with samples from 1993, coupling components for azodyes were found again. In addition *N*-2-cyanoethyl-*N*-(2-phenyl)ethylaniline was found as a new environmental contaminant. Chloropropylphosphates and other pollutants appeared also in the Mulde river but some were observed at higher concentrations as compared to the Spittelwasser, indicating that there exists another source of pollutants in this area. In the Mulde river 5-chloromethyl-4-phenyl-1,3-dioxane was identified for the first time. This is a formaldehydacetal with strong structural similarity to other substances from the sediment and ground water.
The twelve ground water samples showed strong contaminations with chlorobenzenes, chlorophenols, tri-and tetrachlorinated ethanes and ethenes. Other notable pollutants were substituted diphenylureas, as well as chlorinated acetals, which have not been described as environmental contaminants until now.
In conclusion, the Lower Mulde river area is still loaded very heavily with organic pollutants, and the contamination patterns of the surface water points to an entry of extremely contaminated ground water. It can not be excluded that this contamination may increase during the next years by hydrological changes (watering of rest holes, changed water withdrawal).

In the third subject of this thesis non-target-screening was guided by bioassay-directed fractionation in the ISIS-Project. The bioassay-directed fractionation of 7 sediment samples from the North Sea and the Baltic Sea led to different fractionation steps. While for different methodical reasons no exact correlation between substances and toxic effects could be obtained, several compounds were tentatively linked to toxic effects. However, chemical analyses led to the identification of dibromoindole isomers, which seemed to be responsible for at least part of the toxicity of north sea samples in two biological tests systems.