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Simulation of Organic Pollutants: First Step towards an Adaptation to the Malacca Strait

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Abstract: For the simulation of the transport of persistent organic pollutants (POPs), a set of numerical models has been adapted and applied to the Malacca Strait and the adjacent South China Sea and Java Sea. As a first step, a model experiment, namely input of POPs into model region only via rivers, was performed, because realistic input data regarding concentrations, sources and sinks of POPs for the marine environment as well as different other parameters responsible for the fate of POPs in the ocean were not yet available. Firstly, a numerical hydrodynamical model has been applied to the region of interest to simulate the hydrological situations as realistically as possible. Secondly, a numerical model for the fate and transport of POPs has been run on the basis of the hydrodynamical model results to simulate the dispersal of two differently behaving POPs, i.e., γ-HCH and PCB 153, from river input only. It is shown that only a clear seasonal but hardly annual variation is present in the model results for the currents and for the total POP concentrations. Despite permanent riverine input, the seasonal pattern of total POP concentration in water repeats in the simulation results year after year without further accumulation indicating that a quasi-steady state has been reached. Tidal mixing leads to vertically homogeneous concentrations except in deeper areas of northern Malacca Strait. Furthermore, the concentration distributions of PCB 153 in water show similar patterns but lower values than γ-HCH.

Key words: Malacca Strait, circulation, persistent organic pollutants POPs, PCB 153, γ-HCH.

Introduction

"Persistent organic pollutants (POPs) are chemical substances that persist in the environment, bio-accumulate through the food web, and pose a risk of causing adverse effects to human health and the environment." (UNEP, United Nations Environment Programme, http://www.chem.unep.ch/pops/) Ecological aquatic systems are also sensitive to POPs because of their eco-toxic characteristics. POPs are artificially introduced into the nature and the ocean from industry and agriculture via waste water and rivers or atmospheric input. They are persistent meaning that they hardly transform due to biological, chemical and physical processes leading to accumulation within living plants and animals, where they can influence cell growth and the metabolism and harm the ecosystem.

The most common and known POPs are PCBs (poly-chlorinated biphenyls, widely used by industries) and HCHs (hexachlorocyclohexane, widely used in agriculture). In this study, the isomers PCB 153 and γ-HCH (lindane) have been selected as representatives for two different classes of many distinct organic artificial chemicals with very different properties.

POPs (HCH and PCB) have been banned by Indonesia in the first half of the 1990s (UNEP/GEF, 2003), and—on a global scale—the production at least of HCHs has been drastically reduced within the last two decades (Vijgen, 2006). However, there are still thousands of tons of obsolete pesticides stock waiting

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for treatment on destruction (Vijgen and Egenhofer, 2009). Also, high potential use of PCBs due to major stock piles are reported (UNEP/GEF, 2003). For this region, limited data are available on today's import, use, emission and inventory (UNEP/GEF, 2002). Growing industry might still produce PCBs releasing these chemicals via industrial discharge into rivers and coastal waters and into the atmosphere, from where it can be deposited on land and ocean. Besides, Huang et al. (2007) estimated in their global budget from model simulations that SE Asia is a net sink for global PCB in the atmosphere, which was produced in Europe and North America.

It can be concluded that there is still a high potential for increase of POPs in this part of the world even though concentrations are declining already in other regions of the world (e.g. Elbe river, North Sea) (ARGE Elbe, 2003, 2005, 2007, 2008).

The Malacca Strait, which is the focus of our study, is one of the world's most exploited straits, connecting the South China Sea in the south with the Andaman Sea in the north. It is enclosed to the east by West-Malaysia, and to the west by Sumatra. Sumatra is a fast developing island of Indonesia with intensifying use of land for agriculture and growing industries. The major land and population is located on the eastern side of the watershed, which is a mountain range close to the west coast of Sumatra reaching from the NW entirely to the SE tip of Sumatra. More than 70% of the land of the island drains via its largest rivers into the eastern adjacent seas, also the Malacca Strait, with an impact on this marine environment.

To achieve more knowledge about the fate of POPs in the coastal regions of Sumatra, a set of two numerical models is adapted and applied: the first and basic necessity is to simulate the hydrodynamics of the region of interest, i.e. the Malacca Strait and the western part of the Sunda Shelf, to obtain the information about the physical transport rates and pathways. Secondly, a numerical model for the simulation of the fate of certain POPs has been adapted to the same area. For realistic simulations, many POP related input data are necessary to be determined from measurements and used in the numerical simulation (e.g., river loads, atmospheric concentrations of gaseous and aerosol-bound compartments, concentrations of the different compartments in ocean water and in sediment, sinking velocities of SPM). Most of these data are not yet available for the region of interest.

As a first step, the numerical simulation of the dispersal of the two above mentioned congeners was performed by means of a model experiment: starting without POPs in the domain, only input from rivers is allowed.

The aim of this model experiment is to investigate the spreading of fluvial POPs in the Malacca Strait. Even though these are only intermediate results, they give already a useful estimate of the marine region influenced by riverine input of the tracers studied. The most important information, we gain from this model experiment, are the dispersal and the patterns of POPs in water due to hydrodynamics, fluvial sources and sinks from deposition of particle-bound compartments on the sediment. Eco-toxic effects of the POPs on the bio-environment make the knowledge about the pathways of these substances relevant.

The simulated period covers seven years from 2000 to 2006. The applied model system is ready to simulate more realistic situations, when the corresponding key parameters have been determined.

The following section presents a short introductory to the POPs of our interest in the ecosystem. Then, the applied numerical models are briefly described. Thereafter, the hydrodynamical situation will be explained. The next section will then present some interesting results of the POP simulations.

Properties and Transport Processes of γ-HCH and PCB 153

The two distinct POPs investigated in this work are dangerous to the ecosystem, because they can harm health of living animals by influencing the cell growth, the metabolism and the endocrine system (UNEP/GEF, 2002, 2003). PCBs are even supposed to be carcinogenic. They accumulate in different organs of the bodies, where they can stay for long time because they are hardly bio-degradable. Depending on the phase and the environment of the POPs, they have half-lives of weeks to decades, i.e. PCBs: three weeks to two years in air, more than six years in aerobic soils and sediment, over 10 years in fish; HCHs: one year in soils, two years in water (UNEP/GEF, 2002, 2003). The persistency of the POPs enables permanent bio-accumulation.

Another important property distinguishes γ-HCH clearly from PCB 153: the solubility. PCB 153 is much less soluble in water (much more lipophilic) than γ-HCH, meaning that most of the PCB 153 found in nature is bound to particulate organic carbon (POC) and with this to suspended particulate matter (SPM), thus following the pathways of this material, while the majority of γ-HCH is dissolved in water (Ilyina et al., 2006, UNEP/GEF, 2002, 2003) transported directly with ocean currents. Guglielmo et al. (2009) simulated the global distribution of γ-HCH and found less than 0.2% bound to SPM. Besides, hydrophilic (well soluble) POPs like HCHs are less bio-accumulative, because they can be flushed out and leave the body again, while lipophilic POPs like PCBs are stored easily in adipose tissues and accumulate there. Living creatures of a higher trophic level of the food web do bio-accumulate at a higher rate, because they consume already polluted food. ARGE Elbe (2008) report for the year 2007 that the eel living in the German river Elbe is contaminated with POPs sometimes even above the legal limit for human food, while the food of the eel and the water are not.

The fate of POPs in the ocean is influenced by a wide range of interacting biological, physical and chemical processes including land-ocean, atmosphere-ocean and—within the ocean—sediment-water interchange. Figure 1 presents the key processes included in the numerical model for the fate and transport of POPs (Ilyina et al., 2006).

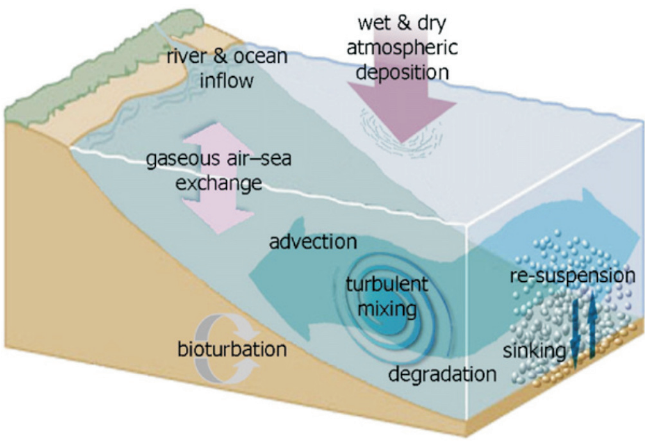

Figure 1: Key processes determining the fate and transport of POPs in the numerical model FANTOM. The transformation of POPs between the two phases – dissolved in water and attached to particulate matter – is included as well.
***Source:* Ilyina et al. (2006).**

For SE Asia and its marine system, the gaseous air-sea exchange and wet and dry deposition of POPs from the atmosphere might play an important role. However, as mentioned before, data are scarce to estimate and simulate reasonable rates. Therefore, in this study, we focus on the dispersal of Sumatran fluvial POPs in the waters of the Malacca Strait.

Applied Numerical Model Systems

Hydrodynamical Model System

For a most realistic simulation of the circulation in the Malacca Strait and the adjacent South China and Java Seas, a nested model system has been set up and applied for a period of 27 years (1980 to 2006). The global ocean circulation model MPI-OM (Marsland et al., 2003, Jungclaus et al., 2006), which was used for the IPCC model simulations for the estimation of the development of the world's climate, simulated the global circulation on a tri-polar grid with a horizontal resolution of 24′ (approx. 44 km in lower latitudes). The vertical grid resolution is based on a z-coordinate system with 40 layers of increasing thickness from 6 m for the most upper layers to a few hundred metre for the lowest layers. Meteorological forcing was taken from the NCEP/NCAR reanalysis data (Kalnay et al., 1996). For the region itself, the 3-dimensional ocean model HAMSOM (Hamburg Shelf Ocean Model) (Backhaus, 1985; Pohlmann, 1996, 2006) was applied with horizontal resolution of 1′ (approx. 1.8 km), also working on a z-coordinate grid with 16 layers of different thickness (5 to 6 m for the upper layers to 7 and 13 m for the lowest layers). The simulations were driven with the same NCEP forcing as the global model. The topography for the regional model was composed of different worldwide data sets (Gebco-Team, 2003; NOAA, 1988), which were partly corrected using satellite images and navigational charts. This was especially done for some of the narrow passages between islands. Figure 2 presents the model area.

Initial temperature and salinity distributions were interpolated from monthly and seasonal data of the World Ocean Atlas (Levitus, 1982), version 2 of 0.25° data (Boyer et al., 2005). At the open boundaries of the regional model, simulation results (daily averages) from the global model were used for the sea surface heights as well as the vertical structure of temperature and salinity.

Tidal forcing was also included. The TPXO7.2 version of the tidal prediction software OTPS of the College of Oceanic and Atmospheric Sciences of the Oregon State University in Oregon, USA, was used with 13 tidal constituents to create their tidal phases and amplitudes superimposed on the SSH open boundary values coming from the global model. A description of the tidal prediction software can be found on the website http://volkov.oce.orst.edu/tides/global.html.

River runoff has to be considered in the regional model runs, because the hydrodynamics of the fairly

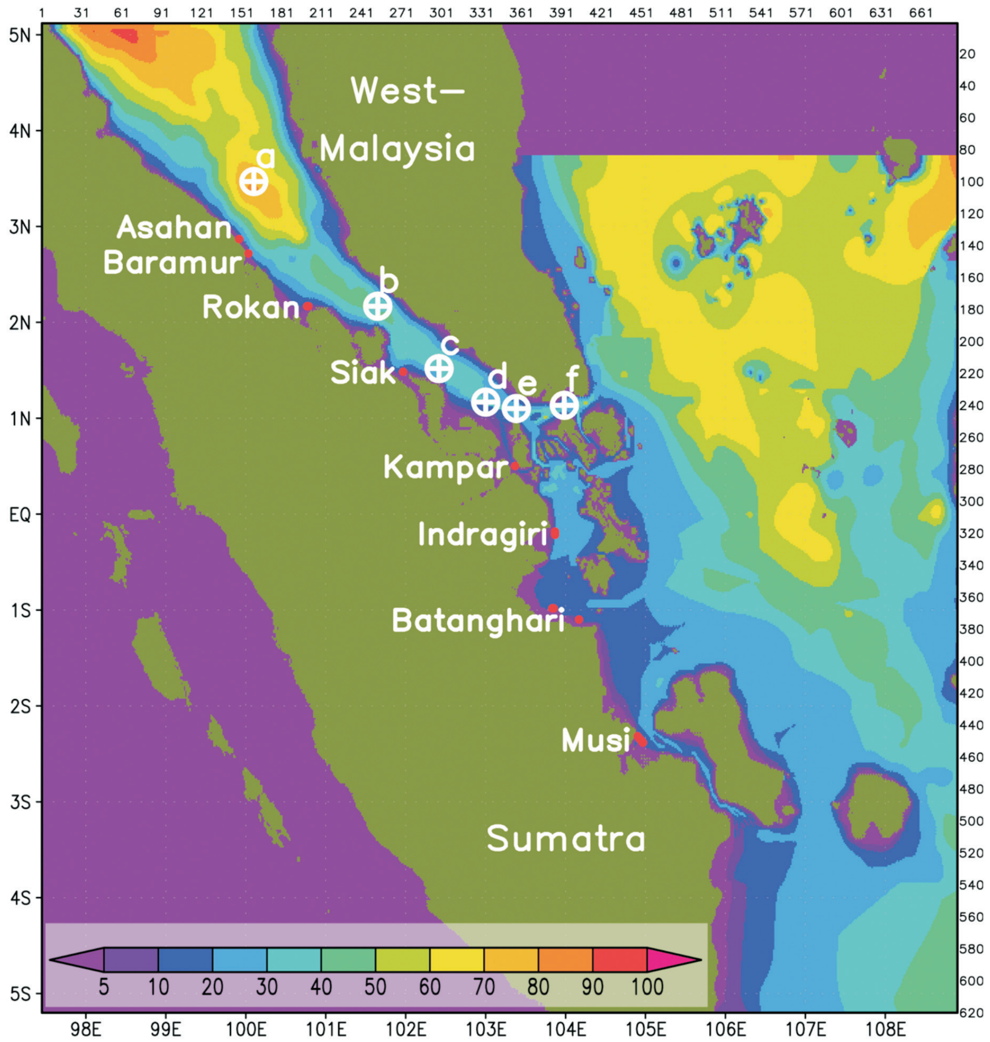

Figure 2: Model area of the regional model HAMSOM for the Malacca Strait and adjacent seas. Bathymetry and scale depth are in metres. Red dots mark the input points for riverine fresh water and POP input. The encircled crosses depict the locations of the vertical Hovmöller diagrams for the temporal development of γ-HCH in Figure 4.

small and narrow Malacca Strait is effected by the fresh water. Besides, for the case study of POP transport in the Malacca Strait and its near-coastal areas, the distribution of POPs due to input from rivers was supposed to be of major interest, since this might become an important source in these regions in the future, when industrial economy and agriculture are growing. Because no reliable time series of river runoff data were available, precipitation data from the Climate Data Centre of the German Weather Service (DWD) have been used (V.1 of the GPCC Monitoring Product, see http://cdc.dwd.de/catalogue). River runoff was then calculated combining the provided daily precipitation data and the estimated catchment areas for the nine most important river basins of Sumatra flowing into the ocean along the eastern coast of the island (Malacca Strait, South China Sea, Java Sea). According to Asdak et al. (1998) and Schellekens et al. (2000), only 55% of the volume raining onto a tropical vegetation reaches the bottom. Assuming that the bottom in tropical regions is saturated, we conclude that this full fraction will be drained into the rivers and into the ocean. A temporal lag between rain fall and river runoff is not taken into account.

The river runoff data were available until end of 2000. For the years 2001 to 2006, climatological daily values were calculated from the available time series and used for the riverine fresh water input.

The same setting of the global and the regional numerical hydrodynamical models has been successfully applied already to a region east of the Malacca Strait, namely the area of the Indonesian throughflow (Mayer et al., 2010). In fact, the same global model data were used here to feed the regional model at its open boundaries.

POP Transport Model

For the simulation of the dispersion of POPs, the numerical model FANTOM, Fate and Transport Ocean Model (Ilyina et al., 2006), has been set up and applied to the region of the Malacca Strait. It is driven with the hydrodynamical data delivered by the aforementioned regional model HAMSOM. For example input data necessary for realistic simulations are:

- concentrations of the different POPs compartments in river water and in the atmosphere (for gaseous exchange of dissolved and wet and dry deposition of aerosol-fixed substances),
- SPM loads in rivers and at open model boundaries,
- content of fine fraction in the sediment for the exchange of POPs at the sediment-water interface and for physical deposition or erosion due to waves and strong currents, and
- other area-specific parameters mentioned in the Introduction section.

Those values influence the bio-geochemical processes involved in the fate of POPs, and hence, they are included in the model FANTOM as presented in Figure 1.

For this model experiment, exchange of substances across the air-sea interface was neglected. As a consequence, losses of POPs in the water due to volatilization as well as gains due to gaseous input or wet and dry deposition from the atmosphere were ignored. One-way transfer from water to sediment (sedimentation) was allowed assuming calm weather conditions and settling velocities for SPM of 0.0003 m/s, which is a little higher compared to background values for the North Sea (Gayer et al., 2006), because the partition of eroded material, which is a part of SPM in ocean water and sinks almost one order of magnitude faster (Gayer et al., 2006), was not considered explicitly here. Weather conditions and strong currents are responsible for erosion of fine fraction in the sediment leading to increase of SPM concentration and with this of particle-bound POPs in the water column (especially important for PCB 153). Again, we are interested in the dispersal of fluvial POPs, and hence, it is justified to neglect these processes.

As a consequence, all possible POP input sources except river input were switched off. The largest rivers of Sumatra were taken into account with non-constant runoffs (see previous section) but with a prescribed constant concentration for γ-HCH or PCB 153 of 1 ng/L, which is of the order of the average European riverine concentration of POPs into the North Sea (ARGE Elbe, 2008; O'Driscoll et al., 2011). UNEP/GEF (2002) reported for HCHs a range of 0.08-22 ng/L in rivers of the region including SE Asia as well as Australia and New Zealand in the 1990s. Neither industries nor agriculture were as developed as they are now in Sumatra.

As a first step, this is sufficient, because the focus of this study was put on the general fate of POPs, which are introduced into the ocean by rivers only, and to investigate how far the discharged tracers disperse in the adjacent ocean.

First Results

Hydrodynamics

To get an idea about the seasonality of the hydrodynamical situation in the Malacca Strait, Figures 3a and 3b show the horizontal distribution of the total transport as monthly average for January and June 2002 with focus on the Malacca Strait, our main investigation area. Figure 3a presents the predominant winter monsoon situation with strong northward transport through the entire Malacca Strait. This occurs, because the northerly winds push water masses from the northern parts of South China Sea towards its southern part and into the Java Sea piling up the water also close to the southern entrance of the Malacca Strait. This produces a barotropic pressure gradient accelerating the currents through Malacca Strait into the Andaman Sea even against the prevailing wind direction. Figure 3b shows a typical summer monsoon situation with indifferent transports within the southern part of the Malacca Strait and a recirculation of Andaman Sea waters in its northern part. The barotropic gradient of the winter monsoon has been relieved, sometimes even reversed, while the wind transports the water masses towards the northwest. Similar results are presented by Pang and Tkalich (2003), who simulated the hydrodynamics for the Singapore Strait, and Rizal et al. (2010), who simulated the hydrodynamics of the Malacca Strait.

There is strong tidal mixing almost in the entire model domain except in northern part of Malacca Strait, where the depth exceeds 50 or 60 m, because of the

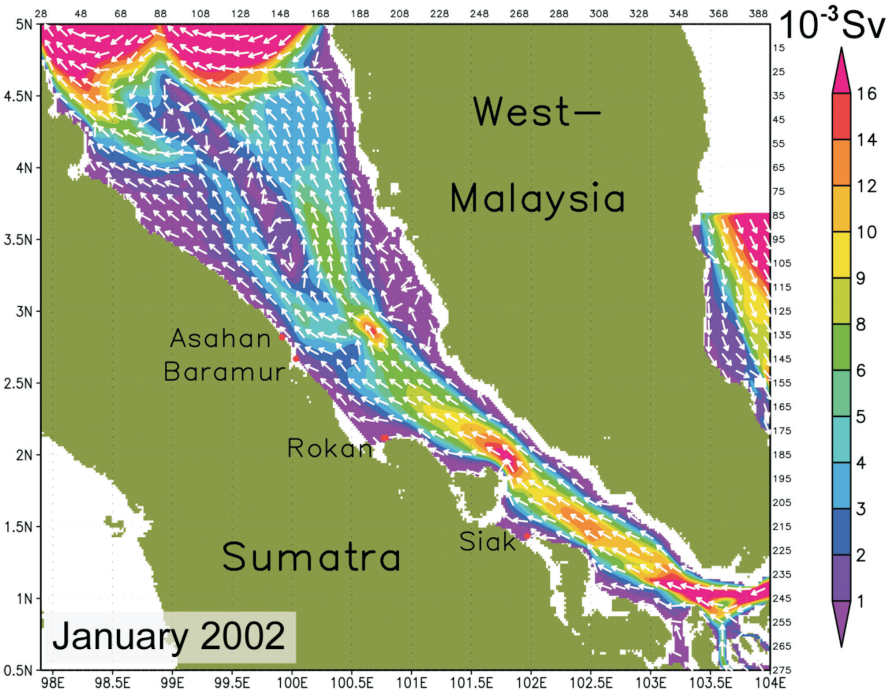

Figure 3a: Horizontal distribution of the simulated total volume transport in the Malacca Strait in 10^3 m^3/s (=10^{-3} Sv) as monthly average for January 2002. Shading colours present the magnitude of the transport, arrows the direction. Note: Scale of shading colours is different to the one in Figure 3b.

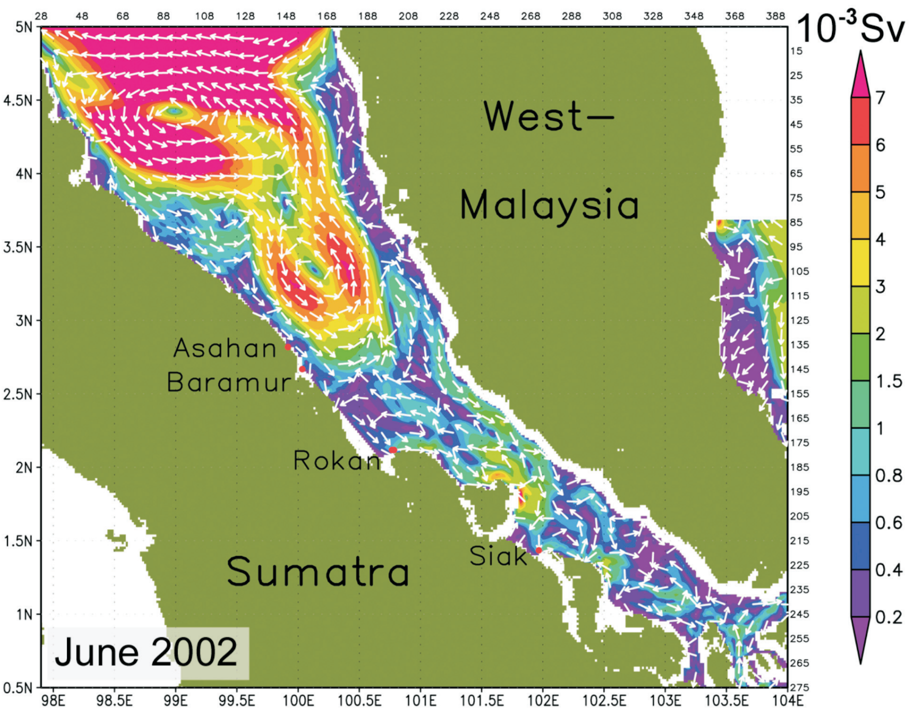

Figure 3b: Horizontal distribution of the simulated total volume transport in the Malacca Strait in 10^3 m^3/s (= 10^{-3} Sv) as monthly average for June 2002. Shading colours present the magnitude of the transport, arrows the direction. Note: Scale of shading colours is different to the one in Figure 3a.

strong tidal currents in quite shallow regions leading to a rather non-stratified water column.

POP Dynamics

The simulated distributions of the POPs will be presented only for the γ-HCH, because there is a more or less constant difference in the model results between the distributions of γ-HCH and PCB 153. The concentration of the latter POP is lower but shows similar patterns and variability. The reason is the above mentioned main differences between the properties of both POPs in half-life time and solubility, which act contradictory for the concentration of PCB 153 in water. While PCB 153 is much longer lasting (half-life is higher), much more of this substance is bound to particles and leaves the water column due to sedimentation. Therefore, we will present only the simulated behaviour of γ-HCH.

The clear seasonal development of the POP concentration in ocean water, if we have only river input, can be seen in the vertical Hovmöller diagram of Figure 4. The positions of the water columns, for which the concentrations are displayed, can be seen in Figure 2 by the white encircled crosses.

The seasonal signal with high concentrations in the boreal summer and low concentrations during the winter monsoon phase corresponds to the seasonality of the circulation driven by the barotropic pressure gradient and wind. During boreal summer, when the pressure gradient between South China Sea and Andaman Sea decreases or even reverses, the northward flow through the Malacca Strait slows down or reverses. This is additionally supported by the prevailing wind direction in the SE monsoon phase. Obviously, at this time the riverine POP accumulates along the coast of Sumatra. During the following boreal winter monsoon season, again the northward water transport through the Malacca Strait is enhanced and the high concentrations are diluted and transported further towards the Andaman Sea.

It is interesting to see from Figure 4 that the POPs are homogeneously distributed over the entire depth because of the strong tidal mixing. Only in the northern regions of the Malacca Strait with greater depths, where occasionally near-bottom southward counter-current occur, a stratification can be observed in the model results with higher concentrations in the upper water column.

Within the period 2000 to 2006, there is no significant interannual variability superimposed to the seasonal variability. However, Figure 4 shows an unusual low concentration of POP at all stations in summer 2003. Further investigation has to be performed to answer the question, if this is connected to the El Niño event of the second half of 2002.

The horizontal distribution of the riverine POPs is presented in Figure 5 as monthly averages of the POP concentration in the surface layer of the model for the year 2002. As mentioned before, there is no vertical gradient in the concentrations, and there is no interannual signal in the patterns of the monthly mean POP concentration. The distribution patterns of the monthly means look very similar for each year as well as for other model layers.

The tracer concentration is highest close to the river input points. In boreal winter, the near-coastal concentrations are lower and wider spread than during summer time, when the water velocities are slower. When comparing the concentration distribution close to the river input points in Figure 5, the Siak River seems to have a rather low impact on the Malacca Strait due to its relatively low runoff, while other rivers develop a larger area of higher POP concentrations around the respective river mouths.

For a closer look to the region of the Siak estuary and the adjacent Bengkalis Strait, Figure 6 magnifies the corresponding part of the Malacca Strait. From the shape of the concentration isolines, we can conclude the mostly prevailing northeastward transport through the Malacca Strait. From the level of the concentrations, we can conclude a low transport rate during late boreal summer time and a higher mass transport during other times of the year.

Summary and Conclusions

A set of numerical models has been applied to the region of the Malacca Strait, the south-western South China Sea and the western Java Sea in order to simulate the dispersal of the persistent organic pollutants γ-HCH and PCB 153, which are in the present study introduced into the marine eco-system by input through rivers only. It has to be noted that only an instructive model experiment with respect to the POP dynamics was performed because of a very thin POP related data base for this region, which has hardly been subject of marine investigation in the past. The first set of models simulated the hydrodynamical current system as realistic as possible. A clear seasonal variation with stronger north-westward flowing water masses in the Malacca Strait in boreal winter season and weaker north-westward or partly southward directed currents during summer season was obtained. The model

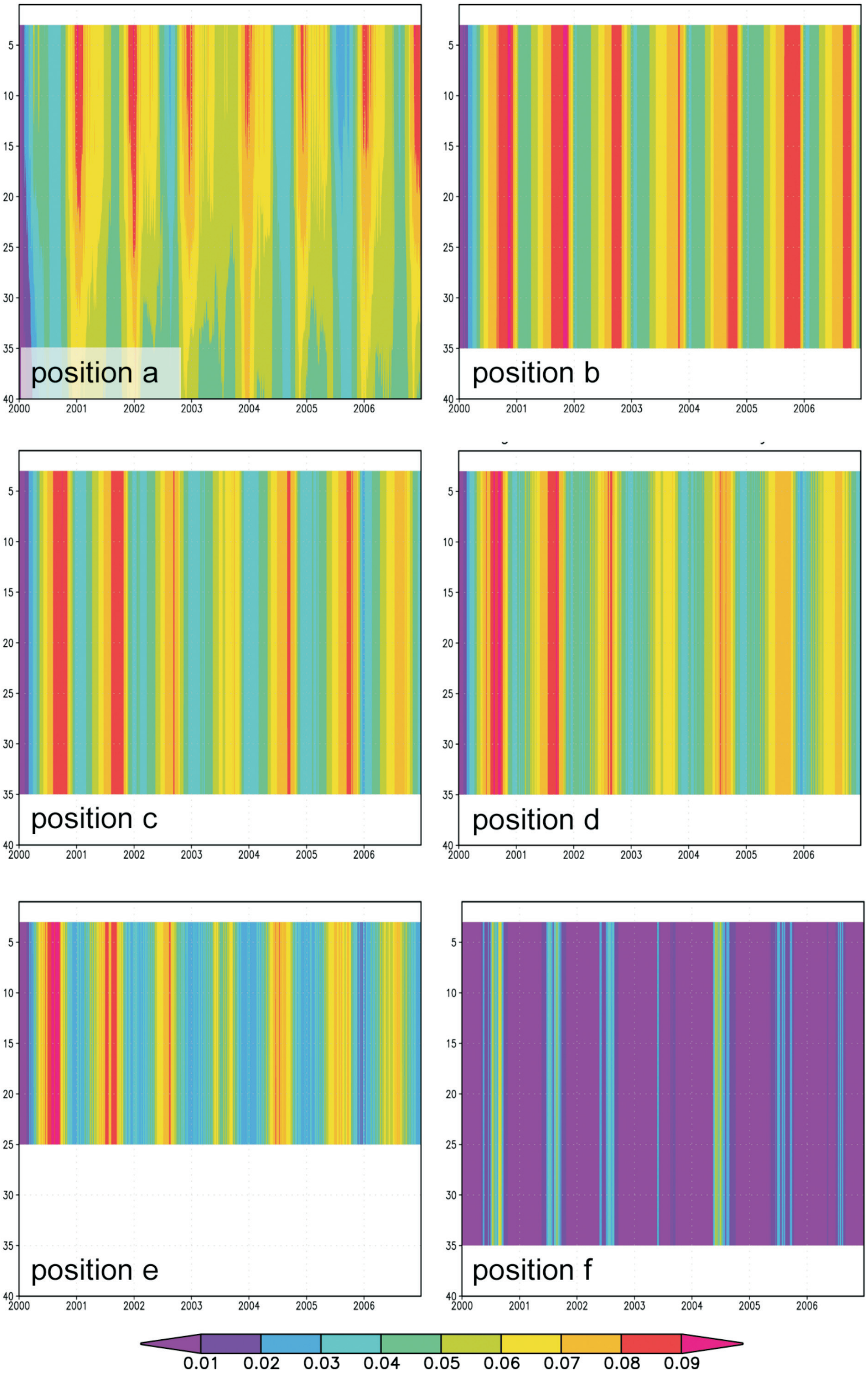

Figure 4: Vertical Hovmöller diagrams for the simulated concentration of γ-HCH in water in ng/L. The locations of the water columns are displayed by the white encircled crosses in Figure 2.

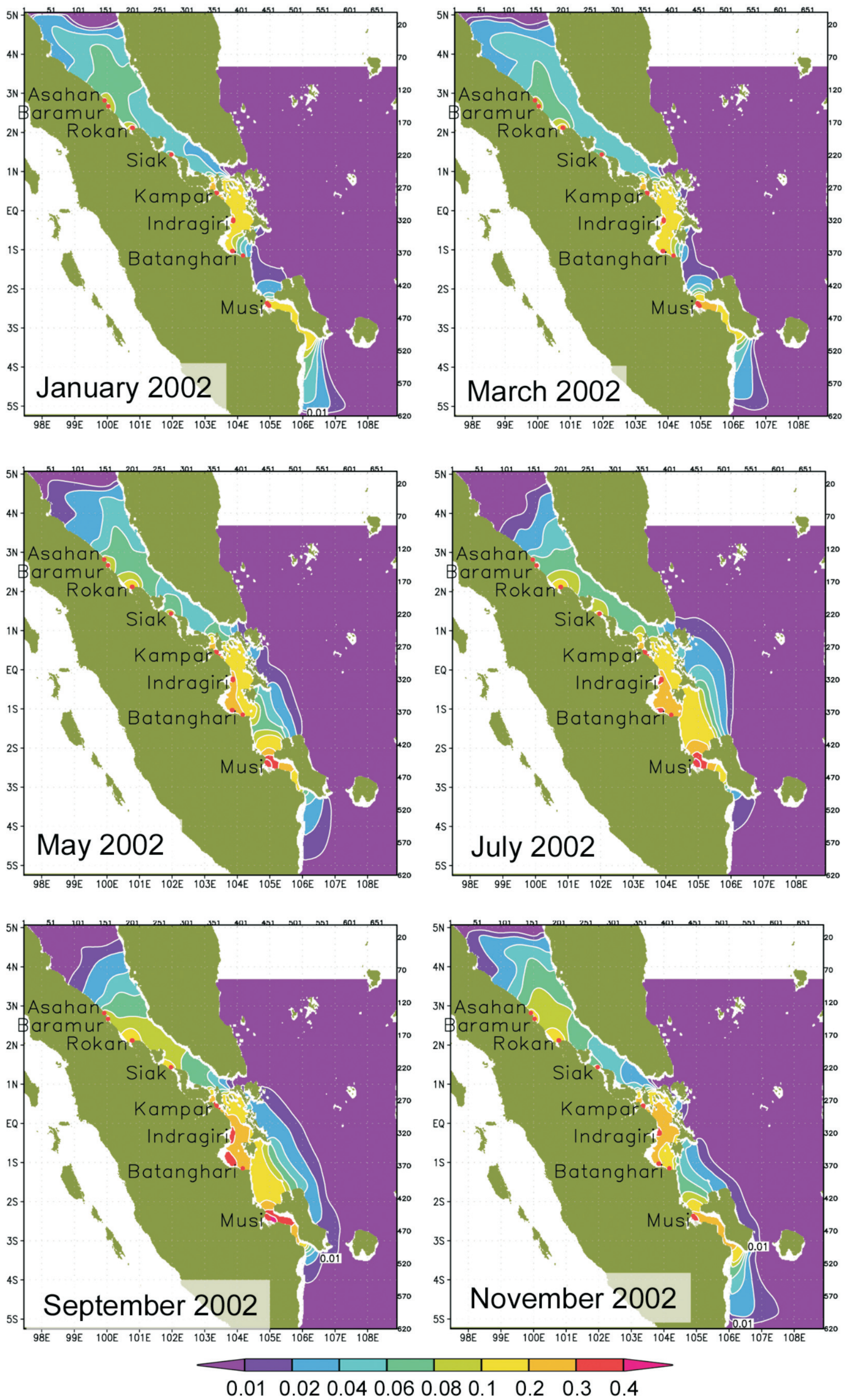

Figure 5: Horizontal distribution of the simulated concentration of dissolved γ-HCH in water (surface layer) in ng/L as monthly average for every second month in 2002.

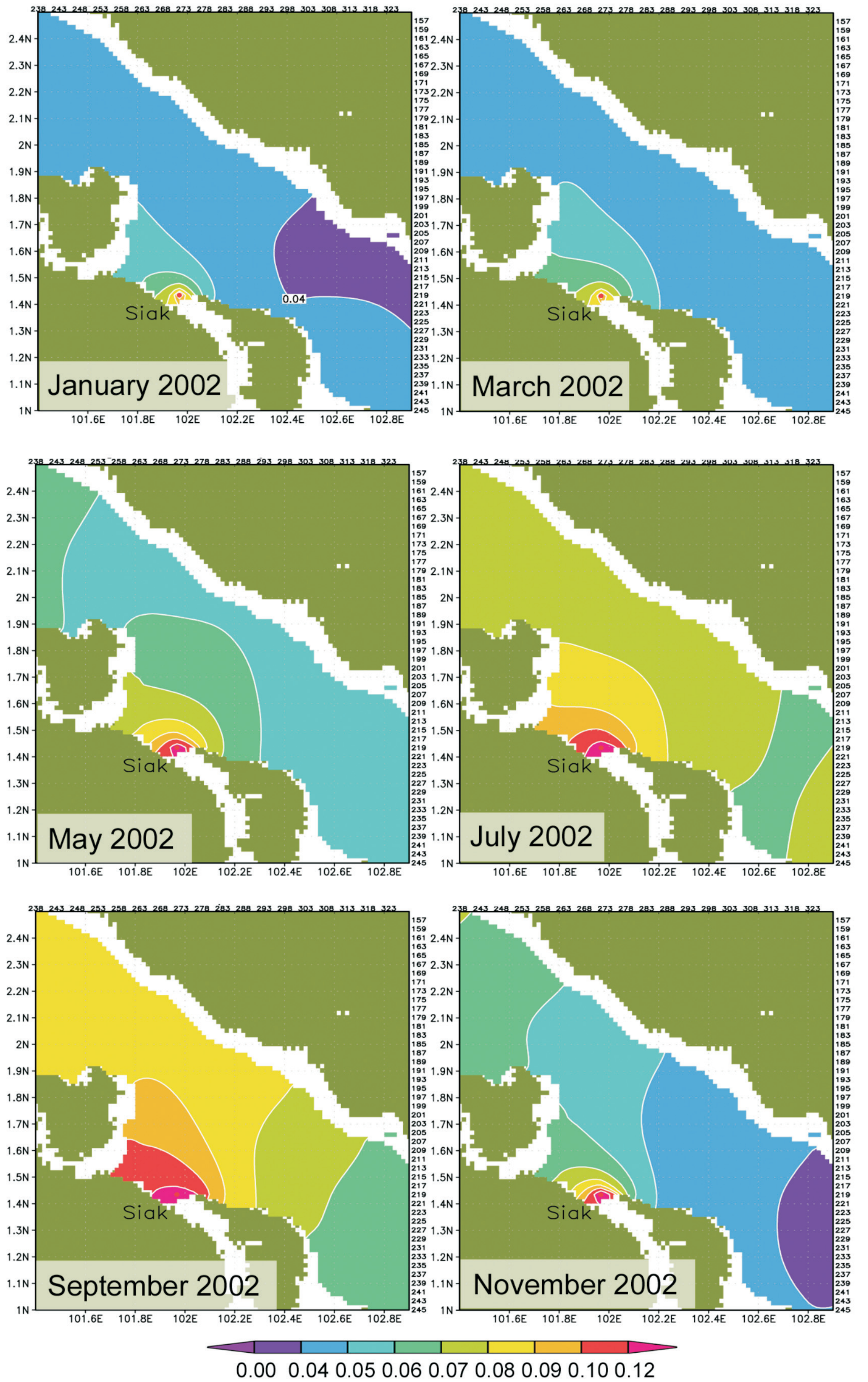

Figure 6: Horizontal distribution of the simulated concentration of dissolved γ-HCH in water (surface layer) in ng/L as monthly average for the region of the Siak river mouth for every second month in 2002.

results were then taken to force the fate and transport model for the POPs. The simulation results showed interestingly that seasonal POP distribution patterns are established without interannual signals and no further accumulation in the water indicating a quasi-stationary state with a seasonal cycle. The source for introducing POP into the model area was obviously of the same order as the sink due to sedimentation of particle-bound compartments, lateral outflow and degradation (the other sink implemented in the POP model, volatilization, as well as other exchange processes at the air-sea-interface were disabled for this simulation).

It was admitted that the model experiment of this study was not intended to provide the most realistic results. Taking all processes into account would probably show much higher concentrations of both POPs in the marine environment. Strong tidal mixing leads to vertical homogeneous concentrations of dissolved POPs; non-dissolved SPM-attached compartments will develop a vertical profile with highest concentrations close to the sea floor, where it will deposit during calm conditions and be eroded in situations with strong (tidal) currents or high waves. A strong impact on the benthic bio-environment is probable. Additionally, the sediment acts as a long-term storage for SPM-attached POPs.

Further investigation should be done using these powerful numerical tools to realistically simulate the development of harmful POPs in the oceanic environment, including the probably high atmospheric input, to estimate the real contamination of the marine ecosystem. These model studies should be accompanied by field campaigns measuring the POP concentration in the marine environment and the atmosphere. The people of Sumatra, West-Malaysia and Singapore are living on marine fish and other "fruits" of the ocean. Following Huang et al. (2007) and the reports of UNEP/GEF, there is a high potential that the concentration of certain POPs in the ocean and with this the contamination of the marine food will increase in future, due to global atmospheric POPs produced in other parts of the world but also due to growing local economy.

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