Model analysis of deoxygenation connected with acetate discharge in the coastal zone

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Consequences of acetate discharge during production of X-ray contrast agents in the coastal waters of the Norwegian coast of the North Sea were analyzed with a set of mathematical models. Firstly contact measurements data were collected in order to verify results of modeling. The baseline seasonal variability of temperature, salinity, advection and turbulence were calculated with FVCOM (The Finite Volume Community Ocean Model) applied to the Southern coast of Norway. These data were used to force a vertical 2-dimensional benthic-pelagic transport model (2DBP) coupled via Framework for Aquatic Biogeochemical Models (FABM) with a biogeochemical model OxyDep, calculating spatial distribution and seasonal variability of phytoplankton, heterotrophs, nutrient, dissolved organic matter, particulate organic matter, and dissolved oxygen (DO). Acetate was considered as a chemical oxygen depletion substrate leading to the decrease of oxygen concentrations. We simulated seasonal variability at a 10 km long vertical transect with spatial resolution of 50 m horizontally and approximately 2 m vertically. These calculations reproduced local minimum in vertical DO distributions in 2 km from the discharge point, that corresponded to the observations data. We conducted numerical experiments on the effects of doubling of the acetate discharge and on formation of acetate complexes. Due to low ion concentrations and small stability constants, complexes with some of the ions presented in the sea water were not considered. That is why calculations of acetate concentration were updated by adding formation of complexes with Mg and Ca into the equation.