A conservative, positivity preserving scheme for advection-diffusion-reaction equations in biochemical applications

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The talk is devoted to the development of a higher order finite volume method for biochemical applications. As eutrophication is a serious problem through giving rise to excessive algae blooms in all types of waters with no or only small current it is crucial in ecological science to understand and predict the coherences of the underlying dynamics. As phosphorus is the limiting nutrient element for most of all algae growth processes an advanced knowledge of the phosphorus cycle is essential. Due to the specific situation in lakes and rivers the governing equations are based on the 2D shallow water equations extended by a profound model is presented taking into account four different species of algae and zooplankton with the particularity of mapping variable phosphorus contents in the biomasses. Furthermore phosphorus in soluted and organic bounded form in the water body as well as in the sediment is considered.

In particular, the examined constituents of the biological system are soluted phosphorus/ PO4- (PS), phosphorus in detritus (PD), inorganic and soluted phosphorus in sediment (PE_I), organic phosphorus in sediment (PE_O), biomass of zooplankton (BZ) and its content of phosphorus (PZ), the biomasses of four different species of algae (BA_A, BA_B, BA_C, BA_D) with their respective content of phosphorus (PA_A, PA_B, PA_C, PA_D). The dependencies as well as transitions are depicted in figure 1. For the sake of simplicity only one biomass algae (BA) and respectively only one phosphorus content (PA) are included. The remaining of both biomasses and corresponding phosphorus can easily be included since their evolution is quite alike.

The considered processes between this members are an enhancement of the phosphorus cycle model proposed in [1]. All dependencies are outlined in the sketch.

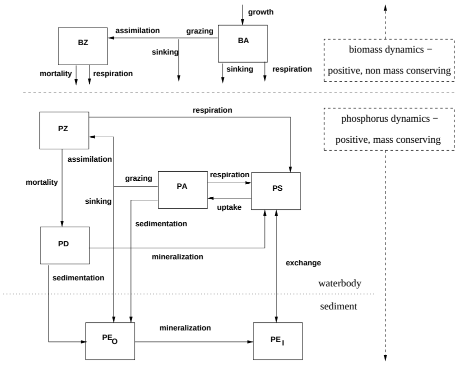

Figure 1: Biological and chemical processes

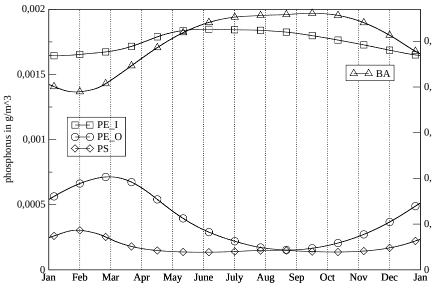

Figure 2: Circle of the year for phosphorus in water and sediment with one biomass algae

Coupling the underlying flow model with the phosphorus and biomass cycle gives

$$\partial_t \mathbf{u} + \sum_{j=1}^{2} \partial_{x_j} \left(\mathbf{f}_j^c(\mathbf{u}) - \mathbf{f}_j^d(\mathbf{u}) \right) = \mathbf{r}(\mathbf{u})$$

where the vector $\mathbf{u}$ contains the water height, velocity as well as all different forms of phosphor and biomass.

Furthermore, the convective fluxes $\mathbf{f}^c$ represent a combination of the shallow water flux with terms describing passive transport of non sediment constituents, $\mathbf{f}^d$ denotes diffusive processes of soluted phosphor and $\mathbf{r}$ represents source terms due to the local transition of the biological constituents.

Dealing with a mass conserving modeled matter cycle and biological and chemical quantities poses severe demands on the used algorithms. Thus to obtain scientific reasonably results a scheme must be which guarantees the positivity for all substantial compartments and which does not generate nor destruct matter. To take advantage of special time integration schemes which yields desirable properties, a second order Strang splitting ansatz is used.

The fluxes, $\mathbf{f}^c(\mathbf{u})$ and $\mathbf{f}^d(\mathbf{u})$, are solved by a TVD-type finite volume scheme, a modification of the code proposed in [2]. It works on a secondary unstructured grid with the HLL flux solver and linear reconstruction on the boxes with two limiters proposed by Venkatakrishnan in [3] and the classical Barth-Jesperson. The diffusive flux is solved via the unique known gradients on each triangle, see [4].

As the considered species hold three different sets of properties a special treatment for each set is required. The water height (H) and the biomasses (BZ, BA_{A-D}) are obviously positive yet not mass conserving with respect to the model used. So the used scheme must ensure positivity for this objects. This attribute holds true for the Patankar Scheme developed in [5]. All phosphorus quantities $(PS, PD, PE_I, PE_O, PZ, PA_{A-D})$ are modeled positive and additionally mass conserving and need therefore a scheme which conserves the mass and maintains the positivity. The modified Patankar Scheme presented in [6] satisfies both positivity and conservativity.

Applications are shown which confirm the theoretical statements. For example the changes of the phosphorus with one biomass algae is presented in figure 2. The scheme gives reasonably results for the change of the phosphorus content over the seasonal changes as can be seen in the graph. The phosphorus concentration augments in the spring. With the rising of the temperature the bacteria in the sediment start to convert the organic bounded, which was accumulated over the winter, into inorganic soluted phosphorus. Through the diffusive exchange between the soluted phosphorus in water and sediment the soluted phosphorus in the water augments and is directly consumed by the starting algae growth BA. In the end of the year the phosphorus concentration PE_O and PS increases due to the decease of the algae BA. PE_O is augmented by the dead biological mass, PS through lesser consumption and exchange between PE_I and PS.

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