Applicability of zero-dimensional equations to forecast nonconservative components concentration in water bodies

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Abstract. The presence of ongoing climate change and their increasing scale have now become apparent. Climate models provide a glimpse of the future. Disappointing forecasts pushing to develop models that would allow rapidly develop measures for adapting to unavoidable environmental conditions and to mitigate impacts, including those related to the deterioration of water quality in natural water bodies and reservoirs.

The most simple and effective models for fast and fairly accurate forecasts regarding waters are the zero-dimensional models. Such models widely used in engineering practice owing to their considerable simplicity which is correct for conservative substances. At the same time, additional limits should be taken into account while forecasting water quality involving nonconservative components which could change its chemical characteristics in particular.

The period during which the concentration of a substance becomes the same over the entire area of a reservoir could be considered as a time scale in which zero-dimensional equations are applicable, the average concentration of substances for the entire body of water can be considered only as of the average over some time not less than determined by the scope of consideration. The expression which is given in the paper allows identifying limits of applicability of zero-dimensional equations for a non-conservative substance concentration as a function of time scale and coefficient of non-conservativeness.

1. Introduction

The object of research was the quality of water in reservoirs, and the subject of research was the zero-dimensional equations of state of water. The aim of the research was to formulate conditions under which zero-dimensional (balance) models could be used to predict water quality. Wind exposures as well as diffusion were considered as the main factors leading to the mixing of both conservative and non-conservative substances in water bodies.

Water is perhaps the primary medium through which the effects of climate change will be felt most tangibly. Water availability is becoming less predictable in many places, and increasing floods threatens to destroy water infrastructure and contaminate water sources.
The main climate change consequences related to water resources are the shifts in precipitation patterns and snow cover, and a likely increase in the frequency of flooding and droughts [1].

Water resources are important for both society and ecosystems. Humankind depends on a reliable, clean supply of drinking water to sustain our health. There is also need for water for agriculture, energy production, navigation, recreation, and manufacturing. Many of these uses put pressure on water resources, stresses that are likely to be exacerbated by climate change.

In many areas, climate change is likely to increase water demand while shrinking water supplies. This shifting balance would challenge water managers to simultaneously meet the needs of growing communities, sensitive ecosystems, farmers, ranchers, energy producers, and manufacturers.

Many areas of the Central Asian downstream countries currently face water shortages. The amount of water available in these areas is already limited, and demand will continue to rise as population grows. At the same time, water quality could suffer in areas experiencing increases in rainfall. Heavy precipitation events could cause problems for the water infrastructure, as sewer systems and water treatment plants are overwhelmed by the increased volumes of water [2]. Heavy downpours can increase the amount of runoff into rivers and lakes, washing sediment, nutrients, pollutants, trash, animal waste, and other materials into water supplies, making them unusable, unsafe, or in need of water treatment [3].

According to the UN World Water Development Report [4], water use has been increasing worldwide by about 1% per year since the 1980s, driven by a combination of population growth, socio-economic development and changing consumption patterns. Global water demand is expected to continue increasing at a similar rate until 2050, accounting for an increase of 20 to 30% above the current level of water use, mainly due to rising demand in the industrial and domestic sectors.

The increasingly evident impacts of climate change at various levels lend the issue a particular sense of urgency to think through about mitigation measures which would prevent catastrophic situations related to both availability of the required volume and quality of water. In this regard, the study of options to quickly assess water quality in natural water bodies and reservoirs seems relevant.

The number of natural disasters associated with climate change has risen sharply over the past decade. The use of existing tools, including computer programs, is associated with a significant investment of time in preparing the initial data for modelling and forecasting. In this regard, the need for the development and practical application of simple but reliable calculation methods and algorithms, including those related to the prediction of water quality in natural water bodies and reservoirs, has increased. Such methods include calculations based on the use of zero-dimensional equations.

2. Method
Perhaps the most effective models for fast and fairly accurate forecasts regarding waters are the zero-dimensional models. That is, such models when the hypothesis of complete, instant mixing of contamination in a reservoir is valid. Such models widely used in engineering practice because of their considerable simplicity [5 - 13].

3. Results and Discussion
Mixing of substances in a reservoir may be initiated by various factors, for example, by wind or by penetrating stream which initiate currents. However, when substances enter into reservoirs, complete mixing in any case cannot happen instantaneously.

Two type of substances were being considered in this paper, namely conservative, i.e. when substance does not change its properties entering a water body and non-conservative.

It takes some time during which a complete mixing of a conservative substance occurs, i.e. concentration of the substance at any point of the reservoir will be the same. This time can be determined in the following way. A source of conservative impurity is placed at some point in the reservoir. The time
During which the concentration of the substance will be the same over the entire area of the reservoir with some precision which should be considered as the required time $T$, which should be considered as the time scale inside which it is permissible to use zero-dimensional equations, i.e. the average concentration of substances for the entire water body can only be considered as the average over a period of time $T$. Inside the time interval $T$, concentrations may vary significantly from average. Thus, it is necessary to use more complete models if there is the need to determine the average values of substance concentrations over a shorter period of time.

It is more difficult to characterize the area of applicability of zero-dimensional equations for a non-conservative substance.

Complete mixing time ($T_c$) can be found by solving a model problem considering a rectilinear channel with length $L$ along which the wind blows with the following properties:

- the wind speed module is constant;
- both directions of the wind are equally probable;
- wind duration distribution function ($t$) is similar to normal probability law (Gaussian probability law). In this case, the flow in the channel is also equally probable and diffusion equation (1) could be used to describe distribution of a substance in the channel as follows:

$$\frac{\partial S}{\partial t} + \frac{\partial}{\partial x} D \frac{\partial S}{\partial x} = -K_{H} S$$

(1)

where:

- $S$ – concentration of substance;
- $D$ – diffusion coefficient;
- $K_{H}$ – destruction coefficient which characterizes the amount of substance destroyed (or changed its properties) for a certain period of time.

**Determination of complete mixing time ($T_c$) for conservative substance**

Let us consider the process at the initial moment of which a substance concentration in the channel is zero. The substance with concentration $S = 1$ is supplied at one of the boundaries and the other boundary is impermeable. In this case, if $K_{H} \neq 0$ the solution of the equation (1):

$$S(x,t) = 1 - \sum_{n=1}^{\infty} C_n \exp \left[ -\left( \frac{n\pi}{L} \right)^2 DT \right] \sin \left( \frac{n\pi x}{L} \right),$$

(2)

where $C_n = \frac{2}{n\pi} (1 - \cos(n\pi))$; and $L \geq 2L$.

For sufficiently large $t$ the series (2) converges very quickly and therefore for estimates it is sufficient to analyse the first term of the series. Then, the time of complete mixing, i.e. the time during which $S$ for all $X$ differs from 1 by a given value $\varepsilon$:

$$\frac{4}{\pi} \exp \left[ -\left( \frac{\pi}{L} \right)^2 DT \right] \leq \varepsilon$$

(3)

and:

$$T_c \geq \frac{4L^2}{\pi^2} \ln \frac{4}{\pi \varepsilon} \frac{1}{D}$$

(4)
Determination of complete mixing time \((T_{\infty})\) for non-conservative substance

Solution of equation (1) for \(\frac{\partial S}{\partial t} = 0\) in (1) and the same boundary conditions:

\[
S = \frac{e^{K \cdot x} + e^{-K \cdot x}}{2 \cdot \cosh(K \cdot L)},
\]

(5)

here \(K = \sqrt{\frac{K_H}{D}}\).

Define \(D\) in \(T_{\infty}\) at \(x = L\) from (5):

\[
S|_{x=L} = \frac{1}{\cosh r}
\]

(6)

here \(r = \frac{\sqrt{K_H T_{\infty} \pi^2}}{\sqrt{4 \ln\left(4/(\pi \cdot \varepsilon)\right)}}\).

The complete mixing hypothesis is true if

\[
S|_{x=L} > 1 - \varepsilon.
\]

(7)

Taking into account (6) and (7):

\[
\cosh r = \frac{1}{1 - \varepsilon}.
\]

(8)

Where, up to small second order:

\[
\frac{r^2}{2} < \varepsilon
\]

and

\[
K_H T_{\infty} < \frac{2\varepsilon}{\pi^2} \ln\left(\frac{4}{\pi \varepsilon}\right).
\]

(9)

It should be noted that if the conditions (9) are not met then zero-dimensional models lead to errors greater than the permissible ones.

4. Conclusions

The studies conducted allowed to formulate the constraints imposed by the specific properties of substances, and in particular, the change in their properties in the aqueous environment. Conditions under which zero-dimensional equations can be applied in engineering practice for forecasting water quality involving both conservative and in particular for nonconservative components which could change its chemical characteristics in water over time were derived.
There were restrictions associated with the destruction coefficient obtained under which zero-dimensional models can be used to forecast water quality in natural water bodies and reservoirs. It was noted that if the conditions are not met then zero-dimensional models lead to errors greater than the permissible ones.

The period of time during which the concentration of a substance becomes the same over the entire area of a reservoir and which could be considered as a time scale in which zero-dimensional equations are applicable was defined, i.e. the average concentration of substances for the entire body of water can be considered only as the average over a period of time not less than determined by the scope of consideration. The analytic expression which is given in the paper allows to identify limits of applicability of zero-dimensional equations for a non-conservative substance concentration as a function of time scale and coefficient of non-conservativeness.

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