Rehabilitation of the Specified-Concentration Boundary Condition for Solute Transport

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ABSTRACT

The specified-concentration boundary condition is also referred to as the Type I and Dirichlet condition. In this study the bold claim is made that there has been a widespread, systematic misinterpretation of fundamental aspects of the Type I boundary condition for solute transport. The objective of the study is to begin the rehabilitation of the Type I boundary condition and to demonstrate that this boundary condition should always be available and sometimes applied in solute transport modeling. The key points of the analyses reported in this paper are summarized below.

1. The Type I boundary condition has been systematically misinterpreted. The Type I boundary condition does not assume that the concentration is fixed through time. Rather, use of the Type I boundary condition requires that the concentration history be known.
2. The Type I boundary condition is mass conservative. The analytical solutions for the Type I boundary condition that are presented in the paper, including the Ogata-Banks solution, satisfy the governing equation, which is a formal statement of the conservation of mass.
3. In its general interpretation, the Type III boundary condition is a statement of mass balance across a boundary. The typical interpretation of the Type III boundary condition invokes the assumption of a “well-mixed” reservoir. This is equivalent to assuming that the influent mass flux has only an advection component.
4. For the case of a constant inflow concentration, the results obtained with a solution for a general interpretation of the Type III boundary condition match those obtained with the Type I condition. The results are completely consistent when the Type III boundary condition is assigned the total mass flux, incorporating both the advective and dispersive mass flux.
5. For the case of a constant mass flux at the inflow boundary corresponding only to the advective mass flux (the “well-mixed” reservoir assumption), the results obtained with a solution for a general interpretation of the Type I boundary condition match those obtained with the Type III condition. The results are completely consistent when the Type I boundary condition is assigned a time-varying concentration that gradually builds up to the concentration in the influent reservoir.
6. Differences between the results from calculations with solutions derived for the Type I and for the Type III well-mixed inflow boundary condition are well established. As far as we are aware, the fundamental source of these differences has not been examined previously. The mass flux from the Type I boundary condition has components of advective and dispersive flux. The concentrations for the Type III well-mixed inflow boundary condition lag those predicted with the Type I condition because the influent mass flux incorporates only the advective component. Results for the two boundary conditions converge as dispersive gradients near the source dissipate.

There is no fundamental weakness in the Type I boundary condition and there are physical situations for which it will be most appropriate. In our opinion, solutions developed for this boundary condition should remain in use, and numerical models should support it. Further analyses with the Type I boundary condition have been developed and will be reported subsequently; these developments highlight the errors that may arise when the “well-mixed” assumption is invoked in interpretations of the typical Type III inflow boundary condition, and the circumstances for which the Type I boundary condition is most appropriate.

It is hoped that this paper will spur a re-assessment of the Type I boundary condition for solute transport. Detailed derivations and all of the codes and input files for the calculations presented are available from the author upon request.