

A brief Report on the article “Mobile and Immobile Gaseous Transport: Embedded Analytical Solutions to Finite Volume Methods. ”

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Abstract: The author derives analytical and semianalytical solutions of convection–reaction equations with general initial conditions. The analytical test functions are embedded into discretization methods for the convection diffusion reaction equation. Further mobile and immobile equations can be treated with splitting methods that allow of reducing the computational complexity and yield higher-order discretization schemes. The author could also verify the new methods with analytical and numerical test examples and present the higher-order results of the underlying schemes.

The convection-dominant equation can be solved with combined analytical and decomposed methods to decouple the complicated equation systems and achieve the accuracy with iterative or analytical embedded methods.

For complex computations of such convection–dominant problems, the author used these methods in the initialization process of the computation and switch after sufficient accuracy to implicit methods with large time-steps. .

Key words and phrases: mobile and immobile Gaseous Transport; advection-reaction equation; analytical solutions; Godunov’s method; Laplace transformation;

Subject Classification : 65M08; 76Rxx; 76Mxx

1 Some questions and remarks ...

1. I still do not understand what meant the author by “Mobile and Immobile Gaseous Transport”

2 Some basic and useful information

1. **Importance.** The article seems interesting since it provides a numerical scheme for an interesting model in Gaseous Transport
2. **Importance again.** The studies are motivated by a desire to model deposition processes based on chemical vapor problems. The model problem is given by a coupled transport–reaction equation with mobile and immobile areas, see [GEI 10].
3. **The model.** The mathematical model is a coupled system of transport equations (given by convection–diffusion–reaction equations) and reaction equations.

4. **Which numerical method is used?** Since the equations involved in the model are transport equations which are conservation law systems, it is suitable to use finite volume methods, see [EYM 00, EYM 01, EYM 02]
5. **Some useful information..** The article contains useful information related to the practical side of problem.
6. **What is the mathematical model ?** In the modeling equation, the author considers mobile and immobile pore water, equilibrium sorption, diffusion and dispersion and chemical reaction of the first-order. The modeling is based on homogenization of the underlying equivalent porous media, [BEA 72, BEA 91]. The equations are coupled with the reaction terms and are presented as follows, for $i \in \llbracket 1, m \rrbracket$.

$$\partial_t R_i u_i + \nabla \cdot v u_i = -\lambda_i R_i u_i + \lambda_{i-1} R_{i-1} u_{i-1} + \beta(-u_i + g_i), \quad (x, t) \in \Omega \times (0, T) \quad [1]$$

$$u_{i,0}(x) = u_i(x, 0), \quad x \in \Omega, \quad [2]$$

$$\partial_t R_i g_i = -\lambda_i R_i g_i + \lambda_{i-1} R_{i-1} g_{i-1} + \beta(-g_i + u_i), \quad (x, t) \in \Omega \times (0, T), \quad [3]$$

$$g_{i,0}(x) = g_i(x, 0), \quad x \in \Omega, \quad [4]$$

where m is the number of equations and i is the index of each component. The unknown mobile concentrations $u_i = u_i(x, t)$ are considered in $\Omega \times (0, T) \subset \mathbb{R}^n \times \mathbb{R}^+$, where n is the spatial dimension. The unknown immobile concentrations $g_i = g_i(x, t)$ are considered in $\Omega \times (0, T) \subset \mathbb{R}^n \times \mathbb{R}^+$. The retardation factors R_i are constant and $R_i \geq 0$. The kinetic part is given by the factors λ_i . They are constant and $\lambda_i \geq 0$.

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