The simulation of a two-dimensional (2D) transport problem in a rectangular region with Lattice Boltzmann method with two-relaxation-time

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Abstract. Transport phenomena are found in many problems in many engineering and industrial sectors. We analyzed a Lattice Boltzmann method with Two-Relaxation Time (LTRT) collision operators for simulation of pollutant moving through the medium as a two-dimensional (2D) transport problem in a rectangular region model. This model consists of a 2D rectangular region with 54 length (x), 27 width (y), and it has isotropic homogeneous medium. Initially, the concentration is zero and is distributed evenly throughout the region of interest. A concentration of 1 is maintained at 9 < y < 18, whereas the concentration of zero is maintained at 0 < y < 9 and 18 < y < 27. A specific discharge (Darcy velocity) of 1.006 is assumed. A diffusion coefficient of 0.8333 is distributed uniformly with a uniform porosity of 0.35. A computer program is written in MATLAB to compute the concentration of pollutant at any specified place and time. The program shows that LTRT solution with quadratic equilibrium distribution functions (EDFs) and relaxation time \( \tau_a = 1.0 \) are in good agreement result with other numerical solutions methods such as 3DLEWASTE (Hybrid Three-dimensional Lagrangian-Eulerian Finite Element Model of Waste Transport Through Saturated-Unsaturated Media) obtained by Yeh and 3DFEMWATER-LHS (Three-dimensional Finite Element Model of Water Flow Through Saturated-Unsaturated Media with Latin Hypercube Sampling) obtained by Hardyanto.

1. Introduction
The study of transport phenomena in porous media has been increased in attention over the past few years, including in modeling heat, fluid flow, and mass transfer through a porous medium. These transport phenomena that are currently being studied is groundwater flow, fluid flow, multi-phase flow, spreading of contaminants, oil and gas movement in the reservoir, saltwater intrusion, radioactive pollutants, viruses, and others [1-3].

Solving the mass transport in the porous media problems to be studied fairly complicated, as it involves complicated equations. Constructed a mathematical equation that usually represents the spatial distribution and evolution of time in accordance with the phenomenon observed, where this equation is usually a partial differential equation (PDE) which can be resolved by various methods, both analytically and numerically. An analytical solution of the transport equation can be obtained only by making simplifying assumptions, such as its geometries, boundary conditions, and idealization.
of the physical quantities [4-5]. Numerically, PDE resolved by approaching and discretization in the spatial domain and time, so that the results obtained are close to the exact solutions [6].

Some numerical methods have been applied to solve the mass transport equation, such as finite difference method (FDM) [7], finite element method (FEM) [8-9], the spectral element method (SEM) [10], and the finite volume method (FVM) [11]. Another method that also can be used to solve the transport equation is the lattice Boltzmann method (LBM) [12-13]. In the equation of groundwater flow and transport phenomena, FDM is the most often applied method. A lot of software with FDM approach that successfully made to solve and visualize the transport phenomena, such as SILK, LEWASTE, and SEAWAT [14]. While the software with FEM-based such as GIS, FEMWATER, and FEMWATER-LHS [15].

Lattice Boltzmann method (LBM) was originally a development of the lattice gas automata (LGA) in computational fluid dynamics [3]. The implementation of a LGA model is straightforward, just a following of the collision-streaming paradigm. The LGA method has some disadvantages, such as the statistical noise arising from the Boolean variables, the violation of the Galilean invariance, the dependence of velocity of the pressure, and difficult implementation in three dimension problem [16]. LBM was first introduced as a numerical method to solve fluid flow by Higuera and Jimenes in 1989 [17]. LBM simulates macroscopic fluid dynamics-based models and microscopic fluid kinetic equation. The LBM is based on the discretization of the Boltzmann equation that comes from statistical mechanics [18].

Chen and Doolen has introduced the LBM in relation to the boundary condition, and some examples of applications such as turbulence, multiphase flow and heat transfer [19]. They approach collision operator with a time of relaxation, better known as the operator LBM Bhatnagar-Gross-Krook (LBGK). To improve the performance of LBM, Ginzburg introduced the collision operator in the form of two relaxation time or better known as Lattice Boltzmann Method with Two-Relaxation-Time (LTRT) [3]. However, the study of comparative LBGK and LTRT in solving the transport equation has not been done. In this work, we analyze a Lattice Boltzmann method with Two-Relaxation Time (LTRT) collision operators for simulation of pollutant moving through the medium as a two-dimensional (2D) transport problem in a rectangular region model.

2. Methods
2.1. Problem Definition

![Figure 1. Problem definition of 2D mass transport problem in a rectangular region model](image)

A two-dimensional (2D) mass transport problem in a rectangular region model was depicted in Figure 1. This model consists of a 2D rectangular region with 54 length (x), 27 width (y), and it has
isotropic homogeneous medium. Initially, the pollutant concentration is zero and is distributed evenly throughout the region of interest. A concentration of 1 is maintained at $9 < y < 18$, whereas the concentration of zero is maintained at $0 < y < 9$ and $18 < y < 27$. A specific discharge (Darcy velocity) of 1.006 is assumed. A diffusion coefficient of 0.8333 is distributed uniformly with a uniform porosity of 0.35.

2.2. Numerical Formulation

To solve the above mass transport problem, which is an advection-diffusion equation, the LTRT method is used with the dimensionless equilibrium distribution function (EDF).

![Flowchart](image)

Figure 2. Flowchart to implement the LTRT to solve the 2D mass transport problem

The steps taken are as follows:

- Determine the initial conditions ($t = 0$) of the associated quantities and other necessary parameters. In this case the concentration conditions $C$, Courant number ($Cr$), lattice Peclet number ($Pe$), relaxation time, lattice spacing $dx$, and time step $dt$.
- Calculate the dimensionless quadratic EDF for all nodes.
- Calculate the particle distribution function at $t = 0$ for each node.
- Do the iteration from $t = 1$ to the maximum time interval:
  - Do the collision phase.
  - Do streaming phase.
  - Include appropriate boundary conditions.
  - Calculate the new $C$ value for each node.
The algorithm can be described in the flow charts as shown in Figure 2.

3. Result and Discussion
A computer program is written in MATLAB to compute the concentration of pollutant at any specified place and time, as the two-dimensional mass transport problems, using the LTRT method. To obtain reliable results, the source code has been verified and validated by using analytical solutions of Gaussian distribution of concentrations, as practiced by Camas [3] and Huang [20-21].

The selected parameters used in this simulation include LBGK relaxation time of 0.8 and anti-symmetric relaxation time for LTRT of 1. This selection is based on the stability of the program's validation result [3]. In addition, the computational domain is divided into 55x28 nodes, with \( dx = dy = 1 \) and an interval \( dt = 0.12 \). Thus, obtained Peclet number of 3.45 and Courant number of 0.345.

![Figure 3. Contour of pollutant concentration at 180-time unit](image)

The concentrations on the left side \((x = 0)\) and the nodes at \(9 < y < 18\), as shown in Figure 3, are maintained at one, while the other nodes are maintained equal to zero. The Dirichlet boundary conditions problem in this case can be solved by applying the periodic boundary conditions on the other nodes referring to the algorithm given by the Sukop [12].

At nodes along \(x = 0\) at the boundary between concentrations 0 and 1 \((y = 9\) and \(y = 18)\) there is a small ripple. This is due to the imposition of the Dirichlet boundary conditions by forcing a certain concentration value on the node by applying approximations of the unknown particle distribution function. As shown in Figure 3, after the simulation runs 180 steps, a concentration of 50% pollutant has occurred in the area along \(x\) at \(y = 9\) and \(y = 18\).

The results are in good agreement with other numerical solution obtained by Hardyanto [22] using the program 3DFEMWATER-LHS (Three-dimensional Finite Element Model of Water Flow Through Saturated- Unsaturated Media with Latin Hypercube Sampling) as shown in Figure 4, and the results obtained by Yeh [14] using 3DLEWASTE (Hybrid Three-dimentional Lagrangian-Eulerian Finite Element Model of Waste Transport Through Saturated- Unsaturated Media) program as shown in Figure 5.
Figure 4. Contour concentrations of 40%, 50%, and 60% on the 2D transport problem obtained by Hardyanto with FEMWATER-LHS [22]

Figure 5. Contour concentrations of 50%, obtained by Yeh [14] with 3DLEWASTE program

4. Conclusion
The Lattice Boltzmann Method with Two-Relaxation-Time (LTRT) has been used to simulate a two-dimensional (2D) transport problem in a rectangular region successfully. The program shows that LTRT solution with quadratic equilibrium distribution functions (EDFs) and relaxation time $\tau_a=1.0$ are in good agreement result with other numerical solutions methods such as 3DLEWASTE obtained by Yeh and 3DFEMWATER-LHS obtained by Hardyanto.

Acknowledgment
We would like to thank Ministry of Research, Technology and Higher Education of the Republic of Indonesia for supporting the study. Our gratitude also goes to member of Computational Physics Laboratory, Physics Department, Universitas Negeri Semarang (UNNES) for permitting the use of the research facilities and for their helpful discussion time throughout the completion of this work.

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