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Tracer diffusion and fluid transport are studied in a model for a geomarine system in which fluid constituents move from regions of high to low concentration. An interacting lattice gas is used to model the system. Collective diffusion of fluid particles in lattice gas is consistent with the solution of the continuum diffusion equation for the concentration profile. Comparison of these results validates the applicability and provides a calibration for arbitrary (time and length) units of the lattice gas. Unlike diffusive motion in an unsteady-state regime, both fluid and tracer exhibit a drift-like transport in a steady-state regime. The transverse components of fluid and tracer displacements differ significantly. While the average tracer motion becomes nondiffusive in the long time regime, the collective motion exhibits an onset of oscillation.

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Gradient driven flow: lattice gas, diffusion equation and measurement scales

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Abstract: Tracer diffusion and fluid transport are studied in a model for a geomarine system in which fluid constituents move from regions of high to low concentration. An interacting lattice gas is used to model the system. Collective diffusion of fluid particles in lattice gas is consistent with the solution of the continuum diffusion equation for the concentration profile. Comparison of these results validates the applicability and provides a calibration for arbitrary (time and length) units of the lattice gas. Unlike diffusive motion in an unsteady-state regime, both fluid and tracer exhibit a drift-like transport in a steady-state regime. The transverse components of fluid and tracer displacements differ significantly. While the average tracer motion becomes non-diffusive in the long time regime, the collective motion exhibits an onset of oscillation.

Key words: Diffusion, Fick's law.

How do fluids and their dissolved constituents move through the often complex pathways within the seafloor [1,2]? While we cannot answer such a difficult question for a real geomarine environment [3], we can address such complex issues via simplified computer simulation models such as interacting lattice gas [4]. The question then arises how to connect the results of idealized models to field measurements. One way to approach this problem is to calibrate the simulation results with the field measurements for a specific quantity such as tracer diffusion [2,5] that is experimentally feasible. Using such calibrated spatio-temporal scale then one can predict the behavior of other quantities such as flow-rate In this paper we attempt to address the validity of our lattice gas simulation with the Fick's diffusion [5] and show how to calibrate our simulation data.

We consider Kawasaki kinetics of Ising (lattice gas) model on a three dimensional lattice of size $L_x \times L \times L$. The reservoir source of fluid is connected to the bottom end ($x = 1$) of the lattice where each site is always occupied by a fluid particle. As in most lattice gas models [6,7], a particle does not necessarily represent a atom or molecule, but a assemblage of constituents such as water molecules, dissolved constituents, and the tracer, e.g. Chloride [2], at a maximum concentration. Thus when all spaces are filled with particles, as the bottom layer of the lattice in this model, the concentration is maximal. Empty sites in the lattice represent assembleges of just water and tracer at minimum concentration. We assume that the sediment grains are inert for this simulation. The diffusion constant for which we calibrate the model is therefore the effective diffusion constant.

The occupation state of a lattice site (i) is described by $S_i = 1$ (occupied), -1 (empty). A site cannot be occupied by more than one particle, i.e., there is a hard-core interaction among the fluid particles. In addition, we consider a nearest neighbor interaction with energy,

$$E = U \sum_{ij} S_i S_j \tag{1}$$

where U is the interaction strength, $U = 1$ in units of the Boltzmann constant (k_B) in this simulation. Note that there is a nearest neighbor attraction between the fluid particle and the empty pore. By varying the interaction one may change the effect of viscosity and instantaneous capillarity. Each particle attempts to move to one of its neighboring site chosen randomly with a Metropolis algorithm. Obviously, a move (hopping) is successful only if the randomly selected neighboring site is empty and energetically feasible with a Boltzmann distribution. A periodic boundary condition is used along the transverse (y, z) direction and a open boundary condition along the x-direction. A particle cannot go below the bottom plane ($x = 0$) and can escape the lattice if it attempts to move beyond the top ($x = L_x$). The attempt to move each particle once is defined as one Monte Carlo Step (MCS).

Initially, the fluid is concentrated at the bottom ($x = 1$) and spreads upward in time. The evolving concentration gradient eventually conforms to an steady-state profile when the rate of mass flow into the system (at the bottom) becomes equal to that of the fluid leaving the top. A typical evolution of the concentration profile is presented in figure 1. Even though there is no external field such as a pressure gradient, the concentration gradient drives the fluid resulting in a net fluid-flux from bottom to top. Note that the morphology of the concentration profile front leads to a percolating network of nearest neighbor fluid particles at the percolation threshold [8] in a gradient percolation [9].

In nonsteady-state, i.e., the time regime in which no fluid particle arrives at the top, the dynamics of the concentration (C) profile is described by the diffusion equation [2],

$$D_m \nabla^2 C = n_c \frac{\partial C}{\partial t} \tag{2}$$

where D_m is the diffusion constant and n_c is the effective porosity. The diffusion equation [2,5] has been used extensively to track down or trace out the diffusion and spreading of chemical species. The realistic time and length scales for the diffusion equation compatible with these specific systems are identified with appropriate parametric constants (D_m, n_c, ...). If we show that our lattice gas simulation reproduces the results of diffusion equation then we verify the validity of discrete lattice approach for diffusive systems. One can then calibrate the arbitrary time and length units of lattice in order to connect it to field measurements.

A typical solution for the concentration profile is shown in figure 2 which resembles closely to the profile emerging from the lattice gas model (see figure

1). By comparing the collective motion of the fluid particles in lattice gas simulation with the diffusion of the concentration front described by equation 2, one can establish a relation between (or calibrate)the MCS time step and the real time and lattice space and the real length units. Figure 3 shows the variation of the collective fluid particles (i.e., the center of mass) with time. We see that the variation of the root mean square (rms) displacements (R_{cm}) with the time is diffusion-like, i.e.,

$$R_{cm} = D_l t^{\nu} \tag{3}$$

where D_l is the lattice diffusion constant and $\nu \simeq 1/2$. Suppose we have the field measurement for the variation of the rms displacement with time for a specific system. We may then calibrate the MCS time step and the lattice constant with the real time and length units by comparing the measured data with our computer simulation (fig. 3). Unfortunately, we do not have such a field measurement. However, there are measurements that determine the diffusion constant for systems such as Chlorine ions (Cl^-) in water. In the following, we attempt to use that data as an input parameter to calibrate our lattice gas simulation.

The variation of fluid transfer with time step is presented in figure 4. We see that the flux-rate has become constant and the system has reached the steady-state. The concentration profile becomes stable and leads to a constant concentration gradient (see figure 5). With such a gradient field, we expect a linear response (Darcy's law) of the fluid-flux (mass current) density (j),

$$j = -D_w \frac{dC}{dx} \tag{4}$$

In steady-state, the density gradient is almost linear (see fig. 5), i.e.,

$$\frac{dC}{dx} \simeq -1/L_x \tag{5}$$

For a typical simulation, $j \simeq 0.338 \times 10^{-2}$ a^2/MCS, $L_x = 50, D_{wl} \simeq 0.169$ a^2/MCS, where a is the distance between nearest neighbors. The measured value of chlorine ion diffusion in water, $D_{wm} \simeq 20.3 \times 10^{-10}$ m^2/s. For our simulation to be valid for Cl^- diffusion, $D_{wl} \sim D_{wm}$. If one lattice constant $a = 1$m, then 1 MCS$\simeq$ 2.64 yrs. On the other hand, if 1 MCS = 1 s, then $a \simeq 10^{-4}$m.

The variation of the rms displacements of the collective fluid particles, i.e., the center of mass, R_{cm} and that of individual particles, i.e., the tracer R_{tr} with time is presented in figure 6. The asymptotic power-law behavior is drift-like for both tracers and the fluid and longitudinal transport dominates over the transverse movement. In the transverse direction (y, z) on the other hand, the tracers motion differs drastically from collective fluid movement (see figure 7). The asymptotic (long-time) motion of the tracer particles seem nondiffusive while the collective motion of particles (fluid) becomes oscillatory.

We are able to verify the validity of our lattice gas simulation by recovering the standard result of the diffusion equation, i.e., the diffusive motion of fluid and its concentration profile. In the steady state such diffusive motion becomes drift. In the transverse direction, the tracer motion is non-diffusive while the collective fluid motion is some what oscillatory. These behavior seem reasonable. Further, we show that the flux-rate increases with temperature as reported before [10].

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Figure Captions:

Figure 1: Concentration profile, i.e., the concentration of fluid with the longitudinal distance (x) from simulation with sample size $50 \times 50 \times 50$ with 32 independent samples at a uniform temperature $T = 2$ (arbitrary unit). The dotted lines are the solution of diffusion equation.

Figure 2: Variation of the RMS displacement of the center of mass of the fluid particles with time on a log-log scale. Sample statistics for the lattice gas data is the same as in figure 1.

Figure 3: Flux versus time on a 30^3 sample with 10-50 independent runs at different temperatures.

Figure 4: Steady-state concentration profile on a 50^3 lattice with 32 independent runs at $T = 2$.

Figure 5: RMS displacement of collective fluid (a) and tracer (b) (longitudinal (x-) component) versus time. Statistics is the same as in figure 3.

Figure 6: Transverse component of collective fluid (a) and tracers (b) displacement versus time. Statistics is the same as in figure 3.

Figure 1

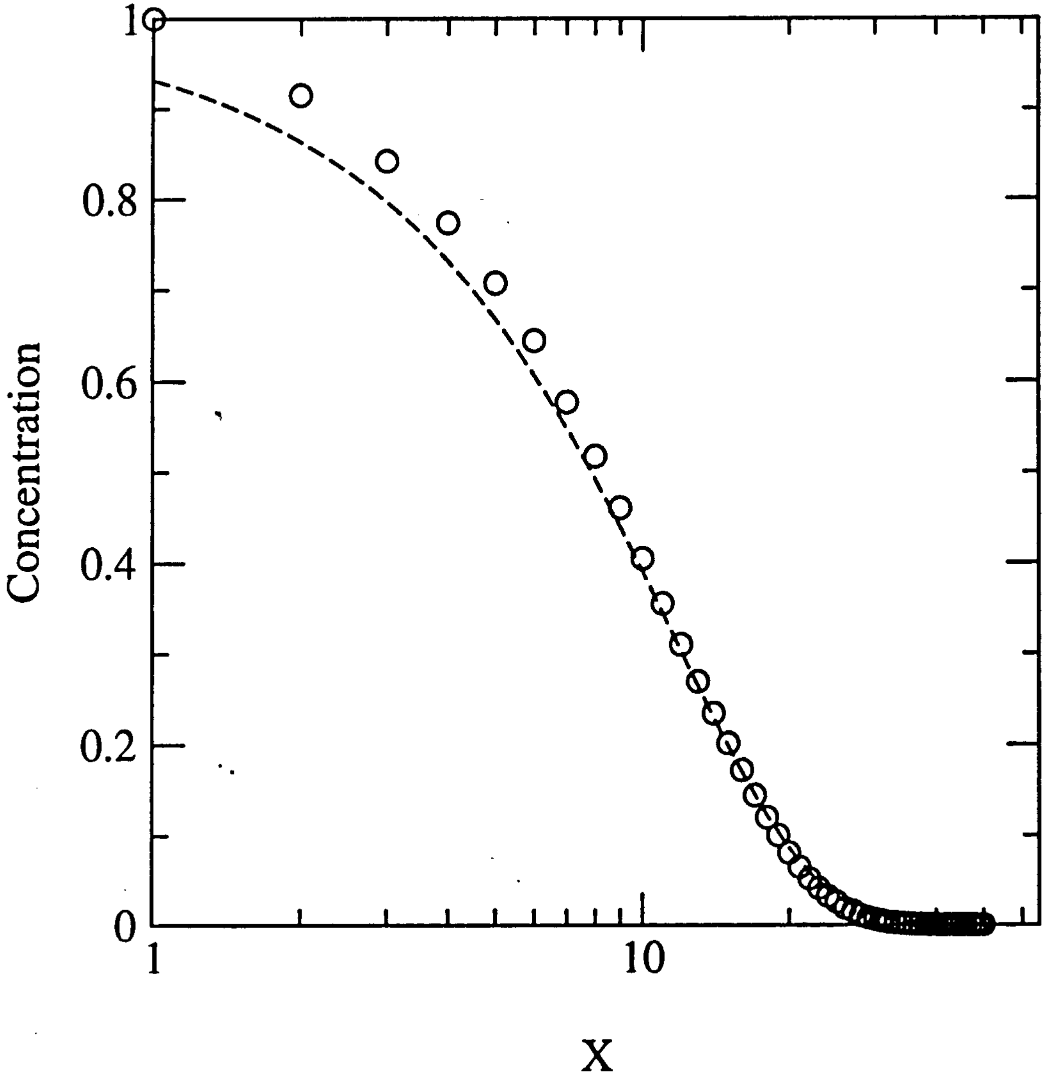


Figure 2

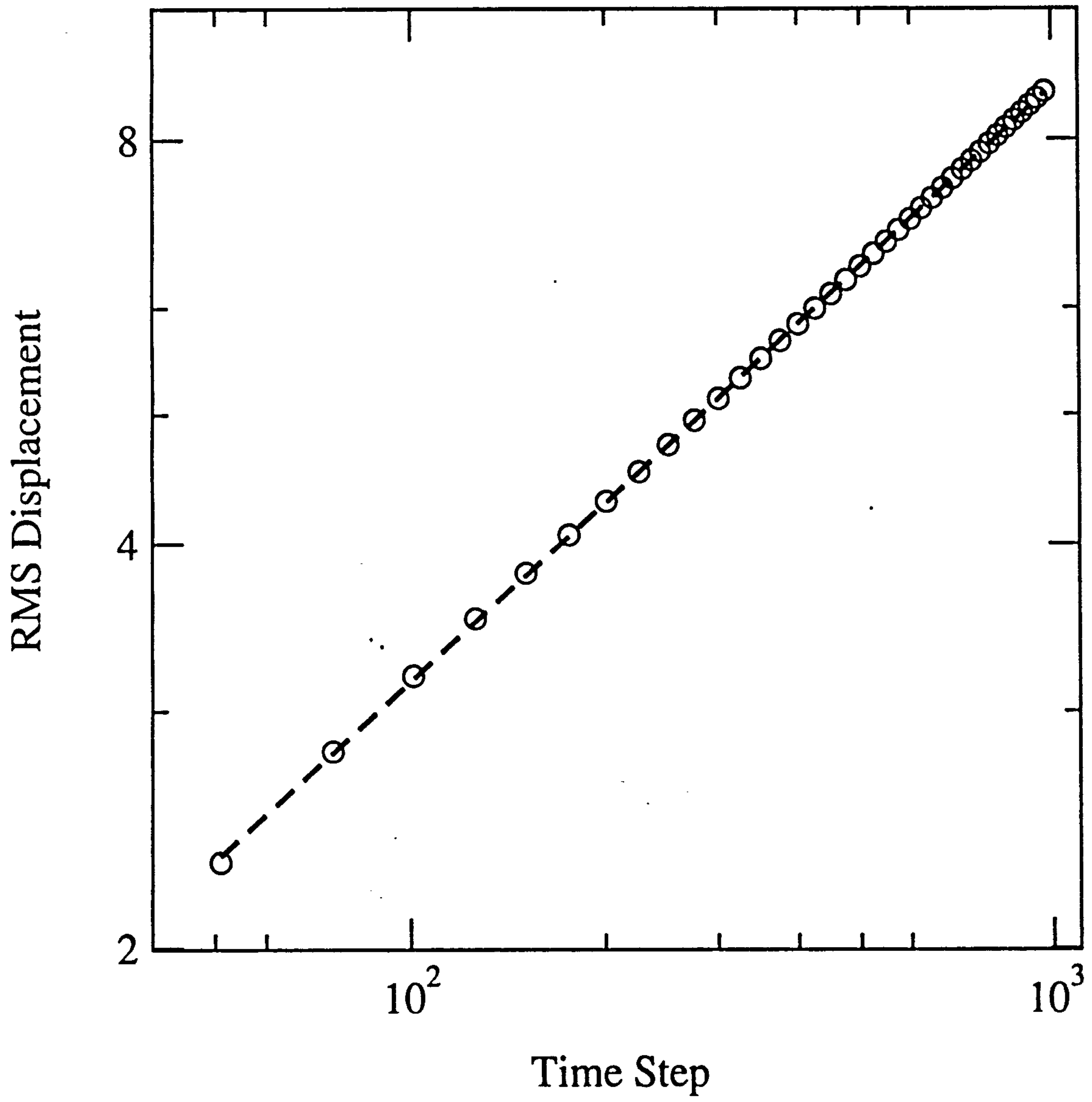
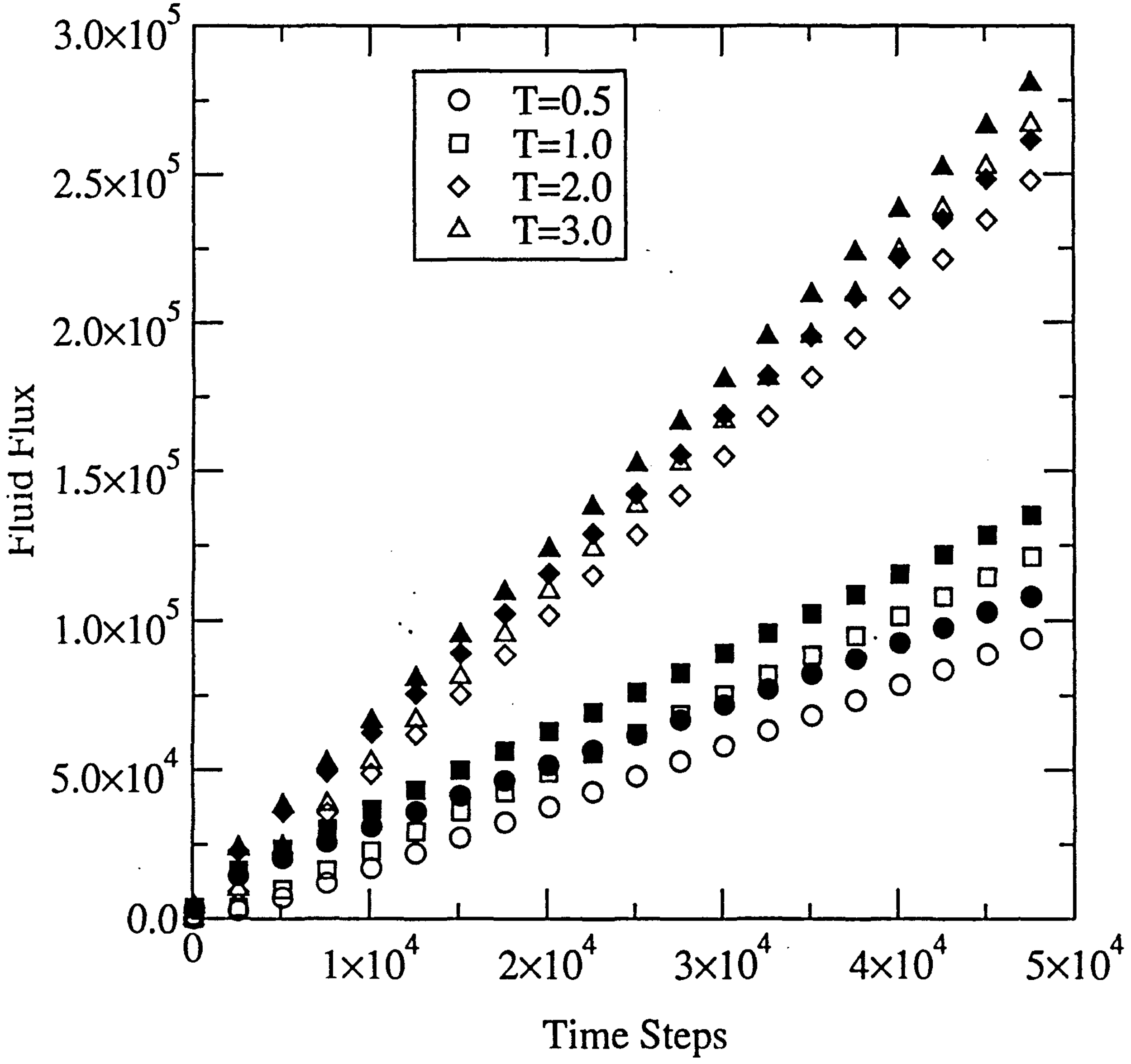


Figure 3



○ T=0.5
□ T=1.0
◇ T=2.0
△ T=3.0
Fluid Flux
3.0×10^5
2.5×10^5
2.0×10^5
1.5×10^5
1.0×10^5
5.0×10^4
0.0
0
1×10^4
2×10^4
3×10^4
4×10^4
5×10^4
Time Steps

Figure 4

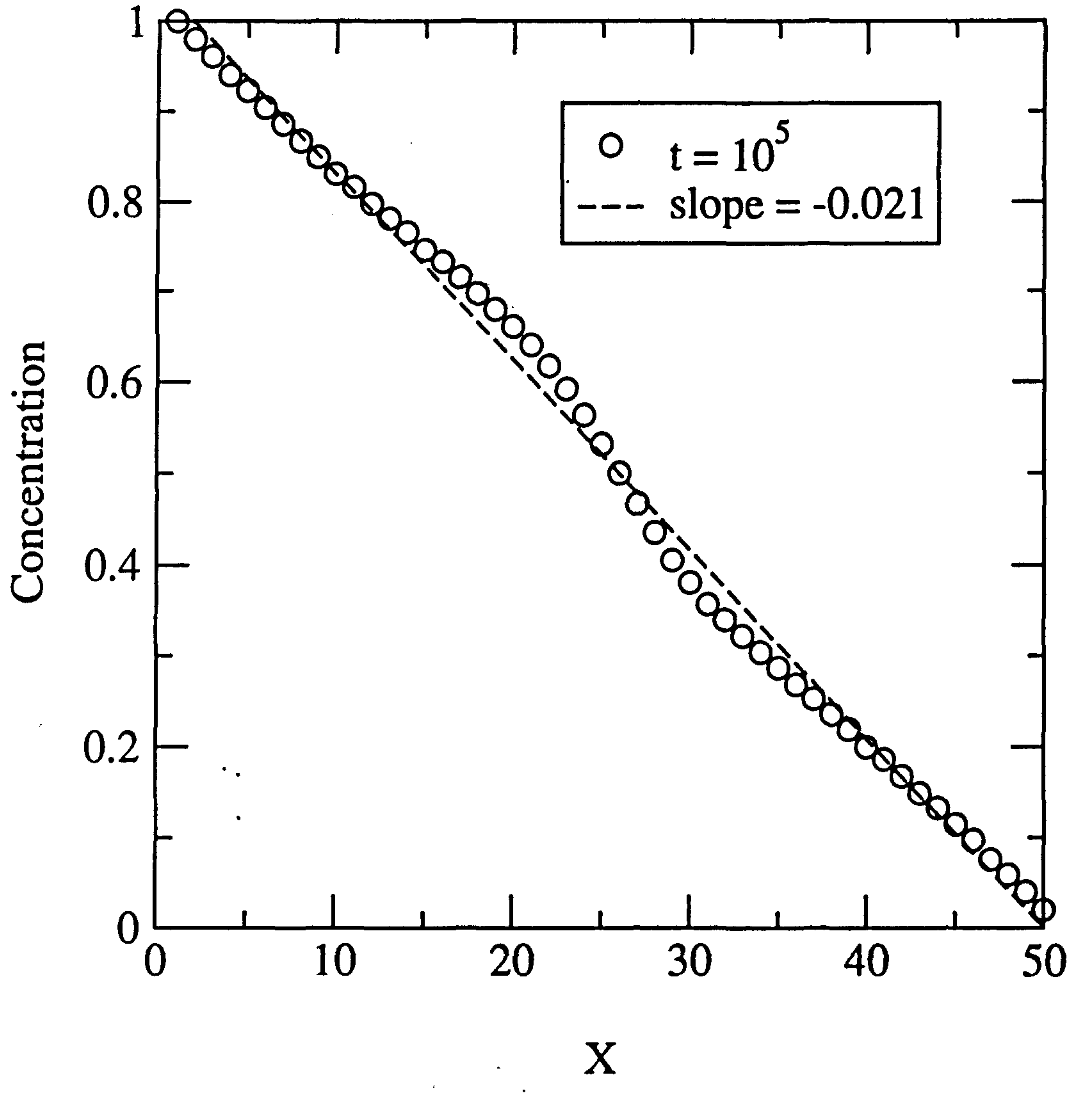
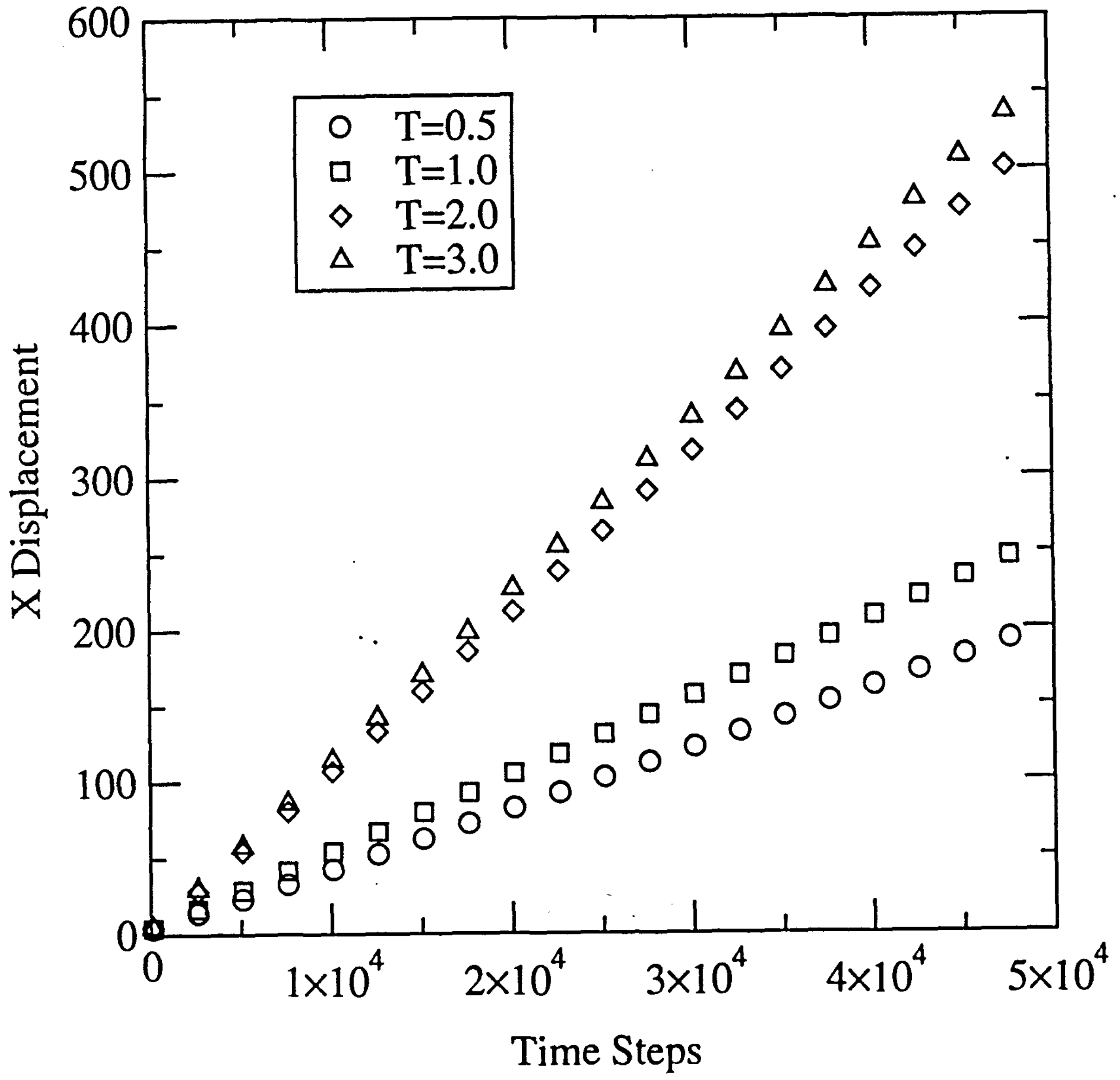


Figure 5(a)



T=0.5
T=1.0
T=2.0
T=3.0
X Displacement
Time Steps
0
100
200
300
400
500
600
0
1×10^4
2×10^4
3×10^4
4×10^4
5×10^4

Figure 5(b)

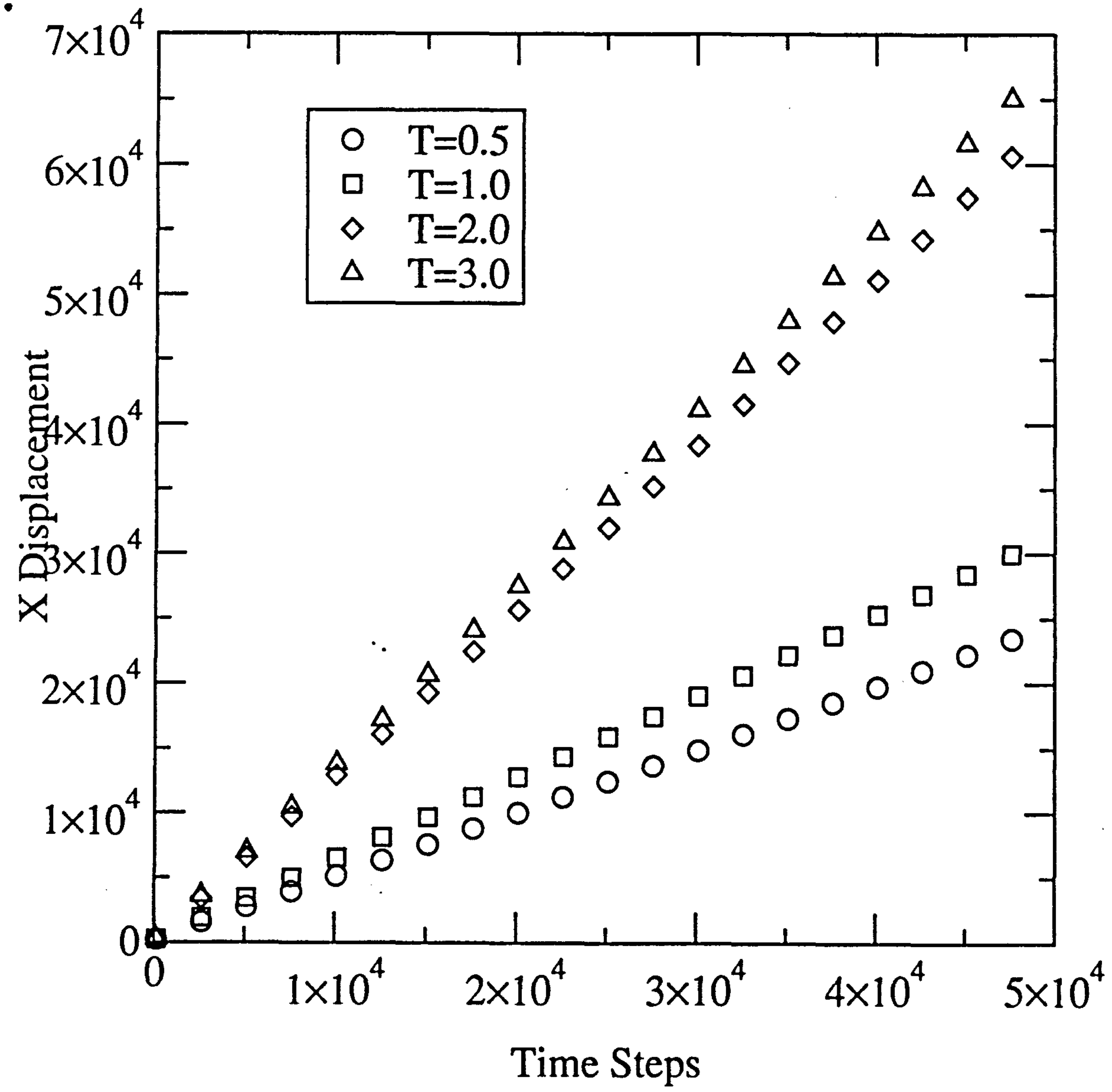

T=0.5
T=1.0
T=2.0
T=3.0
X Displacement
0
1×10^4
2×10^4
3×10^4
4×10^4
5×10^4
6×10^4
7×10^4
0
1×10^4
2×10^4
3×10^4
4×10^4
5×10^4
Time Steps

Figure 6(a)

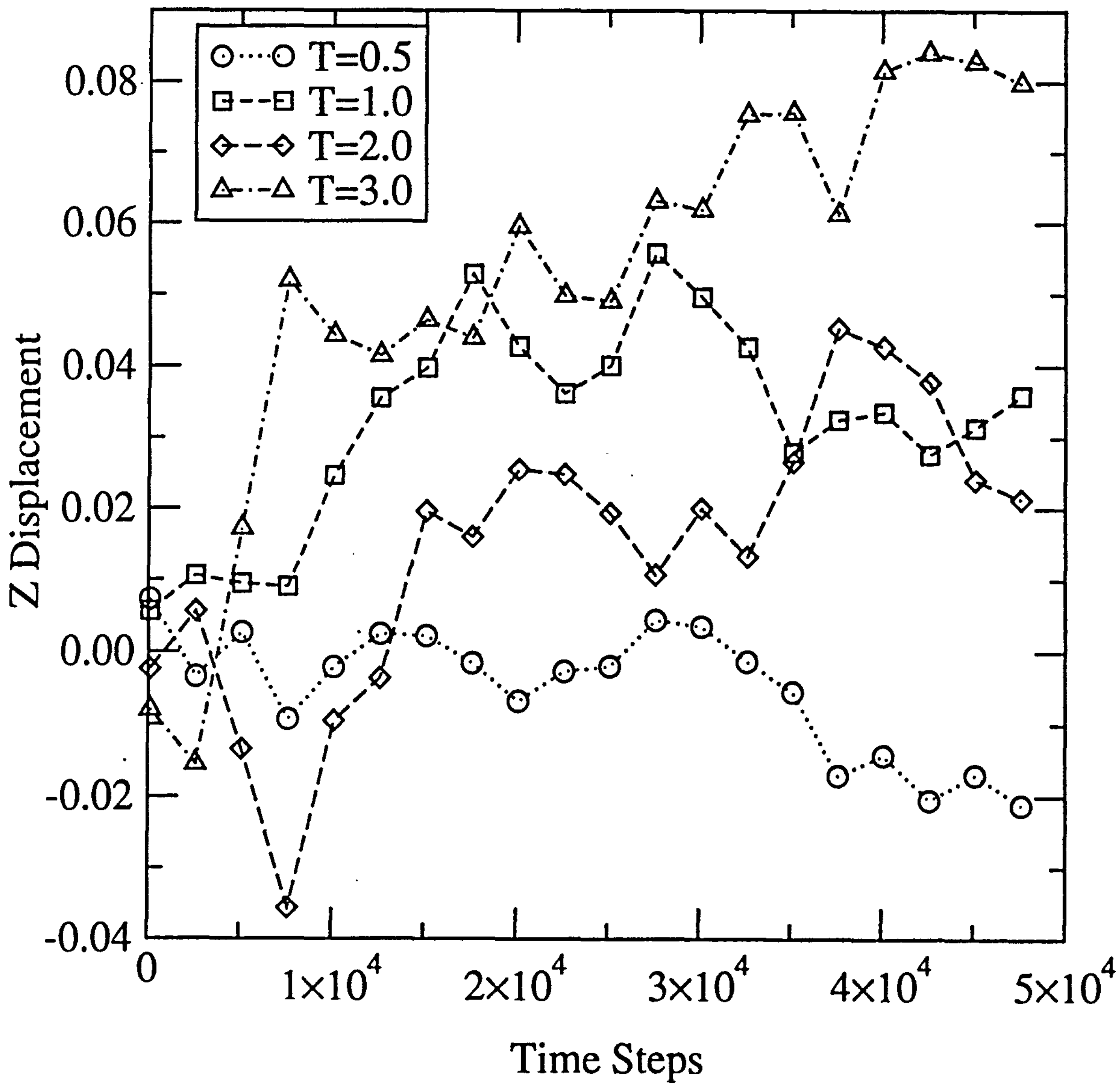
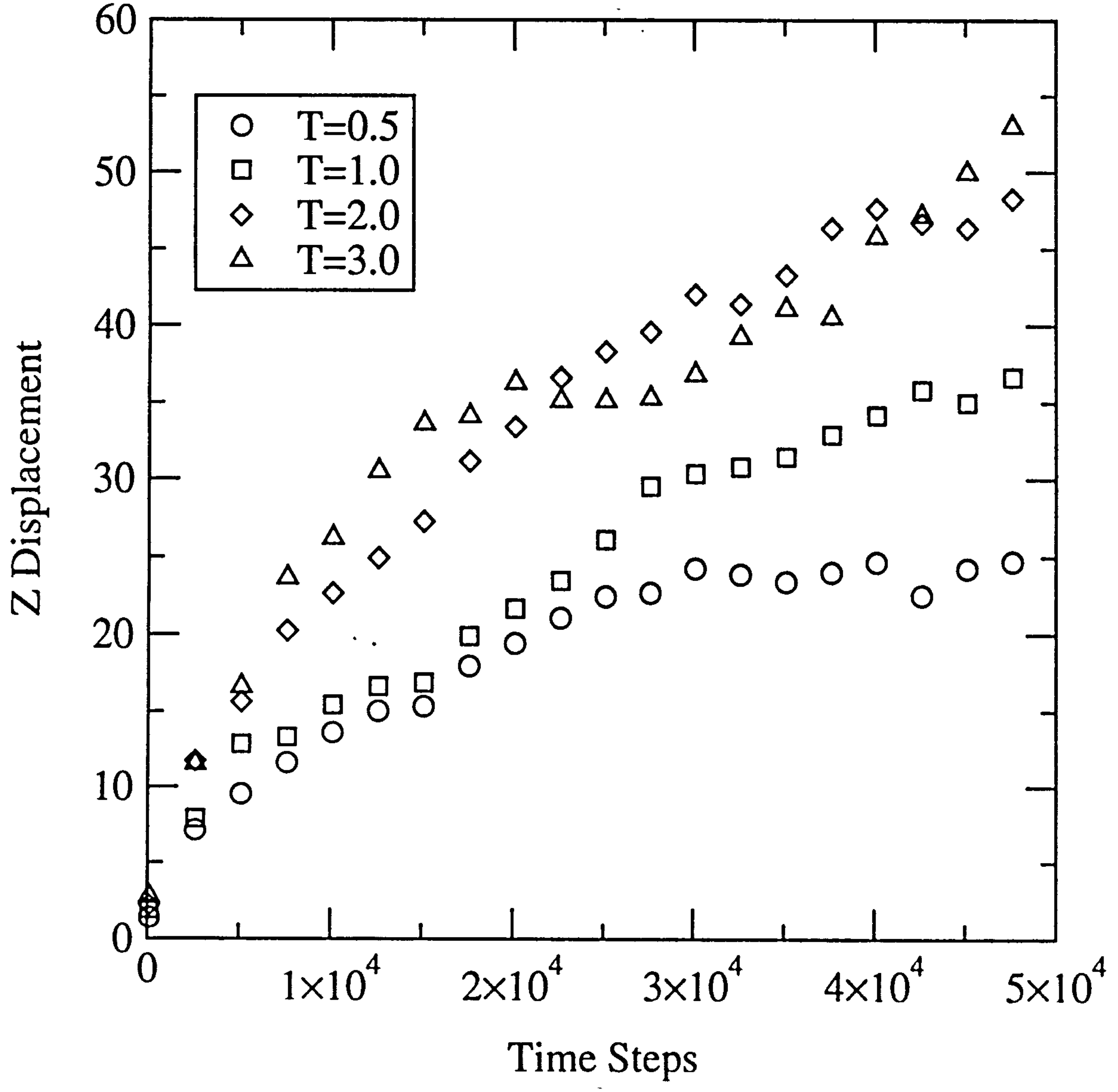

T=0.5
T=1.0
T=2.0
T=3.0
Z Displacement
0.08
0.06
0.04
0.02
0.00
-0.02
-0.04
0
1×10^4
2×10^4
3×10^4
4×10^4
5×10^4
Time Steps

Figure 6(b)



T=0.5
T=1.0
T=2.0
T=3.0
Z Displacement
0
10
20
30
40
50
60
0
1×10^4
2×10^4
3×10^4
4×10^4
5×10^4
Time Steps