IEICE TRANS. INF. & SYST., VOL.E87–D, NO.3 MARCH 2004

PAPER Special Section on Cellular Automata

Discrete Simulation of Reactive Flow with Lattice Gas Automata

Kazuhiro YAMAMOTO[†], *Nonmember*

SUMMARY Normally, flow field is described with governing equations, such as the Navier-Stokes equations. However, for complex flow including multiphase and reactive flow such as combustion, this approach may not be suitable. As an alternative approach, Lattice Gas Automata (LGA) has been used to simulate fluid with mesoscopic particles by assuming that space and time are discrete, and the physical quantities take only a finite set of values. In this study, the model for combustion simulation is proposed, with the reaction probability depending on the local temperature to simplify the chemical reaction. Here, counter-flow twin flames are simulated. In order to validate this approach, some results of non-reactive flow are presented, compared with those by solving Navier-Stokes equations.
key words: *LGA, reaction probability, combustion, counter-flow flame*

1. Introduction

Recently, since computer performance has drastically increased in the last decade, numerical simulation has been a powerful means to investigate combustion phenomena. Especially, direct numerical simulations (DNS) have been widely used [1], [2], because it is possible to examine the phenomena directly without any models. We can select flame characteristics and turbulence freely for modeling turbulent combustion, which is difficult in experimental studies. However, when we simulate turbulent flames with detailed chemistry in two or three-dimensional geometry, the computational costs of such a treatment would be too much. Also, it is tough to handle phase transition in spray combustion. An alternative approach may be needed in combustion simulation.

In conventional CFD code, hydrodynamics are normally described by partial differential equations with the Navier-Stokes equations. Recently, the methods have been proposed to describe the fluid at a more microscopic level by assuming that it is composed by mesoscopic particles. One of them is called Lattice Gas Automata (LGA) [3]–[7]. The space and time are discrete and the physical quantities take only a finite set of values. Properties such as density and velocity are determined by the collective behavior of many particles. This simplified kinetic model is constructed so that the macroscopic averaged properties obey the desired macroscopic equations. It has been applied to complex phenomena such as erosion and multiphase flow. Reactive flow has been also simulated [8], [9]. The reactive lattice gas scheme is well presented in Ref. [10]. So far, this general algorithm for reactive flow is to change the particle number based on the probability regardless of the state of reactive species. In combustion field, the chemical reaction is described using Arrhenius-type reaction, which is strongly affected by temperature.

In this study, the LGA model for combustion field is proposed. Two particles of reactant and product are considered, and the transition between two particles is determined by the reaction probability depending on the local temperature. Here, counter-flow flames are simulated, which is considered to be important for modeling turbulent combustion [11], [12]. In order to validate this approach, some results of non-reactive flow are obtained, compared with those by solving Navier-Stokes equations.

2. Numerical Method

2.1 LGA (Lattice Gas Automata)

LGA is a kind of cellular automata (CA). From this perspective, the lattice gas method is often called lattice gas cellular automata. In the late 1940s, Cellular automata (CA) have been proposed by Neumann to model the mechanisms of self-reproduction in living organisms [13]. This model is an idealization of a physical system in which space and time are discrete and the physical quantities (i.e. the states of automaton) take only a finite set of values. Formally, it can be defined as:
(1) A regular lattice of cells (or sites) covering a portion of a d-dimensional space.
(2) A set of Boolean variables attached to each site of the lattice and giving the current state of automata.
(3) A rule that specifies the time evolution of the cells according to the current state of the nearest neighbor cells. To obtain the state of the automaton at the next iteration, the same rule (homogeneous CA) is applied synchronously to all the cells. The neighborhood (i.e. the range of the rule) is a parameter.

It should be noted that sufficiently large cellular automata often show seemingly continuous macroscopic behavior. Thus, they can potentially serve as models for continuum systems such as fluids. By Frisch et al. [4], [5], the FHP model has been proposed to model a fluid as a fully discrete molecular dynamics. They have used a hexagonal lattice for symmetry of the lattice to succeed in obtaining the correct Navier-Stokes equation by starting from the lattice gas automata. So far, this method has been applied to a large range of scientific problems including diffusion processes,

Manuscript received June 5, 2003.
Manuscript revised October 16, 2003.
[†]The author is with Nagoya University, Nagoya-shi, 464–8603 Japan.

wave propagation, and multi-component fluids [6]. Because of its simple numerical approach, it has been recognized as a powerful way to solve problems with a high degree of data-parallelism, which is appropriate for parallel computation.

2.2 Numerical Approach

In this study, FHP III model is adopted, introduced by Frisch, Hasslacher, and Pomeau [4], [5]. It consists of a hexagonal (triangular) lattice with particles residing on the node (see Fig. 1). A set of Boolean variables, $n_i(x,t)$ ($i = 0$ to 6), describing the particle occupation, is defined. The lattice with unit lattice space, where there are seven directions at each node, are

$$\vec{e}_0 = (0,0),$$
$$\vec{e}_i = \left(\cos\left(\frac{(i-1)\pi}{3}\right), \sin\left(\frac{(i-1)\pi}{3}\right)\right), \qquad (i = 1,\ldots,6),$$

where $\vec{e}_i$ is the local velocity vector, and each particle has the same mass and velocity of unity. As shown in Fig. 1, the local averaging is conducted in sub-domain to obtain macroscopic quantities such as velocity and density.

Starting from the initial state, the configuration of each particle of reactant or product evolves in two sequential sub-steps of collision and propagation. For simulation of reactive flow, the transition between two particles is needed, which is explained later. The first step is *collision*.

$$n_i(\vec{x}, t^*) = n_i(\vec{x}, t) + \Omega_i(n(\vec{x}, t)), \qquad (i = 0,\ldots,6),$$

where, n_i is the Boolean occupation number describing the presence or absence, and Ω_i is the collision operator. This collision occurs just after particles arrive at a node at $t = t^*$. They interact and change their directions according to scattering rules, which preserves mass and momentum (see Fig. 2 (a)). The collision rules are shown in Table 1, listing only the cases such that mass flux in the x- and y-directions, j_x and j_y, are positive. Configurations with four particles and more are obtained by duality replacing particles by holes and holes by particles. The first three columns give the number of particles and the total momentum. The fourth column shows the different configurations, the legal collisions exchanging configurations appearing within the same row, and the last column gives the number of different configurations obtained by the application of the symmetry group.

At the next time step ($t = t + 1$), each particle moves to the nearest node in the direction of its velocity, shown in Fig. 2 (b). It is called *streaming propagation*.

$$n_1(\vec{x} + \vec{e}_i, t+1) = n_i(\vec{x}, t^*), \qquad (i = 0,\ldots,6).$$

Thus, the evolution equation of LGA is as follows:

$$n_i(\vec{x} + \vec{e}_i, t+1) = n_i(\vec{x}, t) + \Omega_i(n(\vec{x}, t)), \quad (i = 0,\ldots,6).$$

To describe the particle motion at the wall, the bounce-back rule is adopted to obtain zero velocity, by which the

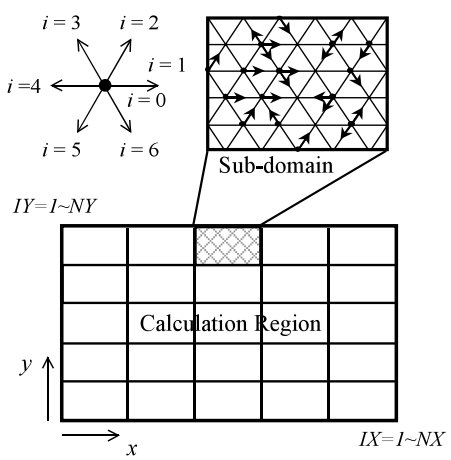


Fig. 1 FHP model and hexagonal lattice.

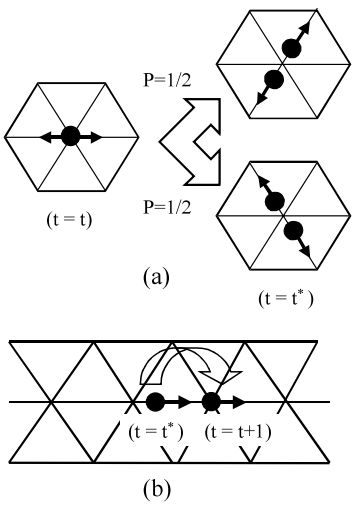


Fig. 2 Microscopic movement of particles, (a) collision, (b) streaming propagation.

Table 1 List of configurations for FHP III.

n	j_x	j_y		Folds
0	0	0		1
1	0	0		1
1	1	0		6
2	0	0		1
2	1	0		6
2	$\frac{3}{2}$	$\frac{\sqrt{3}}{2}$		6
3	0	0		6
3	0	0		1
3	1	0		6
3	$\frac{3}{2}$	$\frac{\sqrt{3}}{2}$		6
3	2	0		6

particle bounces back when it reaches at the wall boundary. The total particle density, ρ, and momentum, $\rho\vec{u}$, are defined and given by

$$\rho = \sum_i n_i,$$
$$\rho\vec{u} = \sum_i \vec{e}_i n_i.$$

For this FHP model, the transport coefficients and Reynolds number are given by

$$c_s = \sqrt{3/7},$$
$$\nu = \frac{1}{28}\frac{1}{d(1-d)}\frac{1}{1-8d(1-d)/7} - \frac{1}{8},$$
$$Re = \frac{UD}{\nu},$$

where d is $\rho/7$, ν is kinematic viscosity, c_s is sound speed, and D is the grid number of the characteristic length. These formulas are useful when we compare the results with those by solving the N-S equation.

Here, the counter-flow flame was simulated by LGA, which has been widely examined for modeling turbulent combustion to investigate the interaction between flame and flow [11], [12]. Figure 3 shows the schematic of counter-flow twin flames. Two-dimensional rectangular coordinate is used. The porous walls for mixture injection are located at $y = L$ and $-L$. The symmetry at the stagnation plane of $y = 0$ was not assumed.

In LGA model, physical quantities are obtained by averaging the particle motion in sub-domain. This procedure is needed to eliminate statistical noise. When we take the large sub-domain, the spatial resolution becomes worse. However, there are the large fluctuation exists when the sub-domain size is too small. Here, the sub-domain of 16×8 nodes was used to obtain velocities and density through averaging procedure. The total computational domain has 257,121 grids (801×321). Thus, there are 50×40 points to determine the physical quantities. The inlet velocity at the wall is 0.09, so that the Mach number, Ma, is 0.137. Then, the Reynolds number, Re, is about 370.

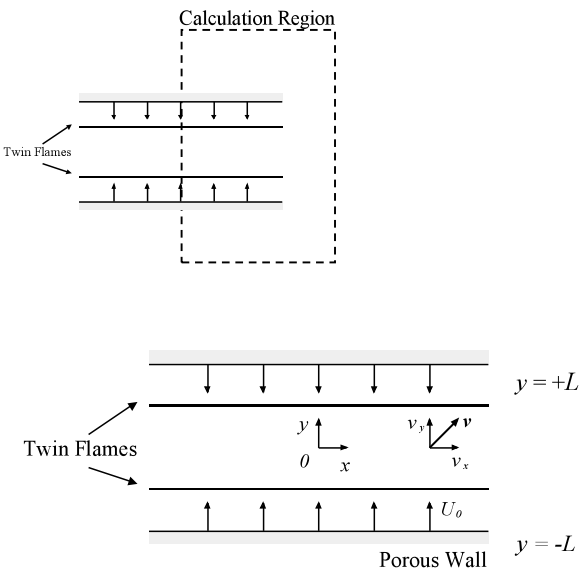


Fig. 3 Schematics of counter-flow twin flames and rectangular coordinate.

3. Results and Discussions

3.1 Non-reactive Flow

First, the flow field in a non-reactive mixture was investigated to examine the velocity fluctuation. The steady state was achieved (about 5000 time steps). Figure 4 shows the non-dimensional axial velocity at $x/L = 2$ and 4. It is found that there exists the velocity fluctuation, which can be eliminated by time-averaging process for 100 time steps.

Also, the counter-flow was simulated with the following Navier-Stokes equations by finite difference method.

$$\partial_t u + (u \cdot \nabla)u = -\frac{1}{\rho}\nabla p + \nu\nabla^2 u$$

Both results are shown in Fig. 5. These velocities are non-dimensionalized with inlet velocity at the wall. As seen in this figure, the fine counter-flow structure is observed in LG simulation, and its flow field is similar to that by solving the Navier-Stokes equations.

Next, these results were quantitatively compared,

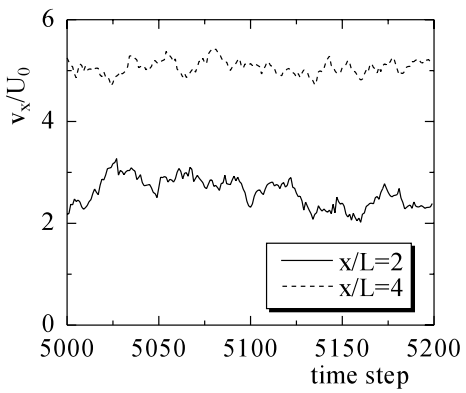
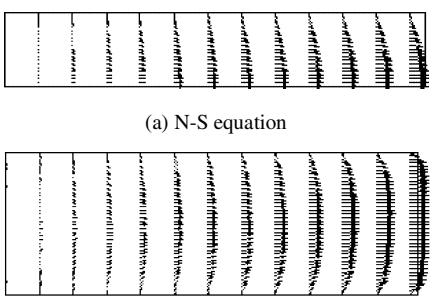


Fig. 4 Non-dimensional axial velocity.



(a) N-S equation

(b) LGA

Fig. 5 Flow field in cold flow.

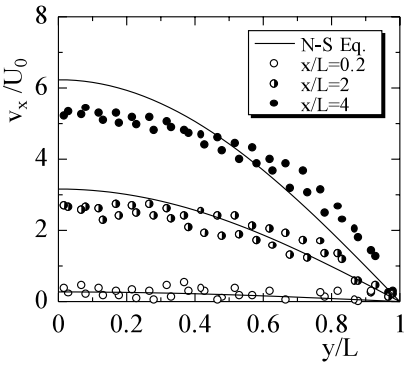


Fig. 6 Distribution of non-dimensional axial velocity.

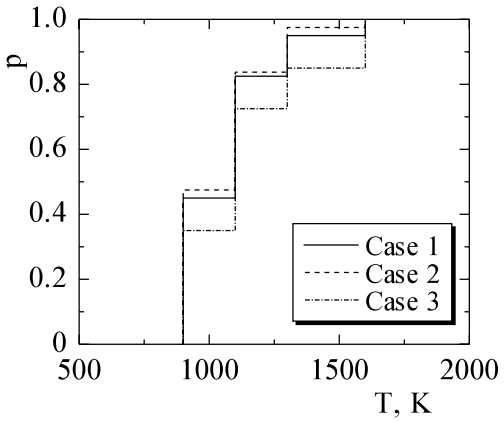


Fig. 7 Variations of reaction probability with temperature.

which is shown in Fig. 6 at three different axial positions. It is found that the velocity obtained by LGA is almost the same as that by N-S equation. Therefore, this counter-flow can be simulated by this discrete model, as well as other flow configurations including a Poiseuille flow and the flow after a backward facing step etc. [6].

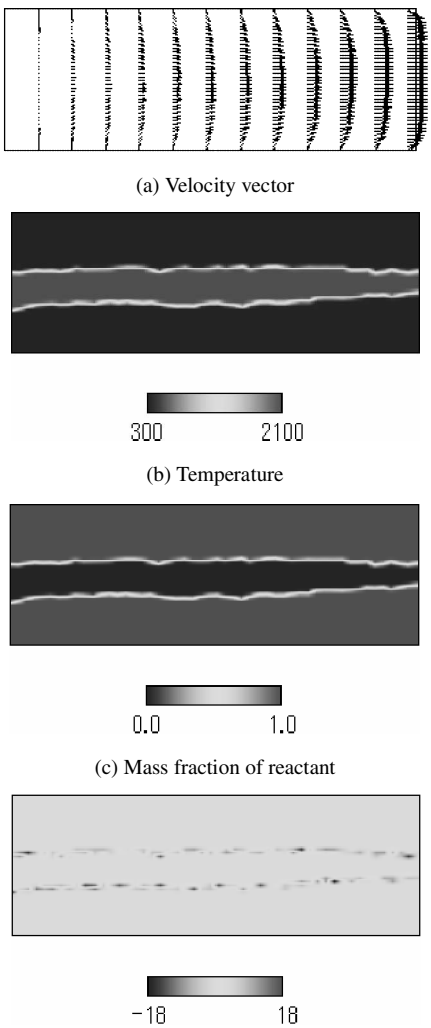
3.2 Reactive Flow

Next, the transition between two particles of reactant and product was included for reactive flow simulation. Reactant, A, and product, B have equal mass, and both temperatures are 300 K (T_A) and 2100 K (T_B), respectively. Therefore, the total mass is conserved even when the reaction occurs. Here, it was assumed that the reaction occur based on the reaction probability. That is, the reactant reacts to become product with probability of p. To avoid the complex collision rules, the backward reaction was also considered so that the reactant and product do not exist together. Then, the product becomes reactant with probability of $(1 - p)$.

$$\mathrm{A} \rightarrow \mathrm{B} \quad \text{(forward reaction with probability of } p\text{)}$$
$$\mathrm{B} \rightarrow \mathrm{A} \quad \text{(backward reaction with probability of } (1-p)\text{)}$$

Usually in combustion field, the reaction rate is changed by temperature. Thus, in this model, the reaction probability depends on the local temperature, T, which is obtained by $(N_A T_A + N_B T_B)/(N_A + N_B)$, where N_i is the number of particle i at the specified node. As seen in Fig. 7, three cases of different temperature dependence were considered.

Results obtained in case 1 are shown in Fig. 8, including the profiles of velocity vector, temperature, mass fraction of reactant, and reaction frequency. The mass fraction of species i is obtained by $\rho_i/(\rho_A + \rho_B)$, where ρ_i is the number density of particles existing per node. In Fig. 8 (a), the unburned gas region exists outside, and burned gas region is inside. The reaction zone, which is determined by reaction frequency, is located at the boundary of two regions. From these profiles, it is considered that reactants flow inward from both walls at $y = L$ and $-L$, and are transformed chemically to products in the reaction zone. Then, both flow outward along the x-direction. This configuration is very similar to the counter-flow premixed flames [14], [15].



(a) Velocity vector

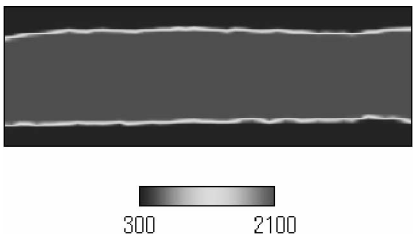
(b) Temperature

(c) Mass fraction of reactant

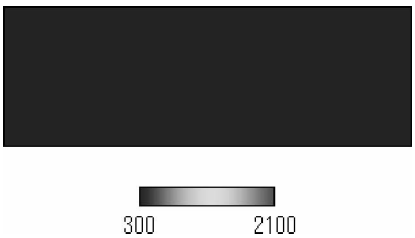
(d) Reaction frequency

Fig. 8 Contour of reactive flow in case 1, t = 5000.

Next, temperature profiles in cases 2 (more reactive) and 3 (less reactive) are shown in Fig. 9. In case 2, where the reaction probability is higher than that in case 1, the high



(a) Case 2



(b) Case 3

Fig. 9 Contour of temperature in cases 2 and 3, $t = 5000$.

temperature region is expanded. When the reaction probability is lower in case 3, the reaction region is extinguished. Thus, the reaction probability controls the reaction intensity. It was concluded that the combustion could be simulated by this two-component LGA model.

4. Conclusions

In this study, Lattice Gas Automata (LGA) was applied for combustion simulation, which simulates the fluid with mesoscopic particles of reactant and product. In the reaction model, the reaction probability was used. Three cases of different temperature dependence were considered. Results show that the flow field in non-reactive flow by LGA is quite in agreement with that by solving Navier-Stokes equations. The flame (reaction region) behavior is similar to the real counter-flow flames. Although, the reaction model may be improved, it is possible to simulate the combustion field by this discrete model.

References

[1] T. Mantel and J.M. Samaniego, "Fundamental mechanisms in premixed turbulent flame propagation via vortex-flame interactions part II: Numerical simulation," Combust. Flame, vol.118, p.557, 1999.
[2] D. Karmed, M. Champion, and P. Bruel, "Two-dimensional numerical modeling of a turbulent premixed flame stabilized in a stagnation flow," Combust. Flame, vol.119, p.335, 1999.
[3] J. Hardy, O. de Pazzis, and Y. Pomeau, "Molecular dynamics of a classical lattice gas: Transport properties and time correlation functions," Phys. Rev. A, vol.13, p.1949, 1976.
[4] U. Frisch, B. Hasslacher, and Y. Pomeau, "Lattice-gas automata for the Navier-Stokes equation," Phys. Rev. Lett., vol.56, p.1505, 1986.
[5] U. Frisch, D. D'Humières, B. Hasslacher, P. Lallemand, Y. Pomeau, and J.P. Rivent, "Lattice gas hydrodynamics in two and three dimentions," Complex Syst., vol.1, p.649, 1987.
[6] G.D. Doolen, Lattice Gas Methods for Partial Differential Equations, Addison Wesley, 1989.
[7] D. Rothman and S. Zaleski, Lattice Gas Automata: Simple Models of Complex Hydrodynamics, Cambridge University Press, 1997.
[8] D. Dab, A. Lawniczak, J.P. Boon, and R. Kapral, "Cellular-automaton model for reactive systems," Phys. Rev. Lett., vol.64, p.2462, 1990.
[9] J.R. Weimar and J.P. Boon, "Class of cellular automata for reaction-diffusion systems," Phys. Rev. E, vol.49, p.1749, 1994.
[10] J.P. Boon, D. Dab, R. Kapral, and A. Lawniczak, "Lattice Gas Automata for reactive systems," Physics Reports, vol.273, p.55, 1996.
[11] L.W. Kostiuk, K.N.C. Bray, and R.K. Cheng, "Experimental study of premixed turbulent combustion in opposed streams. Part II - Reacting flow field and extinction," Combust. Flame, vol.92, p.396, 1993.
[12] L.W. Kostiuk, I.G. Shepherd, and K.N.C. Bray, "Experimental study of premixed turbulent combustion in opposed streams. Part III - Spatial structure of flames," Combust. Flame, vol.118, p.129, 1999.
[13] A.W. Burks, Von Neumann's self-reproducing automata, Essays on Cellular Automata, 1970.
[14] H. Tsuji and I. Yamaoka, "Structure and extinction of near-limit flames in a stagnation flow," Proc. Combustion Institute, vol.19, p.1533, 1982.
[15] S. Ishizuka and C.K. Law, "Effects of Lewis number on extinction behavior of premixed flames in a stagnation flow," Proc. Combustion Institute, vol.19, p.327, 1982.

Kazuhiro Yamamoto is Associate Professor at Nagoya University. His research field is thermal engineering, especially combustion. His recent topic is discrete simulation for fluids including Lattice Gas Automata and Lattice Boltzmann method. In collaboration research with Los Alamos National Laboratory, numerical scheme on combustion simulation has been newly proposed, published in J. Statist. Phys. He is a member of the Japan Society of Mechanical Engineers and the Combustion Society of Japan.