Commun. Comput. Phys.
doi: 10.4208/cicp.441011.270112s

Vol. **13**, No. 3, pp. 741-756
March 2013

Lattice Boltzmann Modeling of Advection-Diffusion-Reaction Equations: Pattern Formation Under Uniform Differential Advection

S. G. Ayodele[1,*], D. Raabe[1] and F. Varnik[1,2]

[1] *Max-Planck Institut für, Eisenforschung, Max-Planck Straße 1, 40237, Düsseldorf, Germany.*
[2] *Interdisciplinary Center for Advanced Materials Simulation, Ruhr University Bochum, Stiepeler Straße 129, 44780 Bochum, Germany.*

Received 31 October 2011; Accepted (in revised version) 27 January 2012

Available online 29 August 2012

Abstract. A lattice Boltzmann model for the study of advection-diffusion-reaction (ADR) problems is proposed. Via multiscale expansion analysis, we derive from the LB model the resulting macroscopic equations. It is shown that a linear equilibrium distribution is sufficient to produce ADR equations within error terms of the order of the Mach number squared. Furthermore, we study spatially varying structures arising from the interaction of advective transport with a cubic autocatalytic reaction-diffusion process under an imposed uniform flow. While advecting all the present species leads to trivial translation of the Turing patterns, differential advection leads to flow induced instability characterized with traveling stripes with a velocity dependent wave vector parallel to the flow direction. Predictions from a linear stability analysis of the model equations are found to be in line with these observations.

AMS subject classifications: 76R05, 76R50, 92C15, 80A32

Key words: Advective transport, differential advection, Turing patterns, linear stability, lattice Boltzmann.

1 Introduction

Spatially and/or temporally varying structures have been observed in a variety of physical [1, 2], chemical [3–5] and biological [6–11] systems operating far from equilibrium. In chemical and biological systems for instance, the macroscopic reaction-diffusion (RD) equations have been proposed as models for morphogenesis [12], pattern formation [6,7] and self-organization [13, 14]. This class of equations usually includes the following two

*Corresponding author. *Email addresses:* `s.ayodele@mpie.de` (S. G. Ayodele), `d.raabe@mpie.de` (D. Raabe), `fathollah.varnik@rub.de` (F. Varnik)

features: (i) a nonlinear reaction between chemical species describing local production or consumption of the species and (ii) the diffusive transport of these species due to density gradients. The properties of structures that arise from this class of systems are determined by the intrinsic transport parameters of the system such as the diffusion coefficient and reaction constants. However, the presence of an external influence such as advection may lead to qualitative changes in the system's behavior and to the emergence of new non-equilibrium structures. This is very important in the experimental investigations of the diffusive chemical instability in gel reactors where the perturbative effect of the feeding flows is not fully suppressed or in tubular reactors where spatiotemporal behaviors might also be of interest. Attempts to understand the role played by advection in spatio-temporal organization of RD systems have led to the discovery of the flow distributed structures (FDS) or flow distributed oscillations (FDO). In this case excitable RD systems with fixed or periodically forced inflow boundary, are known to develop stationary [15, 16] and traveling waves [17, 18] depending on the boundary-forcing frequency. Patterns of these type are known to occur even when the Turing instability condition of unequal diffusion coefficient is not satisfied.

A closely related problem to the boundary forced structures which have received less study in 2D is the interactions between advective fields and a pre-existing sharp chemical gradients produced by reaction-diffusion processes. This means the interaction of already existing instabilities with the instability caused by advection. This interaction can give rise to complex patterns in both chemical and biological systems [19, 20]. In this work we consider the interaction of a uniform flow field with the Turing instability. As a prominent example of an autocatalytic reaction-diffusion pattern forming system we choose the Gray-Scott model [23]. This model has some generic features which can make it adaptable to study some realistic situations such as vegetative patterns, combustion and cell division [21, 22]. We propose a Lattice Boltzmann (LB) method for solving the ADR equations arising from the interaction of the advective fields with the Turing patterns. The LB simulation of the ADR equations shows that while advecting all the species leads to trivial translation of the Turing patterns, differential advection of the species leads to an additional flow induced instability characterized by traveling stripes with a velocity dependent wave vector parallel to the flow direction. These observations are in line with the predictions from linear stability analysis carried out on the model equations. The article is organized as follows. In the next section, we present the model equations. In Section 3 we address the framework adopted for the Lattice Boltzmann modeling of the model equations. The results obtained from the linear stability analysis and numerical simulations are discussed in Section 4. At the end of the same section, we conclude the discussion with a summary of our results.

2 The model equations

In this section we present the governing equations for the Gray-Scott advection-diffusion-reaction (ADR) model. The original Gray-Scott reaction-diffusion model describes the ki-