

ANALYTICAL STUDY OF THE RDME THROUGH THE VAN KAMPEN SYSTEM-SIZE EXPANSION

Pietro de Anna^{*}, Tanguy Le Borgne^{*}, Philippe Davy^{*} and Marco Dentz[†]

^{*} Géosciences Rennes, UMR 6118, CNRS,

Université de Rennes 1, Rennes, France

e-mail: pietro.deanna@univ-rennes1.fr

[†] Institute of Environmental Assessment and Water

Research (IDAEA/CSIC), Barcellona, Spain

e-mail: marco.dentz@upc.edu

Summary. In this work we propose a stochastic formulation of a reactive-diffusive system. We discretize the space into cells positioned at the vertices of a lattice hypercube (i.e. we assume that the number of nearest neighbors of each cell is $2d$, where d is the dimension of space). We define the state of the system by the number of each chemical species at each spatial position at every time. The system evolves through diffusion and reaction. We treat this system as a problem of population dynamics. Transitions of the system from one state to another are expressed in the form of a set of chemical equations. Interpreting the rate of such chemical equations as probabilities, the system is stochastic and evolves from one generic state to another through these transition probabilities, along a chain of stationary Markov processes. The system as a whole is thus described by a Master Equation. Performing the van Kampen's system size expansion of the Master Equation, at the leading order, we recover the macroscopic law described by the deterministic diffusion-reaction equations (the so-called mean field). We perform stochastic simulations, based on the Gillespie's algorithm, allowing us to test the validity and consistency of the stochastic model introduced. This stochastic approach allows us to quantify the relationship between local transition probabilities and the macroscopic diffusion-reaction equations. The next-to-leading order of the van Kampen expansion provides a quantification of the fluctuations around the mean field.