Understanding reaction-diffusion systems using simulations.

Reverse emulsions (water in oil) can be used, for instance, as micro-reactors to produce nanoparticles or to mimic signal transduction and communication. The exchange of mass among drops is governed by diffusion and partition coefficients and by “affinity” factors between the different molecules and the solvents involved. Some coefficients can be measured directly and/or can be inferred from secondary changes in other molecules (chemical reactions). However, because of the many coefficients and variables involved, any attempt to understand a complicated diffusive-reactive system has to consider a computer simulation.

In this talk we show the relevant information necessary to predict, using simulations, experimental data of chemical interaction among micro-reactors. We show the importance of considering physical information as can be the distance between drops as well as chemical information as can be the concentration of different reactants. Finally, we present applications for these systems: nano-particle production with precise size and chemo-mechanical gels.