Effects of Spatial Diffusion on a Model for Prebiotic Evolution. Ben F. M. Intoy[1] (bmintoy@umn.edu), Aaron Wynveen[1], and J. Woods Halley[1], [1]School of Physics and Astronomy, University of Minnesota (UMN) Twin Cities, Minneapolis MN USA.

Introduction: In previous work [1], a Kauffman-like model for prebiotic evolution [2] was used. The model describes 'chemical species' as binary numerical strings consisting of 0's and 1's which are to be interpreted as polymers (e.g., nucleic acids or proteins with only two available monomer types). We include all possible ligation and scission reactions of all possible polymers up to a maximum polymer length of l_{max} with probability p. Each reaction also has an 'enzyme' or catalyst assigned, without which the reaction cannot take place. At differing values of p many chemical reaction networks were generated. For each such generated chemical network we stochastically simulated its dynamics multiple times and considered systems to be lifelike if, in steady state, it was out of chemical equilibrium. That constraint, consistent with intuitive ideas of the meaning of 'lifelike', had a significant impact on the probability of the appearance of lifelike states in the model. The model assumed that the constituent 'molecules' were in a 'well-mixed' reactor so that effects of spatial diffusion played no role. I will review that earlier work [1] and report results of an extension of the 'well-mixed' reactor model on a spatial lattice [3].

The competition between chemical reaction and diffusion leads to various kinds of nonequilibrium steady states, some out of diffusive equilibrium but in chemical equilibrium within each lattice site [diffusively alive and locally dead (DALD)], some in diffusive equilibrium but out of chemical equilibrium on each lattice site [diffusively dead and locally alive (DDLA)] and still others, perhaps the most lifelike, which are not equilibrated in either way but are in dynamic steady states far from equilibrium [diffusively alive and locally alive (DALA)]. Using data from simulations, I will present estimated probabilities of the generation of these various kinds of states as a function of two parameters of the model.

The chemical dynamics within a site in the model is controlled by a parameter p, while the diffusive rate of hopping between sites is controlled by parameter η. The parameter p is the probability that a chemical reaction from a list of all chemical reactions is included in the network and characterizes intra-site reactions. We found that at large η the probability of finding a lifelike steady state for the spatial simulations is similar to the 'well-mixed' simulation results [1]. At low values of η we find with particular interest that DALA states appear at large values of p where the 'well-mixed' model gave mainly chemically equilibrated systems (see figure 1) [3]. Most of these DALA states are due to the explosive population growth of a few sites. In these cases the population growth is quite dramatic, causing systems to go from one metastable steady state to a different one of lower entropy. The details and characteristics of these states will be elaborated upon in this presentation.

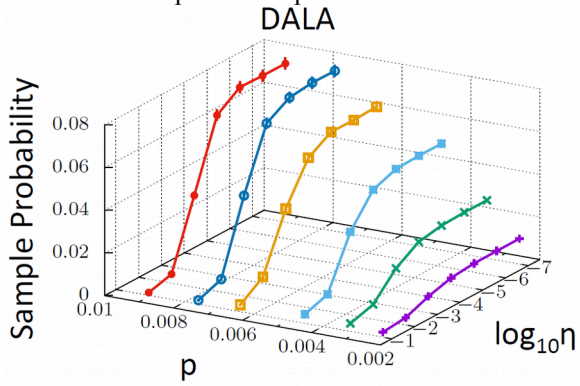

Figure 1: The sample probability obtained from simulation data of forming a DALA steady state given a random chemical network formed with parameter p and simulated with hopping parameter η.

This work is supported by the United States of America National Aeronautics and Space Administration (NASA) through grant NNX14AQ05G. Computational resources used by this project include the UMN Minnesota Supercomputing Institute, the UMN School of Physics and Astronomy Condor Cluster, the NASA Advanced Supercomputing Division, and the Open Science Grid.

References: [1] A. Wynveen, I. Fedorov, and J. W. Halley, *Phys. Rev. E* 89, 022725 (2014). [2] S.A. Kauffman, *The Origins of Order*, Ch. 7 (1993). [3] B. F. Intoy, A. Wynveen, J. W. Halley, *Phys. Rev. E* 94, 042424 (2016).