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ROBUST COMPUTATIONAL ALGORITHM FOR NUMERICAL CONSISTENCY AND CONVERGENCE OF LIESEGANG PATTERNS FORMATION MODEL

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Abstract. Liesegang patterns are coloured bands which are formed in numerous reactions that involve the precipitation of one compound (most frequently salt crystals) produced from the reaction of two specific substances in the absence of convection. Although Liesegang studied these phenomena more than a century ago, currently they are receiving a renewed and increasing interest, as far as they can serve as an alternative for the bottom-up manufacturing of functional nano- and microstructures. Regarding the formation of Liesegang pattern, there exist few models, but the more accepted and used is the Keller-Rubinow model based on the Ostwald's supersaturation theory. Numerical simulation of the dynamics of these processes is a very active research topic due to the discontinuous nature of the pehenomena, which turn the numerical problem to a challenging task. In fact, very recent works still discuss the ill-posedness of such state-of-the-art models, i.e. the numerical implementation of the Keller-Rubinow model. In this work, we propose a complete numerical strategy based on original criteria for adaptive timestepping, adaptive meshing, and definition of supersaturation parameters in order to obtain a well-posed numerical formulation for the Liesegang pattern formation phenomena. The strategy was tested by using a typical case from the literature showing stability and convergence for the proposed scheme.