# Elaboration of cellular automata-based numerical model reflecting condensation kinetics of MTMS-based aerogels

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Condensation is a crucial aspect of silica aerogel preparation by the sol-gel acid-base method. The process is affected by a variety of factors, like the chemical composition of the sample, reaction pH value [1] or temperature of gelation [2]. The formation of aerogel hierarchical structure is a compelling and complex phenomenon: first, polycondensation of precursor molecules into primary particles occurs, then primary particles create aggregates – the secondary particles, that subsequently create a continuous silica network with outstanding properties. An in-depth understanding of this process – on both, experimental and numerical level – would provide the essential knowledge to plan the aerogel synthesis process in such a manner, to precisely control the product's structure, thus its properties. Hence, the goal of the presented research is to prepare a cellular automata-based numerical model that would connect the synthesis parameters with the hierarchical aggregation process.

The presented research includes the basic cellular automata model reflecting the aggregation of secondary particles process, due to the sample concentration and probability of successful collisions. The preliminary results illustrate a model based on classic diffusion/reaction limited aggregation (DLA/RLA) [3] and kinetics curves obtained by this method. Model improvement bases on comparison to an experimentally obtained data. The investigated samples were based on hydrophobic methyltrimethoxysilane (MTMS) precursor, and prepared with a different precursor/anti-solvent ratios to control porosity and morphology of the obtained structures, due to interference into microscopic phase separation.

The crucial parameter, essential for the development of the proposed model is the probability of successful collisions of particles. Base on the collision theory, it is proportional to specific reaction rate and can be connected with the parameters from the Arrhenius equation (activation energy and Arrhenius constant). The preliminary parameters designated by the tilting-test-tube method. The second experimental part was to establish the kinetics curves of gelation by UV-Vis spectrophotometric measurements at particular time intervals.

The conducted studies provided the implementation of cellular automata system reflecting the silica aerogel formulation process. Both numerical and experimental measurements gave characteristic sigmoidal curves of condensation kinetics. Furthermore, the activation energy was successfully designated experimentally. As far as the coefficient related to Arrhenius constant is concerned, due to significant standard deviation values, it was only approximately estimated. For the development of a more accurate, quantitative model, the need for more precise gelation measurement (rheometric investigation).

## References

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