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A rational approach towards kinetic modeling of microbial inactivation

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Since the formulation on the law of disinfection it has been debated, whether, the inactivation kinetics of microorganisms originates from underlying chemical reactions. It is generally assumed that a complex living structure is unlikely to obey simple first order kinetics. Notwithstanding, after more than a century, the classical-D and z-value concept is still the regular framework for quantitative analysis of experimental inactivation data. Complementary to this classical approach is the formulation of empirical inactivation models, which are required for statistical analysis of the collected data. Predictive modeling is used to accurately describe experimental data and accounts for observed shoulders and tailing in kinetic data series. Recently, it has been shown that both approaches aimed at quantifying microbial inactivation can be merged into a single thermos-dynamical model. This was achieved by including quantum theory on molecular dynamics in order to deal with large complexes of interacting molecules and the stochastic nature of protein unfolding. In addition, microorganisms with different resistance towards heat and chemical treatment could be included in the model by assuming Gaussian distributed sub-populations. It is suggested that critical polymer structures, e.g. proteins, omnipresent in bacteria and spores, require unfolding prior to inactivation. These model predictions are in line with the mechanism for inactivation of different species of *Bacillus* spores by wet heat that is found to coincide with the denaturation of key proteins.

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