"MWK" MODEL OF CONFINED NANOSYSTEMS

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The relationship between the reaction constant and the quantum properties of the reactants is a topic at the border between chemical kinetics and quantum mechanics. The reaction constant, usually denoted by k, characterizes the rate at which a chemical reaction occurs; it depends on factors such as temperature, the nature of the reactants, and the activation energy; in the transition state theory, this constant is related to the formation of the activated complex. On the other hand, in the quantum description of particles, the state of motion is characterized by the wave vector k, which is directly related to the momentum by the relation; this concept arises naturally in the theory of quantum scattering, where chemical reactions are treated as collision processes between particles. The present work explores the connection between the reaction constant and the wave vector. Thus, in elementary gas-phase processes, the reaction constant can be expressed as the product of the relative velocity of the particles and the effective reaction cross section. Since the velocity is related to k, and the effective cross section is a function of it, it follows that k-"rate reactions" becomes a function of k – "wave vector", and, although not identical, they are in a functional relationship "k (rate reactions) ~ k (wave vector)"). Even in extreme conditions, such as very low temperatures or ideal quantum systems, this relationship remains of interest. In this new conceptual context, the new relationship as $\Delta m \sim \omega k$ ("MWK" Model) describes a proportional relation between mass change in a nanosystem and the rate constant of a chemical process occurring on its surface. Further quantum Einstein-Planck-De Broglie considerations produced the working quantum-relativistic connection under the momentum form $\hbar = \alpha c\sqrt{p}$ allowing to correctly describing the quantum-system scale factor $[\alpha] = kg^{1/2}m^{1/2}s^{1/2}$; moreover it becomes a quantum length–action hybrid scale $\alpha_{system} = \sqrt{m^*_{carrier} \cdot L_{conf}}$ that encodes effective mass $m^*_{carrier}$ of the relevant carrier (e.g. electron, exciton, proton, quasiparticle), and the characteristic coherence length scale L_{conf} (e.g. MOF pore size, tunneling distance, active exciton length site size) in nanosystems. The study of these relationships contributes to the development of nanotechnology and a better understanding of chemical and biochemical processes at the (sub)microscopic scale, e.g. enzyme nanokinetics (understanding reaction rates in confined biological environments), nanoreactors (designing systems where reaction rates are maximized under unity conditions), quantum biology (exploring wave effects in biochemical processes), or biosensing (interpreting signal generation at low molecular numbers). Relevant numerical examples are correspondingly given.

Acknowledgements. This work has been supported by West University of Timisoara (DEVELOP Programme 2026) and by National Institute of RD for Electrochemistry and Condensed Matter (INCEMC-Timișoara "Nucleu" Programme 2026), respectively.