# Efficient quasi-spectral numerical method to integrate chemical master equation

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Chemical Master Equation (CME) approach is typically used to estimate the rate coefficients of elementary chemical reactions on the level of molecular dynamics [1]. At present, existing conventional methods to treat this problem especially for multi-well systems are semi-empirical and remain rather computationally demanding [2]. The conventional method leads to a linear but highly dimensional systems of equations, which are employed to evaluate estimations for elementary reaction rates [2, 3]. In our study a quasi-spectral method to integrate single-, multi-well CMEs systems is presented [4]. For a given reaction system, CMEs are integrated such that the evolution over the energy range of entire populations of the species involved in the mechanism can be determined. Afterwards the detailed solution can be used to define the rates of elementary reactions in a systematic manner. For this a method to estimate reaction rate constants of a phenomenological model is proposed as a generic solution of an inverse problem for these rates.
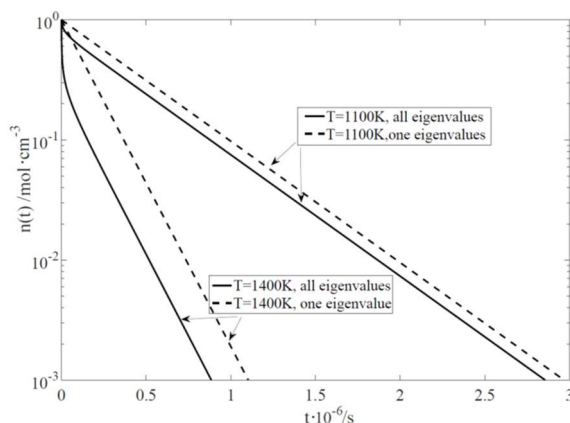


Fig.1. Concentration evolution of the allene, dashed lines show the phenomenological model based on the standard estimation approach, while actual concentration evolution is shown by solid lines for different initial temperature and normal pressure.

The suggested approach is implemented and illustrated by the problem of the allene isomerization into propyne through cylcopropene [3, 5]. The comparison of the allene concentration evolution given by conventional method and the proposed method is presented in Fig. 1. The figure shows transparently possible over estimations of the concentration produced by conventional method.

## References

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