Investigating mechanisms: Is this what you need?

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Areas of chemical kinetics using large reaction mechanisms, such as combustion, atmospheric chemistry and metabolic modelling need reliable, wide coverage program packages. Having analyzed the requirements for such a package, we have been writing [1] codes in *Mathematica* to solve more and more problems arising in the practice of kinetic modelling. Our package has a modular structure and everyone may download it who is interested in.

Here we show how to use our program package for dealing with the following problems:

- visualizing various graphs of reactions,
- performing theoretical operations, like union, complementation, and differencing of sets of elementary reaction steps,
- calculating numerical characteristics beyond (or before) numerically solving the kinetic differential equations of a given mechanism,
- trying to find the ignition time etc.

The methods above will be presented using combustion mechanisms as examples.

[1]] A. L. Nagy, D. Papp and J. Tóth: ReactionKinetics: A *Mathematica* Package with Applications, *Chemical Engineering Science*, **2012**, http://dx.doi.org/10.1016/j.ces.2012.01.039 (2012).