ADGenKinetics: An Algorithmically Differentiated Library for Biochemical Networks Modeling via Simplified Kinetics Formats

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This work demonstrates a comprehensive overview of a compact but powerful freely available Modelica library for descriptive modeling of biochemical reaction networks using a specific subset of enzyme kinetics referred to as simplified kinetics formats. These subsets of enzyme kinetics are represented by generalized structured kinetic formulas suitable for biochemical reactions with arbitrary number of substrates, products, inhibitors and activators [2]. While existing powerful works and guidelines for modeling biochemical reaction networks already exist [4], in this work a first attempt of utilizing the power of Modelica constructs for providing a compact implementation of such generalized structured formulas is presented. This gives the opportunity of realizing biochemical reaction networks using few number of reaction components, in contrast to libraries based on classical mechanistic kinetics which require hundreds of reactions components.

ADGenKinetics[1] is the first algorithmically differentiated library by which algorithmic differentiation (AD) techniques [3] are directly applied at the library level [1]. The resulting additional subpackage contains extended components with which parameter sensitivities, i.e. derivatives of model variables w.r.t. model parameters, are represented. By importing these types in base models, the dynamics of the underlying biochemical reaction network together with the parameter sensitivities, i.e. the derivatives of all variables w.r.t. the specified input parameters, are simulated. The underlying novel equation-based AD techniques which have been especially designed for *ADGenKinetics* have also the potentials to be employed by other Modelica libraries.

References

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[1] The open-source *ADGenKinetics* library is provided under the Modelica License 2