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About choice of interface language for the solution of problems of mathematical modeling of chemical and technological processes

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The vast majority of the known program complexes applied in simulation modeling uses this or that kind of language of very high level which allows to set computer procedures specific for the model without writing special program module for each kind of the systems of ordinary differential equations (SODE). Software for the solution of direct and reverse problems of chemical kinetics is no exception.
The authors are sure interface language most closely resembling to the notation accepted in chemistry to describe the mechanism of stepwise reactions corresponds to such tasks most accurately. Formation of the right parts of SODE on the assumption of the mass action law provides their accordance with Lipschitz's criterion and also gives a chance to calculate Jacobian determinants explicit that reduces operating time of the integrating units with implicit schemes by times and orders.
The available operation algorithm of entry interface contains the main blocks:
1) All substances, including intermediate, are given in the form of the identification list in the convenient notation. The declaration of all significant substances makes it possible to avoid casual mistakes at the earliest stage and guarantees against appearance of "twins".
2) Initial concentrations of substances are determined as well. Default zero concentration are substituted for the final products of reaction and active intermediates. In the overwhelming majority of cases in most cases "in manual mode" nonzero concentrations of two or three initial substances are assigned.
3) The overall scheme or the mechanism of reagents interaction is formed in the standard for chemical kinetics notation. The choice of participants in the scheme is made strictly according to the identification list declared in item 1. Natural and obligatory restriction is that total number of involved particles can't exceed three neither among reagents, nor among products of the elementary act of interaction that follows from requirements of formal kinetics.
4) All introduced reactions have default zero specific reaction rate. Before the calculation it is necessary to insert reference or guess values. It's never too late to remove reactions with zero rates, however in some cases it's not unreasonable to reserve them in order to complicate and correct the model in future.
Examples of solution of "non-chemical" models using formal chemical and kinetic language are given.

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