On Global Quasi Linearization (GQL) in model reduction of chemical kinetics

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In the present work a novel approach for simplifying chemical kinetics models, the so-called Global Quasi Linearization method (GQL) is suggested. A key mathematical concept for the novel reduction is that of Singularly Perturbed Vector Fields (SPVF), where the theory of Singular Perturbed Systems (SPS) is reviewed and extended with special emphasis on the coordinate free approach. Accordingly, the main idea of the approach is to find a new coordinate system (change of the system coordinates), which gives a decomposed system in the standard SPS form. A number of advantages make the method more robust and easy to implement. First of all, it allows a global approximation of the system decomposition. The most important point of the developed method is the proper identification of the fast subsystem behaviour, because it is not reflected by a slow manifold structure. Thus, the problem of many approaches dealing with decomposition into fast/slow is overcome. The method is implemented within a code for the standard ILDM method and it is compared to the standard ILDM as well as to the detailed system solution.

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