REDIM based model reduction of the decomposition of urea-water-solutions in films and droplets

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In order to fulfil strict environmental regulations concerning emissions of nitric oxides (NOx) selective catalytic reduction (SCR) with urea-water solution (UWS) is often used in automotive industry. The urea from UWS decomposes to isocyanic acid and ammonia that present the NOx reduction agent in the gas phase and on the catalyst surface. Several drawbacks of using the urea reduce the performance of a SCR system. Incomplete deposition leads to formation of residuals affecting efficiency of the exhaust gas systems. The complete decomposition of urea and possibly homogenous distribution of the resulting ammonia in front of the SCR catalyst are necessary [1]. To investigate the process of the urea deposition for exhaust gas conditions numerical methods, which have to include multiphase processes at largely differing time scales and spatial scales, need to be employed. Recently more detailed chemical mechanisms for the decomposition of urea in the liquid phase have become available [3]. Using such mechanisms, the decomposition of urea can be captured more accurately. However, these mechanisms require a large amount of computational (CPU) time. A typical approach to cope with the complexity of chemical kinetics are automatic model reduction methodologies.

The method of Reaction Diffusion Manifold (REDIM) [2] has been developed for the reduction of the detailed chemical kinetics. In this work the developed concept of REDIMs is further extended to describe reduced the gas phase chemical kinetics and mixture composition near the droplet / film surface. For this, the boundary conditions at the phase interface are modified and account for influence of chemical reactions in the liquid phase. By using these boundary conditions, the REDIM is developed and validated for simple reference cases (plane for films and spherical for droplets geometries) under typical SCR conditions. Being compared to the detailed model, it is shown that the proposed reduced model captures the urea decomposition very accurately.

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