A chemical species transport model with variable gas properties for gas dynamic calculation of internal combustion engines

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Abstract

The use of after-treatment systems in internal combustion engines has become an standard in recent years. Diesel oxidation catalysts, diesel particulate filters or selective catalyst reduction systems are required to cope with current and future emission regulations. The inclusion of these systems in 1D gas dynamics codes for internal combustion engine modelling demands the development of a chemical species transport model to account for the influence of chemical species conversion along the engine flow-path on emissions and flow thermal properties.

This paper presents a chemical species transport model to account for variable composition and gas properties along the engine flow path. It is described the numerical solution to adapt the gas dynamic model to chemical species transport in boundary conditions by means of the method of characteristics and in volumes by means of a filling and emptying model. The importance of gas diffusion against convection terms in the flow governing equations in ducts is analysed. The performance for chemical species transport of sock capturing methods, such as the two-step Lax&Wendroff method and the Sweby's TVD scheme considering several flux limiter definitions, is carried out by means of sock-tube tests representative of flow conditions in internal combustion engines. The gas modelling both as perfect and non-perfect gas is performed to evaluate the numerical methods features against variable gas composition and properties and the influence of these flow characteristics on sock-tube results.

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Abstract submitted to Mathematical Modelling in Engineering & Human Behaviour 2011 *March 14, 2011*