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Sommario/riassunto

This work focuses on gaseous reactive flows in ideal and non-ideal reactors. The objective of this research is the development of models for the numerical simulation of homogeneous reactive flows under vacuum carburizing conditions of steel with propane and acetylene. These models can be used for further investigations of heterogeneous reactions during vacuum carburizing of steel to predict the carbon flux on the complex shaped steel parts to understand and, eventually, optimize the behavior of the whole reactor.arburizing is the case-hardening process in which carbon is added to the surface of low-carbon steels at temperatures generally between 850 and 1050 °C. In the conventional gas carburizing at atmospheric pressure, the carbon potential is controlled by adjusting the flow rate of the carburizing gas. Carbon potential of the furnace atmosphere can be related to partial pressure of CO2 or O2 or vapour pressure of water by equilibrium relationships and a sensor can be used to measure it. This method of carbon-potential control cannot be used for vacuum gas carburizing due to the absence of thermodynamic equilibrium which is one of the main difficulties of the vacuum carburizing process. The formation of soot during carburization isalso undesirable and the process parameters should be selected such that the formation of soot is minimized. The amount of carbon available for carburizing the steel depends on the partial pressure of the carburizing gas, carbon content in the carburizing gas and the pyrolysis reactions of the carburizing

gas. The pyrolysis reactions of the carburizing gas are also affected by the contacting pattern or how the gas flows through and contacts with the steel parts being carburized. This work focuses on gaseous reactive flows in ideal and non-ideal reactors. The objective of this research is the development of models for the numerical simulation of homogeneous reactive flows under vacuum carburizing conditions of steel with ropane and acetylene. These models can be used for further investigations of heterogeneous reactions during vacuum carburizing of steel to predict the carbon flux on the complex shaped steel parts to understand and, eventually, optimize the behavior of the whole reactor. Two different approaches have been used to model the pyrolysis of propane and acetylene under vacuum carburizing conditions of steel. One approach is based on formal or global kinetic mechanisms together with the computational fluid dynamics (CFD) tool. The other approach is based on detailed chemistry with simplified or ideal flow models. Two global mechanisms developed at the Engler-Bunte-Institut for pyrolysis of propane and acetylene respectively were used in this work. One detailed mechanism developed at the Institute of Chemical Technology by the research group of Professor Deutschmann was used for modeling the pyrolysis of both the propane and acetylene. Experimental data from investigations on vacuum carburizing conducted at the Engler-Bunte-Institut were used to validate the modeling results.