PREFACE

Automotive Emission Control

Automotive emission control is certainly one of the success stories of our profession. Faced with both acute and chronic environmental problems such as smog and acid rain, in the seventies of the last century industry in general and car manufacturers in particular engaged in a major research and development effort. Since then, environmental regulations have become more stringent with so-called zero emission vehicles as ultimate goal. To meet this challenge it was not sufficient to limit progress to the internal combustion engine front alone. It soon appeared that catalytic oxidation of the non-combusted hydrocarbons (function 1) and carbon monoxide (function 2) as well as the reduction of nitrogen oxides (function 3) was required. The three-way catalytic converter was born. It can be safely stated that today this is the most abundant catalytic reactor in the world. From it a lot of other technologies evolved, the most common being NO_x storage and reduction catalysts and selective catalytic reduction (SCR) catalysts both for lean NO_x removal, diesel oxidation catalysts for lean CO and hydrocarbon removal and (coated) diesel particulate filters for soot removal, or combinations of those. Moreover the range of conditions at which these devices are operating is much broader than that of any chemical reactor in the process industry.

Of course, a key to this success has been the design of catalysts combining different functions and resistant to the harsh reaction conditions. That is why the first contribution of this issue, the most "chemical" one, illustrates the present approach with respect to so-called three-way catalysts and NO_x storage practised by the largest car manufacturer in the world. Issues related to oxygen storage and release, to the sintering of the precious metals group catalyst components as well as to the details of the NO_x storage and reduction are discussed. The present level of understanding is impressive and the expectation is for further progress.

This volume, however, emphasises the role of chemical engineering in automotive emission control. Clearly the development of mathematical models describing the different functions of the converter(s), as well as their interaction, has been and still is crucial. Each of the contributions advocates the implementation of the latter, combined with experimental validation, rather than engaging into elaborate experimental programs. The developed reactor models are capable of covering the wide range of operating conditions. Even more challenging, they cover quite a spectrum of time and length scales. They are, e.g. accounting for the transient operation connected to both the cold start-up of the engine and the periodic changes of the composition of the engine outlet induced by the interaction between the engine and the converter. Needless to say, in view of the computational costs, any implemented feature of the models has been carefully assessed as to its benefits. This has, e.g. lead to the choice of Langmuir–Hinshelwood–Hougen–Watson rate equations rather than of microkinetics, i.e. of kinetics accounting implicitly rather than explicitly for every significant elementary reaction. Still, these models have empowered the involved research themes in their efforts aimed at catalyst and/or reactor development and optimization. In doing so, it was and is important to realize that the emissions control system does not function in isolation, but in combination with the engine. Combining computational fluid dynamics with chemical kinetics, e.g. to investigate the effect of flow maldistributions at the diesel particulate filter, is emerging.

The second contribution comes from a major catalyst manufacturer and illustrates how insight in the reaction paths involved in three-way conversion leads to a fundamental, i.e. based on first principles, model. The emphasis in this contribution is on the chemistry rather than on the reactor model, i.e. on the description of the physical phenomena occurring in the monolith reactor. In this sense, this contribution is the bridge from the first to the third contribution.

The latter elaborates further on the monolith reactor model. It is the result of a long collaboration between a major car manufacturer and two academic groups indicating the degree of effort required to reach the present state-of-the-art. It elaborates further on the monolith reactor model and is the result of a long collaboration between a major car manufacturer and two academic groups indicating the degree of effort required to reach the present state-of-the-art. It is in this section that the reader will find the detailed description and modelling of different lean exhaust aftertreatment technologies. The reactions taking place in the diesel oxidation catalyst and the different steps involved in the removal of NO_x from the lean engine exhaust are covered. The NO_x storage and reduction catalyst as well as SCR technology is discussed in depth.

The last contribution illustrates the progress concerning the removal of particulate matter. It is the most "physical" of the four. In contrast to the first three it comes exclusively from an academic group. Its very strong collaboration with the automotive industry is clearly apparent, among other things from the long list of Society of Automotive Engineers (SAE) technical papers. I am convinced that the present volume will help to position this work in the archival literature. The combination of state-of-the-art computational techniques with heuristics is an example for the chemical engineering community.

Before concluding, let me remind you that the aim of *Advances in Chemical Engineering* is to provide the reader with *personal* views of authorities in the field. These should allow assessment of the state-of-the-art in a particular domain and to develop a feeling of its further evolution without claiming to be exhaustive. This is particularly true for the present volume. I was very happy that major players in the field have accepted to contribute and to allow us to have a look into their ''kitchen''. For the involved companies this is not obvious and I am very grateful to them.

Finally, I would like to dedicate this issue to Jozef Hoebink, my former colleague at Eindhoven University of Technology. Jozef has been active in the field of automotive emission control for more than fifteen years before he left us too soon. Those who have met him will not forget his warm personality and his enthusiasm for our profession.

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