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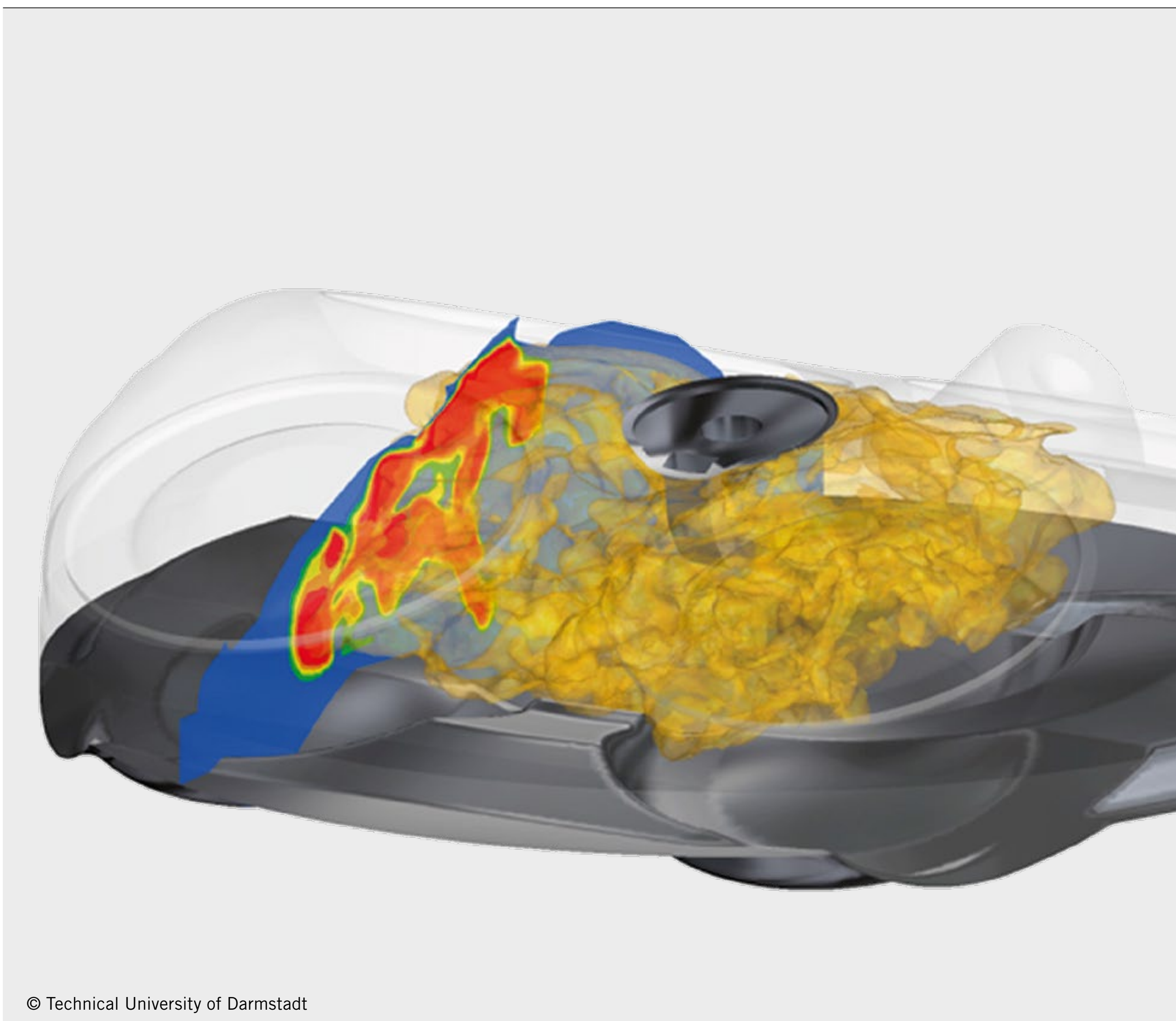
Scale-resolving Simulations for Combustion Process Development

In the academic community, Large Eddy Simulation is an established research approach while simulations based on Reynolds-Averaged Navier-Stokes equations are mostly used in industry. Since many stochastic engine phenomena such as cycle-to-cycle variations, knock or misfire can only be predicted qualitatively using this approach, there is an increasing interest in the industrial sector in also establishing Large Eddy Simulation. As part of the FVV research project 1215, the Technical University of Darmstadt evaluated the current degree of utilization of the Large Eddy Simulation in the academic and industrial environment.



1 MOTIVATION

Scale-resolving Simulations (SRS) are an established research approach at universities for the investigation of non-reactive and reactive flows. In many areas, it has become the de facto standard, replacing Reynolds-averaged Navier-Stokes (RANS) simulations almost entirely. Significant scientific progress has been achieved due to the transition from RANS simulations to SRS. To a large extent, this can be attributed to the improved resolution of the flow and especially to the mixing and non-stationary interaction with local flame structures. Combined with high-resolution (temporal and/or spatial) experimental data, the scientific understanding of turbulence-chemistry interaction has improved significantly and corresponding models have been developed. These models have been applied successfully in Large Eddy Simulations (LES) of stationary combustion processes. As an example, LES of combustion in gas turbine chambers is widely used not only at the university but also in the industry.

There is also an increased interest in LES for internal combustion engines in the academic community in particular. Reviews of recent development can be found in [1, 2], with [2] focusing specifically on combustion process development. The main motivation to use LES rather than RANS simulation is that cycle-to-cycle variations, knock or misfire can be investigated. These high-resolution simulations allow fluctuations to be analyzed for a specific operation point along the cause-and-effect chain. For example, it is possible to quantify how different phenomena interact with each other and how this leads to cyclic fluctuations. Regarding this, results were published for non-reactive [3] and reactive cases [4, 5].

There is a clear and ever-increasing trend toward higher resolutions, such that the modeled part of the flow and the mixing can be reduced or the processes in the near-wall regions can be described more accurately. This, however, requires substantial computational resources, and simulations are usually carried out on high-performance clusters or supercomputers. Especially in Europe, access to these facilities for academic research is provided through a number of national and international programs.

By contrast, RANS simulation is the standard tool for industrial combustion process design and development. The emphasis here is on investigating multiple operating conditions or geometry variations rather than analyzing a single operating point in detail. Thus, RANS approaches can only provide qualitative results for a limited number of today's most pressing questions, such as highly stochastic combustion cycles (knock, misfire, super knock) or lean combustion concepts which operate at the lean burn limit.

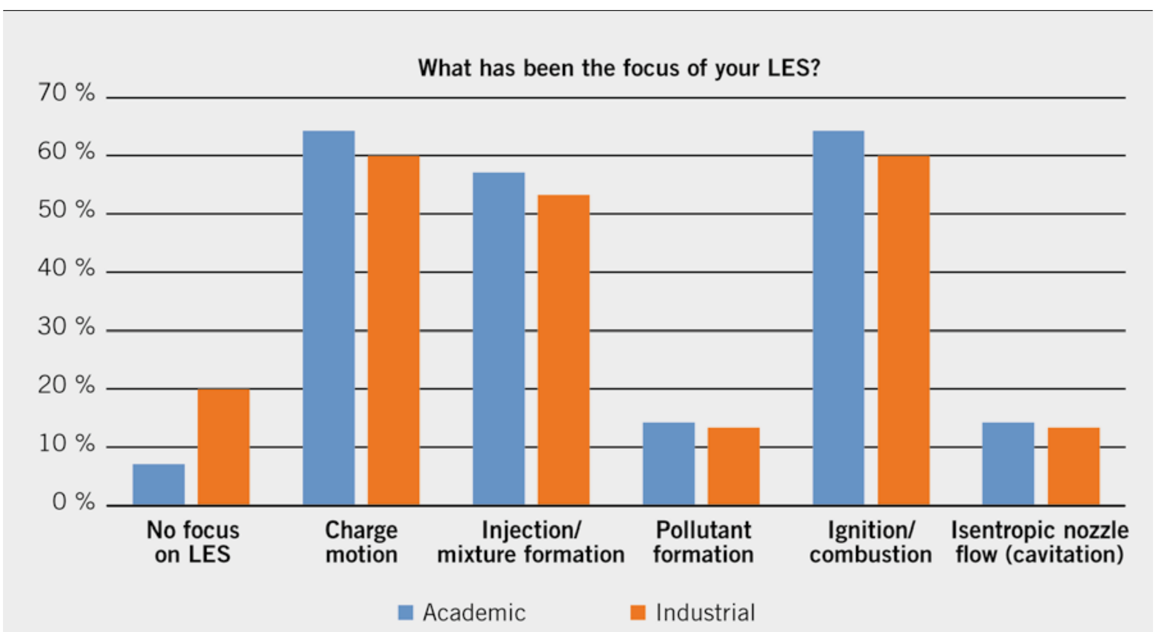


FIGURE 1 Focus of LES (© Technical University of Darmstadt)

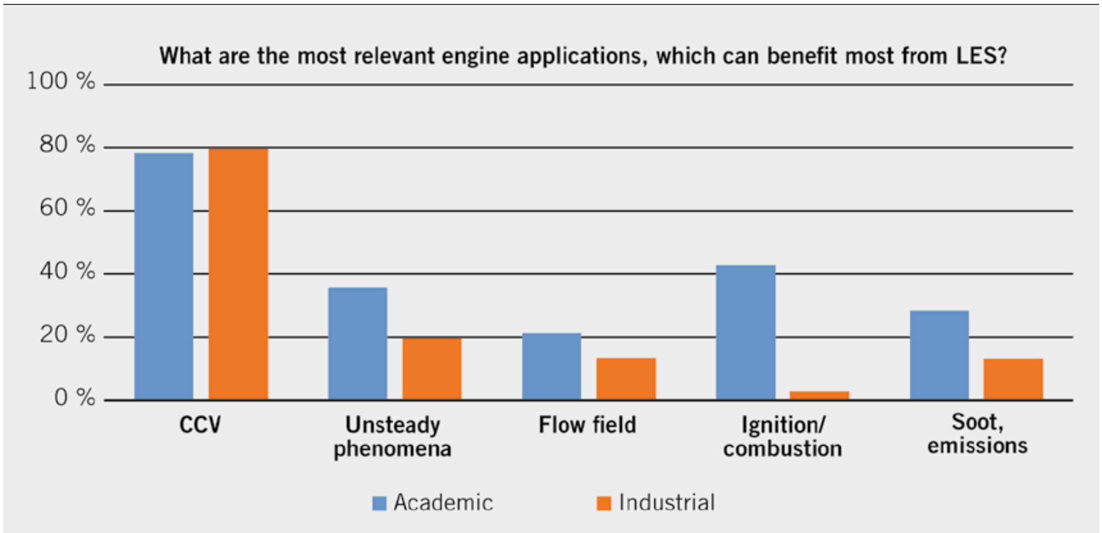


FIGURE 2 Advantages of LES compared to RANS simulation (© Technical University of Darmstadt)

Collaborations in the field of SRS between industry and academia, for example regarding flow-spray interaction analysis [6, 7], confirmed the high potential for improved understanding as well as impact on industrial development. Here, hybrid unsteady RANS (URANS)/LES or Very Large Eddy Simulation (VLES) are especially attractive due to their reduced computational requirements. However, it is not clear whether these approaches are suitable for such complex phenomena. Despite common interests it seems likely that the gap between university and applied research might further grow rather than diminish in the future. Thus, there is an urgent need for collaboration. Further, there is currently no knowledge transfer from high-resolution simulations towards hybrid or VLES model development. Therefore, the overarching goal of the FVV project 1215 was to propose a 3-D CFD simulation strategy roadmap.

2 RESULTS AND DISCUSSION

As a starting point and first part of the study, a detailed assessment and analysis of the current level of understanding of key engine-related processes was needed. Based on discussions with the FVV working group, nine topics were identified as most relevant for the SRS of engine processes: premixed flames, non-premixed flames/auto-ignition, multiphase modeling, pollutants including soot, near-wall modeling, spark ignition, knock, benchmark experiments for model validation, and quality criteria/quality assessment in internal combustion engines, respectively. The detailed topical reviews can be found in [8]. The second part of the study is a survey to assess the current use of LES in academia and industry, to identify future needs and critical issues.

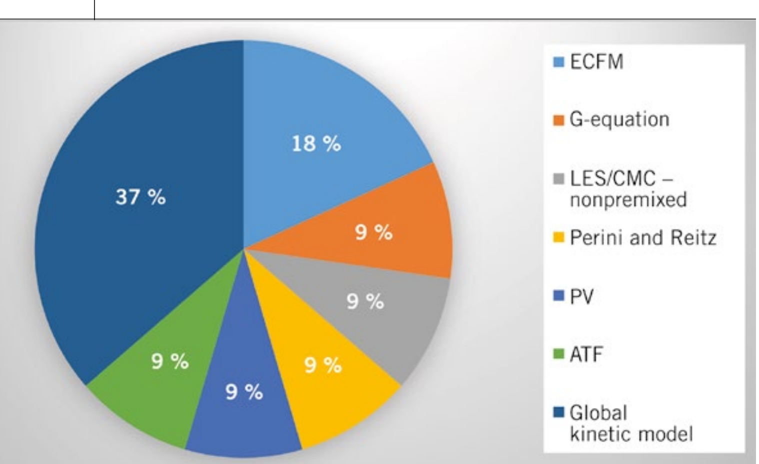


FIGURE 3 Combustion models applied (© Technical University of Darmstadt)

2.1 QUESTIONNAIRE: INTRODUCTION AND ORGANIZATION

The main aim of the FVV project was to develop a roadmap for 3-D CFD simulations in internal combustion engines using scale-resolved simulation methods. This roadmap should cover a period of 10 years and provide the basis for the FVV research and development strategy in this field. Besides the profound experience of the authors in this field, the research and development strategy should reflect and incorporate a broad range of opinions from relevant industrial and academic institutions alike. One well-accepted method of preventing the overemphasis of individual opinions and ensuring the incorporation of the communities involved is a well-designed questionnaire.

Following intense discussion and several iterations within the FVV working group and with selected members of the scientific community, a questionnaire was designed consisting of 29 identical questions for the academic and industrial communities. An additional 8 questions address the specific conditions of the industrial application of scale-resolved simulations. 14 of the academic partners (in some cases only one answer for multiple, closely collaborating institutions) and 15 of the industrial partners responded. The entire questionnaire is listed in the full report of this research project [8].

The questionnaire was subdivided into four parts. The first part is engaged in the current use of scale-resolving simulations and corresponding experience. The subjects addressed were general aspects such as the focus of LES, pre- and post-processing,

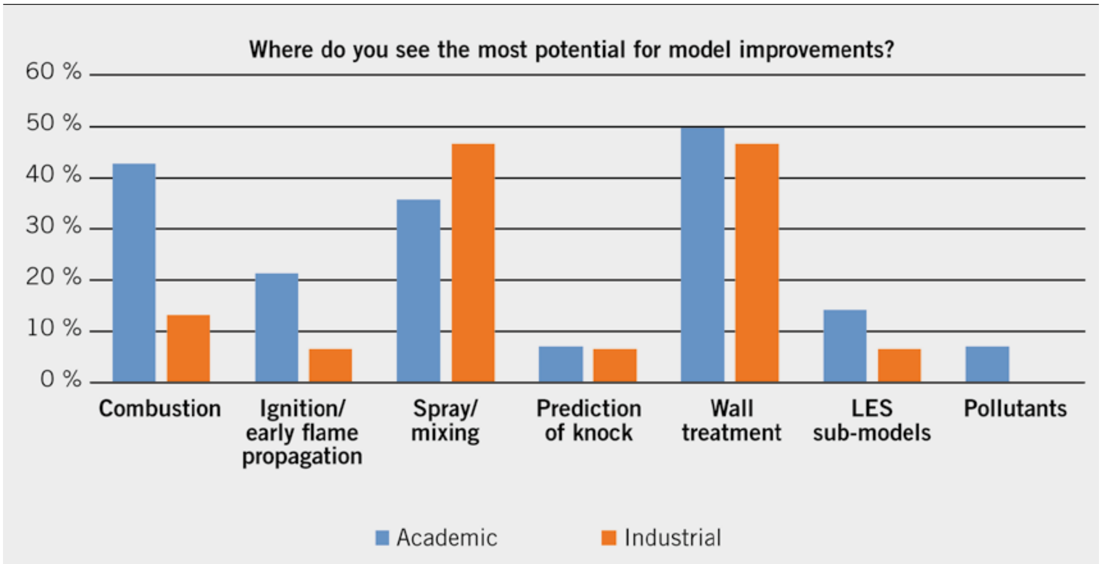


FIGURE 4 Topics where significant model improvements are required (© Technical University of Darmstadt)

solvers and applied models, for example subgrid-scale quantities, two-phase flows, combustion, ignition and numerical aspects. The second part aims at the relevant examples where RANS models fail and scale-resolving simulations offer advantages. The third part covers future topics, where industrial and scientific communities were asked to provide their opinions regarding perspective model development as well as shortcomings in the validation data and numerical methods. The identification of the weakest elements of the entire simulation framework was one key issue here. In the last part of the questionnaire, the next steps to establish LES for engine development in the industry were reviewed. These questions were only posed to the industrial partners and focused in particular on the availability of software and computing resources, their own experience and robust workflows.

2.2 QUESTIONNAIRE: SELECTED RESULTS

The most important findings of this survey are summarized in the following, with questions and answers using the acronym LES as a synonym for scale-resolving simulation.

LES is focusing on a wide range of applications in internal combustion engines. It was predominantly applied to predict the charge motion, injection and mixture formation, ignition and combustion. In contrast, LES has been less often used to predict pollutant formation and nozzle flow. Interestingly, the application range in academia and industry is nearly identical, **FIGURE 1**. Further, both academia and industry see LES as having clear advantages compared to RANS simulations for simulating cycle-to-cycle variation, unsteady phenomena and flow field prediction. In addition, academia sees benefits of LES regarding the simulation of ignition, combustion and the prediction of emissions, **FIGURE 2**. In general, applications were dominated by classical modeling approaches, for example the subgrid scale modeling by the Smagorinsky model, the two-phase flow modeling by classical Eulerian, Lagrangian or Eulerian-Eulerian models and combustion modeling by global kinetic descriptions. The combustion models applied are shown in **FIGURE 3** by way of example. As another important finding, both academia and industry see a distinct need for improving models in the near-wall region and describing the spray and mixing, **FIGURE 4**. Further, improvements in combustion, ignition and pollutant modeling are supported by the academic community, as these aspects are currently not in the focus of industrial LES applications, **FIGURE 2**. In addition to model improvement, both communities identified a strong need for reliable validation data under well-defined conditions. Both communities are interested in these data and are willing to participate in the definition of such experimental setups, **FIGURE 5**. As a last finding of the survey, the identification of challenges regarding industrial use of LES is pointed out here. Though computer resources and software are available, the industrial community identified necessary development activity to address excessively long turnaround times, the robustness of the method, the availability of workflows and suitable post-processing. As an example, **FIGURE 6** demonstrates the lack of availability of a robust work flow identified by 70 % of industrial users.

3 ROADMAP FOR SCALE-RESOLVING ENGINE SIMULATIONS

Based on the response to the questionnaire and the analysis of the literature, three major challenges can be identified: lack of validation data, transfer of sophisticated models to the context of internal combustion engines, and submodel development for phenomena with high technological relevance, respectively. Following, steps to establish LES in the industrial community are outlined.

3.1 LACK OF VALIDATION DATA

The most serious deficiency observed in this study is the lack of experimental validation data from engines with optical access in different operating conditions. This deficiency was addressed by both the academic and the industrial communities. Data is especially required on first-and second-order moments (mean, variance) of velocity, key scalar quantities such as concentrations and temperature, spray conditions, heat transfer under engine-like conditions, flame speed and charge motion. Global quantities such as the pressure are important but not sufficient. Based on the authors' experience, validation data has to satisfy condi-

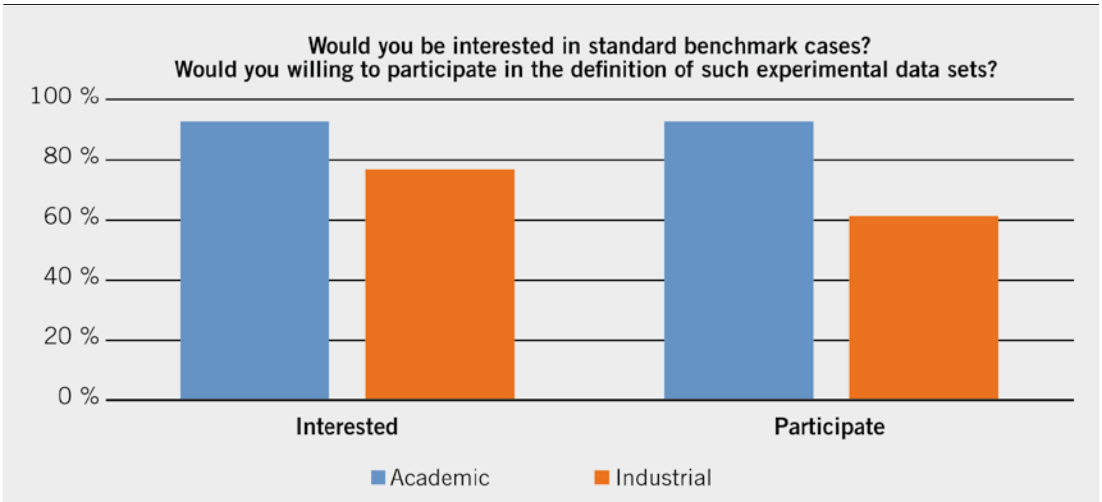


FIGURE 5 Relevance of benchmark experiments (© Technical University of Darmstadt)

tions like reliability, completeness and open access. That is to say, the measurement methods must be state-of-the-art, carefully designed by experienced researchers in the field, as exact as possible and require the indication of precision and accuracy errors. Further, the data must cover a sufficiently large parameter space. Finally, data must be made available to academic and industrial partners. In addition, reference simulation data on these validation experiments is needed as a digital twin. These simulations are indispensable as a reference for all future projects. This data should show the sensitivity of the results to initial and boundary conditions and to the grid resolution, plus the main model sensitivities. These two data sets – the experimental data and the reference simulation – have to be used as benchmarks for existing models and for defining deficiencies with respect to future model development.

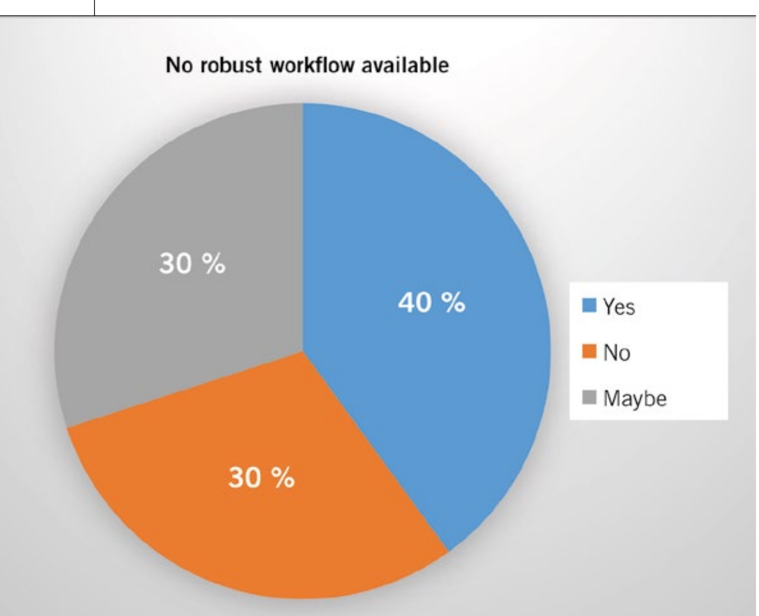


FIGURE 6 Deficiency in industrial application (© Technical University of Darmstadt)

3.2 TRANSFERRING SOPHISTICATED MODELS TO THE CONTEXT OF INTERNAL COMBUSTION ENGINES

As shown for example in **FIGURE 3**, relatively simple models are applied using LES for the context of internal combustion engines. However, it is undisputable that more sophisticated models are needed to predict the phenomena discussed in chapter 2. For example, predictions of pollutants or soot require an accurate modeling of the radical pool of a combustion system. Therefore, it is not possible to apply global kinetic models for this purpose, for instance.

A large number of sophisticated models is available in the scientific literature on combustion. These models have demonstrated superior properties in relatively simple environments such as laboratory flames or in the framework of different technologies such as gas turbines. Examples of these sophisticated models include carefully reduced models of the flamelet or REDIM family based on a limited number of control variables. It is a challenge for future research and development to modify these models and transfer them to the context of internal combustion engines. Again, the first step in dealing with this second challenge is the availability of reliable validation data in combination with reference simulations.

3.3 SUBMODEL DEVELOPMENT FOR PHENOMENA WITH HIGH TECHNOLOGICAL RELEVANCE

Driven by technological developments such as downsizing, increases in energy density or rigid environmental laws, the survey reveals the need for model development in a number of fields. The most important fields of future activity are:

- near-wall modeling with respect to the flow and scalar fields
- pollutant formation and heat transfer
- spray modeling and mixture formation in the combustion chamber, spray-wall interaction
- prediction of early flame kernel development (important for stability phenomena)
- prediction of knocking and detonation processes
- prediction of pollutant formation including soot, NO_x, CO and unburned hydrocarbons.

4 SUMMARY AND OUTLOOK

The results of a survey conducted by a joint research group from two departments of Technical University of Darmstadt as part of an FVV research project were summarized and analyzed in the article. The main goal of this survey was to assess the current level of LES usage in academia and industry and to identify future needs as well as critical issues. Based on this, a roadmap for 3-D CFD simulations in internal combustion engines using scale-resolving simulation methods was outlined. Regarding this, the lack of validation data for model development and validation was identified as a key issue. Further, collaborations between industry and academia confirmed the high potential and substantial impact on industrial development and should therefore be pursued in the future.

The survey shows that a number of actions will be necessary in the future to establish LES as an industrial design tool. The most important aspects are the methods' lack of robustness, excessively long simulation turnaround times, insufficient workflows and lack of experience in dealing with these methods. The authors are convinced that these deficiencies could be remedied by future collaboration projects with a code provider on one hand and experienced academic research institutions on the other.

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