Chapter 1

Introduction

Combustion processes play an important role in the life of mankind because they ensure its survival. These days the primary source of energy production is based on processes involving combustion. However, the composition of the source of energy is quite varied and is constantly subjected to change. While solid fuel was the important source of energy in 1994, today gas and heating oil cover our demand for energy by more than fifty percent. Additionally, as is well known, the ingredients of pollutants have also changed.

Another no less important factor is the wish of human beings to be mobile. This can be substantiated by the annual increase in road use and number of cars. However, at the same time, concerns with respect to health and the environment have also changed. Because of these concerns, laws in various jurisdictions were passed restricting the concentration of the major pollutants like CO, hydrogencarbons (HC), NO_x, SO_x and particles for Diesel and Otto engines.

In addition there is another problem which has had a bearing since the events of the 11th September 2001 when planes crashed into the World Trade Centre in New York. Scientists stressed that the condensation trails caused by planes had an effect which was not in consciousness of mankind. Previously it was impossible to prove this hypothesis because of the constant air–traffic. Only the prohibition of flights in the US proved this connection. The effect called global dimming can be defined as the decreasing intensity of sunlight reaching the surface of the earth. The first examination into this phenomenon was made by Gerry Stanhill in Israel who compared the radiation measurements of 1950 with those of 1980. Evaporimeters were used, establishing that the evaporation of water has decreased all over the world.

The reason for this development can be found with the smallest particles absorbing light. Condensation processes in the atmosphere also play an important role. Clouds were formed where the sunlight is reflected.

It follows that for a considerable time, a complicated connection between air pollution and the green house effect has existed. It can be stated that the decreasing intensity of sunlight is responsible for a cooling effect. On the other hand the green house effect means a saving of heat equal to the loss in temperature by global dimming resulting in the heating of the atmosphere. By destroing this balance the average temperature rises slowly. During the three days after 09.11. when no aircraft was flying in the USA, the radiation from the sun without condensation stripes in the air was measured by American scientists. The difference between the lowest and the highest temperature increased by more than $1°C$ [71].

This leads to the conclusion that the steps taken so far to minimize the green house effect are not enough. On the contrary, by reducing air pollution through the introduction of filters and exhaust systems this effect has increased leading to higher radiation by sun light and summers with higher temperatures.

In the last few years a number of laws was implemented to enforce the reduction of carbon dioxide, which is related to fuel consumption levels. The union of European automobile producers (ACEA) has committed itself to lowering fuel consumptions by about 25% with all cars sold by one producer in the period from 1995 to 2008. This means that in 2008 not more than 140 g/km carbon dioxide would be produced.

The statistics show that previous efforts only lead to a decrease of the pollutants but not to a decrease of CO_2.

To solve the problem of pollutants and carbon dioxide emissions an improved aftertreatment system and impetus are necessary. But this can only be achieved by a very thorough understanding of the physical and chemical processes involved. This must be combined with an improvement of the mathematical models in order for monitoring to be more exact. Basic physical laws without so–called "tuning parameters" must be applied. However, at the moment the presented models are not exact and in a lot of cases numerically motivated making the application of fitting parameters necessary.

The mathematical models of many real world phenomena are presented in the form of differential equations. Therefore numerical methods are important in order to analyse and improve automotive processes. The simulation with Computational Fluid Dynamics (CFD) can produce results related to, for example, flow fields, the distribution of temperature, the transformation of educts into products concerning chemical reactions as well as the generation of pollutants, and represents a transition technology between natural science and industrial application.

However, the physical complexity of the processes and the mathematical problems arising from the numerical transformation of the model equations raise the question of the importance of the quality and authenticity of the produced results. To explain this situation more carefully H. V. Cosey [56] discussed an example in which the pressure difference in a suction pipe behind a water turbine was calculated and compared with the results which were measured. It was determined that 41 results were obtained by applying different CFD-codes, different turbulence models at two working points of the system. Based on this 30% of the results differed by 10% of the experimental value. Most of the results did not coincide with the experimental result. Despite a simulation with the same code and the same turbulence model, but with different persons, there was a discrepancy among the results or with the experimental result.

Figure 1.1 shows the numerical treatment of a process simulation. First, the physical model is described by a system of differential equations. For the application of a numerical solution they must be separated and transformed to a system of algebraic equations which has to be solved. The result is the numerical solution. Furthermore, the type of mistake which can appear during each step can be seen.

One of the methods for studying the properties of differential equations is group analysis. Differential equations usually contain parameters or functions that are determined experimentally and hence are not strictly fixed. Group analysis not only helps to achieve exact solutions but also to classify the differential equations with respect to these arbitrary parameters and functions.

Figure 1.2 shows how symbolic and numerical calculations can work together. Here, the simulation starts with a physical model which is mapped in most cases onto a system of partial differential equations with initial and boundary conditions. The symbolic approach consists of an analysis of the algebraic and geometrical structure of the differential equations, for example, with point symmetries. By using an invariance criterion the original equations can be mapped into one which possesses one order of derivatives less than before. By solving this, analytically exact solutions can be produced, and asymptotes or singularities can be investigated ([151]).

The numerical way starts with the calculation of the Jacobian matrix which can be done in a symbolic or numerical way. This will be used to transform the original problem into difference equations, for which numerically approximated solutions for one initial and several boundary conditions can be found. By combining all methods presented above analytical methods can be used in order to minimize all mistakes except for those originating in the mathematical modelling. Accordingly it becomes possible to discuss the influence of approximations and assumptions made in order to develop the model equations.

The last decade has produced a high number of analytical results concerning hydrodynamics and flow processes which can be found, for example, in [4], [6], [12],[31],[37],[81],[87],[88],[100], [127], [128],[131],[132],[145],[156], [170],[189], [199],[212]. A lot of results also can be found in the proceedings of

- the International Conference of Symmetry in Nonlinear Mathematical Physics and
- the International Conference of Modern Group Analysis.

It is an interesting fact that almost nobody dealing with Computational Fluid Dynamics has neither known nor used these results so far except for the working groups leaded by N.

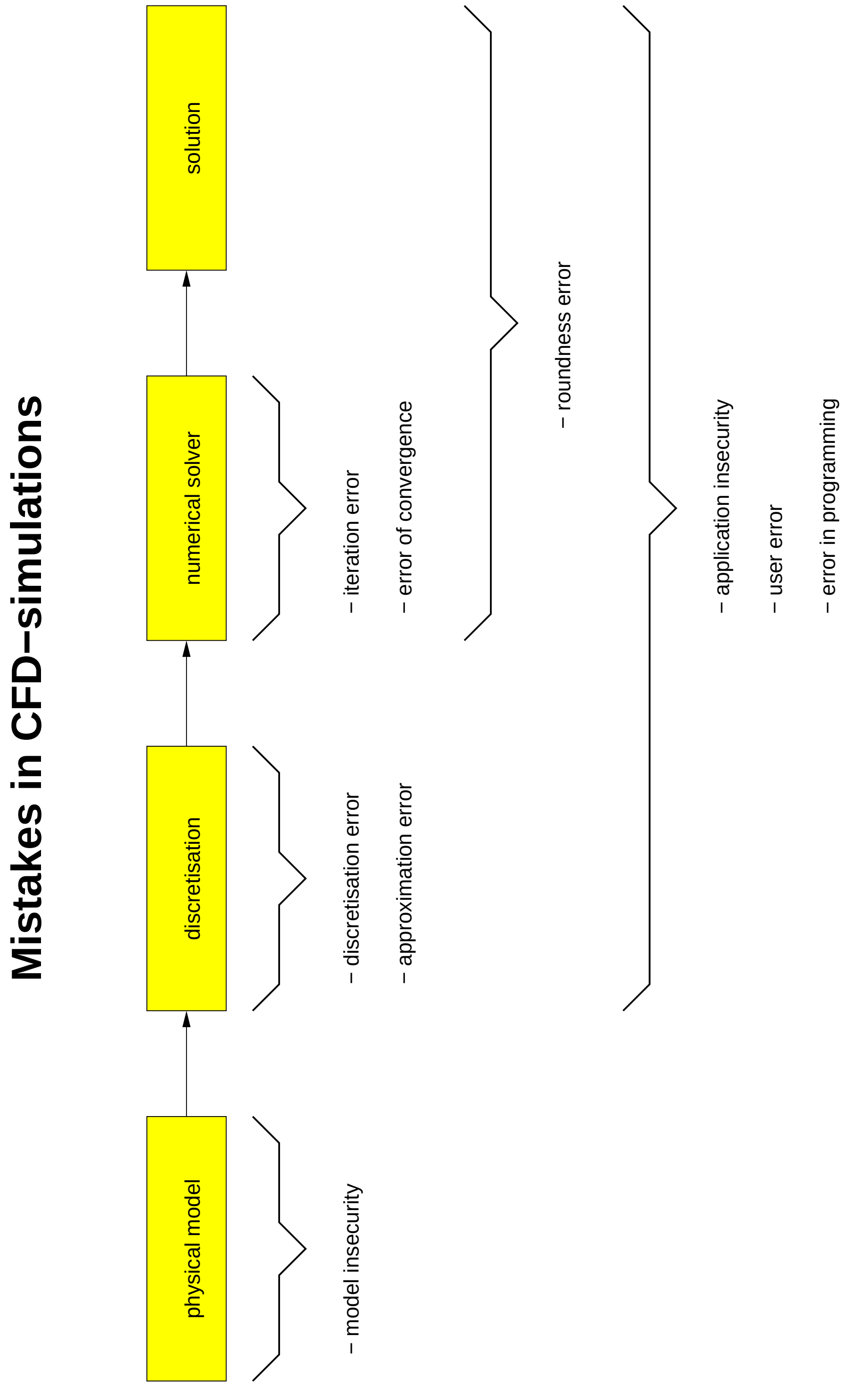

Figure 1.1: Mistakes in numerical simulations

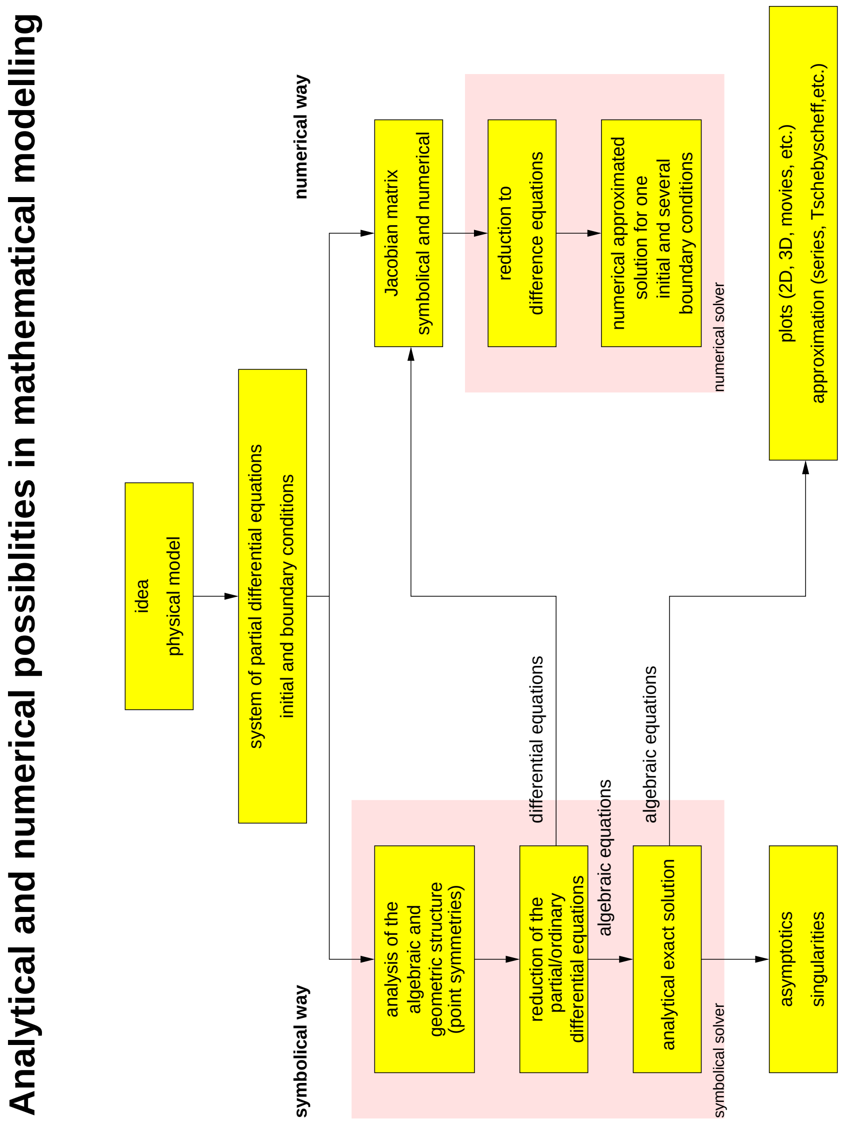

Figure 1.2: Overview of the connection between symbolical and numerical calculations

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So it seems to be necessary to demonstrate the applicability of group analysis in order to construct solutions, to classify equations concerning arbitrary parameters and functions and to create systems of model equations this way.

The concept for this thesis originates in the problems which occurred during the numerical treatment of the model equations describing such a catalytic converter. The used numerical algorithms did not converge, the calculations were unstable, and the computer programs were crashed. The idea was to solve a part of the original system by analytical methods in order to shorten the calculation time and to stabilize the computer codes.

The application of group theoretical methods is the main idea for the entire dissertation in order

- to show, that the application of this approach can produce solutions for industrially relevant problems related to exhaust systems.
- to apply the group theoretical approach to formulate and to develop mathematical models. This can, for example, be done by preliminary group classification introduced by Ovsiannikov ([151]). Experience shows, that most models were formulated by numerical motivation in order to run solution algorithms. When trying to apply analytical methods physically motivated models can be dealt with based on the physical properties of a system.
- to relate different equations. This leads to a reduction of physical effects to an important one, to make equations attractive for numerical calculations.

After presenting an overview of the detailed description relating to exhaust systems, investigations connected with Three-Way-Catalytic-Converters will be focused on. In chapter 4 a simple combustion model describing, for example, the transformation of fuel into a product via a one–step reaction is investigated.

- Equations for the concentration of the species and the temperature are considered by methods of group theory. Here, the possibilities to transform the basic equations into ordinary ones are demonstrated.
- The first method is a step–by–step method, where the number of independent variables are reduced by using two intermediate results.
- In contrast to this, the one–step method will be used in order to obtain an ordinary differential equation immediately.

In both cases the solutions are presented. Because of the fact that chemical reactions were taken into consideration the Arrhenius ansatz has to be used in order to describe the dependence of the reaction velocity on the temperature.

- It can also be shown that a substitution of this ansatz by the logistic one will produce quite the same so–called Lie algebra.

The second main part is devoted to the investigation of particulate traps. Therefore, the 5th chapter is dedicated to the consideration of a family of special mathematical models describing particle filters.

- Starting from a model described in literature it will be pointed out how it can be modified in order to introduce more realistic assumptions.

- The application of the group theoretical approach is discussed in order to construct solutions, to describe the main physical effects and to show how group analysis can be used to model physical effects. The basic description uses a flow model which only takes into account the flow in a channel, the flow through a porous medium, and the pressure difference between an inlet and outlet channel.

Finally, a conclusion will presented at the end of this work.