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Computer Modeling

4.1 COMBUSTION MODELING

There are many reasons to model a combustion system. The most obvious is to gain insight into a particular configuration in order to optimize it. Optimization means different things to different people. It may mean maximizing thermal efficiency, minimizing pollutant emissions, maximizing throughput, minimizing operating costs, or some combination of these. Another reason to model is in the development of new technologies. New geometries can be tested relatively quickly compared to building an entire combustion system. Ideally, modeling is done in conjunction with experimentation to validate a particular new design. Doing modeling first can save considerably on prototype development time and costs by eliminating particular designs without having actually to test them. However, in most cases it is not possible to eliminate prototype testing completely because of the uncertainty and limitations of combustion modeling, especially when it comes to new configurations that may never have been tried before.

Another reason for modeling is to aid in scaling systems to either larger or smaller throughputs. Simple velocity or residence time-scaling laws often do not apply to complicated combustion problems [1]. Modeling can be used for predictive purposes to test different scenarios that may be too risky or expensive to try in an existing operational industrial combustion system. For example, a glass producer may want to evaluate the impact of replacing an existing air preheat system with pure oxygen.

Another reason to do combustion modeling is to help determine the location for instrumentation. For example, models can be used to help decide where to locate thermocouples in a furnace wall at potential hot spots in order to prevent refractory damage. Although experiments are normally used to validate modeling results, the opposite may also be true. In industrial combustion systems, large-scale probes may be necessary due to water-cooling requirements for survivability. These large probes can cause significant disturbances in the process, which can be simulated with models. The model results can then be used to determine the relevance of experimental measurements. Models can also be used to simulate potentially dangerous conditions to assess the consequences in order to design the proper safety equipment and procedures.

A more recent use of computer modeling is for control of processes where the models are used to predict the results under the given conditions and then adjust the operating parameters to produce the desired results. This includes the use of artificial intelligence where the control system has a large database of past operating conditions and the associated results so that the system can then predict and adjust itself to meet new operating conditions. Examples include making adjustments as equipment ages and deteriorates as well as for new materials being processed. In the past, these adjustments would have been based on the knowledge and experience of the operators and were often trial-and-error. Newer control systems promise more sophisticated and systematic evaluation of the given operating conditions and desired results.

One of the risks of computer modeling is that too much faith may be placed in the results. Some tend to believe anything generated by a computer. However, if the computer models have not been properly validated, then the results may be highly suspect. For the foreseeable future, it is likely that models will continue to use various approximations (e.g., turbulence) in order to obtain solutions in a reasonable amount of time. Therefore, the user must exercise good judgment and not try to overextend the results beyond what is warranted. For example, in many cases models are very useful in predicting pollutant emission trends but are often very inaccurate in predicting the actual emissions. Knowledge of the model's capabilities helps one understand which results are more reliable and which ones are less reliable. The bulk fluid flow and heat transfer in a combustion system can usually be predicted with a high degree of accuracy, while the small-scale turbulence and trace species predictions may be less reliable. Therefore, it is recommended that computer modeling of combustion systems only be done by those who have been properly trained in that area.

Patankar and Spalding [2] note some of the important aspects of the problem statement for industrial combustion modeling problems:

- Geometry of the combustion chamber
- Fuel and air input conditions
- Thermal boundary conditions
- Thermodynamic, transport, radiative, and chemical–kinetic properties
- The desired outputs of models:
  velocity, temperature, composition, etc. throughout the chamber
  heat flux and temperature at the wall

Figure 4.1 shows a schematic of the elements of computational fluid dynamics (CFD) modeling [3].

A number of books have been written on the subject of modeling combustion processes. However, very few have specifically concerned large-scale industrial combustion systems. Khalil [4] presented modeling results for six large-scale industrial furnaces with published experimental data for comparison. These six studies involved burners with and without quarls (burner tiles); methane, natural gas, and propane fuels; firing rates ranging from 0.74 to 13 MW (2.5–44×10^6 Btu/hr); furnace lengths ranging from 4.5 to 11 m (15–36 ft); and swirl numbers ranging from 0 to 5.0. The modeling results using the k–ε turbulence model were in good agreement with the published experimental data. Oran and Boris [5] have edited a large book on combustion modeling. Part 1 of the book concerns modeling the chemistry of

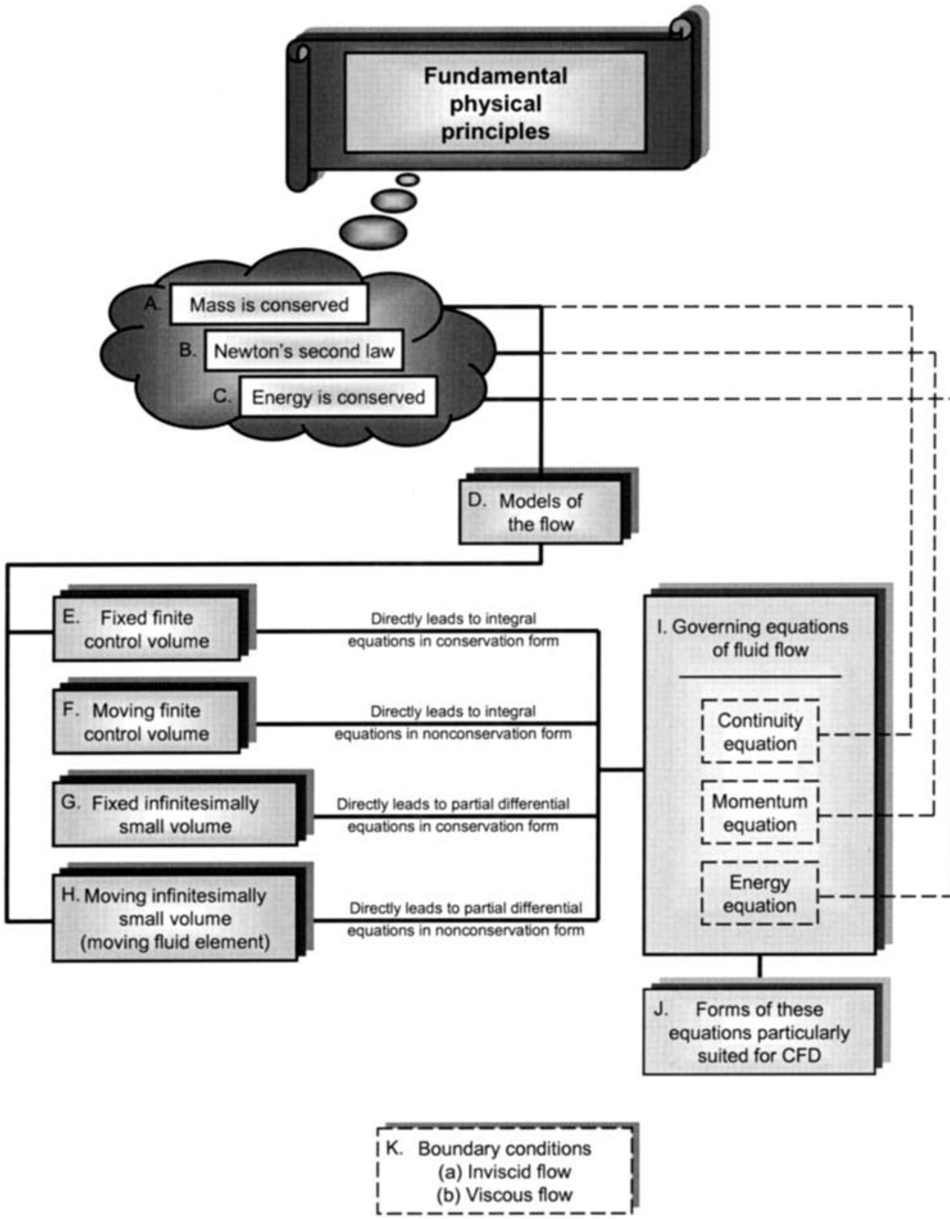

Figure 4.1 Elements of CFD modeling. (From Ref. 3. Courtesy of John Zink.)

combustion. Part 2 contains information on flames and flame structure. Part 3 is on high-speed reacting flows. Part 4 is humorously entitled "(Even More) Complex Combustion Systems" and has chapters on liquid and solid fuel combustion, as well as on pulse combustion. This book is more theoretical in nature and is intended for aerospace combustion. However, it does have some useful information pertinent to industrial combustion, which is referred to later in this chapter.