Accurate pollutant prediction with Equivalent reactor networks

by Fabio Villa
EnginSoft

The simulation of reacting flows is critical for developing competitive products in diverse industries: transport, power generation, materials processing, the chemical industry, and many others. Improving designs for these cases is difficult because they often consist of systems with complex geometries, boundary conditions, and physics, including large networks of chemically reacting species, turbulence, and radiation.

Using the appropriate fuel model enables exploratory design particularly to predict:

- Ignition delay and fuel efficiency
- The effects of varying fuel composition
- Emissions, including soot particle number and size
- Undesired auto-ignition effects (such as knocking, reliability, noise, and operability limits)

The more accurate the fuel model, the more realistically the fuel performance of your design can be predicted. Ansys Chemkin couples Multiphysics simulations incorporating advanced physical models with an advanced chemical solver to provide full simulation capabilities for reacting flows. Many tools have recently been included in the Ansys CFD enterprise license.

Ansys Chemkin

Depending on the complexity and chemical detail of the combustor application, there are several reactive CFD methods to choose from:

- Direct integration
- Table look-up with CFD progress variables
- Equivalent reactor network

The first two methods use a classical (3D) CFD application solver (such as Ansys Fluent/CFX) and are better choices if geometric details are to be included in the simulation, but may be expensive in terms of CPU time if a detailed mechanism is included, or if an extensive design-of-experiments campaign is to be created.

In these cases, equivalent reactor networks (ERNs Fig. 1) which mimic flow but allow for fully detailed chemistry are a viable method that combines high-fidelity flow simulation with detailed kinetics (Fig. 2). Manually generated ERNs, which are linked 0-D models, have long been used to provide high fidelity.

Ansys Chemkin is a standard for solving complex chemical kinetics and surface chemical reaction problems used in the conceptual development of combustion systems. It has evolved since its inception as the Sandia National Laboratory combustion kinetic code (Chemkin II) and has been extensively validated over several decades and is frequently cited in peer-reviewed technical journals.
Engineers can quickly explore the impact of design variables on performance, pollutant emissions, and flame extinction by simulating real-world combustors, burners, and chemical reactors, permitting emissions to be predicted most efficiently with detailed chemistry in minutes.

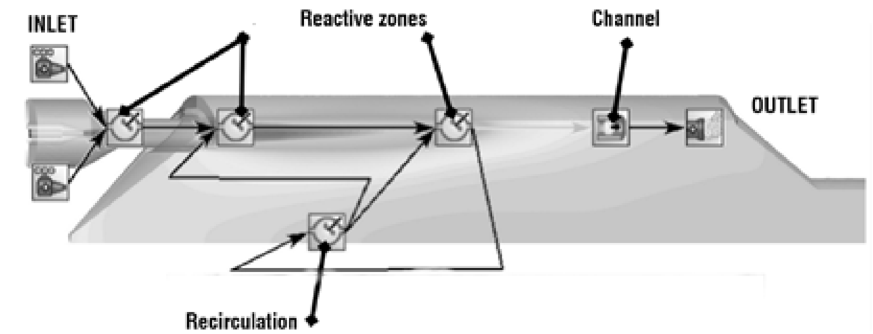

Fig. 1. Equivalent Reactor Networks.

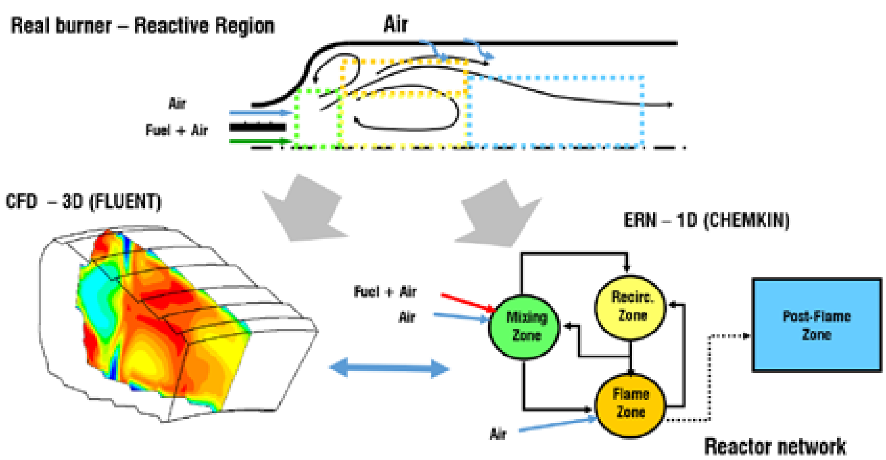

Fig. 2. Burner simulation to link detailed combustion chemistry and CFD.

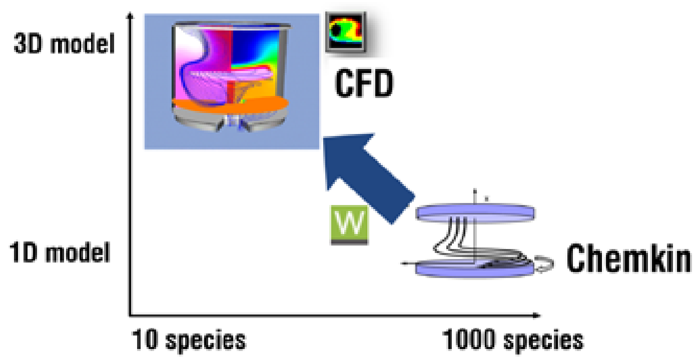

Fig. 3. Standard mechanism reduction process in Ansys CFD.

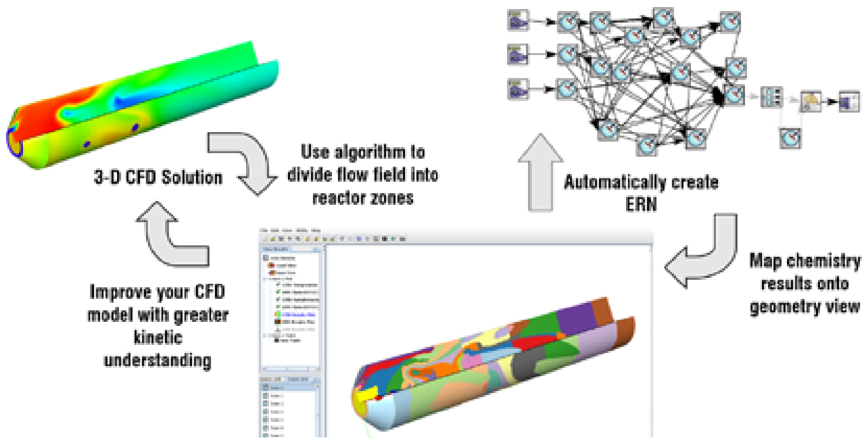

Fig. 4. Automatic generation of an ERN from 3D CFD results using Energico.

ERN simulations yield fast and accurate emissions and stability predictions, particularly for applications that may be challenging to conduct directly in CFD due to complicated flows. Another advantage over other combustion methods is that you can quickly explore operating conditions, fuel effects, and fuel load without having to run large CFD simulations every time, saving design time.

Ansys Model Fuel Library - CFD

A fuel model is defined by two components: its composition and its chemical kinetics or 'mechanism'. The Ansys Model Fuel Library (MFL) is a source of over 65 well-validated fuel mechanisms (H2 is included) and is the result of a ten-year collaboration with industry, academia, and national laboratories.

Compared to public data, it provides consistent rules for reaction rates and validated fuel-blending behaviour. Detailed soot kinetics have been validated from scratch, ensuring accuracy in predicting the multistage emission formation process.

The generation of a surrogate fuel from the MFL mechanism allows designers to accurately match fuel properties including chemical class, heating value, octane/cetane number, H/C ratio, boiling points, and soot threshold index. Using raw data from the public domain may not be as predictive.

Ansys Reaction Workbench

A master chemical mechanism, directly from the model fuel library, may be too complex to be used in a CFD simulation. However, a manual reduction of such a mechanism is not simple and may provide undesirable results.

One way to avoid oversimplification of the chemistry is through automated chemistry reduction, which converts the detailed fuel model to a smaller size suitable for calculation, while maintaining the accuracy required for specific engine or fuel conditions or key predictions of engine performance (Fig. 3). Ansys Chemkin-Pro Reaction Workbench for example automatically generates the smallest skeletal mechanism that meets selected specifications, such as target parameters and acceptable error tolerances.

Ansys Energico

Manually-generated equivalent reactor networks (ERNs) for a combustor are also commonly difficult and error-prone. Today's advanced specialized software tools allow designers to quickly explore ERN strategies and sensitivities, resulting in fast, accurate and predictive system models.

For example, Ansys Energico simulator accelerates combustion system design and allows detailed chemistry to be used even if you do not have an indepth understanding of complex kinetics (Fig. 4).

The resulting ERNs simplify design exploration easier such as setting up automated parameter studies for variations in important operating conditions. The method is appropriate for the design of furnaces, burners, gas turbines, boilers, and flares. It is a quick way to include better chemistry without compromising CFD quality.

Conclusion

The incorporation of detailed kinetics into CFD simulation is the baseline for any recent application in the combustion field. The correct combination of methodology described here, and technology enables you to predict important parameters such as fuel effects, ignition, combustion phase, and emissions.

Ansys simulation tools eliminate the traditional trade-off between accuracy and speed by using the right methods and the right chemistry for your specific application.

For more information:
Fabio Villa - EnginSoft
f.villa@enginsoft.com