reaction DESIGN

ENERGICO

Predicting Emissions from Chemical Processing with ENERGICO

Faster computers and better knowledge of fluid dynamics and combustion chemistry have allowed CFD to become integrated into the combustor design process and to provide valuable design assistance. However, modern CFD codes provide limited chemistry information. While today's computers are fast enough to handle chemical process design models with several million cells, they are still not fast enough to incorporate all of the detailed combustion chemistry of the fuel. Consequently, applying detailed fuel chemistry in combustion simulation requires a simplification of the geometry.

Representing the combustor with a series of idealized reactors allows use of detailed chemistry with a reasonable amount of computational time. ENERGICO automatically converts a complex chemical process geometry into an Equivalent Reactor Network (ERN). Once the ERN is created, a fully detailed chemical mechanism can be used to provide an understanding of combustion performance and emissions such as NO_x, CO and Unburned Hydrocarbons (UHC).

Setting Up in ENERGICO

ENERGICO reads in the reacting flow CFD solution of a generic chemical process burner (Figure 1). A series of filters are applied to the variables in the CFD solution to divide the process geometry into regions that have similar conditions that are important for the desired results (e.g., temperature, oxygen concentration, fuel concentration when looking at NO_x emissions). A set of these filters comprises an ERN algorithm. ENERGICO can also automatically apply previously developed ERN algorithms to help save time and eliminate errors.

ENERGICO allows each reactor zone to be defined as either a Perfectly Stirred Reactor (PSR) with the temperature fixed to the average temperature in the CFD, a PSR with the energy equation turned on, or a Plug Flow Reactor (PFR). ENERGICO then creates the reactor network automatically and solves it using the detailed chemistry mechanism.

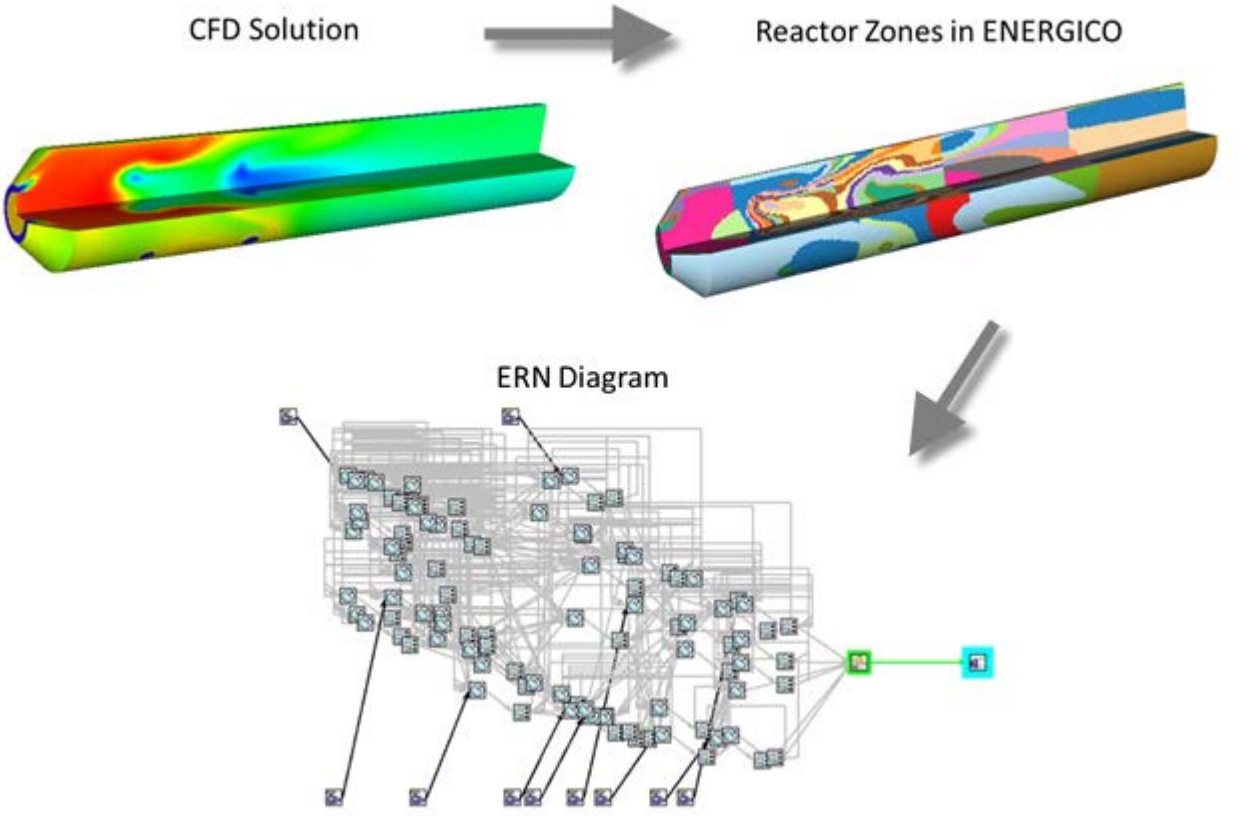

Figure 1. ENERGICO workflow starting from a CFD solution, dividing the chemical process into Zones that become reactors in the ERN.

Results

Results for CO, NO, NO_2 and UHC emissions at the exit are presented in a table. They also can be plotted on top of the chemical process geometry. The high NO_x concentration occurs in the dome region of this chemical process burner (Figure 2). As ENERGICO uses the full detailed mechanism, it is also possible to plot the NO_x formation rate and discern if the NO_x is thermal or non-thermal NO_x.

The CO emissions show high concentrations in the dome regions as expected from the primary combustion of the fuel (Figure 3). It is helpful to plot the CO emissions at the exit of the chemical process to see where peaks of CO are located. The peak in CO concentration can then be traced back upstream to see if it is occurring because the flame is too long or quenching along the walls from cooling flows.

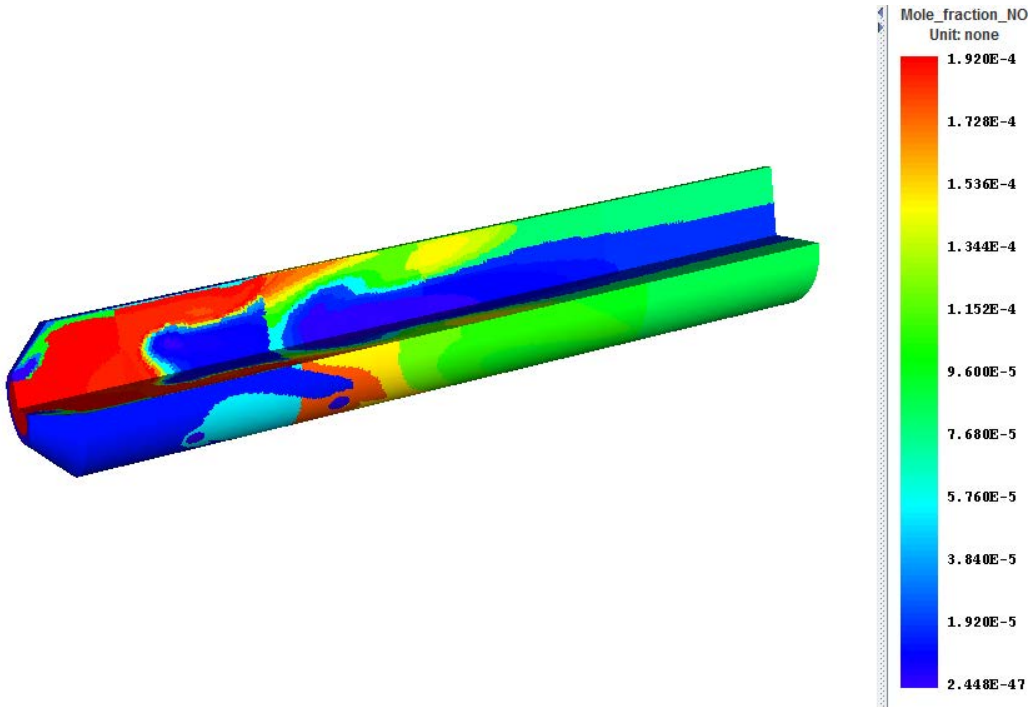

Figure 2. NO emissions on the chemical process.

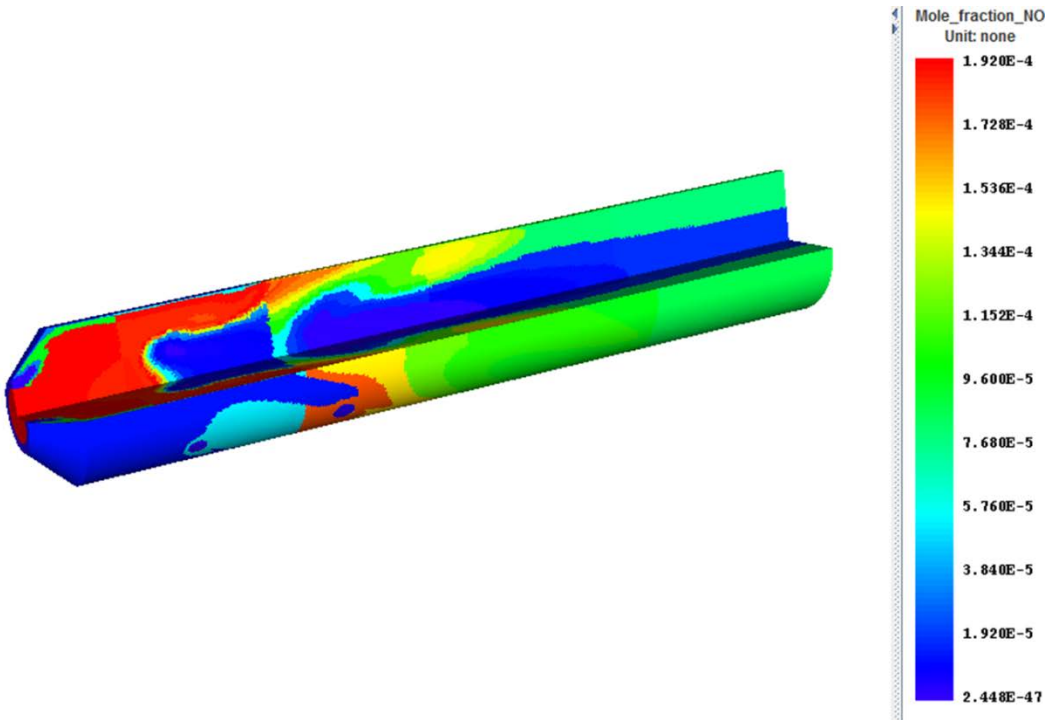

Figure 3. CO emissions on the chemical process.