ENERGICO can be used to simulate liquid fueled combustion systems, such as aircraft gas turbines, boilers, furnaces and rocket engines. Usage of Liquid fuels with ENERGICO requires additional data from the CFD solution to define the spray mass source. Modern CFD simulations are capable of resolving complex combustor geometries and of producing complex flow and temperature fields, but they provide only limited chemistry information. In particular, such simulations do not incorporate the level of detail in the fuel combustion chemistry that is required for accurate emissions predictions.

ENERGICO creates Equivalent Reactor Network (ERN) models from the CFD solution and has been shown to accurately predict emissions for gaseous-fueled, continuous-combustion systems, using fully detailed chemistry. Liquid-fueled combustion presents similar simulation challenges for emissions predictions as in the case of gaseous fuels but with the added complexity of spray modeling in the CFD and even more complex chemical kinetics.

**Setting Up in ENERGICO**

ENERGICO predicts pollutant species such as NO\textsubscript{x}, CO and UHC and presents the results in terms of Emissions Indices, which are mass measurements of corresponding species normalized by the fuel mass input (i.e., grams of pollutant per kilogram of fuel). High-power conditions typically produce higher levels of NO\textsubscript{x} and very low emissions indices for CO and UHC. On the other hand, low-power emissions performance concerns are focused on CO and UHC, due to the lower temperature, lower pressure and reduced mixing in the combustor.

The first step in using ENERGICO to simulate emissions performance is to read in the CFD solution (Figure 1) and to define a detailed chemistry set that will be used in the ERN solution. For CFD cases involving liquid fuel injection, or discrete phase models, a source term variable may be supplied for each species in the CFD system. The source term variable should contain the mass flow rate of the given CFD species variable originating in each cell due to vaporization of the discrete phase. ENERGICO automatically creates an ERN from a reacting-flow CFD solution, using algorithms specifically designed for accurate NO\textsubscript{x}, CO and unburned hydrocarbon (UHC) emissions simulation (Figure 2).
After creating the ERN with ENERGICO, CHEMKIN-PRO displays the ERN and all the information regarding the individual reactors and the links between them (Figure 3). At this point, the ERN can either be solved using the full detailed chemistry solution for the nominal conditions, or a Parameter Study can set up on the ERN to introduce changes for further exploration of the system design.
Results

The resulting ERN can then be solved with detailed chemical mechanisms for the fuel with accurate simulations of emissions of trace species such as NO\textsubscript{x}, CO and UHC. The results of the ERN can also be overlaid on the combustor geometry, allowing the user to visualize where each reactor’s results are within the combustor and providing guidance on how to optimize the combustor design for performance and emissions targets.