Predicting Emissions for Liquid Fueled Combustors with ENERGICO

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Overview

This application note describes how to use the ENERGICO Simulation Package to simulate liquid fueled combustion systems, such as aircraft gas turbines, boilers, furnaces and rocket engines. There are some differences in the set-up requirements for liquid fuel combustion compared to gaseous fuel combustion, when using equivalent reactor networks (ERNs) in ENERGICO. Specifically, liquid fuels require additional data from the CFD solution to define the spray mass source. Also, we recommend the use of some additional, geometry- based filters in the algorithm that defines the ERN to isolate regions more effectively for these types of combustors. . Finally, a liquid fuel requires a different fuel surrogate than natural gas, which means a different detailed chemical mechanism that is appropriate for resolving the combustion behavior of that fuel surrogate under liquid-fuel combustor conditions ENERGICO can be used with liquid fueled combustion systems to predict NOx, CO and unburned hydrocarbons (UHC) over the power range of the combustor.

This application note supplements the ***Predicting Emissions with Auto-generated Equivalent Reactor Networks*** application note by addressing the specific additional inputs, reaction mechanism, and ERN filtering approaches that are required when modeling liquid-fueled systems.

Challenges in Liquid Fuel Combustion Simulations

The use of Computational Fluid Dynamics (CFD) to model combustion has become standard practice in the industry. Modern CFD simulations are capable of resolving complex combustor geometries and of producing complex flowand temperaturefields, 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 but with the added complexity of spray modeling in the CFD and even more complex chemical kinetics.

Designers of liquid fueled combustion systems face different challenges than those designing gaseous fueled systems. For example, liquid-fueled gas turbines are used in aviation where there are much greater demands on the engine than in gas turbines targeted at power generation, including requirements to operate over a much wider power range. Aircraft gas-turbine engines are also to different regulations than those that apply to power-producing, gaseous-fueled engines. The

International Civil Aviation Organization (ICAO) regulates global engine emissions for NO_x, CO, UHC and particulates (i.e., soot). Pollutant species such as NO_x, CO and UHC are measured in terms of Emissions Indices, which are mass measurements normalized by the fuel mass input (i.e., grams of pollutant per kg of fuel). The ICAO estimates an emissions metric from a Take-Off and Landing cycle. This is done by first measuring the emissions at 4 power points: 7%, 30%, 85% and 100% power. These power points represent idle, approach, climb-out and take-off power settings, respectively.

High power conditions typically produce higher levels of NO_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.

Figure 1. CFD Solution of a Gas Turbine Combustor

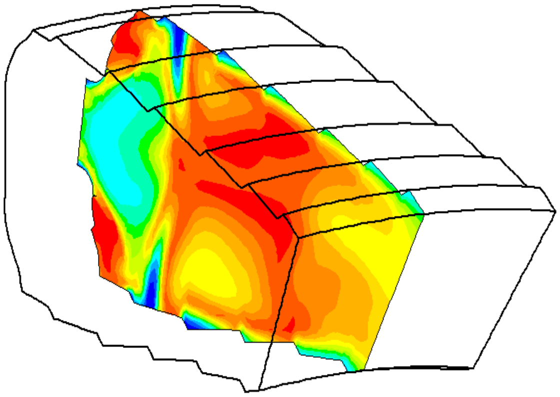
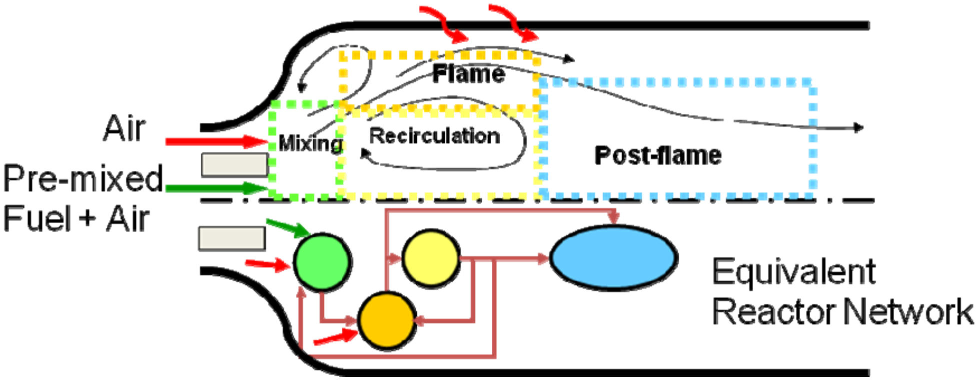


Figure 2. Equivalent Reactor Network Derived from CFD Solution



Producing ENERGICO Input Files for Liquid Fueled Systems

The CFD solution file format expected by ENERGICO is a CGNS file, which is a solution-export option supported by all major CFD vendors (see Figure 1). For Liquid-fueled system, it is important to include in this export the information from the CFD solution that provides the locations and the amounts of the fuel vapor that result from the CFD spray/vaporization model. This is typically in the form of discrete-phase mass source terms in the CFD that are selected for output to the CGNS file. The parameters required for export in liquid fueled systems to the CGNS file are (where the bolded item is the additional need for liquid-fueled systems):

- X, Y, Z Coordinate information
- *Mass* fractions of all species
- Absolute Pressure (or Static Pressure)
- Static Temperature
- Density
- X Velocity
- Y Velocity
- Z Velocity
- Turbulent Kinetic Energy (k)
- Turbulent Dissipation Rate (ε)
- **Mass source from the fuel-spray model for each fuel species (kg/sec)**

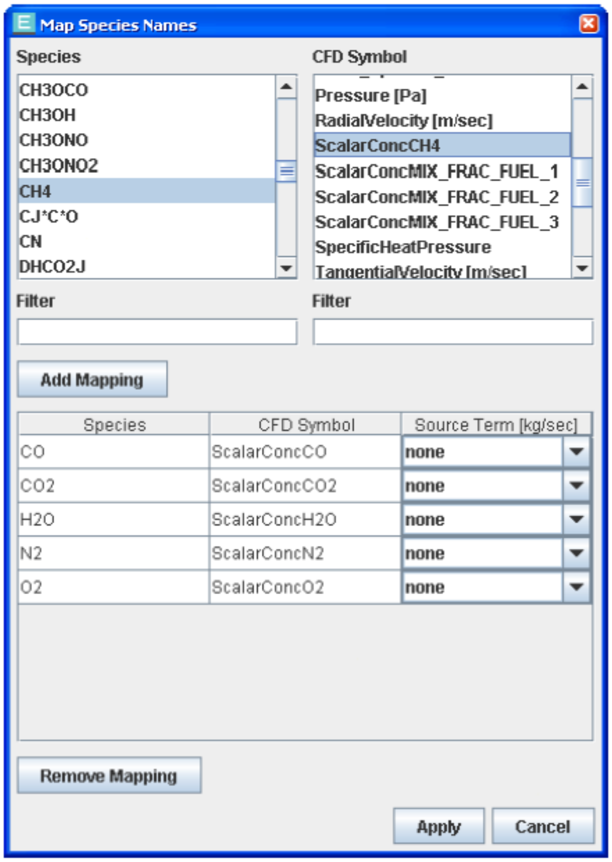
All of these values are required at each cell-center location. It is important to note that ENERGICO tracks the gaseous flow and reactions that occur in the combustion device. The CFD software has spray models to account for the distribution and evaporation of the liquid fuel to define how much vapor is delivered at specific locations in the combustor. ENERGICO takes this spray-vapor distribution as an input and models the gaseous reacting-flow system. ENERGICO assumes that the vaporization of the fuel is adequately modeled in the CFD simulation.

Initial Model Setup in ENERGICO

The ENERGICO Simulation Package automatically creates an ERN from a reacting-flow CFD solution, using algorithms specifically designed for accurate NO_x, CO and unburned hydrocarbon (UHC) emissions simulation. The first step in using ENERGICO to simulate emissions performance is to read in the CFD solution and to define the 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. The only non-zero terms are usually for the fuel species. When present in the CGNS file, this information is used to produce additional sources represented as inlets in the generated ERN.

Figure 3: Map Species dialog box



Species	CFD Symbol	Source Term [kg/sec]
CO	ScalarConcCO	none
CO2	ScalarConcCO2	none
H2O	ScalarConcH2O	none
N2	ScalarConcN2	none
O2	ScalarConcO2	none

First map the species names in the detailed mechanisms to the species identified in the CFD symbols list, for all CFD species (scalars), as shown in **Error! Reference source not found.**. To identify a source term for a fuel species, use the Source Term pull-down list in the right column of the Mapped-Species table in the lower half of the Map Species Names dialog (see **Error! Reference source not found.**). From the pull-down list, select the CFD variable name that represents the discrete-phase mass source term that corresponds to that species. In some cases this will be auto-mapped, if the CFD species name is included in the CFD source-variable name.

Specifying Fuel Properties for Discrete-phase Source Terms:

For fixed-temperature ERNs in ENERGICO, no further information is required. However, in the case where the energy equation will be solved within the ERN, more information about the liquid-fuel properties and injection conditions are needed to provide an accounting of heat transfer required to bring the fuel up to the boiling point at the conditions in the combustor. Use the **Spray Source Properties** panel to specify the properties of the liquid-phase fuel species, which allow an accurate energy balance for reactor networks that employ the energy-equation option.

This set of properties should be specified for each fuel species when the energy equation is used in the ERN calculations:

- **B.P. @ Operating Pressure [K]**

  This specifies the **boiling point** of the fuel at the **operating pressure** of the combustor. The temperature specified here is used as the inlet temperature for source term inlets appearing in the ERN.

The following three properties are optional but are recommended to obtain the most accurate energy balance:

- **H.O.V. [kJ/kg]**

  This is the heat of vaporization of the liquid fuel species. Specifying a value will add a heat-loss term to reactors with inlets derived from the liquid-fuel source terms, to account for the heat lost during vaporization of the fuel.

- **Inlet Temperature [K]**

  This is the inlet temperature of the liquid-phase fuel in the CFD model. An additional heat-loss term is added to reactors with inlets derived from the liquid-fuel source terms, to account for heating of the fuel from this temperature to the boiling point.

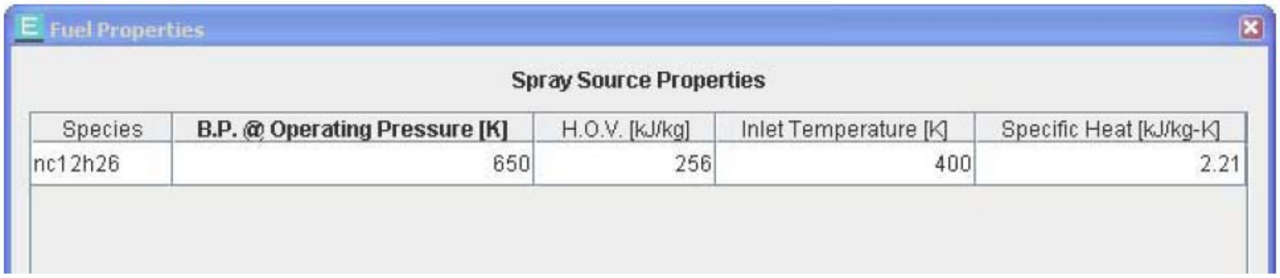
- **Specific Heat [kJ/kg-K]**

  This is the specific heat used to calculate the energy that is lost to heat the fuel from the liquid inlet temperature to the boiling point.

Once ENERGICO has read in the CGNS file, an automatic mapping occurs to associate species and variable names used in the CFD simulation to those that will be used by ENERGICO. You can verify this mapping and make any corrections or additions, in case non-standard names are used in the CFD simulation. The next step is to identify which boundaries are associated with which boundary types (i.e., inlet, outlet, wall, or periodic) for each of the boundary regions found in the CFD solution. The periodicity parameters for any periodic boundaries are then defined, thus completing the model setup in ENERGICO.

Specifying the liquid fuel detailed chemical mechanism: The detailed chemistry set can be any CHEMKIN-compatible chemistry description for combustion of any fuel. There is no limit on the number of species or reactions that can be included in the chemistry set.

Figure 4: Spray Source Properties panel



Spray Source Properties

Species	B.P. @ Operating Pressure [K]	H.O.V. [kJ/kg]	Inlet Temperature [K]	Specific Heat [kJ/kg-K]
nc12h26	650	256	400	2.21

For liquid fuel combustors, a 3-component surrogate mechanism for Fischer-Tropsch fuels NOx formation is packaged for convenience with ENERGICO. [NASA report, the Turbo Expo paper, and a Western States Combustion Institute paper]

Once the Model Setup is complete, the next step towards emissions predictions is to employ an algorithm to divide the combustor flow field into zones that will form the basis of the ERN.

Creating a Reactor Network from a Liquid Fuel CFD Solution

The first step in creating the ERN from the CFD solution is to divide the combustor flow field into zones that will then become reactors linked together to form the ERN.

Liquid fuel reactor network algorithms benefit from a “blocking” approach where the combustor domain is first sliced along its geometry to subdivide regions for further ERN filters. This helps minimize unintentional mixing of downstream conditions with upstream flow. Once the geometry filter has been applied, additional filters can be superimposed. Such additional filters typically are Oxygen and Temperature or Axial Velocity and Temperature, depending on the overall objectives for the ERN simulation.

Once the Zones have been created and the reactor types have been defined, users can create and view the ERN. ENERGICO seamlessly links with the CHEMKIN-PRO software package to view and solve the ERN. Clicking on “Create and View ERN” in ENERGICO, immediately launches CHEMKIN-PRO and the ERN is displayed (see Figure 5). ENERGICO performs all of the necessary calculations to determine mass fluxes across the zone boundaries and constructs the ERN with an accurate accounting of all the forward and recirculating flows between zones.

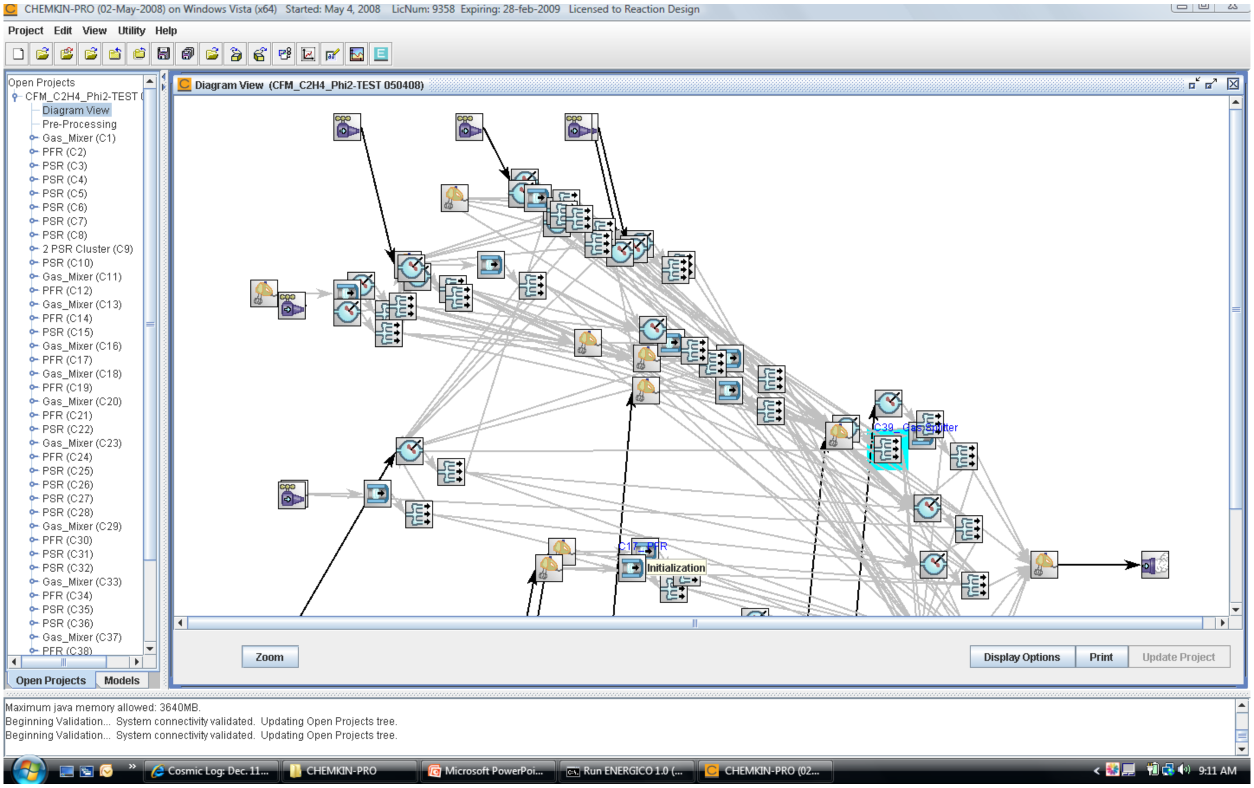
Reviewing Results with ENERGICO

After creating the ERN with ENERGICO, the CHEMKIN-PRO software package displays the ERN and all the information regarding the individual reactors and the links between them. 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 explororation of the system design.

Once the ERN is solved using the detailed chemical mechanism, you post-process the results and they are overlaid upon the combustor geometry in ENERGICO. There you can create tables for the exit emissions in Emissions Indices for NOx, CO and UHC. You can also create tables of the local species concentrations and temperatures for the individual reactors.

Important points about Emissions Index results: The Emissions Index (EI) is a method of reporting emissions that are normalized based on the fuel input. The typical units for an emissions index are grams of pollutant per kg of fuel. When using EI, you do not need to correct for oxygen content as you do with power producing turbines or boilers. However, you do need to be careful to use the correct mass basis for the EI calculation. This is particularly true for EINOx and EIUHC calculations where NO_x and UHC emissions contain species with different molecular weights, unlike EICO. ENERGICO reports the EINOx and EIUHC following the convention called for by the ICAO. EINOx is reported on a NO_2 weight basis and EIUHC is reported on a Carbon atom basis.

Figure 5. Viewing and Solving ERN in CHEMKIN-PRO



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Maximum java memory allowed: 3640MB.
Beginning Validation...  System connectivity validated.  Updating Open Projects tree.
Beginning Validation...  System connectivity validated.  Updating Open Projects tree.
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Summary

This application note describes how ENERGICO can be used to develop Equivalent Reactor Networks (ERNs) directly from liquid fueled reacting-flow CFD 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_x, CO and UHC. The results of the ERN can also be overlaid upon the combustor geometry allowing the user visualization of where each reactor's results are within the combustor, providing guidance on how to optimize the combustor design for performance and emissions targets.

About Reaction Design

Reaction Design helps transportation manufacturers and energy companies rapidly achieve their Clean Technology goals by automating the analysis of chemical processes via simulation and modeling solutions. Reaction Design is the exclusive developer and distributor of CHEMKIN, the *de facto* standard for modeling gas-phase and surface chemistry, providing engineers ultra-fast access to reliable answers that save time and money in the development process. Reaction Design's ENERGICO product brings accurate chemistry simulation to combustion systems using automated reactor network analysis. Reaction Design also offers the CHEMKIN-CFD software module, which brings detailed kinetics modeling to other engineering applications, such as Computational Fluid Dynamics (CFD) programs. Reaction Design's world-class engineers, chemists and programmers have expertise that spans multi-scale engineering from the molecule to the production plant. Reaction Design serves more than 350 customers in the commercial, government and academic markets.

Reaction Design can be found online at www.reactiondesign.com.