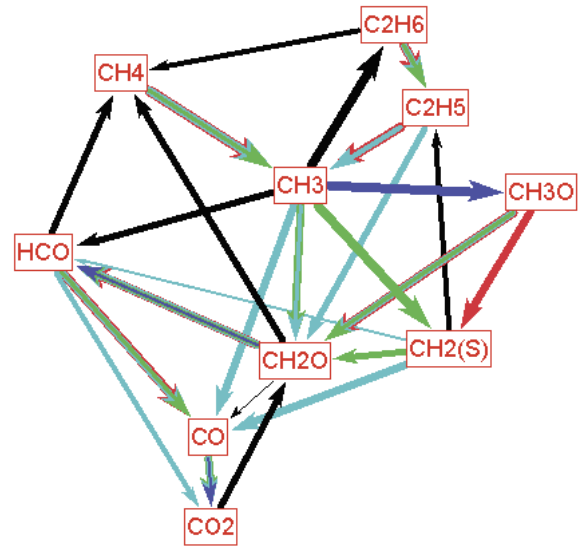# ANSYS®

Chemkin-Pro

**CHEMISTRY SIMULATION FOR
MORE EFFICIENT DESIGNS**

ANSYS

Chemistry Simulation for More Efficient Designs

Visualize reactions with the Reaction Path Analyzer.

Understanding and predicting the effects of chemistry in a system are key to developing competitive products in transportation, energy and materials processing applications. As designers of gas turbines, boilers and piston engines strive to meet low-emissions regulations with ever widening fuel flexibility requirements, they must also maintain, or even improve, their system's performance. Similarly, designing high-throughput materials and chemical processes with high yield and quality must be done with minimal byproduct or waste. Relying on testing alone for accurate performance validation is prohibitive, given today's complex designs and shortened design cycles. Effective simulation of the underlying detailed chemistry is often critical for cost-effective design of systems with reduced pollutant emissions or undesired byproducts.

ANSYS Chemkin-Pro — The gold standard simulation software for complex chemical processes
ANSYS Chemkin-Pro is the gold standard for modeling and simulating complex gas phase and surface chemistry reactions that are used for the conceptual development of combustion systems in cars, trucks, jet engines, boilers, chemical and materials processing equipment, and refining applications. Chemkin-Pro's wide array of accurate, fast and robust kinetic models make it the most trusted kinetic simulation tool for asking "what if" questions in the conceptual design phase. Engineers can quickly explore the impact of design variables on performance, pollutant emissions and flame extinction using large, accurate fuel models

to obtain the results they need to make key product development decisions.

Chemkin-Pro evolved from its origin as a Sandia National Laboratory combustion kinetics code (Chemkin II) into today's commercial-quality software suite with a user-friendly interface, industry-leading time-to-solution performance, and unparalleled accuracy. Chemkin-Pro models have been extensively validated over several decades and frequently cited in technical peer-reviewed journals.

See a whole new view
To help you gain key insights into kinetics dependencies, Chemkin-Pro includes the Reaction Path Analyzer. Employing an interactive visual display, the Reaction Path Analyzer provides a clear view of dominant reaction paths, facilitating mechanism development and reduction.

Use reactor networks to model complex flow-fields
Equivalent Reactor Networks (ERNs) allow simulation of real world combustors, burners and chemical reactors, enabling the most efficient prediction of emissions with detailed chemistry.
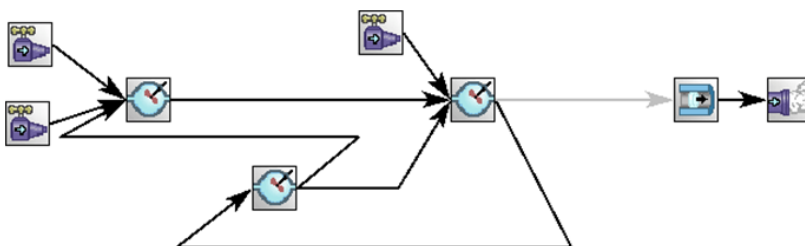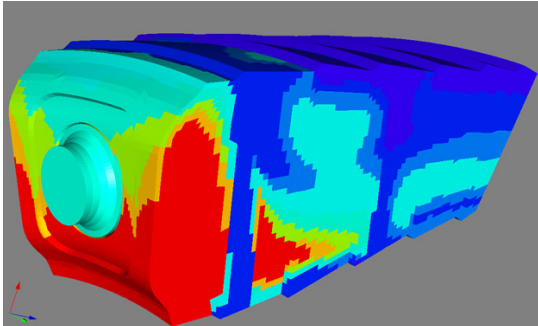
Zones used to define an Equivalent Reactor Network in a combustor

Gain better understanding of low emissions combustion stability
The Chemkin-Pro Extinction Model accomplishes fast, accurate calculations of the extinction strain rate used to determine a system's combustion stability. This is important in premixed low-NOx combustion systems.

Understand and predict particle formation
The innovative Particle Tracking feature of Chemkin-Pro follows particle nucleation, growth, aggregation and oxidation. Two separate tracking approaches allow the prediction of average particle size and number density and/or detailed information on the particle size distribution, which can be used to predict soot emissions or to optimize particle production.

Easily create CFD flamelet tables with speed and accuracy
Many combustion system developers use combustion models that depend on flamelet table lookups in their CFD simulations. Chemkin-Pro provides a robust and fast method to create these flamelet tables for input into CFD models.

Explore how input uncertainties affect simulation results
Enhance the robustness of simulation results with the ability to calculate error bars based on user-defined input accuracy ranges.

Analyze with the IC Engine cases in Chemkin-Pro Engine models
Chemkin-Pro offers multiple in-cylinder engine models: Single Zone HCCI Engine Model, Multi-Zone HCCI Engine Model, and the Spark Ignition Engine Model.

Use the Single Zone and Multi-Zone HCCI models to optimize the analysis of key combustion effects, including ignition, NOx, CO, HC and soot emissions.

| # Species	Flame Speed	Ignition Time	NO$_x$ Emissions
189	<5%	<5%	<5%
113	<5%	<5%	<5%
77	<5%	<30%	<30%
49	<5%	<30%	>30%

Use the Spark Ignition (SI) Engine Model to understand:
• Knock intensity
• Onset of trace knock
• Sensitivity of engine performance on combustion phasing
• Prediction of emissions trends
The SI Engine Model is a zero-dimensional (0D) two-zone combustion model using detailed chemistry to predict end-gas auto-ignition and intensity. It is targeted as an early development tool to gain insights and design directions into combustion performance criteria and trade-offs.

ANSYS Reaction Workbench — Automation and accuracy for fuel surrogate formulation and mechanism reduction
Using the right fuel model for the job is critical to getting the right answers in an optimal amount of time. Reaction Workbench is an extension to Chemkin-Pro that enables the creation of optimal surrogate fuel blend models to match both the physical and chemical properties of the

Reaction Workbench mechanism reduction example for Fischer-Tropsch liquid fuel from a master fuel model with 949 species, showing the impact on accuracy for selected simulation targets
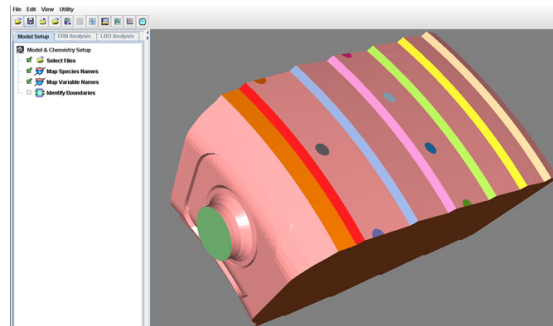
Combustor geometry and flow field imported from CFD
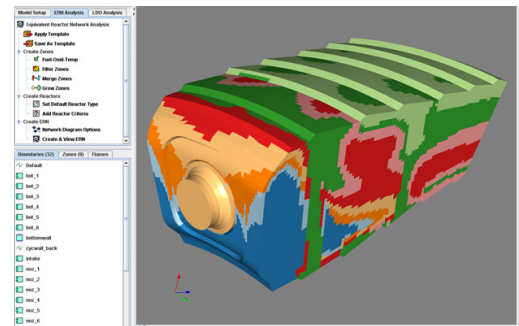
Reactor zones created from CFD solution

fuel. Master mechanisms can be automatically blended from component mechanisms, or sub-mechanisms can be extracted, using Reaction Workbench Mechanism Utilities. For mechanism reduction, Reaction Workbench allows full user control over the automated process. Users select the specific simulation targets of interest (e.g., flame speed, ignition delay, NOx, soot, etc.) and the maximum allowable error for each target. Reaction Workbench automates the application of a series of mechanism reduction techniques to meet those simulation objectives. The result is a mechanism that is optimum for the job and a direct measure of the reduced mechanism's accuracy relative to the original.

Reaction Workbench offers a complete set of software utilities that provide both full control over the reduction process and the ability to create the right mechanism for a specific application. Reaction Workbench includes a Surrogate Blend Optimizer utility that allows you to specify the proper blend of pure components that match specific physical and chemical properties. Blending master mechanisms to create different surrogate fuel compositions is also easy with Reaction Workbench. Then, you can decide what key simulation results (e.g., flame speed, ignition delay, NOx, soot, etc.) are of interest and specify a maximum allowable error in that reduction. Reaction Workbench automates the use of a series of well-established mechanism reduction strategies to build a mechanism that meets the specific criteria for an application, and can be used in any Chemkin-compatible product such as the Forte CFD or ANSYS Energico for gas turbine applications.

ANSYS Energico - Predictive analysis tools for clean-combustion design

ANSYS Energico gives you the power to seamlessly link detailed combustion chemistry and computational fluid dynamics (CFD) for accurate simulation of combustion behavior. This extraordinary software tool lets you take advantage of full combustion reaction mechanisms without sacrificing the resolution of complex fluid dynamics. Used at its full potential, Energico
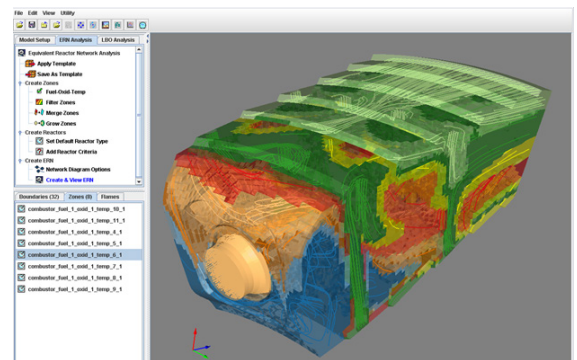

Display CFD results with ERN overlay

speeds combustion system design, allows you to use detailed chemistry without requiring specialized understanding of complex kinetics, and requires fewer, better-directed experimental tests to validate system design.

Energico can be applied to:
• Gas-turbine combustors
• Burners for boilers and furnaces
• Flares and incinerators
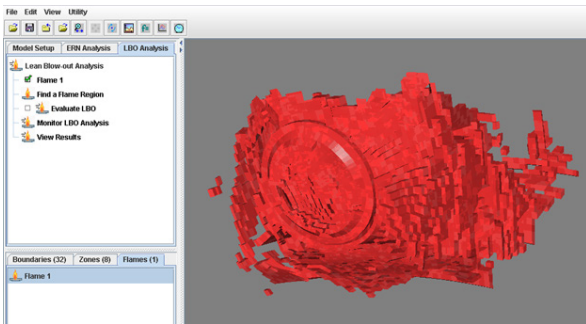
CFD flame for LBO analysis

Key benefits of Energico include:

- Chemistry performance simulation for any continuous-flow combustion system, using virtually any fuel
- Rapid, accurate, prediction of emissions for modern combustors
- Straightforward determination of flame blowout tendency
- Evaluation of the impacts of variations in operating conditions, such as fuel composition on combustion performance
- Direct reading of ANSYS Fluent cas/dat files for quick and easy setup

Accurate emissions prediction with chemistry

Combustor design simulation requires resolution of complex geometry, turbulent flow patterns, heat transfer and detailed chemistry. While CFD can simulate the reacting flow in realistic geometries, it requires the use of severely reduced, global chemistry models that are too simple to accurately simulate emissions and operational stability. The reduced chemistry typically used in CFD cannot represent trace pollutant species such as NOx, CO and unburned hydrocarbons (UHC). To resolve these species requires the use of detailed reaction mechanisms with hundreds of species and thousands of reactions.

nergico software maps idealized chemical reactors to the flow field so you can apply detailed combustion chemistry in an efficient manner to simulate trace species formation and destruction. The use of Equivalent Reactor Networks (ERNs) allows the flow field of the combustor to be represented as a group of Perfectly Stirred Reactors (PSR) and Plug Flow Reactors (PFR) with associated connecting streams. Energico translates the results of a CFD simulation directly into an ERN that captures the dominant flow patterns and recirculation zones. Energico includes automated

templates for every step, and also offers a variety of configuration options that can be used to address your specific requirements.

Lean Blow Off analysis

Lean Blow-Off (LBO) is one of the most challenging combustion stability problems in low-NOx combustor design. LBO occurs when the heat generated by chemical reactions is no longer sufficient to ignite the incoming fuel/air mixture to sustain the flame. In low-NOx combustor design, the low NOx limit is often bound by the onset of combustion instability in the form of LBO. Identifying the onset of LBO is critical in combustion system design. Because this condition is dictated by real chemistry and fluid dynamics, the reduced chemistry intrinsic to most CFD tools cannot provide the necessary accuracy.

Energico uses the well-documented concept of evaluating the relative time-scales for chemical reaction and fluid mixing to predict when LBO will occur. In conventional uncontrolled combustors, the combustion is limited by the degree of mixing occurring within the combustor, as chemistry is typically much faster than mixing. However, as the flame temperature is decreased to reduce NOx, the chemical reaction slows to the point where temperature becomes the rate-limiting factor and the onset of LBO may be triggered.

To help designers determine the propensity of their system to experience LBO, Energico captures the specific region in the combustor flow field that represents the flame front based on the CFD solution. An analysis is then performed, using detailed chemistry and the CFD flow field, to evaluate the viability of a flame in that location.

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If you've ever seen a rocket launch, flown on an airplane, driven a car, used a computer, touched a mobile device, crossed a bridge or put on wearable technology, chances are you've used a product where ANSYS software played a critical role in its creation. ANSYS is the global leader in engineering simulation. We help the world's most innovative companies deliver radically better products to their customers. By offering the best and broadest portfolio of engineering simulation software, we help them solve the most complex design challenges and engineer products limited only by imagination.
Visit www.ansys.com for more information.