Using Detailed Chemistry in ANSYS Chemkin-Pro for More Accurate CFD Combustion and Reacting Flow Simulations

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Outline

• ANSYS portfolio related to combustion and engine simulations
  – New Chemkin Enterprise product

• Chemkin-Pro reactors and tools
  – Demo of flame speed calculations

• Reaction mechanisms (fuel libraries)

• Build a surrogate fuel model

• Reduce a reaction mechanism

• FLUENT-Chemkin integration for CFD

• Auxiliary capabilities:
  – Demo of reactor networks for soot predictions
  – Automated reactor networks (Energico)
  – Internal Combustion (IC) engine simulations (Forte)

• Demo: How to learn and get help?
Chemkin family of products complements ANSYS CFD

<table>
<thead>
<tr>
<th>CHEMKIN-PRO &amp; REACTION WORKBENCH</th>
<th>• 0-D, 1-D reactor models and flames with full chemistry detail, surrogate creation (reactor networks, flame speeds, flamelets)</th>
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</thead>
<tbody>
<tr>
<td>Model Fuel Library</td>
<td>• Complete and validated fuel chemical mechanism set</td>
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</table>
| ANSYS CFD (Fluent & CFX)        | • Flow simulation (Turbulent flows, steady/unsteady)  
• Solid or liquid fuels (droplet, coal particles, etc.)  
• Full range of combustion models (premixed, partially premixed, non-premixed)  
• Radiation modeling  
• Real Gas modeling  
• Pollutant modeling |
| ENERGICO                        | • Equivalent Reactor Networks for emissions  
Gas turbines combustion, furnaces, coal combustion, reformers, boilers, materials, chemical vapor deposition, chemical processing |
| FORTÉ CFD                       | • IC Engine CFD  
• Automatic meshing  
• Flame-front tracking  
• Particle size
New Product: Chemkin Enterprise

CHEMWIN Enterprise

- Introduced in R19.0
- Single License
  - Chemkin-Pro
  - Reaction Workbench
  - Model Fuel Library
  - Energico
  - Forte CFD
  - CFD Pre- and Post-processing (including SpaceClaim Direct Modeler and Ensight)
  - 4 HPC cores

~ANSYS Inc\v191\reaction\data\ModelFuelLibrary\Reduced
Chemkin-Pro focuses on chemistry, using engineering approximations of the flow

- 0-D, 1-D and 2-D approximations of industrial flow conditions

![Equilibrium Calculator](image1)

![Perfectly Stirred Reactor (PSR), 0-D](image2)

![Plug-flow Reactor (PFR), 1-D](image3)

![Opposed-flow Diffusion Flame, 1-D](image4)

![Pre-mixed Flame, 1-D (burner-stabilized)](image5)

![Flame-speed Calculation, 1-D](image6)
Reactor models in Chemkin cover various applications

- **0-D and multi-zone reactors**
  - IC engine models, well mixed and partially mixed reactors, plasma reactor

- **Flow reactors**
  - Plug flow, shear flow, honeycomb monolith reactor

- **Flame simulators**
  - Laminar flame speed, opposed flow, stagnation flow, flame extinction model, flamelet generation for CFD

- **CVD* reactors**
  - Stagnation flow and rotating disk, LPCVD

* Chemical Vapor Deposition
A Chemkin project is quick to set up

- Choose a reactor model
- Define or select a chemistry set:
  - Reactions and reaction rate constants are key inputs to Chemkin
    - Thermodynamic data
    - Gas-phase reactions
    - Surface reactions
    - Transport-property data
- Define the domain size
- Specify operating conditions (Ideal Gas or Real Gas)
Models predict varying state of gas and/or surface

- Thermodynamic state of the gas
  - Temperature / Enthalpy / Entropy
  - Pressure / Density
  - Rate of heat transfer to the environment

- Chemical state of gas / surface / solid
  - Gas-phase composition
  - Surface site coverage
  - Species production rates
  - Rate of progress of individual reactions

- Local fluxes of heat, mass & species
  - Instantaneous deposition rates
  - Multicomponent molecular diffusion
  - Convection, conduction, radiation

- Solution sensitivity to parameters

Predicted as a function of:
- Time
- Distance
- Zone #
- Parameter
Visualize all important aspects in **path analyzer post processor**

Color by
- Side species
- Heat flux
**Mechanism Inspector** can identify issues with thermo and rate parameters

Users can check unphysical data in chemistry sets (e.g., discontinuity in Cp)
Property Estimator for transport and critical properties

Estimator can generate inputs for:
- 1-D reactors
- Real gas model

![Molecular structure of a compound with an oxygen atom]
Demo
Laminar Flame Speed Calculations
Combustion fuels are changing and highly variable

- Blends and dual-fuel strategies
- Shale-oil derived fuels
  - High in aromatics
- Natural Gas local variability
- Biodiesels
  - High in methyl esters
  - Sources differ regionally and are changing
- Biomass-derived, Waste fuels
- Coal-derived, F-T fuels
- Fuel additives
- Specialty, tailored fuels
The **Model Fuel Library** is a large set of validated fuel-component mechanisms

~ 65 Validated Fuel Models

- Common core chemistry
- Consistent rules for reaction rates
- Validated fuel-blending behavior

**Biodiesel Components**

**Diesel and Jet-Fuel Surrogates**

**Gasoline Surrogates**

**Gaseous Fuels**

**Detailed Particle-based and Pseudo-gas Soot Models**
Mechanisms are validated through comparison to fundamental experiments

• Over 500 sets of published experimental results
  – Varying fuels, fuel blends, stoichiometry, temperature, pressure

• Experiments designed to focus on the kinetics
  – Easily modeled flow configurations

1 hanson.stanford.edu
2 crf.sandia.gov
3 afl.mcgill.ca
4 dlr.de
5 itv.rwth-aachen.de
A detailed soot-kinetics model is a key component of the Model Fuel Library

- Validated systematically
  - Fundamental experiments
  - Particle size studies in flames
  - Optical engine data
  - Engine-out data
Particle Tracking Capabilities Available

- Particle Tracking is available for most reactor models
  - Chemistry based via surface chemistry input
  - Nucleation, growth, and oxidation all handled through surface chemistry
- Two options available
  - **Method of Moments:** tracks the average properties of a particle distribution; i.e. particle number density, particle diameter, growth rate
  - **Sectional Method:** more detail, computes the size distribution; i.e. particle size vs. particle number density
- Aggregation, coagulation, and particle radiation heat transfer available in both models
Liquid fuels can be characterized by their content, in terms of molecular classes.

- **Normal alkanes**
- **Branched alkanes**
- **Cyclic alkanes**
- **Aromatics**
- **Others**

*Fuel data from: C. Westbrook presentations*
Prepare a fuel model for use in CFD with ANSYS Chemkin-Pro / Reaction Workbench

- Accurately mimic:
  - Combustion & emissions behavior
  - Chemical and physical properties

Fuel properties to match:
- Chemical properties
- Octane, Cetane numbers
- Distillation Curve

Surrogate Blend Optimizer

Model-fuel blend

Mechanism Reduction

Fuel Model ready for ANSYS CFD
Example of European diesel surrogate

- Surrogate mimics physical and chemical properties

<table>
<thead>
<tr>
<th>Targeted Property</th>
<th>Targeted Value</th>
<th>Optimized Property</th>
</tr>
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<tbody>
<tr>
<td>Liq. density (g/cm³)</td>
<td>0.83</td>
<td>0.83</td>
</tr>
<tr>
<td>CN</td>
<td>54</td>
<td>54</td>
</tr>
<tr>
<td>H/C Ratio</td>
<td>1.875</td>
<td>1.870</td>
</tr>
<tr>
<td>LHV, MJ/kg</td>
<td>43.8</td>
<td>43.76</td>
</tr>
<tr>
<td>T50, K</td>
<td>499</td>
<td>498.5</td>
</tr>
</tbody>
</table>

Composition used for CFD and to create reduced mechanism

<table>
<thead>
<tr>
<th>Component</th>
<th>Mass %</th>
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<tbody>
<tr>
<td>n-Hexadecane</td>
<td>36.0</td>
</tr>
<tr>
<td>1-Methylnaphthalene</td>
<td>9.7</td>
</tr>
<tr>
<td>Heptamethylnonane</td>
<td>15.4</td>
</tr>
<tr>
<td>Decalin</td>
<td>38.9</td>
</tr>
</tbody>
</table>
CFD applications require smaller mechanisms for faster turn-around times

- 7+ mechanism reduction methods implemented
- Multiple targets: ignition time, flame speed, emissions species
- Smallest mechanism produced with specified accuracy
Mechanism reduction works with any reactor model in CHEMKIN-PRO

Example of a 4-component surrogate mechanism reduction

Reduction tool automatically meets required user specified accuracy

4000 Species >> ~200 Species

Reduce mechanism and validate!
FLUENT – Chemkin Integration

FLUENT can utilize:

- Advanced Chemkin-CFD solver for detailed finite rate chemistry (built-in, no license is needed)
- Reduced mechanisms from Reaction Workbench (MFL or user mechanisms)
- Flamelets generated in Chemkin for PDF-based combustion models (FGM, steady diffusion flamelet)

Example: Combined Dynamic Cell Clustering (DCC) with ISAT using Chemkin-CFD solver GRI-Mech mechanism (53 species)

Sandia Flame D

Temperature contours
Number of cells: 16590, Number of iterations: 5000
Reactor networks represent complex systems while allowing detailed kinetics.

Essence of flowfield in complex geometry can be represented by reactors with mass-flow connections.

Gas turbine example

Air
Pre-mixed Fuel + Air

Mixing
Recirculation
Flame
Post-flame

Equivalent Reactor Network
Demo
Reactor Network for Soot Formation & Growth with Surface Chemistry
Automatically create many reactor networks in Energico

- Detailed kinetics used for emissions and lean blow-out predictions

ANSYS CFD Solution

Build algorithm to divide flow field into reactor zones

Improve CFD model with greater kinetic understanding

Solve the ERN with Chemkin-Pro

Map chemistry results onto geometry view
ANSYS FORTE for IC-Engine Simulations

- Set up tailored to IC Engines
- **Automatic mesh generation**
  - On-the-fly, dynamic
  - Solution-adaptive mesh refinement
- **Fast chemistry solver**
  - Predict ignition, emissions, fuel effects
  - Predict flame-front location and knocking in SI engines
  - Particle size tracking (soot)
- **Well validated spray and spray-wall models**
  - Capture physics accurately and robustly with mesh insensitivity
Additional ANSYS FORTE Capabilities

ANSYS Ensight

Large Eddy Simulations

Multi-Cylinder

Arbitrary Sector

GT-Suite Coupling
Demo
How to learn and get help?

https://support.ansys.com

Customer Portal

https://studentcommunity.ansys.com/

Student Community
Join the simulation conversation!

Read. Comment.

Join the conversation!

The ANSYS blog is live at: blog.ansys.com