Introducing CHEMKIN-PRO

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CHEMKIN in Combustion Workshop

August 3, 2008

CHEMKIN-PRO is designed for the advanced user – more features and performance

- **More modules included in package**
  - Uncertainty, Particle Tracking, Reaction Path Analysis
- **Advanced analysis options**
- **New reactor models and features**
- **Performance improvements**
  - Solver speed
  - Solution post-processing
- **Enhanced work-flow / user experience**

reaction DESIGN

Outline – the Highlights

- **Advanced analysis modules**
  - Reaction path analysis
  - Uncertainty analysis
- **Advanced reactor models and features**
  - Multi-zone (HCCI) Engine Model
  - Particle formation and tracking capabilities extended
- **Focus on performance for large, complex systems**
  - Improved solver robustness and speed
  - Advanced methods for accurate ignition calculations
  - More automated Flame-speed Calculator set-up
  - Tear-stream algorithm for heterogeneous reactor networks
- **Improved work-flow, interactivity, efficiency**

reaction DESIGN

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reaction DESIGN

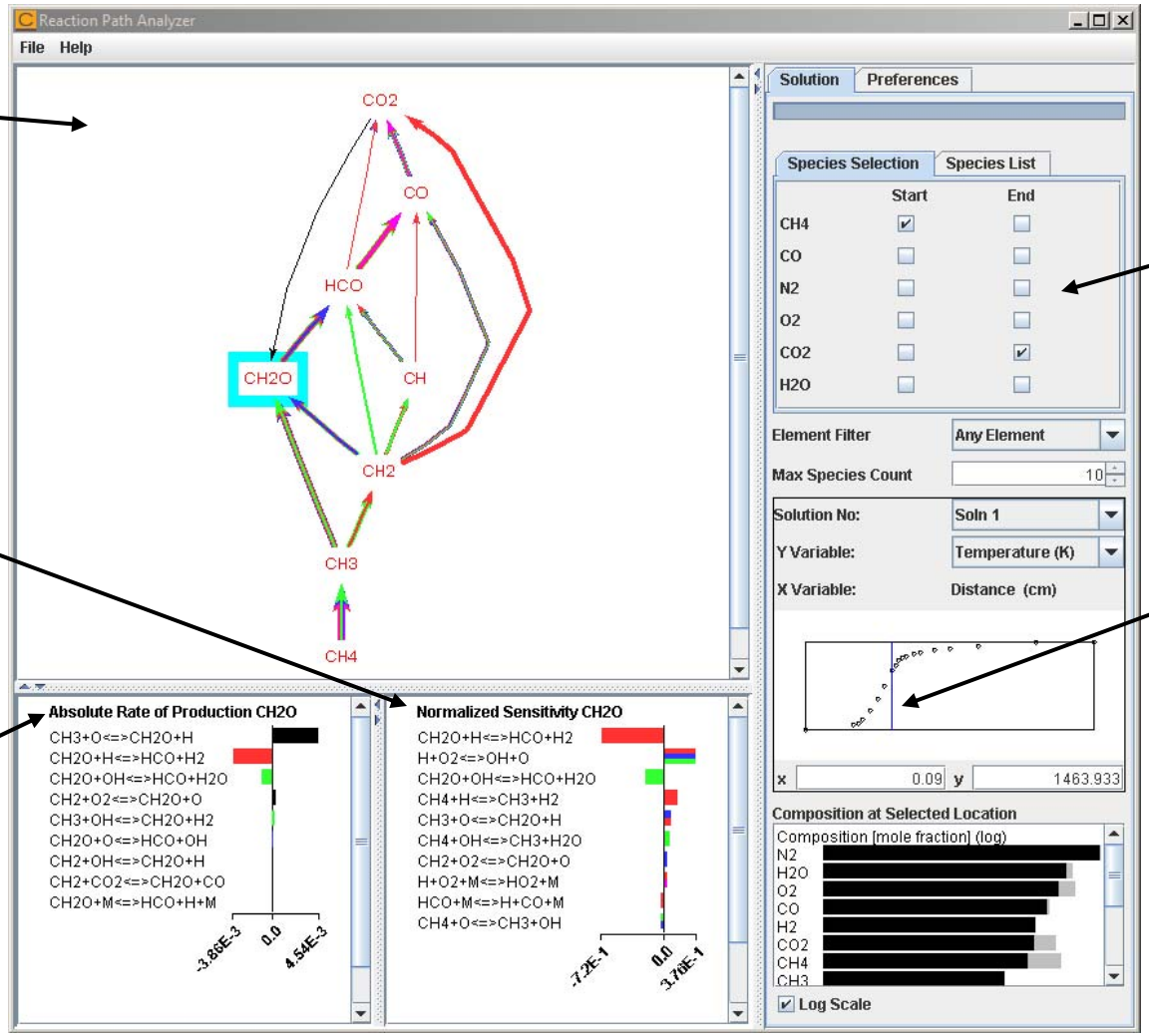
The new Reaction Path Analyzer (RPA)

Example: analysis of reaction paths in CH_4/air flame

Reaction path diagram with color-coding for "side" species (e.g. radicals)

Species Sensitivity bar chart

Species ROP bar chart



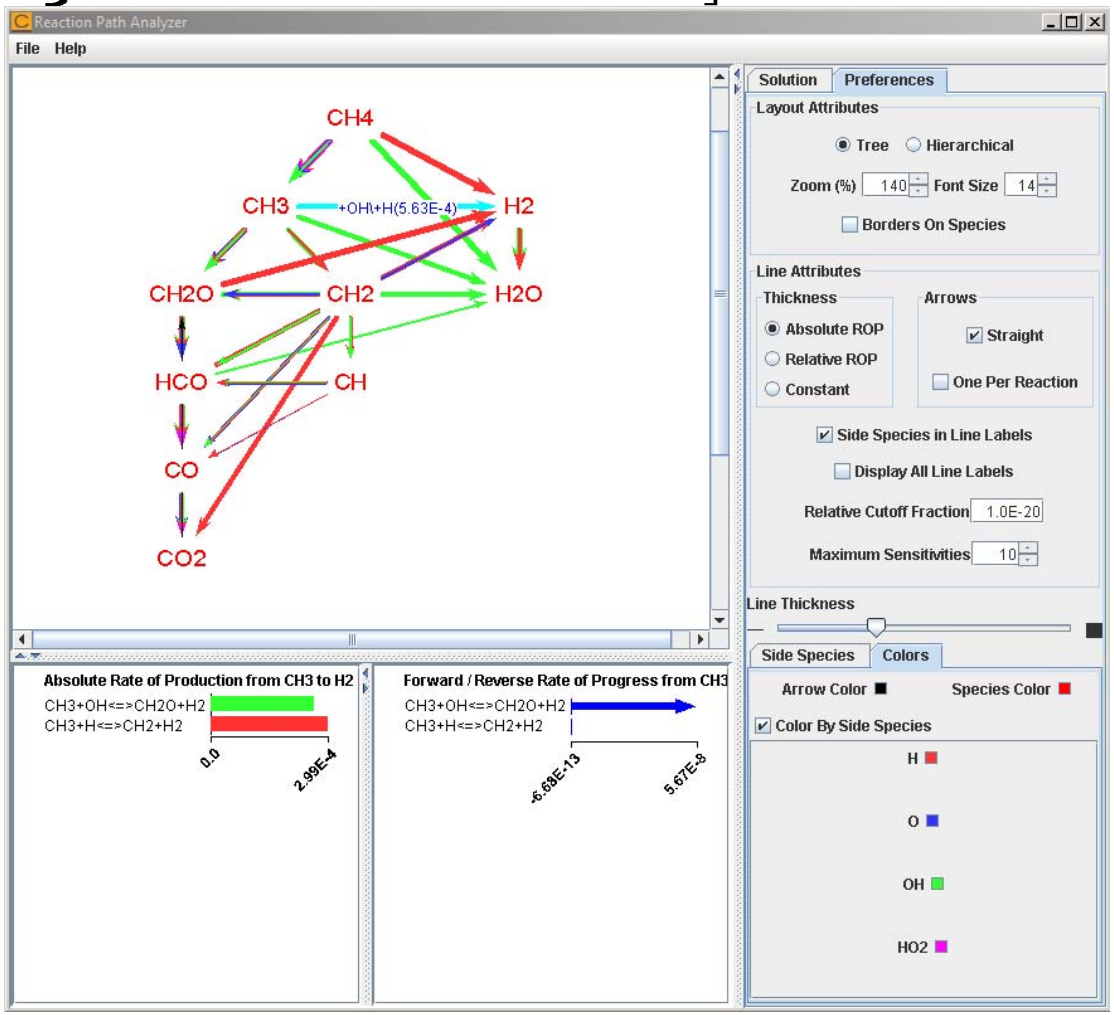
Control of what reaction paths are displayed

Dynamic selection of location in solution

reaction DESIGN

The RPA provides interactive control over layout and the way information is presented

- **"Tree" view (vs. hierarchical)**
- **Reaction focus (vs. species)**
- **Line-thickness gives visual cue for contribution**
  - Absolute or relative scale
- **More in Demo later…**



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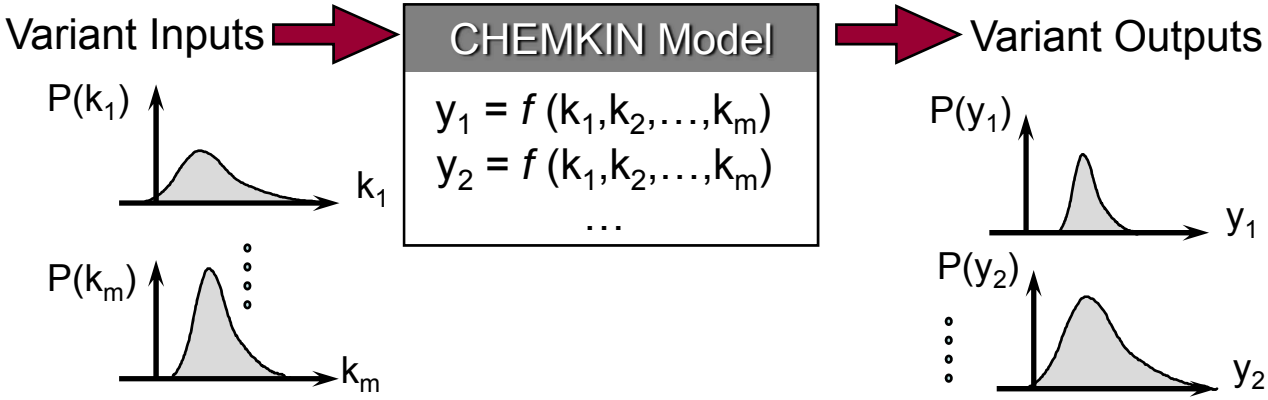
The RPA is available for use with any of CHEMKIN-PRO's reactor models

- **All transient or steady state models**
  - Step through solution points in time
  - Select solution distance for 1-D models
- **Apply to results from any case in a parameter study**
- **Apply to results from any "Cluster" in a reactor network**
- **Includes print options for all graphs**

reaction DESIGN

Uncertainty analysis provides a way to assess the effects of unknown model inputs

- **Based on polynomial chaos expansion theory and collocation methods**
- **Can be used with any CHEMKIN project**
  - Any input parameter can be identified as “uncertain”
  - Any output variable can be identified as a target for which we want to know the uncertainty impact
- **Includes quantitative variance analysis**
  - Which inputs contribute most to the target-output uncertainties



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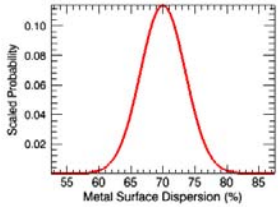
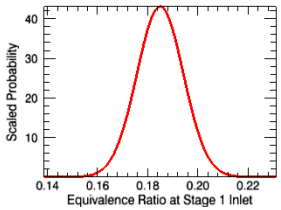
Example: 2-stage combustor with catalytic and homogeneous combustion

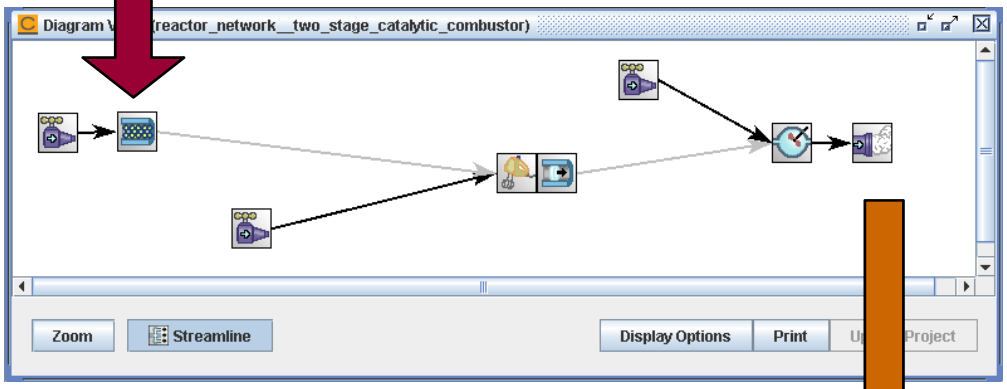
Variant Inputs

(1) % Catalyst dispersion
- Gaussian distribution
- Std deviation = 5%

(2) Fuel-air equivalence ratio
- Gaussian distribution
- Std deviation = 5%



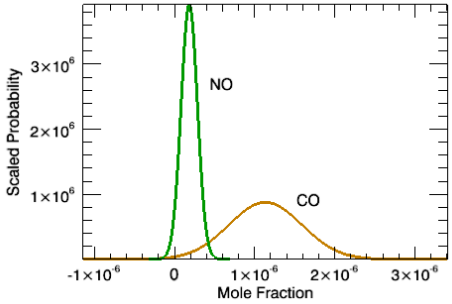




Determine variance of outputs

(1) NO exiting the combustor

(2) CO exiting the combustor



Variance contributions

Input	NO	CO
% Cat. Disp.	53%	39%
Equiv. Ratio	47%	61%

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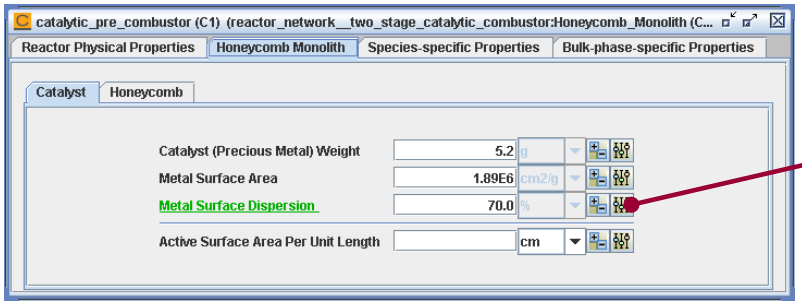
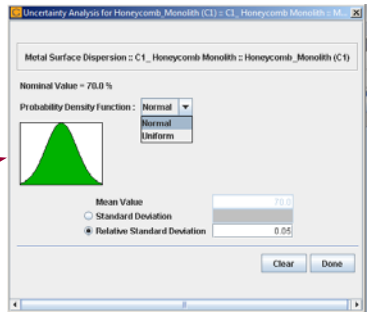
Setup and analysis are guided through the CHEMKIN-PRO user interface

1. Indentify uncertain inputs

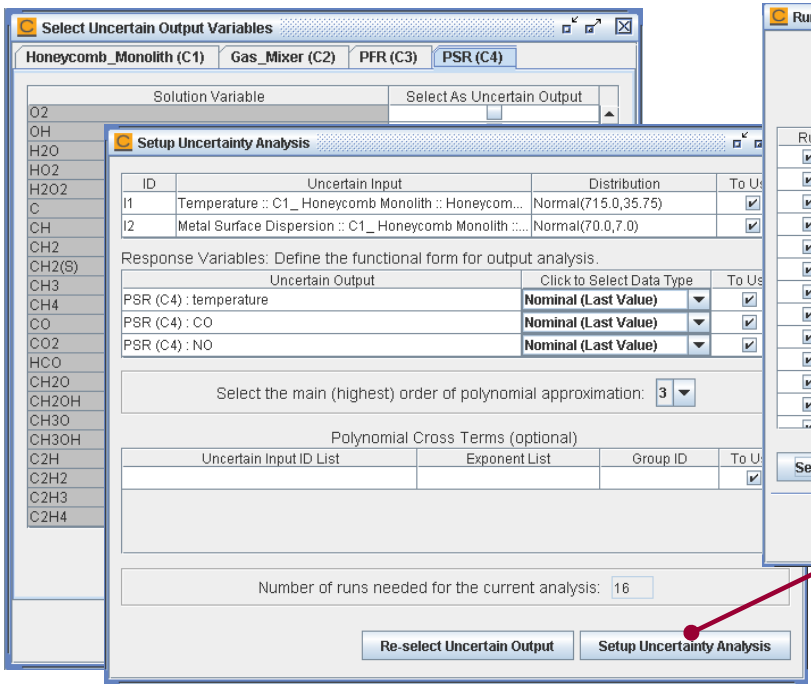


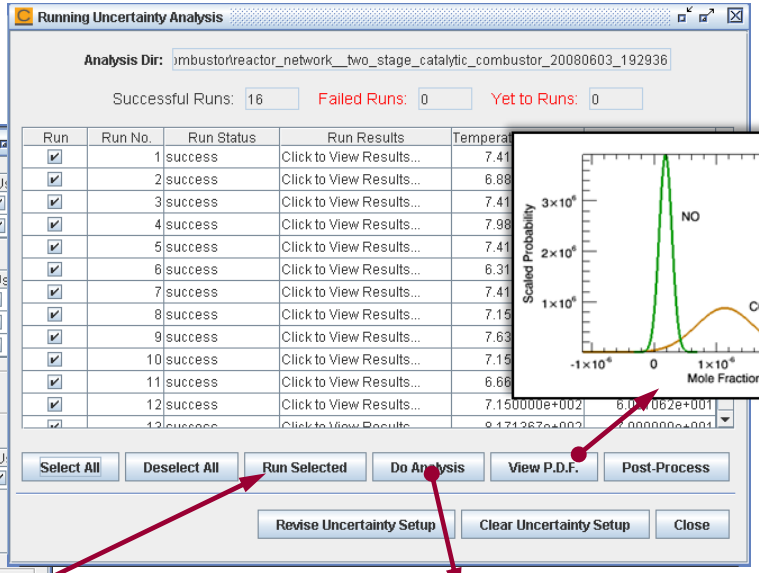


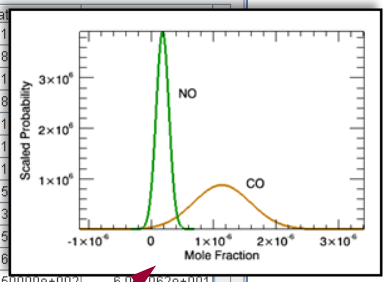
2. Define input PDFs

3. Select target outputs

4. Provide max order of PCE







5. Run model cases

Input	NO	CO
% Cat. Disp.	53%	39%
Equiv. Ratio	47%	61%

6. Analyze results

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Outline

- **Advanced analysis modules**
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reaction DESIGN

New HCCI Multi-zone Engine model allows better prediction of ignition, emissions

- **Permits the use of detailed combustion chemistry**
  - Ignition timing
  - pollutant formation
- **Addresses in-cylinder temperature and/or composition stratifications**
  - Different heat loss for different regions
  - Imperfect mixing of residual or recycled exhaust gas
- **Facilitates parametric studies**
  - Engine/operating parameters
  - Mechanism reduction

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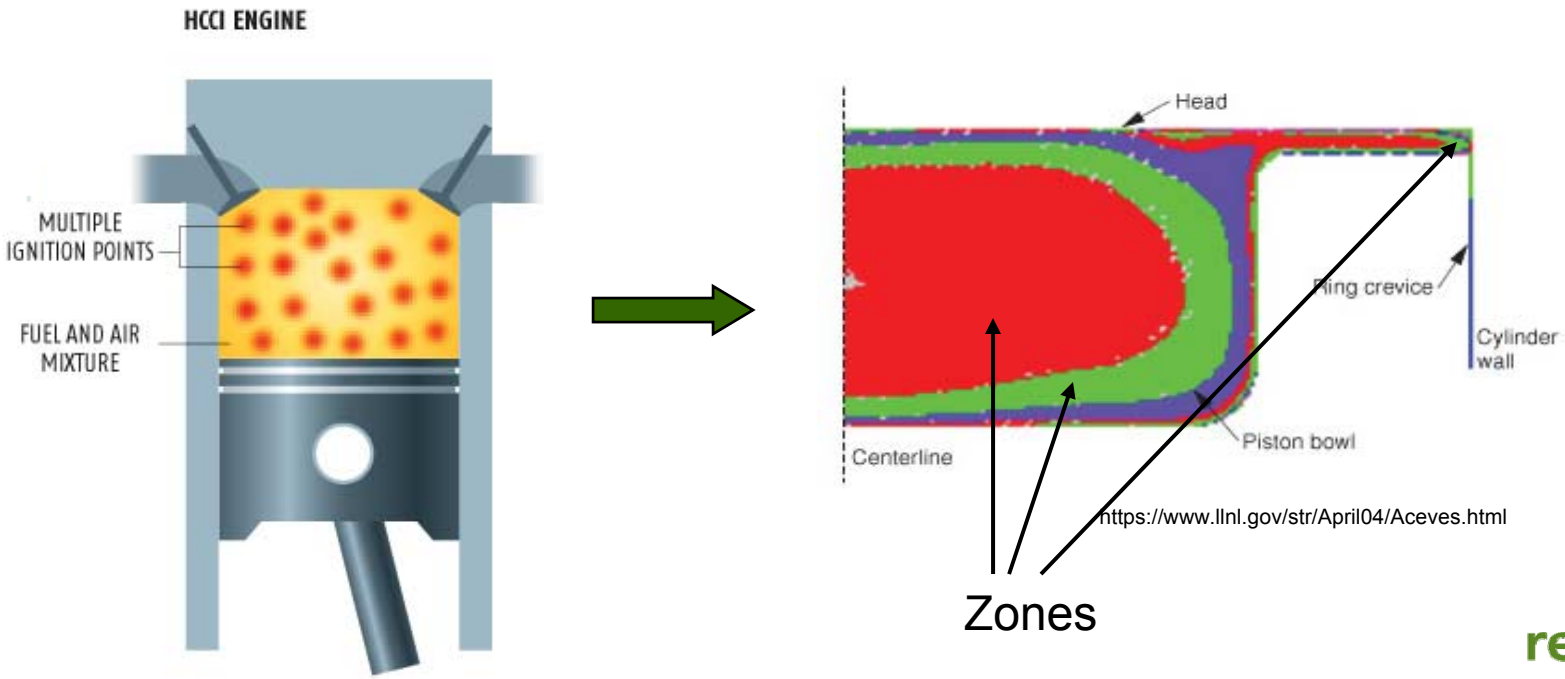
The concept is based on previous models reported in the literature

- **Aceves, et al. (SAE 2000-01-0327)**
- **Zones are conceptual regions**
  - Floating and non-contiguous
  - Total zone volume must equal to cylinder volume
  - Can be derived from a cold-flow CFD model



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Zones interact through pressure work

- **Pressure is uniform inside the cylinder**
- **No mass or heat transfer takes place between zones**
  - Zones can exchange heat with wall
- **Zones interact with each other through pressure work**
- **Each zone can exchange heat with cylinder wall**
  - Each zone has its own wall heat transfer rate
  - Zone wall surface area is given as a constant fraction of instantaneous cylinder wall
    - Zero surface area fraction will make the zone adiabatic

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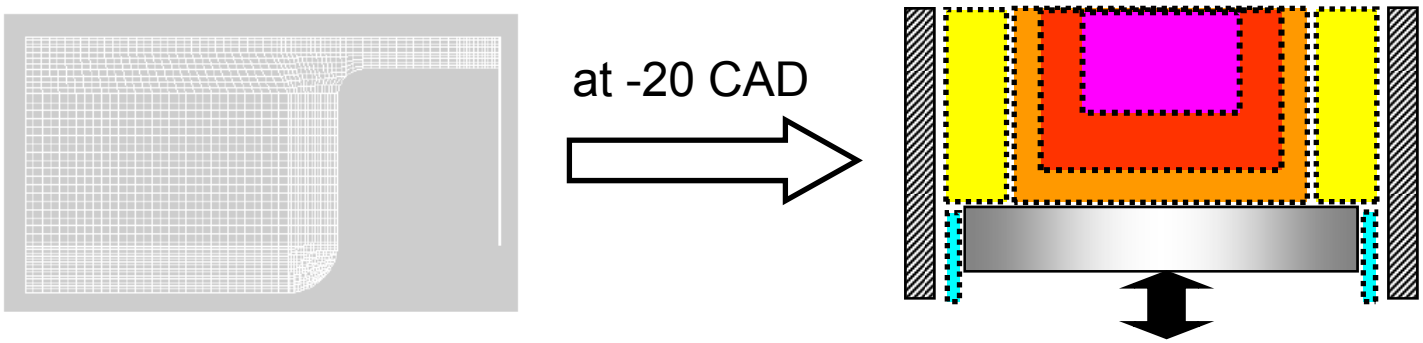
We include the option to use a two-step solution approach employing CFD data

- **Two step hybrid approach**
  1. **Cold-flow CFD simulation determines in-cylinder conditions before chemical kinetics become important**
     - No chemistry, hence very short CFD simulation time
     - Account for temperature variations due to compression / mixing
     - Use temperatures at specified crank angle to define zones
  2. **Use the multi-zone model with fully detailed kinetics**
     - Energy equation to compute zone temperatures
     - Predict combustion phasing
     - Predict emissions



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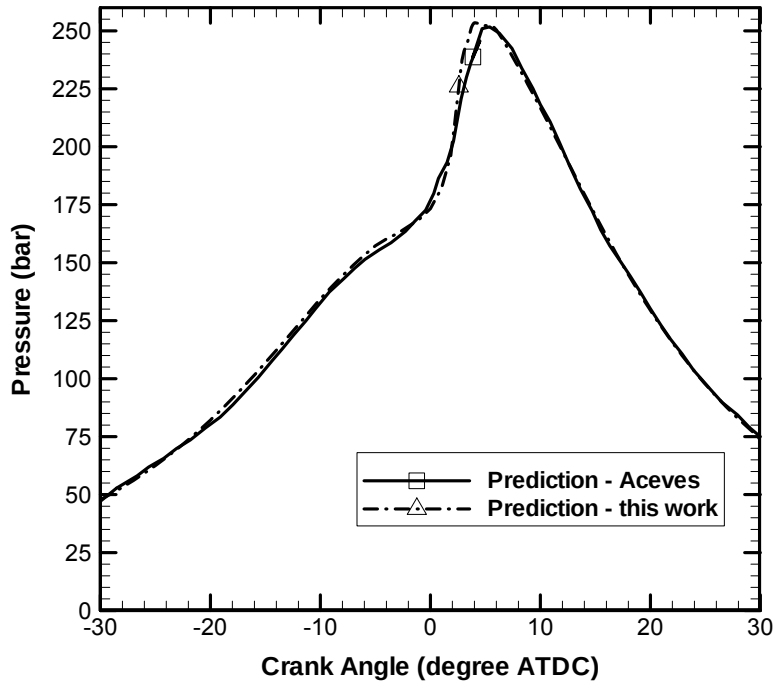
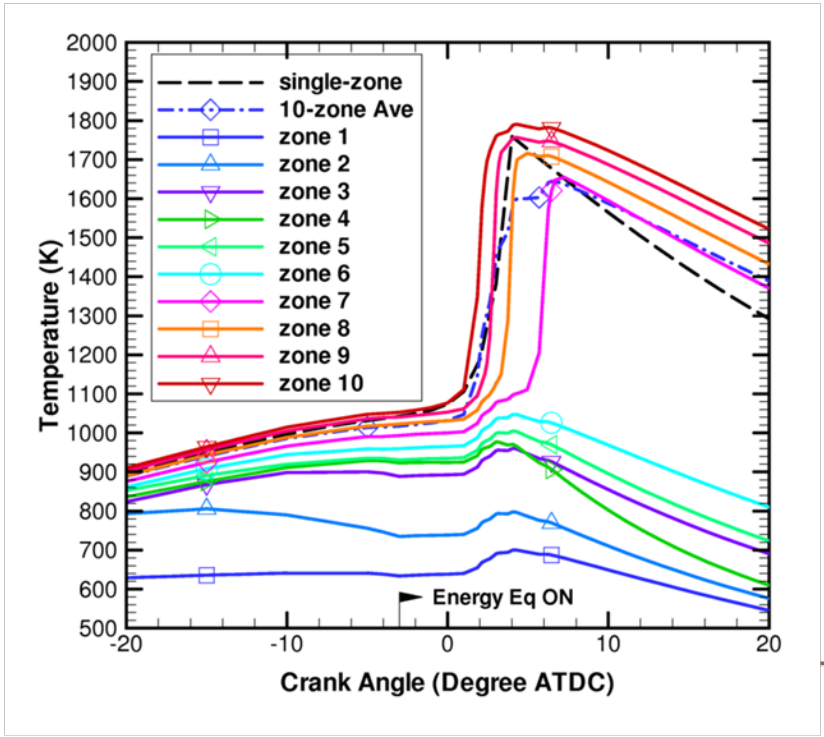
Results compare well to published model of Aceves et al., for natural gas engine

- **Hybrid approach used for temperature solution**
  - Constrained temperature profile used up to user-specified crank angle
    - Temperature could be obtained from CFD simulation
  - Fully coupled energy equation solved after transition
- **Same kinetics mechanism used for comparison**





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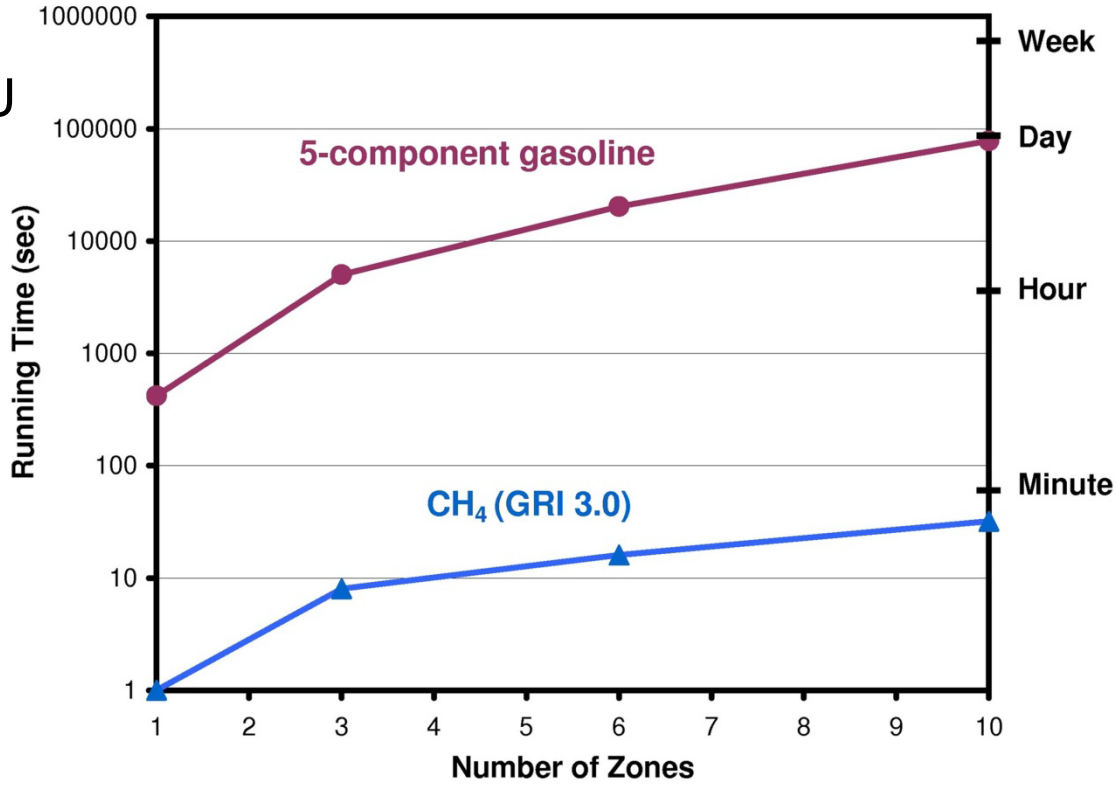
Solution speed allows use of fully detailed surrogate-fuel mechanisms

- **Hardware**
  - 64-bit Linux
  - 2.8 GHz Intel Xeon CPU
  - 6 GB RAM
- **Mechanisms**
  - 5-component gasoline
    - 1380 species
    - 6138 reactions
  - CH4 (GRI 3.0)
    - 53 species
    - 325 reactions



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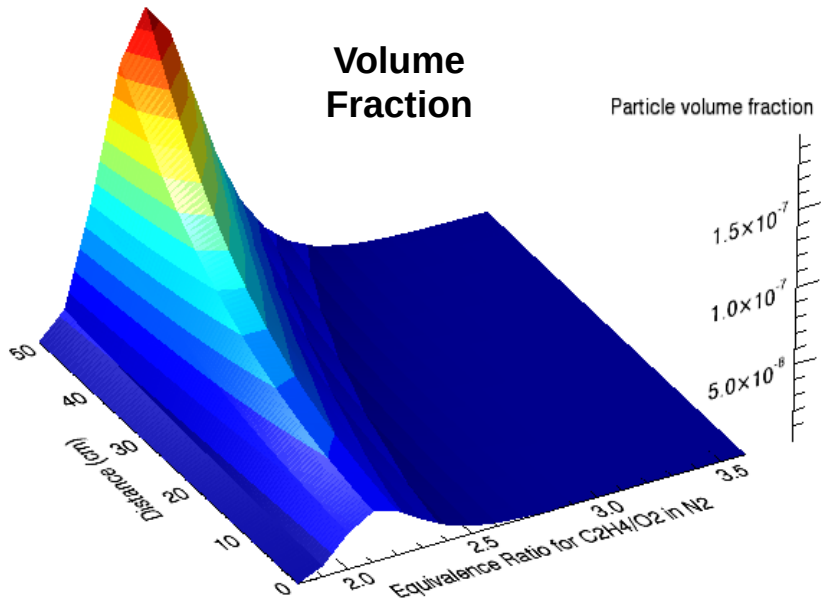
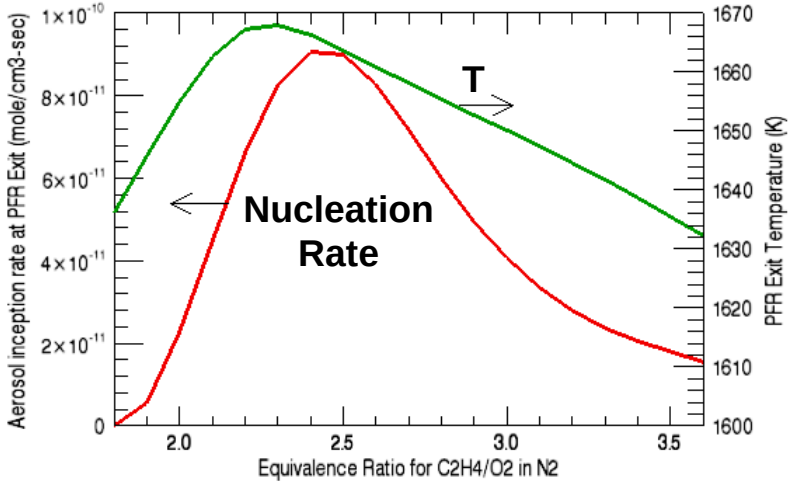
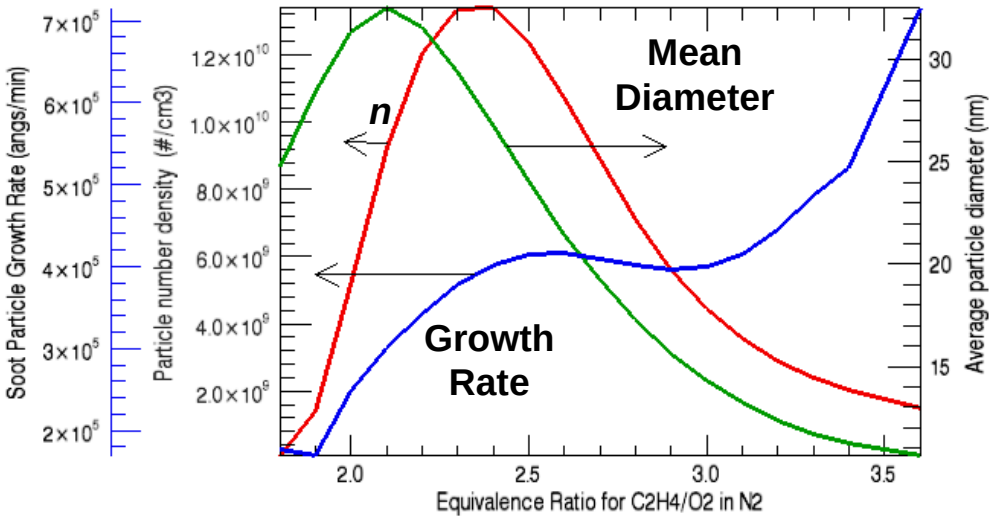
The Particle Tracking Module allows detailed kinetics of particle nucleation and growth





Soot particle predictions for variation of fuel:air for $C_2H_4/O_2/N_2$ combustion



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Moments of the particle size distributions are solved, with kinetics data as input

Coagulation

Particle collision frequency

Nucleation reactions

Surface reactions

Precursor collision frequency

$$\frac{DM_r}{Dt} = R_r + G_r + S_r$$

R_0, R_1, $\vdots$, R_r

G_0, G_1, $\vdots$, G_r

S_0, S_1, $\vdots$, S_r

- Oxidation
- Growth
- Condensation

Moment Equations

reaction DESIGN

Kinetics data is provided through surface-chemistry input file

- **Nucleation of particles from gas-phase species**
  - e.g., poly-aromatic hydrocarbons (PAHs) for soot
  - Rates controlled by collision frequencies
  - Multiple nucleation events, precursors allowed
- **Growth and reduction by general surface reactions**
  - Vapor-deposition type reactions
  - Condensation of large species
- **Tracking of particle state includes surface state**
  - Provides particle mean diameter, mass & volume fractions
  - Average surface state and total surface area

reaction DESIGN

In CHEMKIN-PRO, particle tracking is now available for all flame models

- **Models that can use particle tracking:**
  - 0-D Closed Homogeneous Reactors
  - Perfectly Stirred Reactors
  - Plug-flow Reactors
  - Shear-layer Flow Reactors
  - Premixed, burner-stabilized flames
  - Flame-speed Calculator
  - Counter-flow flames

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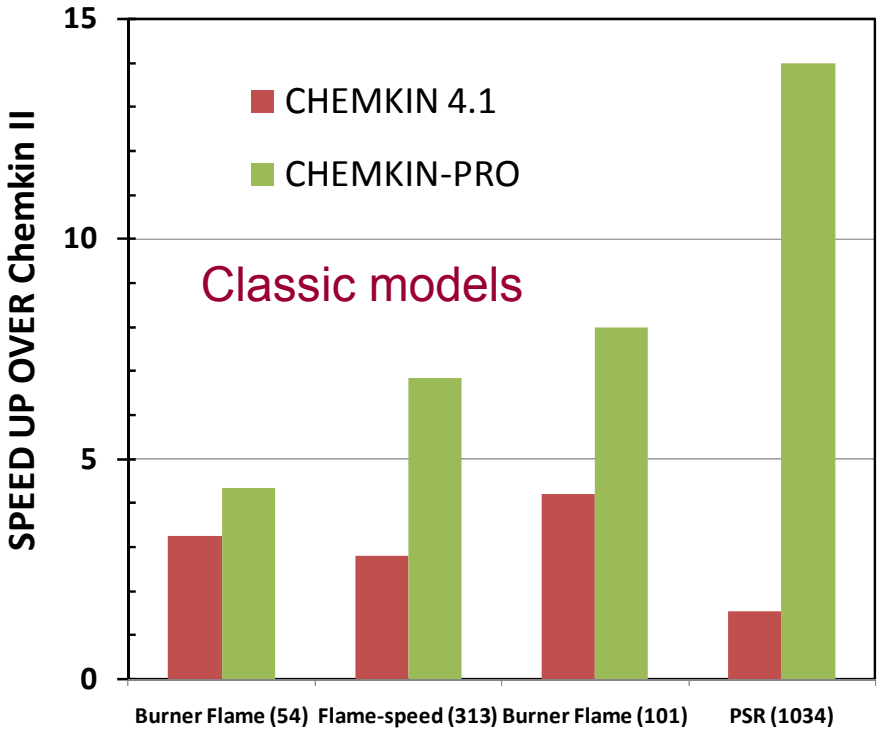
reaction DESIGN

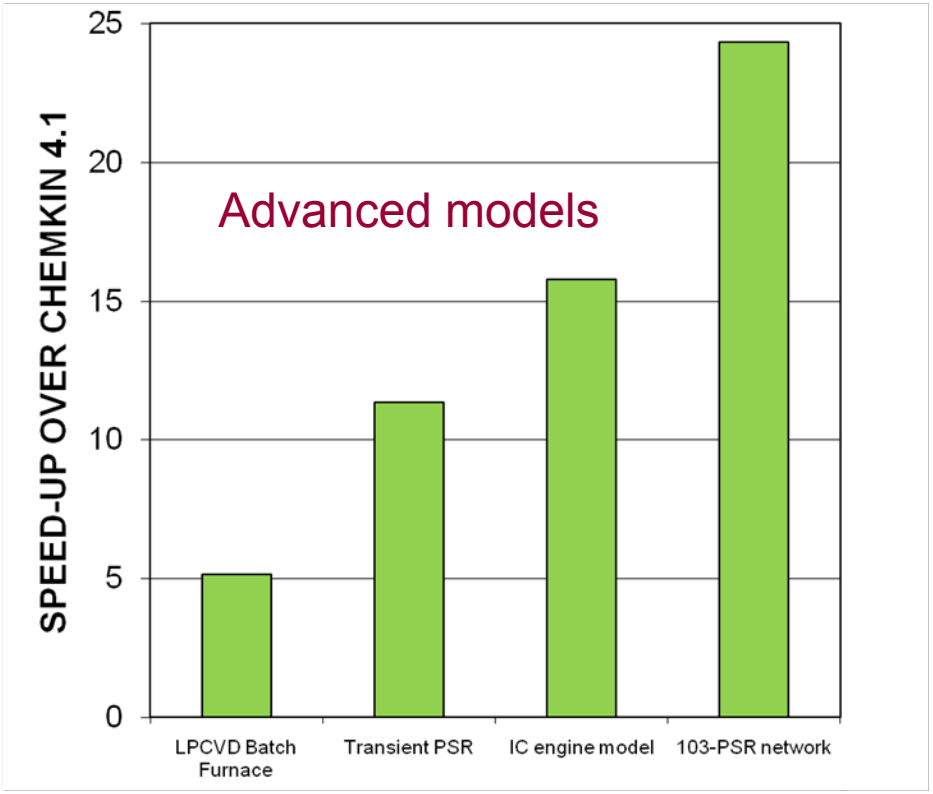
We have made major improvements to the core solver technology in CHEMKIN-PRO

- **Both steady-state and transient solvers accelerated**
- **Net result: ~2X to 20X speed-up & more robust**

Benchmarks vs. Chemkin II



Benchmarks vs. CHEMKIN 4.1



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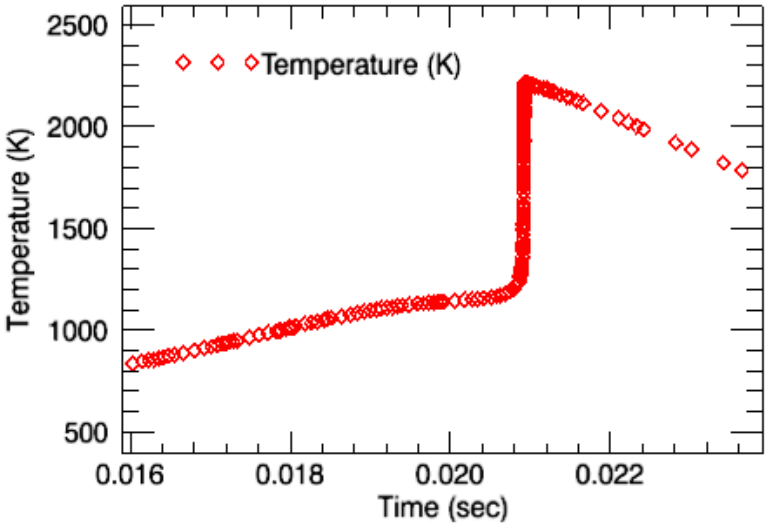
Adaptive stepping for output of solution data facilitates accurate visualization and analysis

- **Important for ignition problems**
  - Avoid huge solution files that were previously required for output at fixed time-steps
  - Accurate post-processing of ignition-delay behavior
- **Assures accuracy of output**
  - consistent with the adaptive solver
  - Default: output every 20 solver-integration steps
- **Options to control adaptation**
  - Every xx solver-integration steps
  - Every yy delta in specified solution variable value



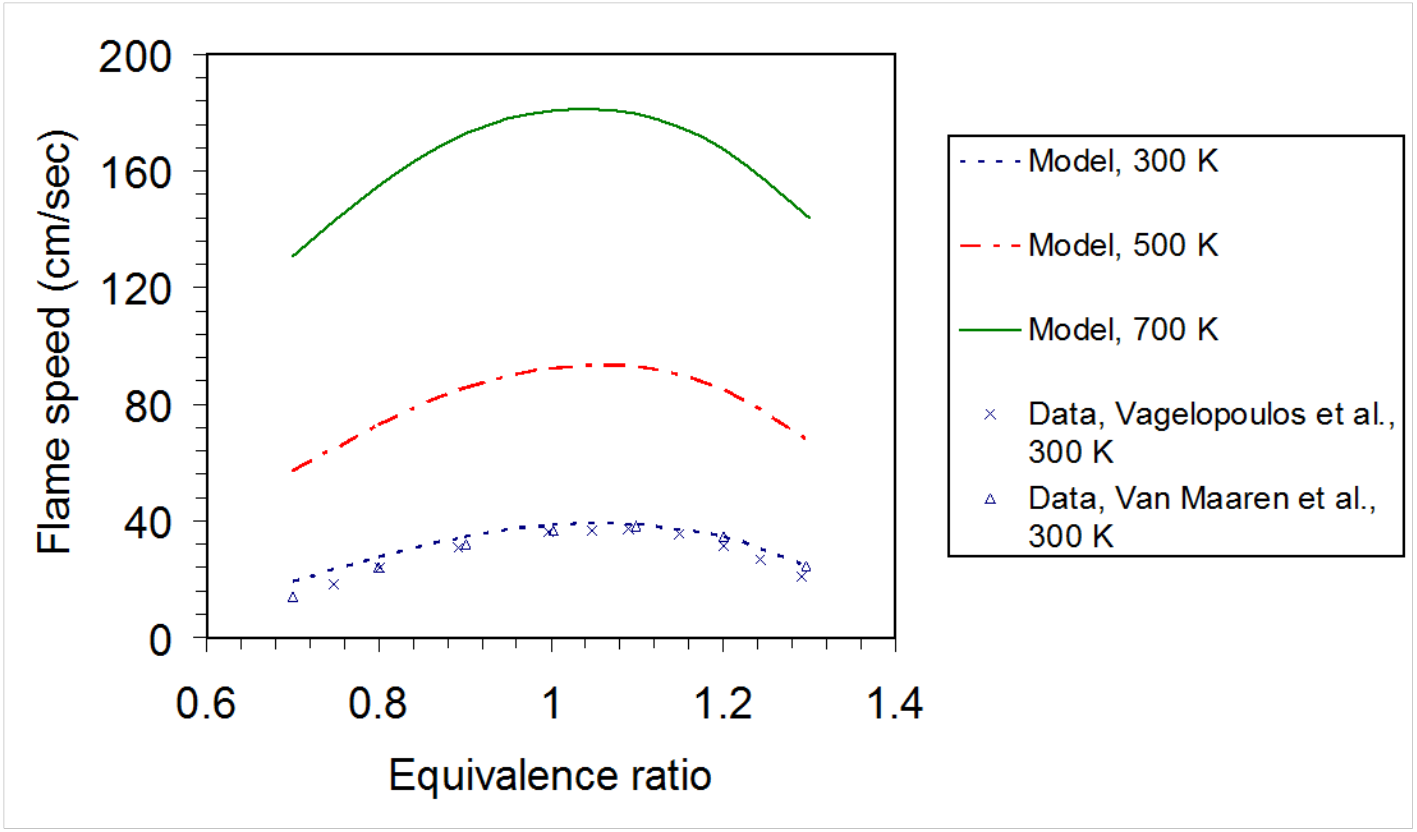
The set-up for flame-speed simulations has been simplified for better convergence

- **Auto-determination of:**
  - Initial temperature profile, including max (flame) temperature
  - Initial species profiles (products, intermediates)
  - Initial grid and domain for accurate solution
  - Appropriate solver parameters
- **User only provides**
  - Un-burned gas temperature
  - Reactant fractions
- **Provides convergence and accuracy for most cases, with no need for continuations**

reaction DESIGN

Results for GRI-mech show convergence in all cases without user intervention

- **84 cases run- all converged, with default solver settings**



- **Similar results found for n-heptane**
  - Required tighter tolerances and setting a few intermediates

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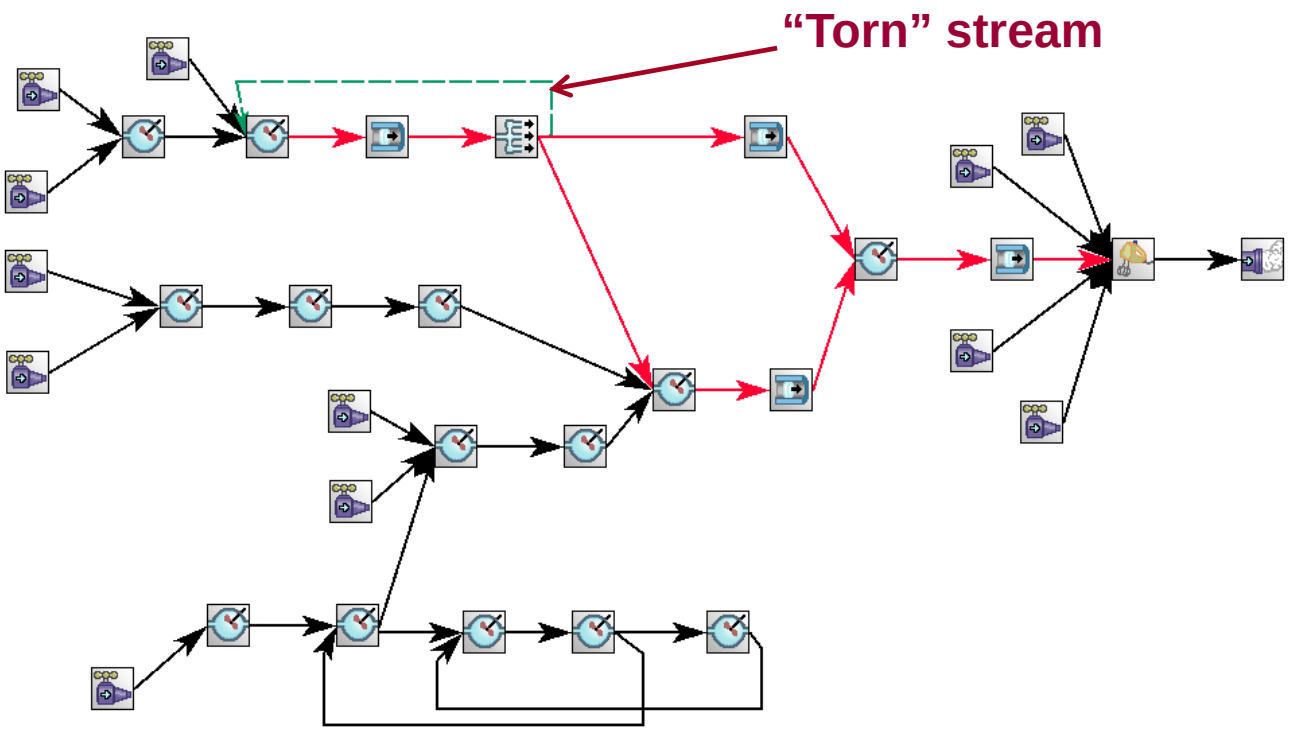
New “tear-stream” algorithm allows recycling in heterogeneous reactor networks

- **Iterative solver to converge “recycling” streams**
- **Multiple and nested “tears” are allowed**
- **Parallel “streams” allowed**



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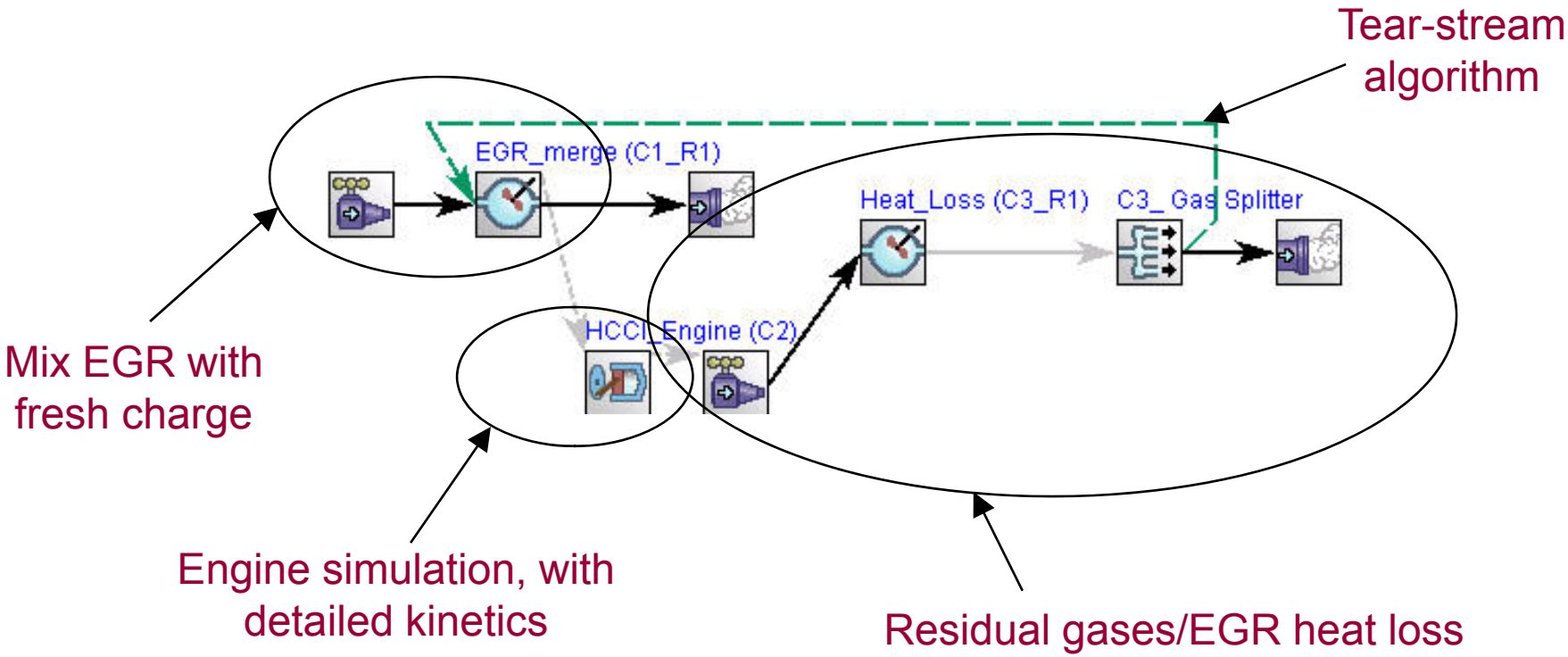
Example use of tear-stream: calculate IVC conditions for IC engine with EGR

- **Accounts for steady-state after several cycles**



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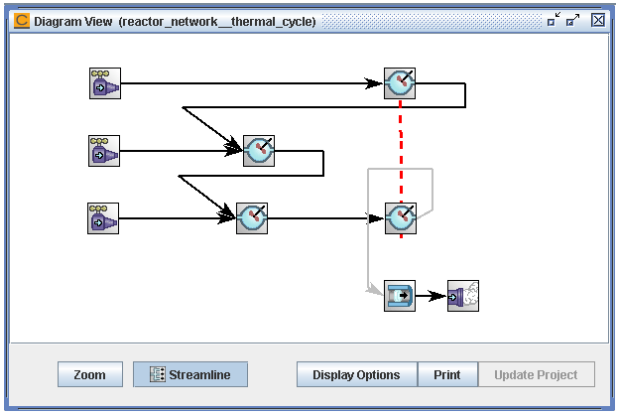
There have been many enhancements for reactor diagramming interactivity

- **Diagram enhancements**
  - Undo (Ctrl-Z) and Redo (Ctrl-Y) for all diagram actions
    - Multi-select, move, add/delete reactors, add/remove connections, straighten lines
  - Zoom option on Diagram View
  - Reactor "running" indicator
  - Click, Double-click and Right-click options
    - Highlight reactor node on Project Tree (click)
    - Direct link to input panel (double click)
    - View results (right click)
    - Analyze results with Graphical Post-processor (right click)
  - Option to streamline flow connections
    - Minimize splitter and mixer icons in complex diagrams
  - Context-sensitive mouse option
    - Non-modal method of switching between move and flow-connection operations



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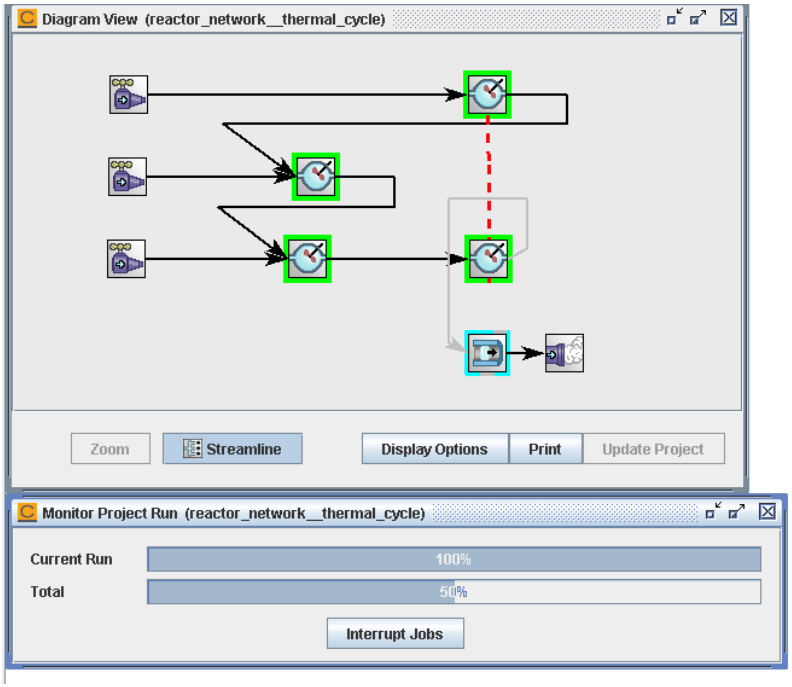
Other User Interface Enhancements

- **Progress indicators**
  - For transient problems
    - Progress vs. end time
  - For steady-state cases
    - Progress vs. grid-resolution criteria
  - For networks
    - Progress of tear-stream convergence
    - Per reactor as well as total project
  - For parameter studies
    - progress for each run and for all runs



- **Improved work-flow in project tree**
  - Project “clone” option to easily copy project
  - Run / Analyze options are grouped logically
    - Nominal case vs. Parameter-study options at each step
- **Export all data to Excel Workbook in one click**

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Summary of CHEMKIN-PRO

- More analysis capability
- More advanced reactor models
- More speed
- Better robustness
- Better work flow and interactivity

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