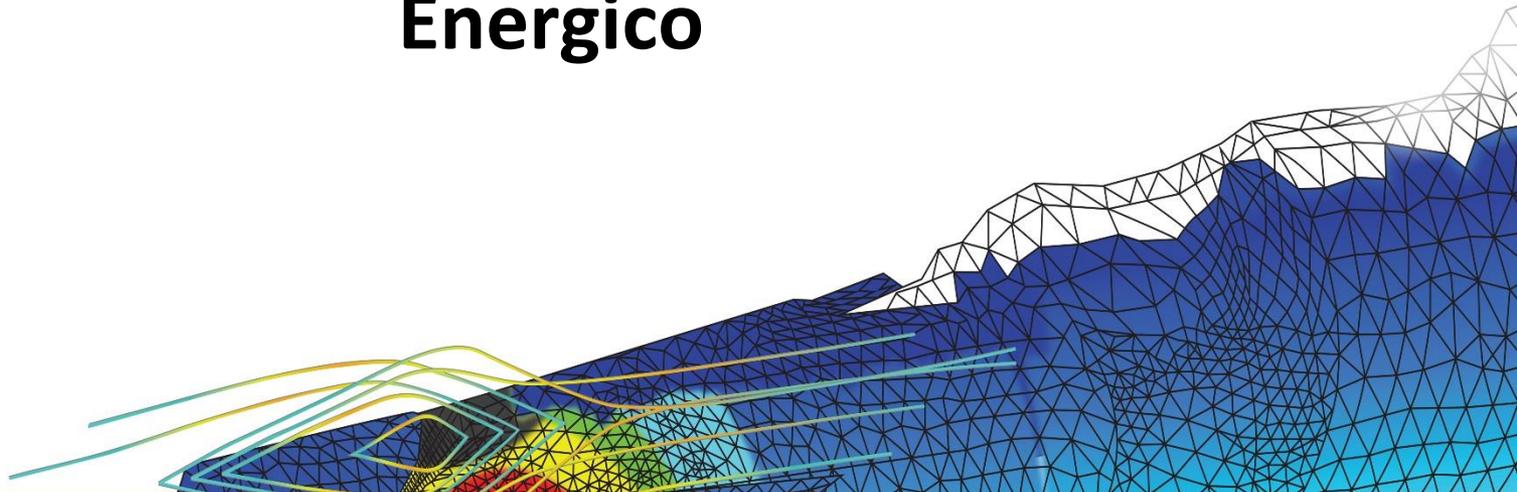


**ANSYS®**

**2019 R1 –  
ANSYS Chemkin-Pro,  
Reaction Workbench and  
Energico**

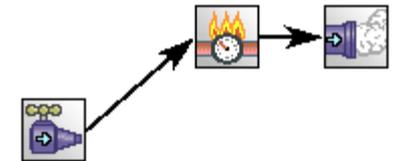
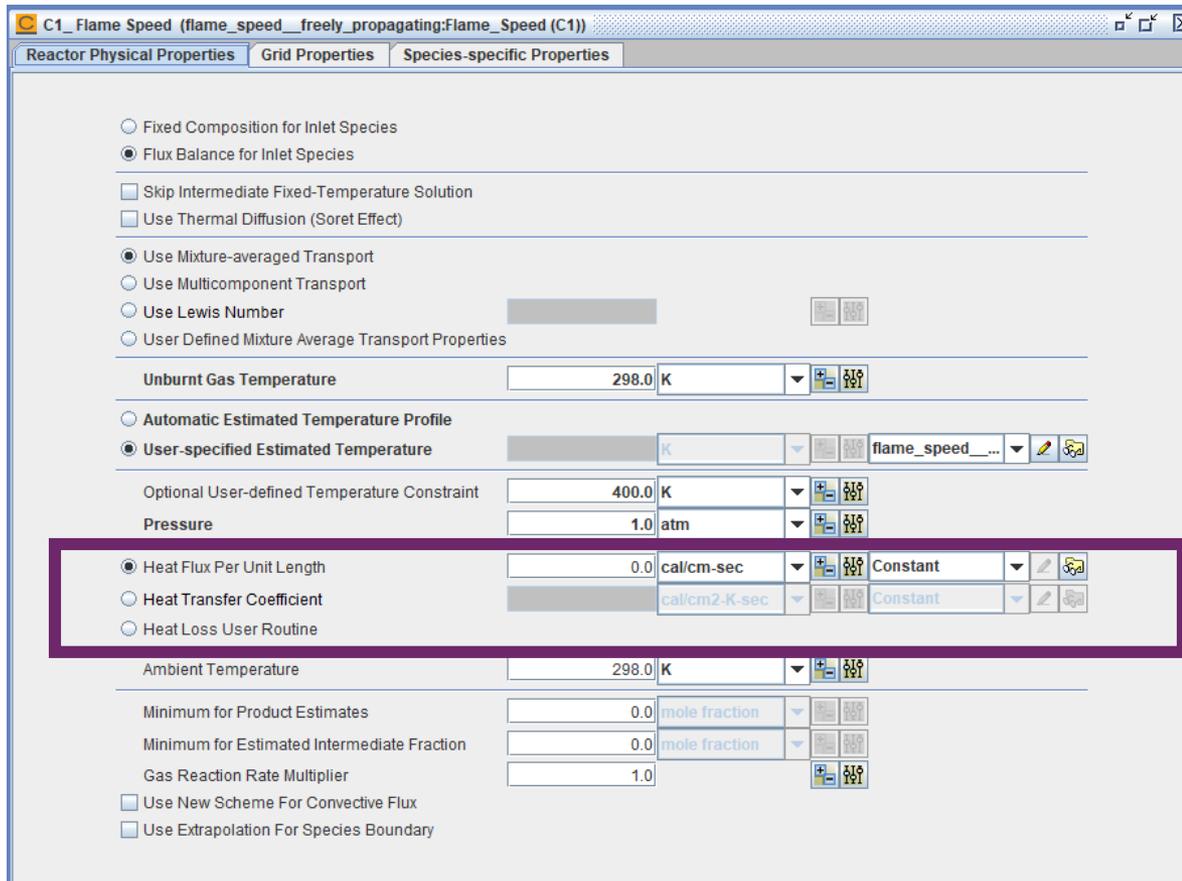


# Overview of new capabilities in 2019 R1

- **Enhancements for flame and flamelet simulations**
  - New heat-loss options for premixed Flame Simulators
  - Ability to specify an enthalpy deficit for Opposed Flow Flames
- **Improved CVD Reactor simulations**
  - More robust convergence with less sensitivity to initial grid
- **Usability enhancements**
  - Ability to specify the delimiter in \*.csv files used in Chemkin
  - Support of European number formats (allow non-standard radix)
  - Ability to save Reaction Path Analyzer (RPA) results for future analysis
- **Improvements to the Surrogate Blend Optimizer (SBO)**
  - Guidelines and recommendations for SBO fuel selections are now built into the UI
  - Improved estimation of RON/MON for blends with ethanol
- **Ability to handle internal walls in Energico**

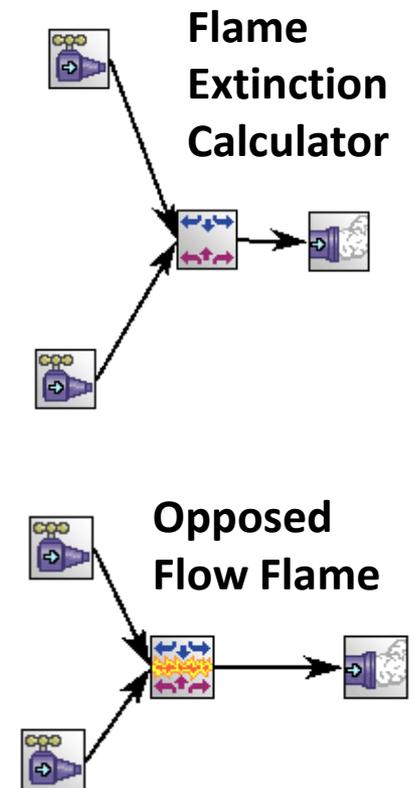
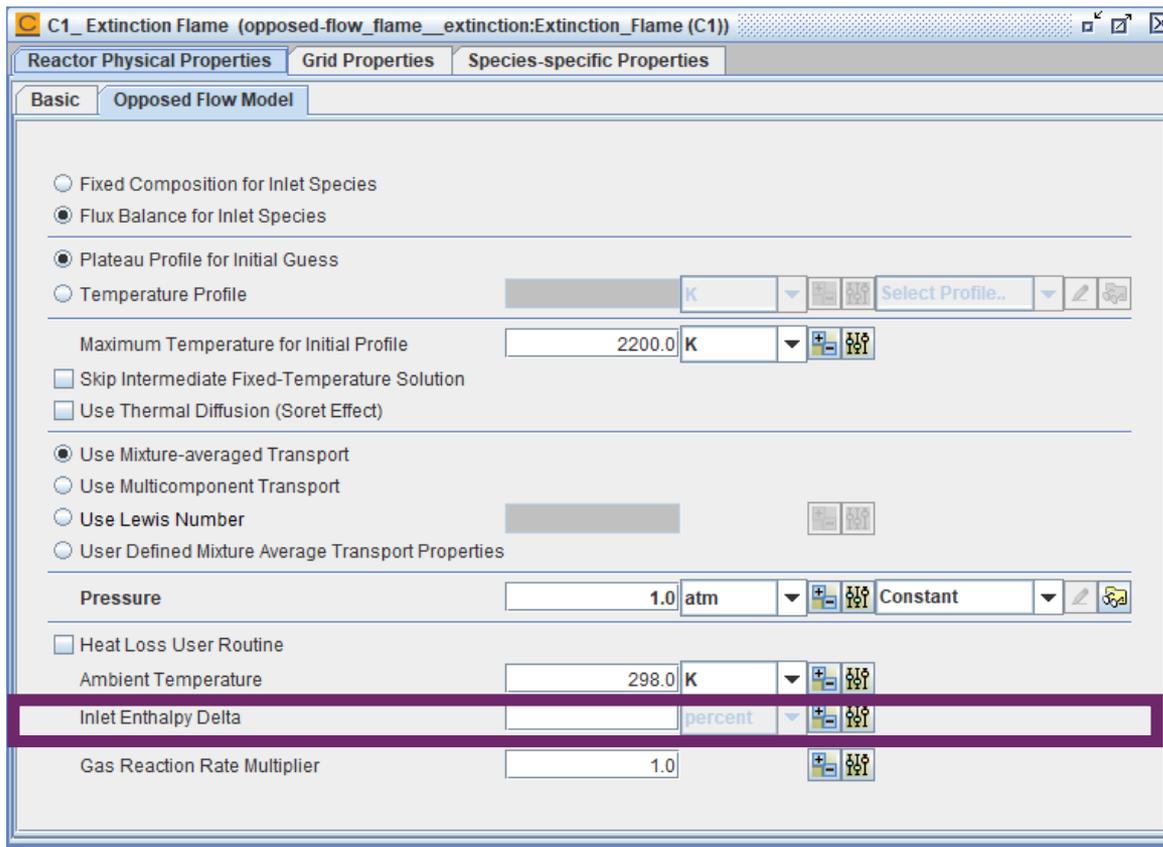
# New options for flame simulations: premixed flames

- Include effects of heat losses for non-adiabatic flames and flamelets using the Flame Speed Calculator



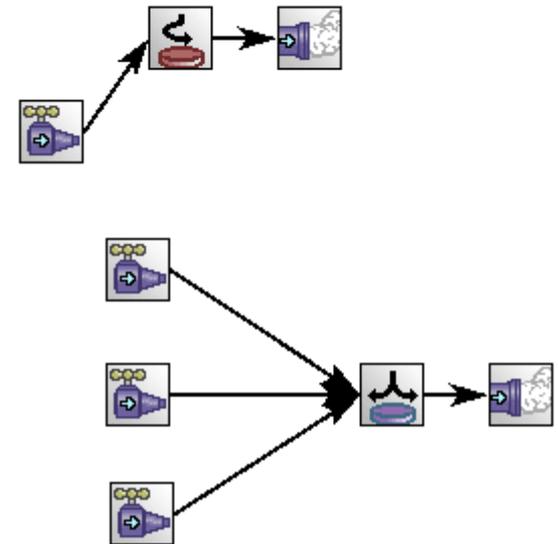
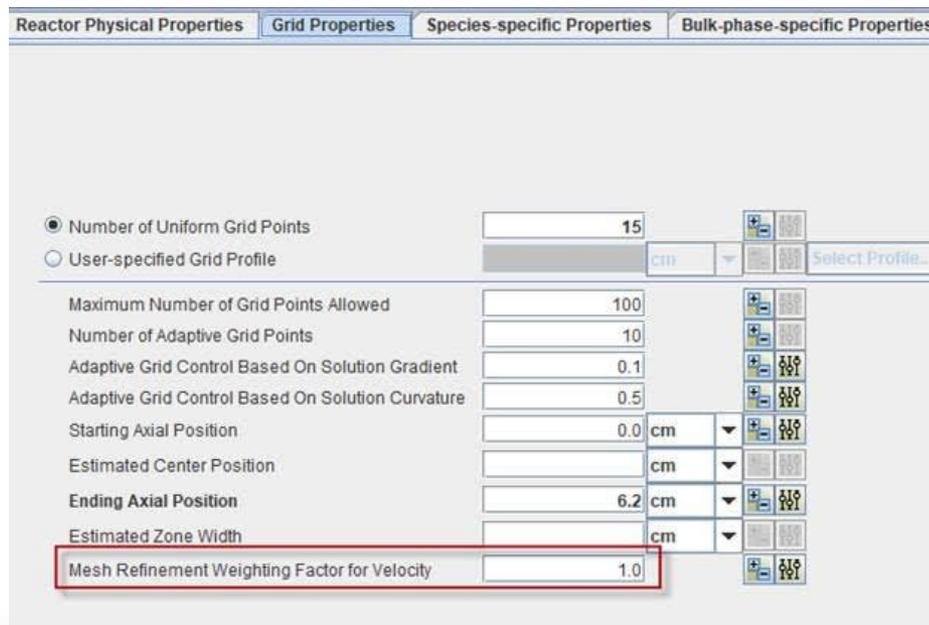
# New options for flame simulations: non-premixed flames

- Include effects of heat losses for non-adiabatic flames and flamelets by specifying an inlet “delta”
  - “delta” = percent of inlet enthalpy to be removed from the domain

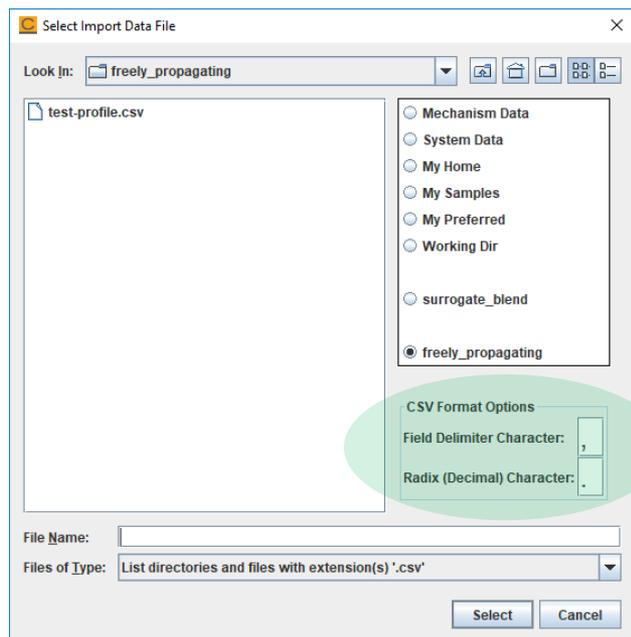


# New option improves convergence for CVD Reactors

- A grid that resolves the velocity profile is key to good convergence behavior for stagnation flows and rotating disk simulations
- A new option allows weighting the velocity profile gradients in the grid adaption to improve velocity resolution
  - A value  $> 1.0$  will increase the weight (recommended value is 2 for most cases)
  - Removes sensitivity of convergence to the initial grid and grid-adaption criteria

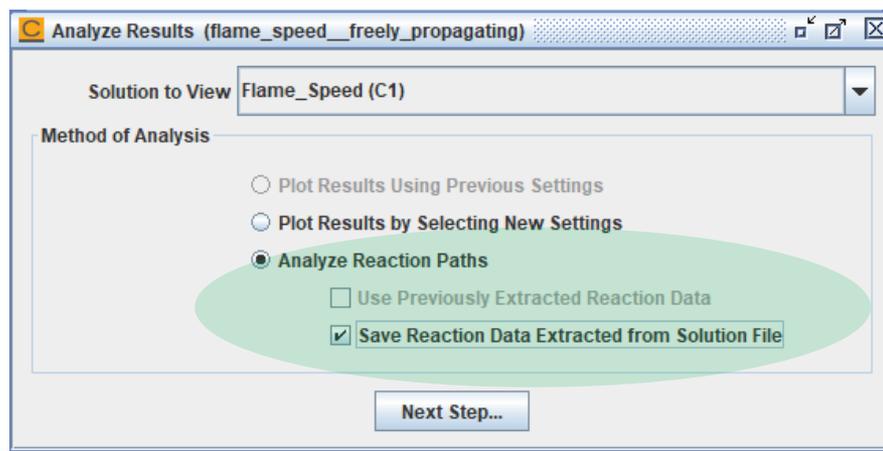


# Usability improvements in Chemkin-Pro



- **Flexibility in CSV formats**
  - Specify preferred delimiter
    - Default is comma
  - Radix (decimal) character can be set to something other than '.'

- **Ability to save and revisit Reaction Path Analyzer results**
  - Eliminate the need to reparse solution



# In Reaction Workbench, built-in guidance for blends

- Select from the recommended components (from the Model Fuel Library) for a complex (>3 components) or simple surrogate

The screenshot shows the 'Surrogate Blend Optimization' window with the 'Select Fuels' tab active. The window contains a table of fuel components with checkboxes for selection and numerical values. The 'mch' component is highlighted in yellow. Below the table, there are radio buttons for 'Gasoline', 'Jet Fuel', and 'Diesel', and a 'Recommendation Level' dropdown menu set to 'Complex'. A summary at the bottom states '4 fuels have been selected. c6h5ch3, mch, ic8h18, nc7h16'. Navigation buttons 'Previous' and 'Next' are at the bottom.

Category	Component	Value
Cycloalkanes	<input type="checkbox"/> decalin	Decalin 44
Cycloalkanes	<input checked="" type="checkbox"/> mch	Methylcyclohexane 22.5
Ether	<input type="checkbox"/> ETBE	Ethyl tert-butyl ether 24
Ether	<input type="checkbox"/> ch3och3	Dimethyl ether (DME) 55
Ether	<input type="checkbox"/> mtbe	Methyl tert-butyl ether (MTBE) 24
Hydrogen	<input type="checkbox"/> h2	Hydrogen 0
Methyl-ester	<input type="checkbox"/> mb	Methyl butanoate 30
Methyl-ester	<input type="checkbox"/> mb2d	Methyl crotonate 0
Methyl-ester	<input type="checkbox"/> mhd	Methyl palmitate 85.9
Methyl-ester	<input type="checkbox"/> mod	Methyl stearate 101
Methyl-ester	<input type="checkbox"/> mod9d	Methyl oleate 57
Methyl-ester	<input type="checkbox"/> mod9d12d	Methyl linoleate 38.2
Methyl-ester	<input type="checkbox"/> mod9d12d15d	Methyl linolenate 22.7
Sulfur compounds	<input type="checkbox"/> h2s	Hydrogen sulfide
iso-Alkanes	<input type="checkbox"/> hmn	Heptamethylnonane 15
iso-Alkanes	<input type="checkbox"/> ic12h26	iso-Dodecane 9
iso-Alkanes	<input type="checkbox"/> ic4h10	iso-Butane 0
iso-Alkanes	<input type="checkbox"/> ic5h12	iso-Pentane 25
iso-Alkanes	<input type="checkbox"/> ic6h14	iso-Hexane 34.0
iso-Alkanes	<input checked="" type="checkbox"/> ic8h18	iso-Octane 14

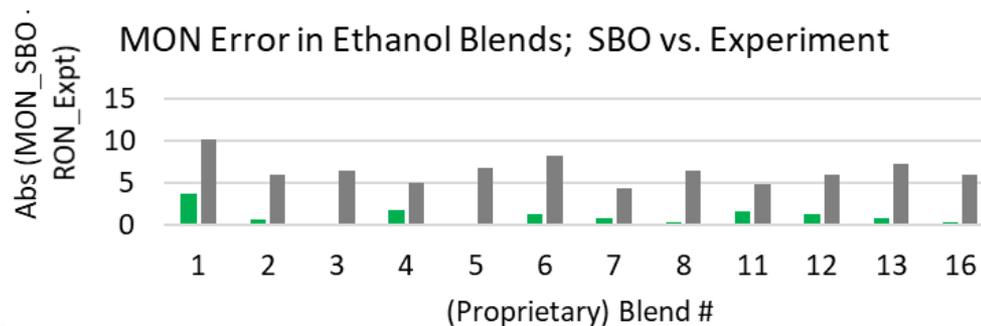
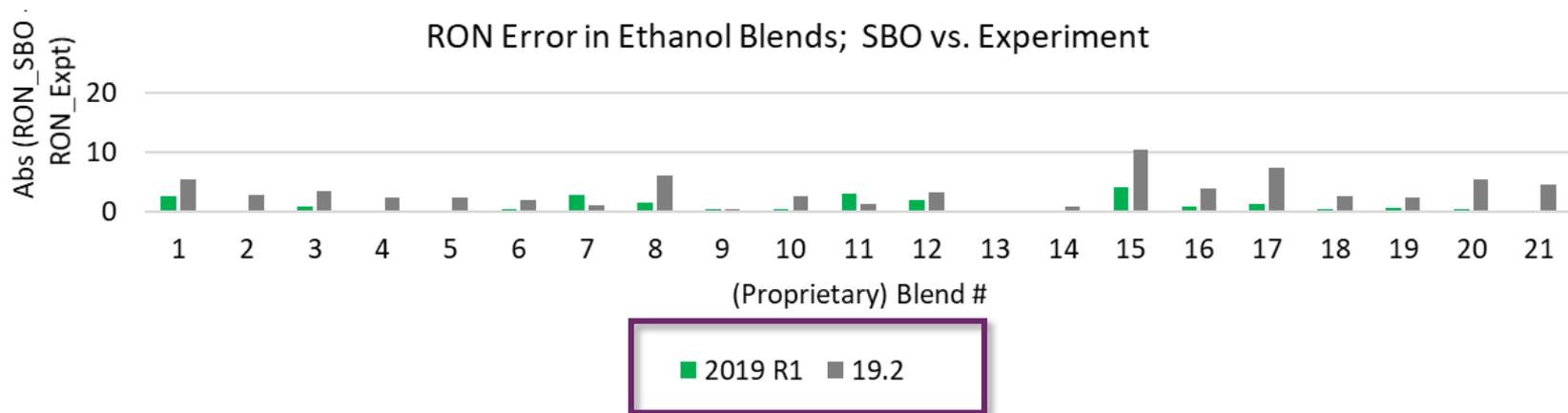
Highlights show recommended components for the target fuel

Select the target fuel and desired level of complexity

Summary of selections

# Improved RON/MON estimation for ethanol blends

- Updated the non-linear blending rules based on new data for ethanol-gasoline blends
- Average error for blends reduced to  $< 1.5\%$  for RON and MON



# Improved flexibility for Energico applications

- Energico now recognizes zero-thickness walls within the CFD simulation
  - Will enforce separation of fluid regions during zone creation

