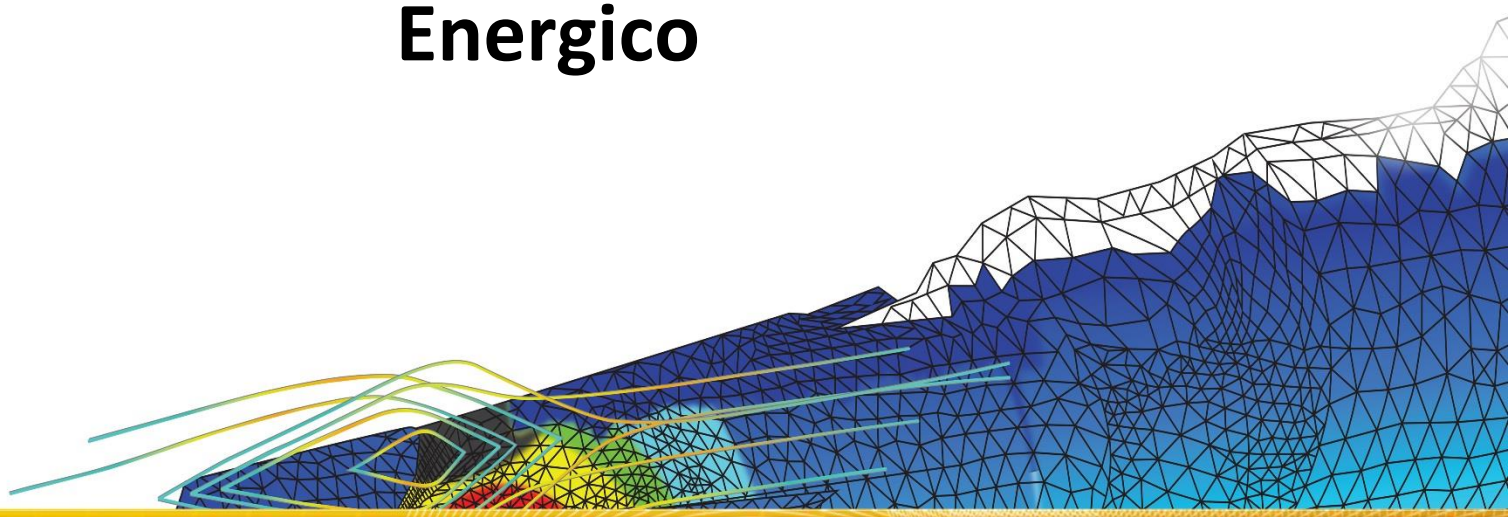
# 2019 R1 – ANSYS Chemkin-Pro, Reaction Workbench and Energico



# 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**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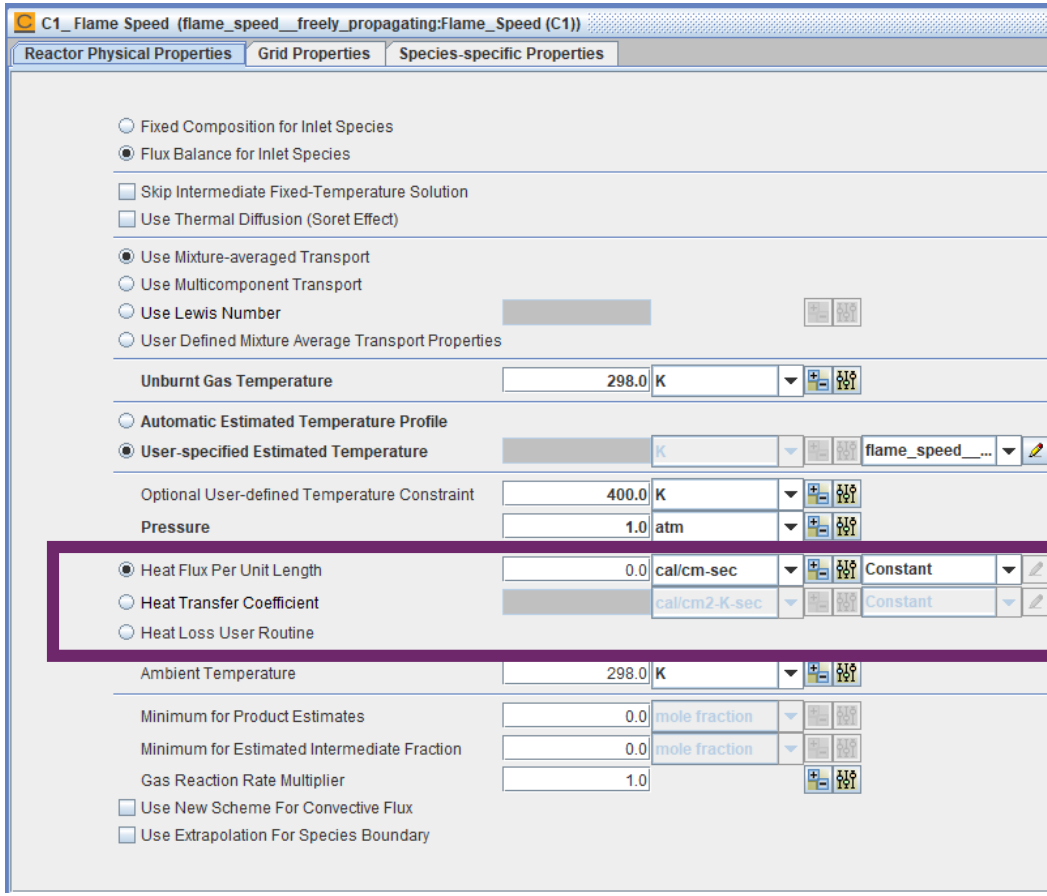
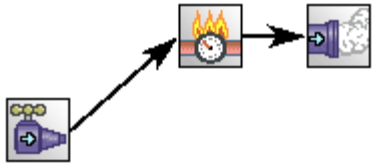
# New options for flame simulations: premixed flames

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

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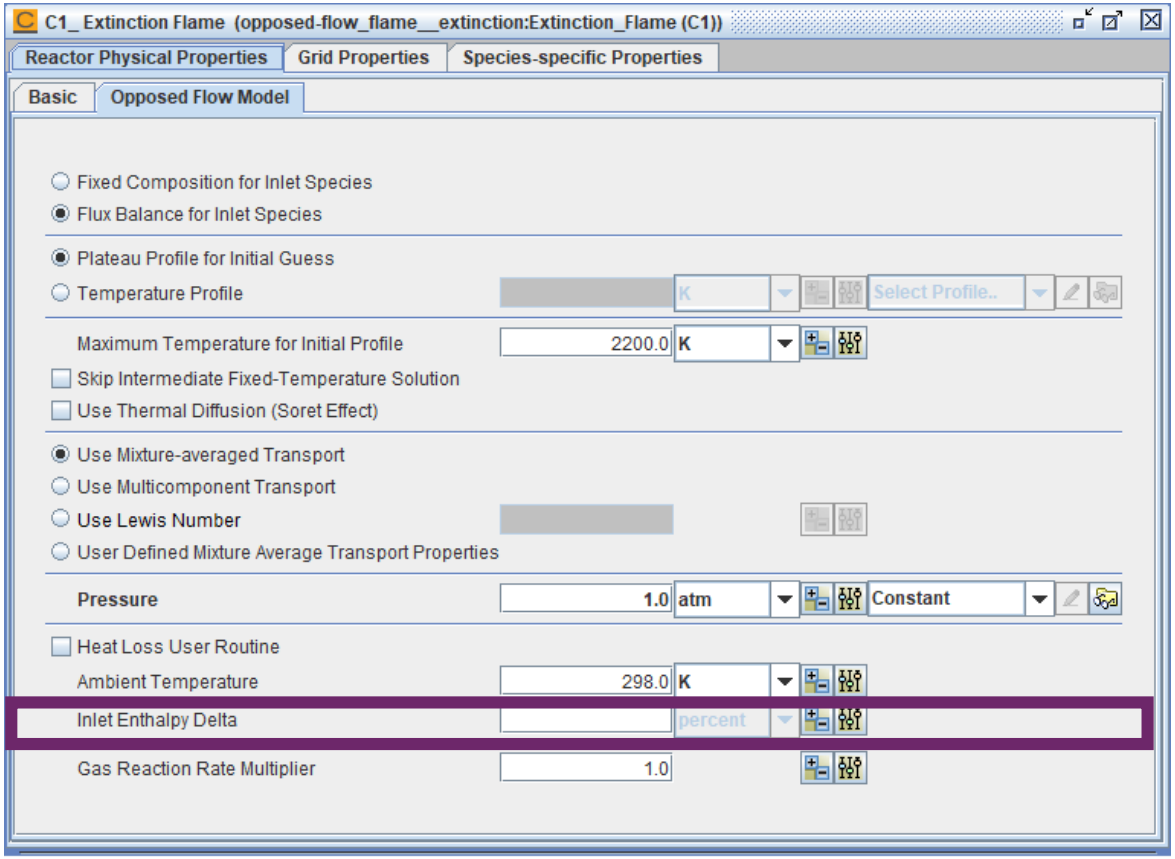
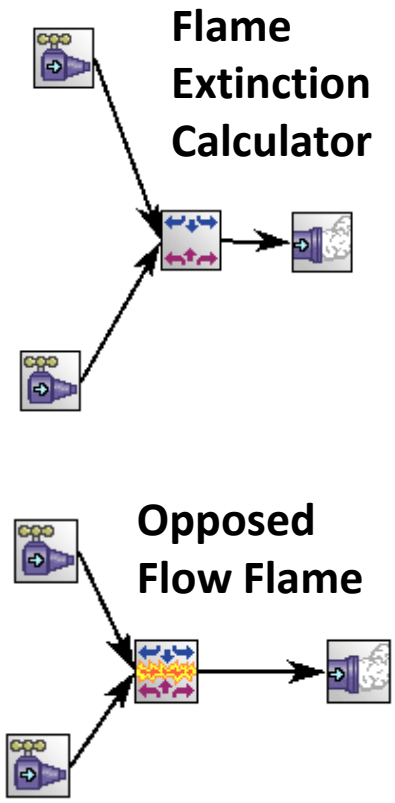
# New options for flame simulations: non-premixed flames

- **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**





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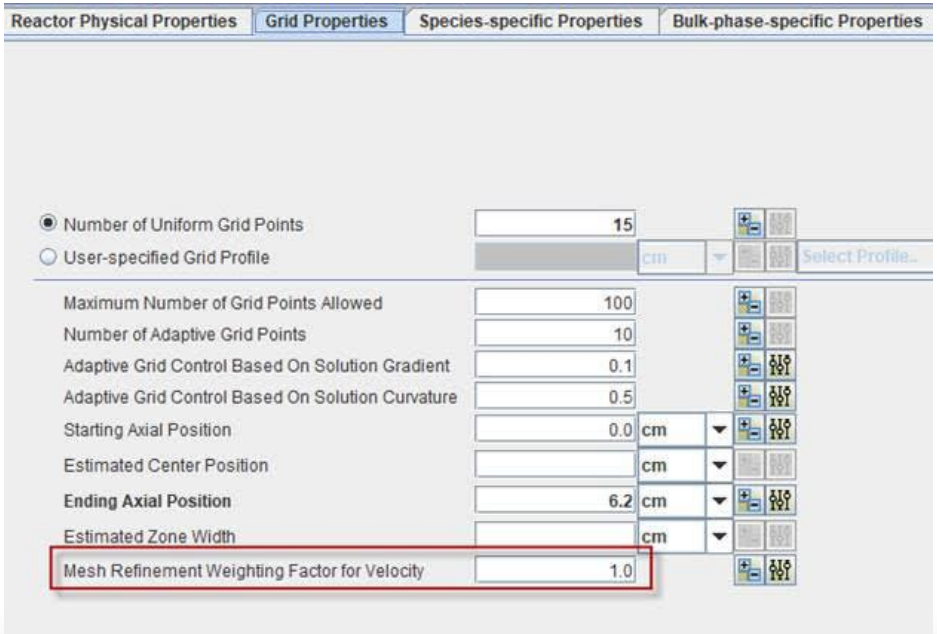
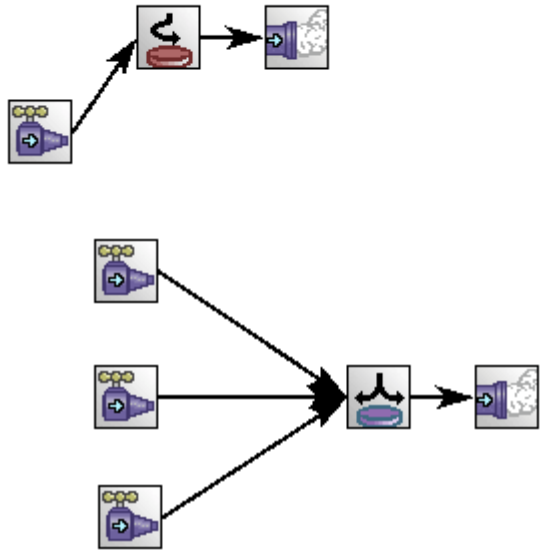
# New option improves convergence for CVD Reactors

- 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

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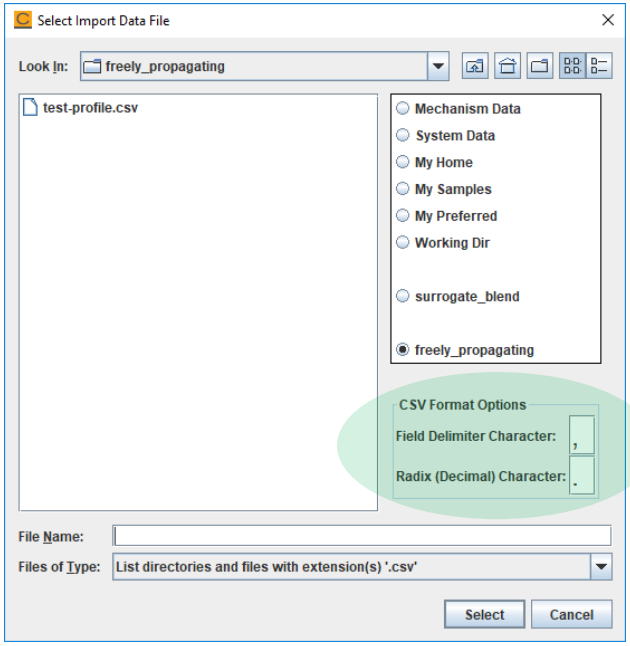
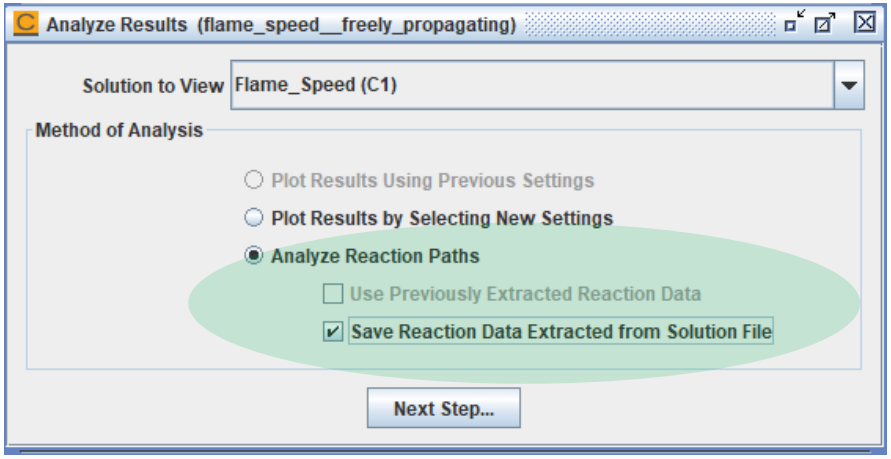
# Usability improvements in Chemkin-Pro




- **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**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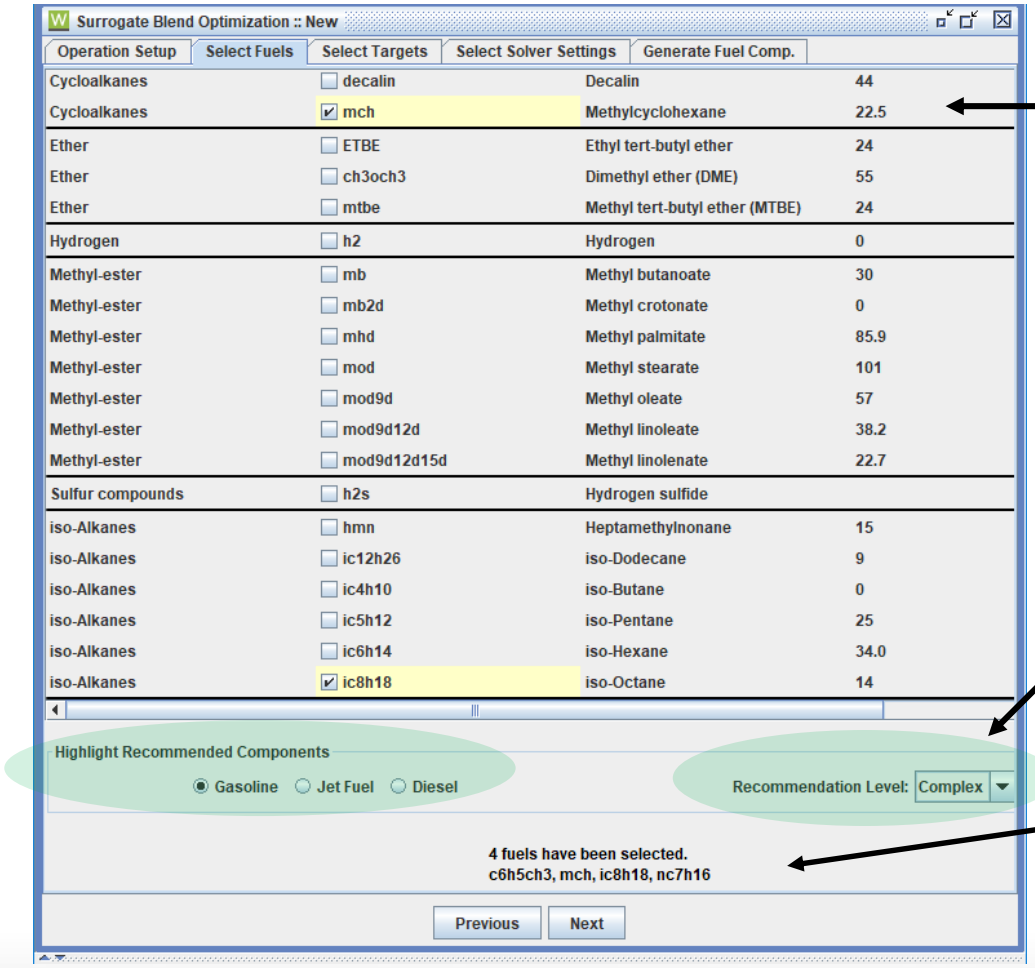
# In Reaction Workbench, built-in guidance for blends

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




Highlights show recommended components for the target fuel

Select the target fuel and desired level of complexity

Summary of selections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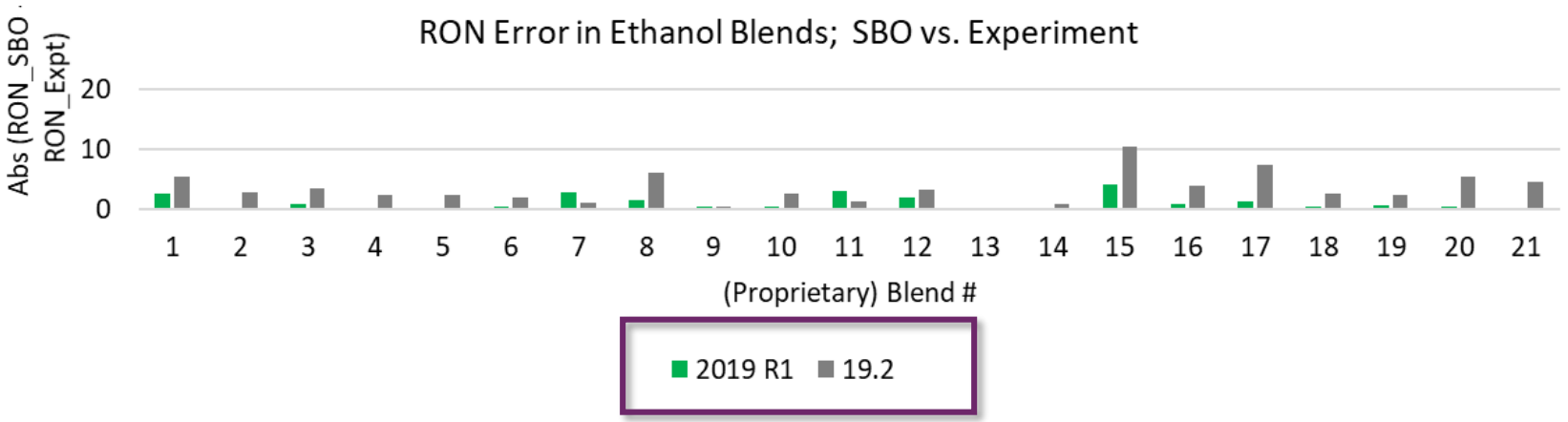
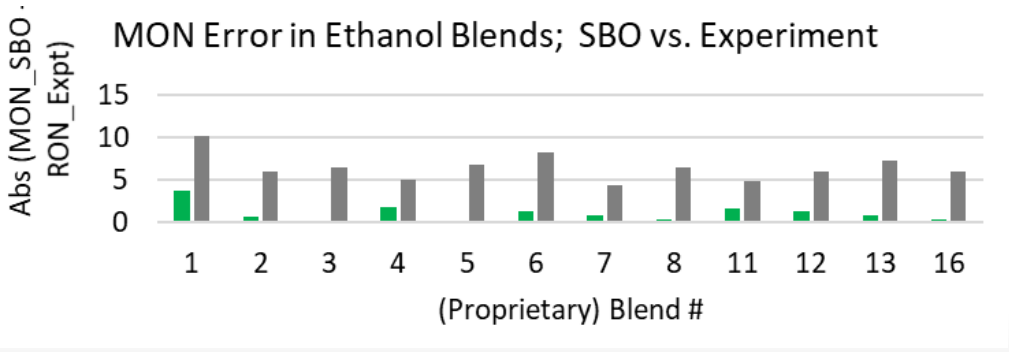
# Improved RON/MON estimation for ethanol blends

- **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**





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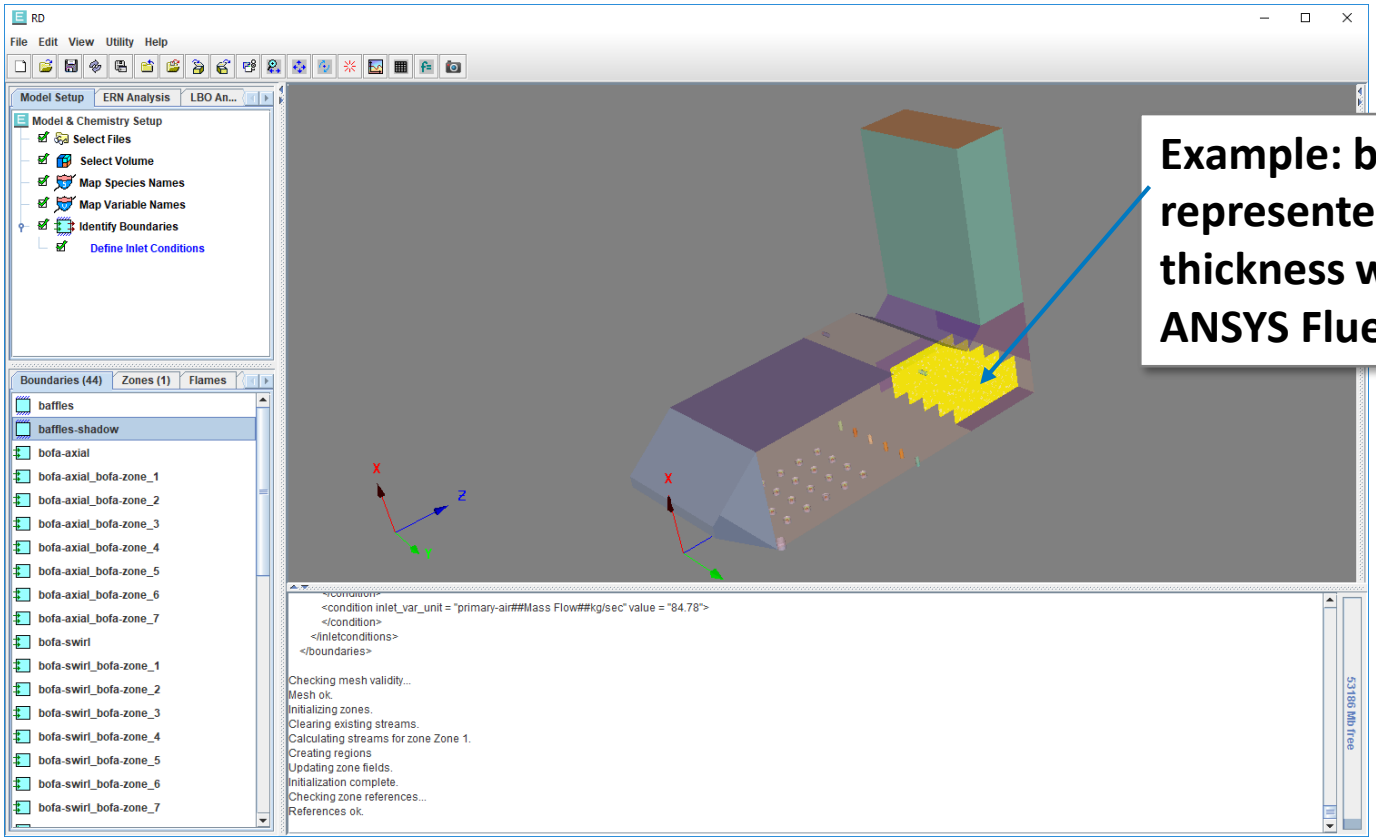
# Improved flexibility for Energico applications

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




**Example: baffles represented as zero-thickness walls in ANSYS Fluent**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