Realize Your Product Promise®



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

C1_Flame Speed (flame_speed_freely_propagating:Flame_Speed (C1))								
Reactor Physical Properties Grid Properties Species-specific Properties								
0) Fixed Composition for Inlet Species) Flux Balance for Inlet Species] Skip Intermediate Fixed-Temperature Solution							
	Use Thermal Diffusion (Soret Effect)							
) Use Mixture-averaged Transport) Use Multicomponent Transport) Use Lewis Number) User Defined Mixture Average Transport Properties	5						
	Unburnt Gas Temperature	298.0	к	▼ [*] - [*] →				
C @) Automatic Estimated Temperature Profile) User-specified Estimated Temperature		к	▼ 🔢 ∰ flame_speed ▼ 🗶 🗞				
	Optional User-defined Temperature Constraint Pressure	400.0	K atm	▼ *- ₩9 ▼ *- ₩9				
) Heat Flux Per Unit Length) Heat Transfer Coefficient) Heat Loss User Routine	0.0	cal/cm-sec cal/cm2-K-sec	▼ ■ Image: Second stant ▼ ∠ Image: Second stant ▼ ■ Image: Second stant ▼ ∠ Image: Second stant				
	Ambient Temperature	298.0	к	▼ 💾 ₩				
	Minimum for Product Estimates Minimum for Estimated Intermediate Fraction Gas Reaction Rate Multiplier] Use New Scheme For Convective Flux] Use Extrapolation For Species Boundary	0.0	mole fraction					





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

Fixed Composition for Inlet Species Flux Balance for Inlet Species Plateau Profile for Initial Guess Temperature Profile K E Select Profile. Z	Extinction Calculator
Maximum Temperature for Initial Profile 2200.0 K ▼ Image: With the second seco	
○ Use Multicomponent Transport ○ Use Lewis Number ○ User Defined Mixture Average Transport Properties Pressure 1.0 atm	Opposed Flow Flame
Heat Loss User Routine Ambient Temperature 298.0 Inlet Enthalpy Delta percent Gas Reaction Rate Multiplier 1.0	



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

Select Import Data File	×
.ook In: freely_propagating	▼ A C B B E
🗋 test-profile.csv	O Mechanism Data
	System Data
	O My Home
	My Samples
	My Preferred
	Working Dir
	surrogate_blend
	freely_propagating
	C SV Format Options
	Field Delimiter Character:
	Radix (Decimal) Character:
1	
ile <u>N</u> ame:	
iles of <u>Type</u> : List directories and files with e	extension(s) '.csv'
	Select Cancel

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

C Analyze Results (flame_speed_freely_propagating)						
Solution to View	Flame_Speed (C1)					
Method of Analysis						
O Plot Results Using Previous Settings						
O Plot Results by Selecting New Settings						
Analyze Reaction Paths						
Use Previously Extracted Reaction Data						
Save Reaction Data Extracted from Solution File						
Next Step						

- 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

W Surrogate Blend Opti	imization :: New		r⊏ ⊠	
Operation Setup Sel	lect Fuels Select Targets Select Solv	ver Settings Generate Fuel Comp.		
Cycloalkanes	decalin	Decalin	44	
Cycloalkanes	<mark>⊮ mch</mark>	Methylcyclohexane	22.5	Hignlights show
Ether	ETBE	Ethyl tert-butyl ether	24	wa a a wa wa a a ala al
Ether	ch3och3	Dimethyl ether (DME)	55	recommended
Ether	mtbe	Methyl tert-butyl ether (MTBE)	24	
Hydrogen	h2	Hydrogen	0	components for
Methyl-ester	mb	Methyl butanoate	30	the toward final
Methyl-ester	mb2d	Methyl crotonate	0	the target fuel
Methyl-ester	mhd	Methyl palmitate	85.9	-
Methyl-ester	mod	Methyl stearate	101	
Methyl-ester	mod9d	Methyl oleate	57	
Methyl-ester	mod9d12d	Methyl linoleate	38.2	
Methyl-ester	mod9d12d15d	Methyl linolenate	22.7	
Sulfur compounds	h2s	Hydrogen sulfide		Select the target
iso-Alkanes	in hmn	Heptamethylnonane	15	
iso-Alkanes	ic12h26	iso-Dodecane	9	/ tuel and desired
iso-Alkanes	ic4h10	iso-Butane	0	
iso-Alkanes	ic5h12	iso-Pentane	25	level of complexity
iso-Alkanes	ic6h14	iso-Hexane	34.0	
iso-Alkanes	<mark>⊯ ic8h18</mark>	iso-Octane	14	
Highlight Recommended	d Components asoline	Recommend	lation Level: Complex 💌	Summary of selections
	4 Tues c6h5c Previous	h3, mch, ic8h18, nc7h16		

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



