

# Reaction Path Analyzer in CHEMKIN-PRO



**reaction**  
DESIGN

CHEMKIN Workshop

August 3, 2008

LEADING THE WAY TO CLEAN COMBUSTION DESIGN

# Reaction Path Analyzer.

## A powerful tool for kineticists and engineers

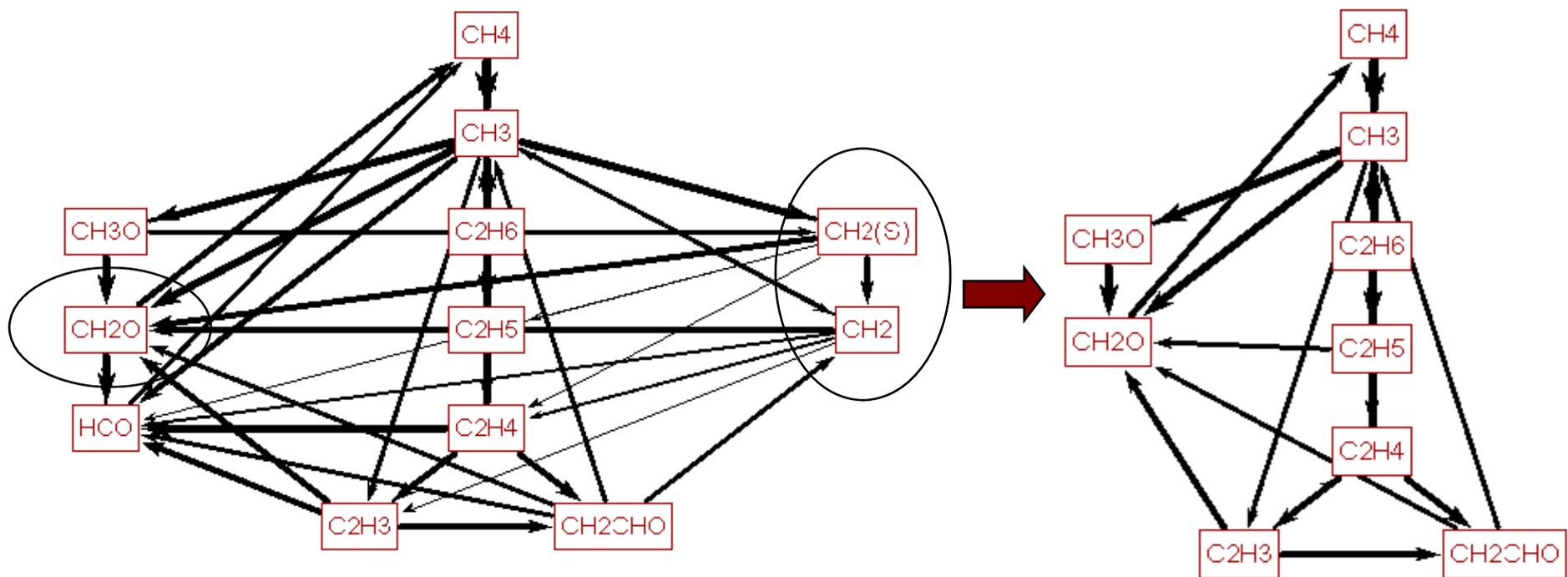
- **Graphically describe the pathways and relative contributions in the formation and depletion of chemical species**
- **Quickly analyze chemical pathways in a particular simulation**
- **Drastically reduces the analysis time**

# Reaction Path Analyzer: Seamlessly integrated with all reactor models

- **Based on Rate of Production (ROP) analysis**
  - No need to do any special calculation
- **Included in “Analyze Result” panel**
- **Load several solutions from a continuation run**
- **Load all zone solutions from a multizone model**
- **Select specific run from a parameter study**
- **Simple use with user controls**
  - Conceptual entity Side Species
  - Colors characterizing reaction pathways
  - Dynamic interface

# Concept of Side Species makes viewing major flux easier

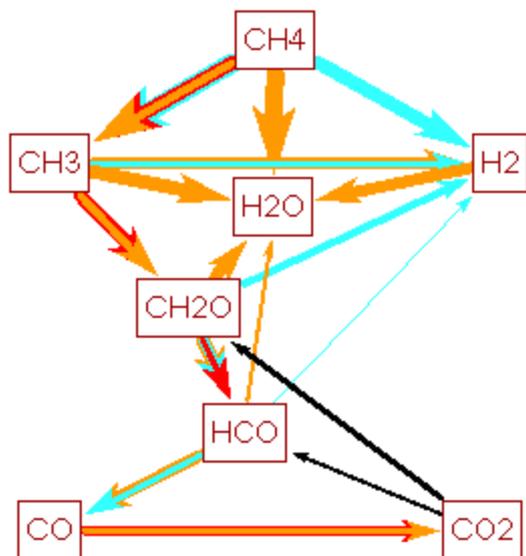
- **Side Species not drawn explicitly on the diagram**
  - E.g. radical pool H, OH, O, etc.



# Reaction pathways are colored based on Side Species

- Identify species involved just by looking at the color of an arrow

\* Example: H: cyan, O: red, OH: orange



Absolute Rate of Production from CH4 to CH3

$\text{CH}_3 + \text{H} + \text{M} \rightleftharpoons \text{CH}_4 + \text{M}$   
 $\text{CH}_4 + \text{O}_2 \rightleftharpoons \text{CH}_3 + \text{HO}_2$   
 $\text{CH}_4 + \text{H} \rightleftharpoons \text{CH}_3 + \text{H}_2$   
 $\text{CH}_4 + \text{O} \rightleftharpoons \text{CH}_3 + \text{OH}$   
 $\text{CH}_4 + \text{OH} \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}$



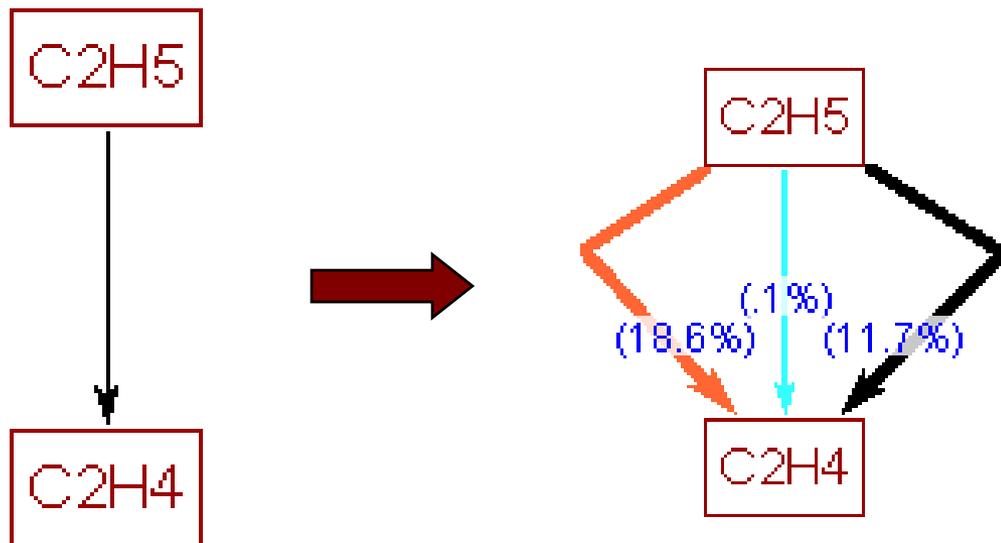
# Controls for display of reactions

- **Splitting Reaction Pathways**

- One line per reaction

- **Relative Rate of Production**

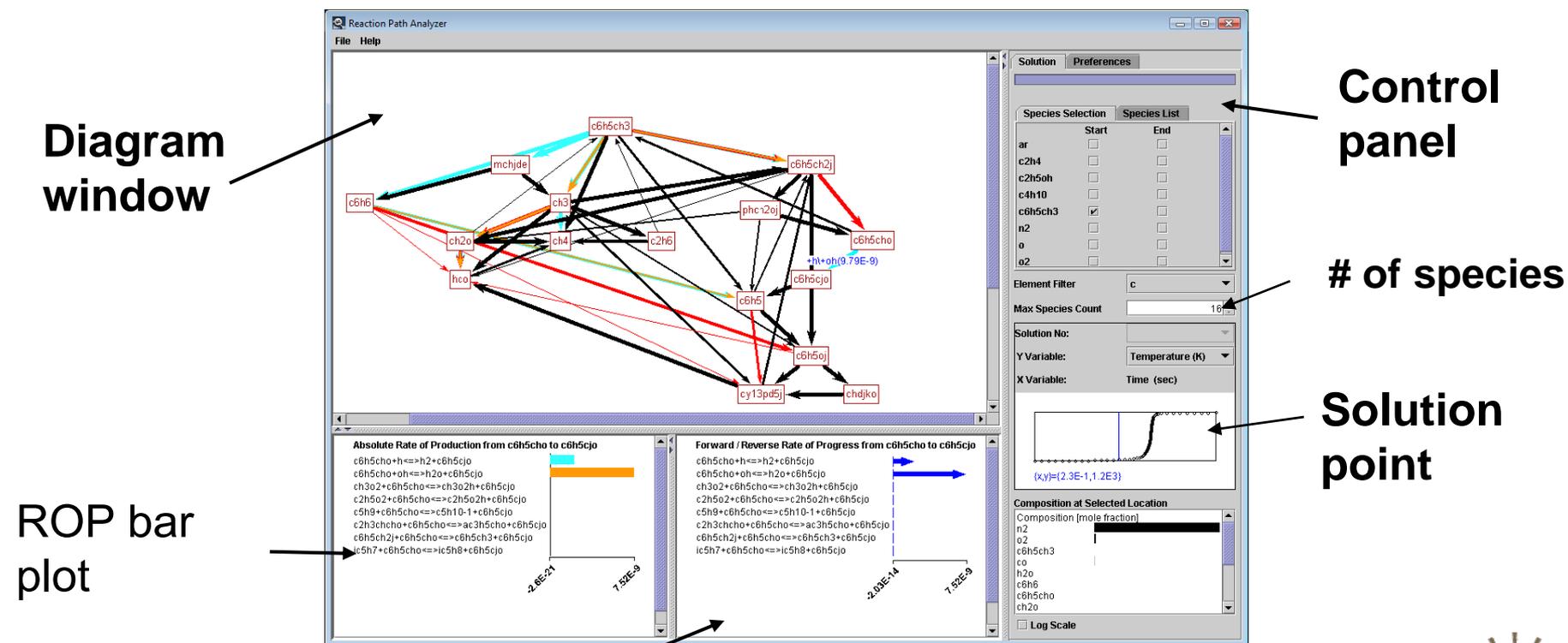
- Per reaction basis



# Controls, diagram, rate, and sensitivity analysis results in one window

## ● Dynamic controls

- Immediate effect on preference controls resulting in easier to use interface



Forward & reverse rate of progress OR Sensitivity plot



# Flexible controls. Dynamic zoom, relative cutoff fraction, labeling, and more

Reaction Path Analyzer

File Help

Solution Preferences

Layout Attributes

Tree  Hierarchical

Zoom (%) 100 Font Size 17

Borders On Species

Line Attributes

Thickness

Absolute ROP  Relative ROP  Constant

Arrows

Straight  One Per Reaction

Side Species in Line Labels

Display All Line Labels

Relative Cutoff Fraction 1.0E-16

Line Thickness

Side Species Colors

(ic5h7)2  
a1c2h  
a-ac5h10o  
a-ac6h12o  
a-bc5h10o  
a-bc6h12o  
ac3h4ch2cho  
ac3h4ch2coch3  
ac3h4coc2h5  
ac3h4coch3  
ac3h5chcoch3  
ac3h5cho  
ac3h5co  
ac3h5coo  
ac3h5oo  
ac5h10

Add Remove Clear

Absolute Rate of Production c6h6

c6h6+ch3<=>mchjde  
c6h5ch3+h<=>c6h6+ch3  
c6h6+oh<=>c6h5+h2o  
c6h6+o<=>c6h5oj+h  
c6h6+h<=>cyc6h7  
c6h6+oh<=>c6h5oh+h  
c6h5ch3+c6h5<=>c6h5ch2j+c6h6  
c6h6+h<=>c6h5+h2  
c6h6+h<=>linc6h7  
c6h6+o<=>chdko  
c6h6+o<=>cy13pd5+hco

Types of views

Zoom & font settings

Display Labeling of pathways

Relative Cutoff Fraction

Side species selection and coloring

- **Flame Simulator: Methane flame speed**