Coupling Fluid Dynamics and Chemistry

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REACTION DESIGN

STAR-CD User Conference
May 1-2, 2000
Detroit, Michigan

Outline of Presentation

- **Opportunities for CFD and chemistry**
  - *Broad spectrum of chemical reacting flows*
  - *Expectations for more physically accurate models*
- **Plans for detailed chemistry using CHEMKIN in STAR-CD**
  - *Introduction to CHEMKIN and Reaction Design*
  - *Hierarchical modeling approach*
  - *Integration of CHEMKIN into STAR-CD*
  - *Preliminary results*
- **Value of a Hierarchical Approach to Chemistry Modeling**
- **Conclusions**

Acknowledgements

John Deur, Sreenadh Jonnavithula, Greg McRae

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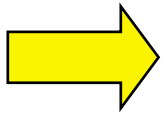
Computational Fluid Dynamics (CFD) software has impressive capabilities

- 3-D computational fluid dynamics in complex geometries is commonplace
- Visualization technology addresses 3-D flows, streamlines, particles
- Adaptive meshing greatly enhances speed of problem solving



While there has been much progress in advancing the state of the art of CFD -- there is a missing piece

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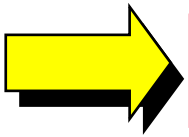
Incorporation of detailed chemistry is critical to many key industries

- Combustion
- Air pollution, climate
- Microelectronics
- Advanced Materials
- Petrochemicals
- Pharmaceutical production

All involve chemically reacting flows in complex geometries



Industry requires cost-effective solutions.

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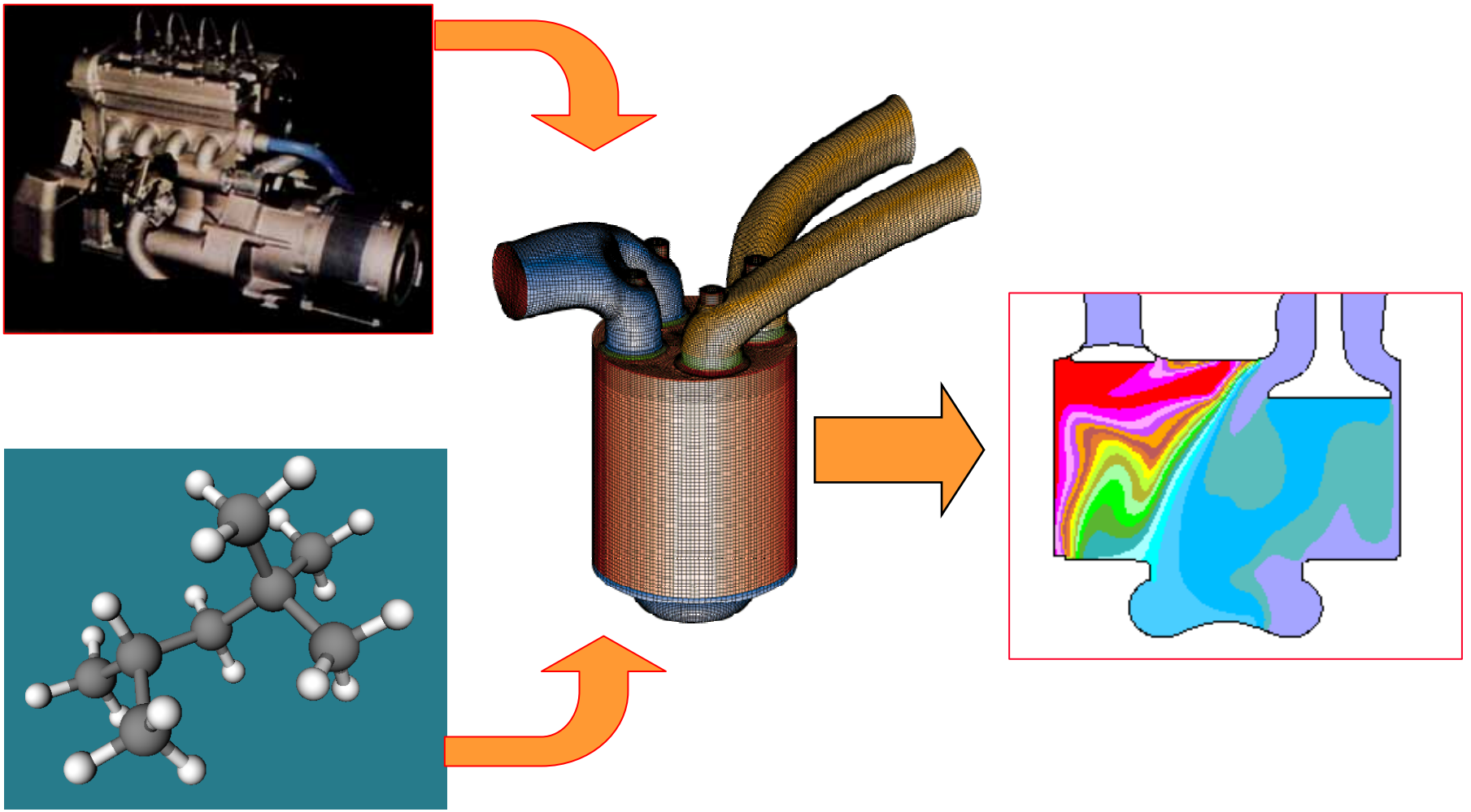
Fuels and Energy Management



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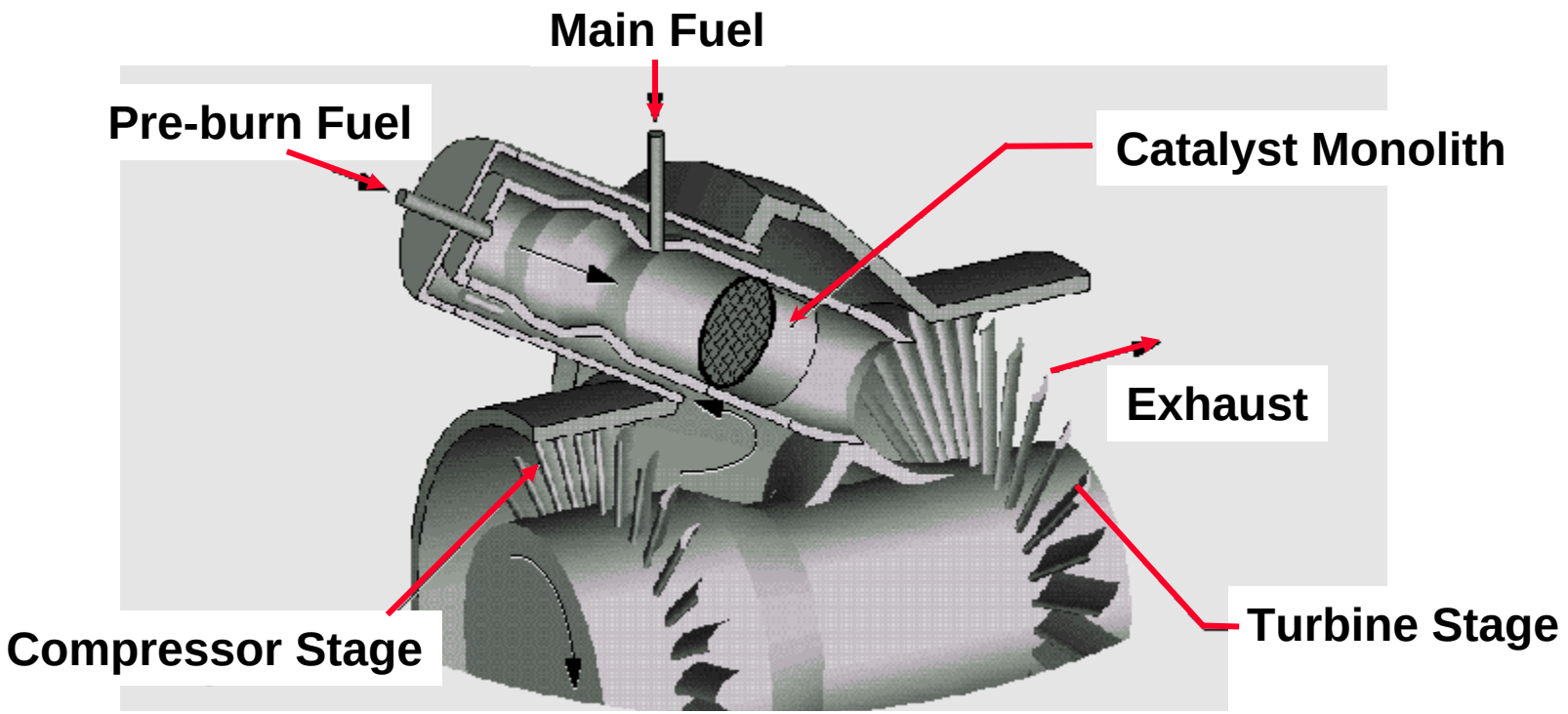
Catalytic combustion in turbines

The Challenge: Improve efficiency and reduce pollutant emissions (NO_x)



Main features of GE and Allison Systems Designs

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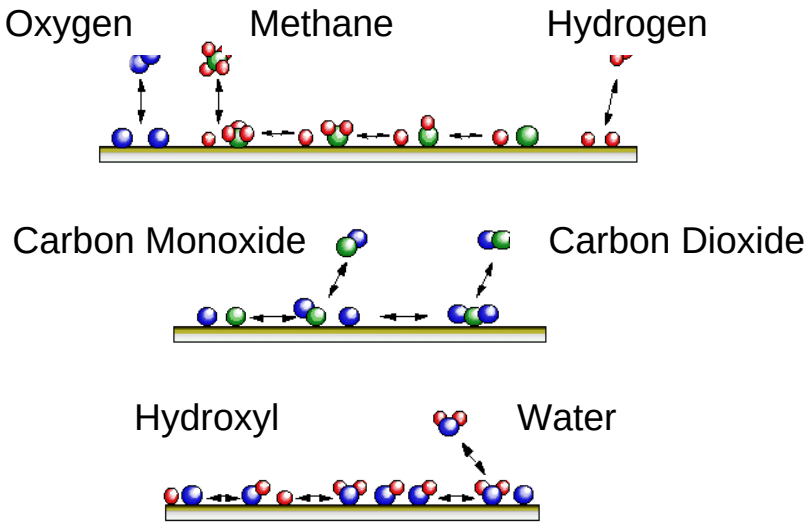
Detailed surface reaction mechanisms describe the combustion process

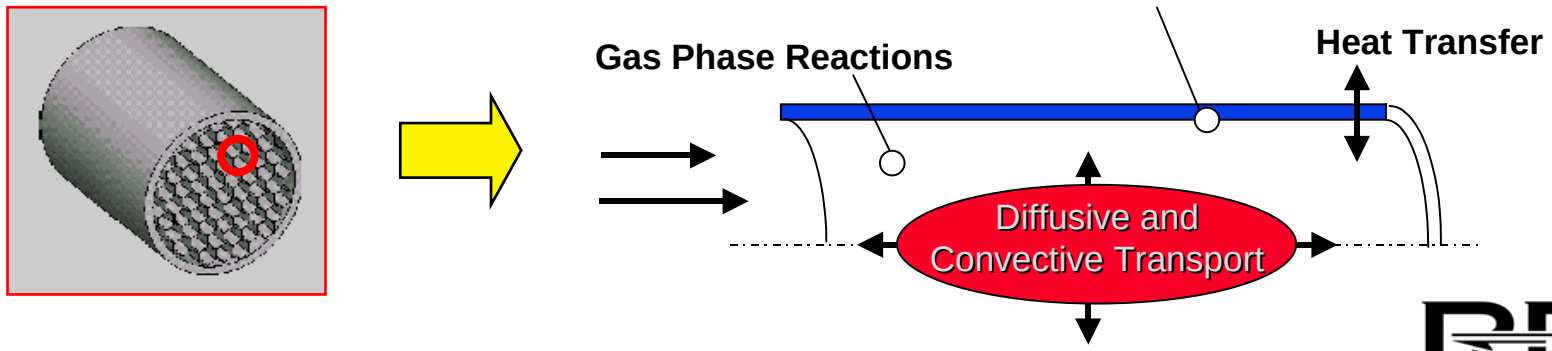
Surface Processes



Reaction Mechanism

Reaction	A	b	E(J/mol)
H2 + 2PT(S) => 2H(S)	0.046	0.0	0
2H(S) => H2 + 2PT(S)	3.70E+21	0.0	67400
H + PT(S) => H(S)	1.00	0.0	0
O2+ 2PT(S) => 2O(S)	1.80E+21	-0.5	0
O2+ 2PT(S) => 2O(S)	0.023	0.0	0
2O(S) => O2 + 2PT(S)	3.70E+21	0.0	213200
O + PT(S) => O(S)	1.00	0.0	0
H2O + PT(S) => H2O(S)	0.75	0.0	0
H2O(S) => H2O + PT(S)	1.0E13	0.0	40300
OH + PT(S) => OH(S)	1.00	0.0	0.0
OH(S) => OH + PT(S)	1.00E13	0.0	192800
H(S) + O(S) = OH(S) + PT(S)	3.70E+21	0.0	11500
H(S) + OH(S) = H2O(S) + PT(S)	3.70E+21	0.0	17400
OH(S)+ OH(S) = H2O(S) + O(S)	3.70E+21	0.0	48200
CO + PT(S) => CO(S)	0.84	0.0	0
CO(S) => CO + PT(S)	1.00E+13	0.0	125500
CO2(S) => CO2 + PT(S)	1.00E+13	0.0	20500
CO(S) + O(S) => CO2(S) + PT(S)	3.70E+21	0.0	105000
CH4 + 2PT(S) => CH3(S) + H(S)	0.01	0.0	
CH3(S)+ PT(S) => CH2(S)s + H(S)	3.70E+21	0.0	20000
CH2(S)s + PT(S) => CH(S) + H(S)	3.70E+21	0.0	20000
CH(S) + PT(S) => C(S) + H(S)	3.70E+21	0.0	20000
C(S) + O(S) => CO(S) + PT(S)	3.70E+21	0.0	62800
CO(S) + PT(S) => C(S) + O(S)	1.00E+18	0.0	184000

Geometry and Fluid Flow



Ref: Deutschmann, Goralski, Schmidt, Raja & Kee; 27th Symposium (International) on Combustion, 1998

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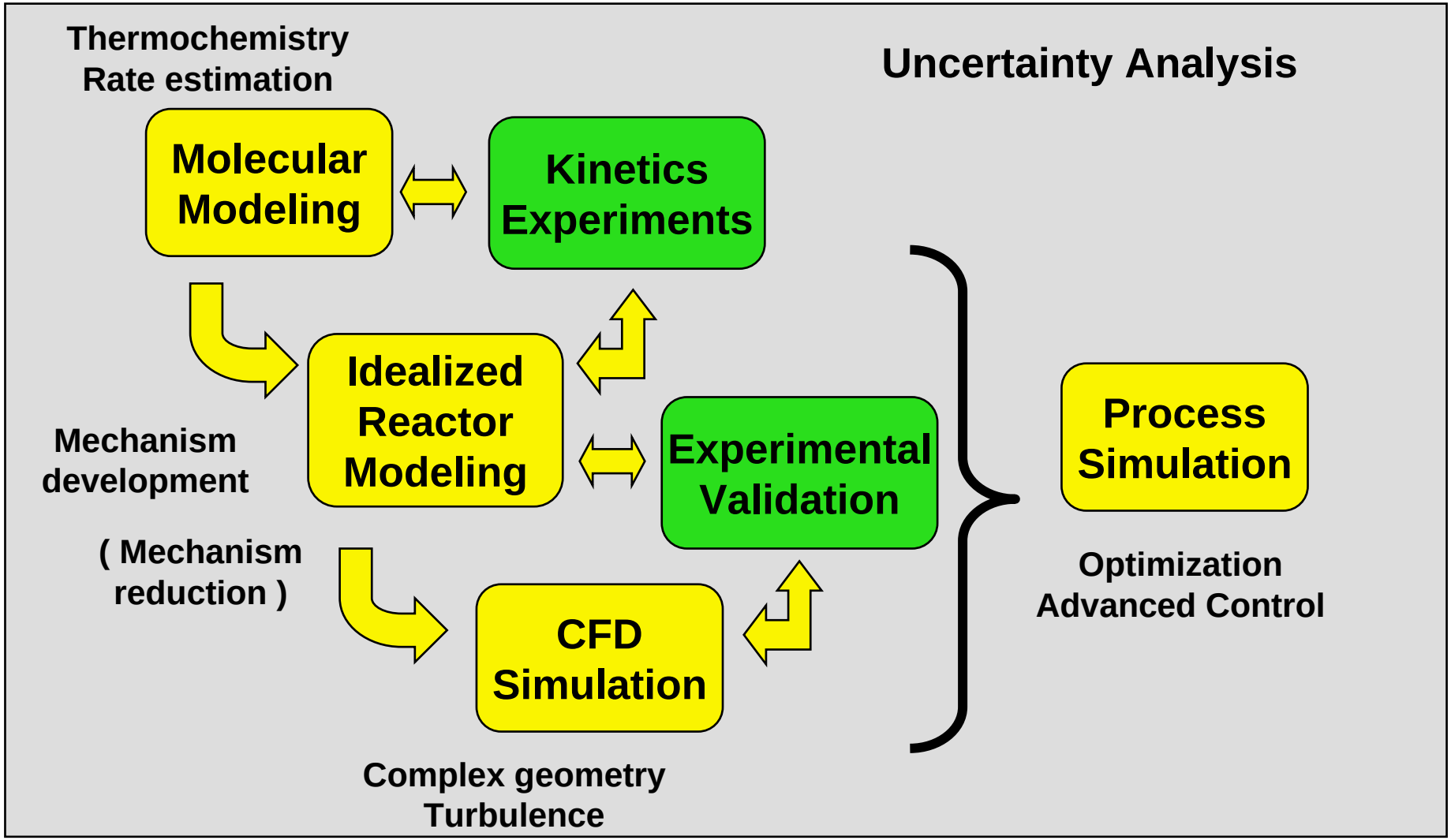
Reaction Engineer "Workbench" requires integration across many disciplines



REACTION DESIGN

SUCCESS WILL DEPEND ON:

- Seamless coupling of fluid flow models to detailed treatment of chemical and physical phenomena
- Integration across length & time scales
- Improved numerical algorithms
- Commercialization of new methods

Adapco/CD has teamed with Reaction Design to develop new chemistry capability

- **CHEMKIN is a *de facto* standard in describing and modeling chemically reacting systems**
- **Reaction Design is the exclusive worldwide distributor of CHEMKIN**
- **Reaction Design will provide a "plug-in" to STAR-CD to allow inclusion of detailed kinetics capability**
  - *Ability to read CHEMKIN input files*
  - *Use of CHEMKIN gas-phase, surface, and transport libraries*
  - *Implementation of "stiff" equation solution methods for transient and steady-state reacting flows*
  - *Surface chemistry module for solving surface site coverage*
  - *Expected release: September, 2000*

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Linkage Between Adapco and Reaction Design (STAR-CD + CHEMKIN)

STAR-CD

- Navier-Stokes Equations
- Energy Transport
- Species Transport
- Turbulence models

+

CHEMKIN 3.5

- Gas-phase Chemistry
- Surface Chemistry
- Multicomponent Transport
- Property databases

STAR-CD + CHEMKIN

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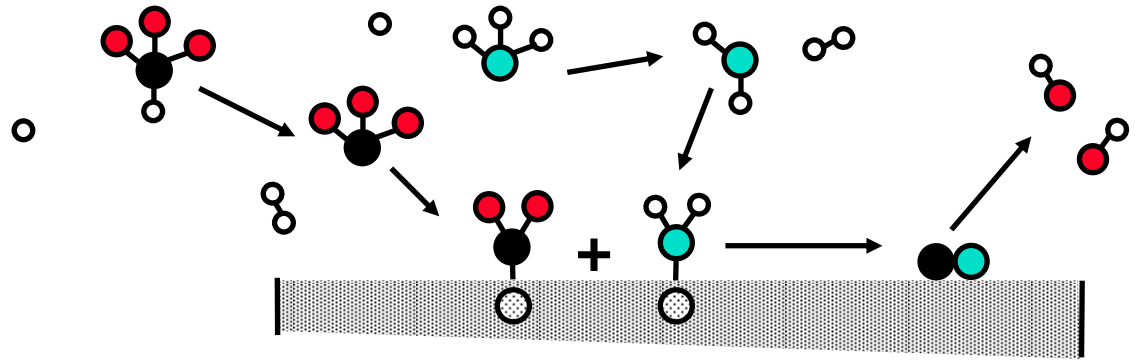
CHEMKIN has many unique features

- Ability to treat detailed surface kinetics
  - Surface-species coverage dependence
  - Multiple materials
- Robust “stiff”-equation solvers
- Extensive error-checking for reaction sets
  - Mass balance
  - Charge balance
  - Site balance
- Rigorous multi-component transport treatment
- Multitude of reaction-rate formulation options
  - Elementary or Global reactions
  - Pressure dependence
- Ability to treat plasma kinetics and plasma-surface interactions

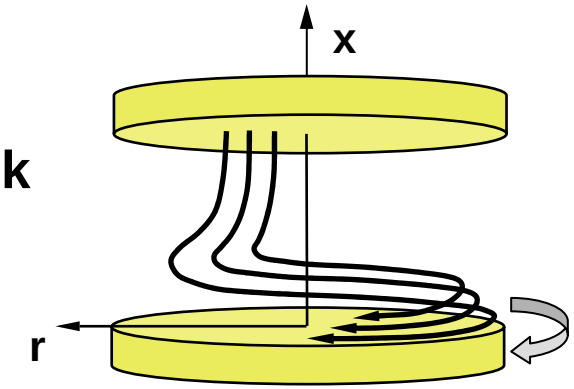
REACTION DESIGN

CHEMKIN: A set of tools designed to model complex chemical kinetic processes



- CHEMKIN Applications are programs built from these tools to represent specific reactor types
  - Example: SPIN

Rotating Disk Reactor

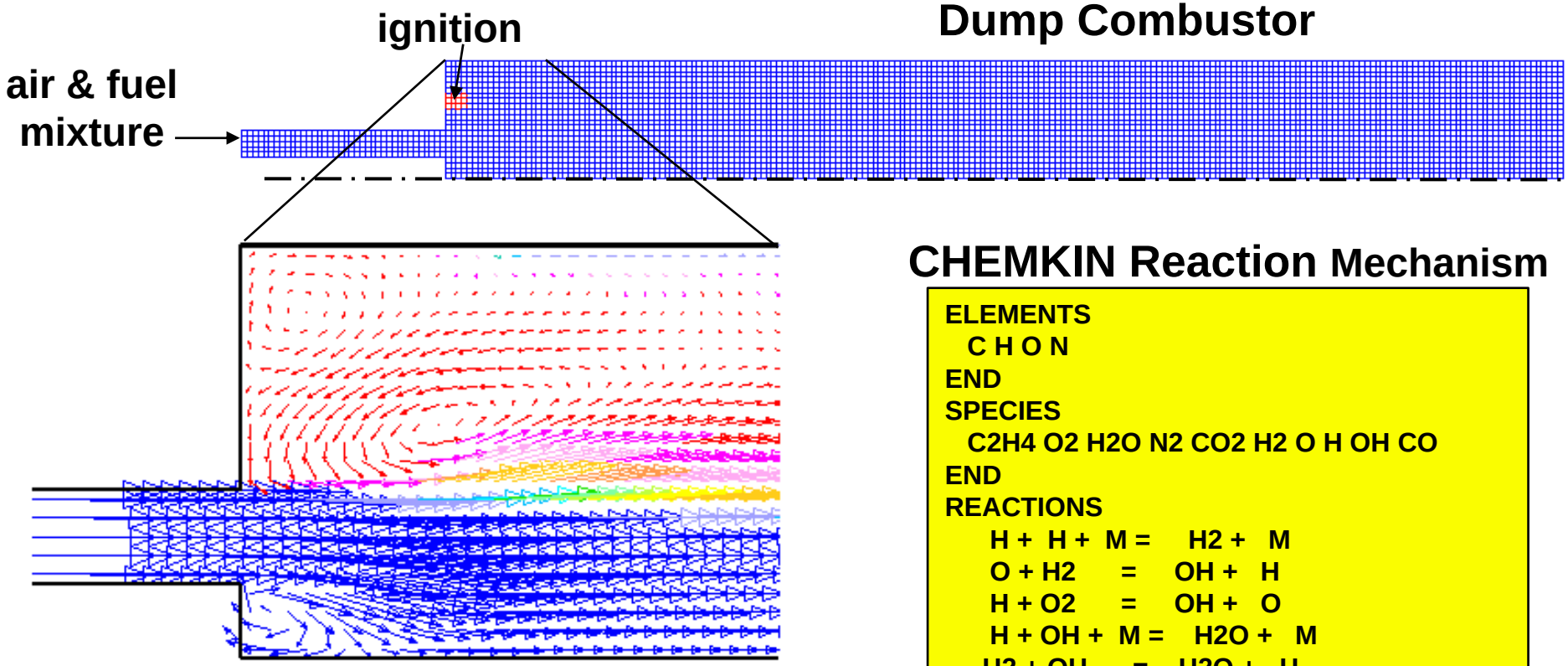


REACTION DESIGN

How will CHEMKIN 3.5 be incorporated into STAR-CD?

1. Incorporate fast, robust solver for gas-phase kinetics
   - Cell-by-cell
   - Optimized for “stiff” kinetics
   - Transient and Steady-state
2. Incorporate surface chemistry solver module
   - Closely couple with gas species boundary flux
   - Allow coverage-dependent surface chemistry
   - Determine surface species site fractions
3. Incorporate multicomponent molecular transport model for determination of diffusion coefficients, thermal conductivity, and viscosity
4. Access latest CHEMKIN databases for thermodynamic and transport properties

Test problem with preliminary solver shows coupling of turbulence and kinetics



- 4788 cells
- Flowfield includes recirculation
- Reversible reaction kinetics
  - 10 species
  - 8 reversible reactions

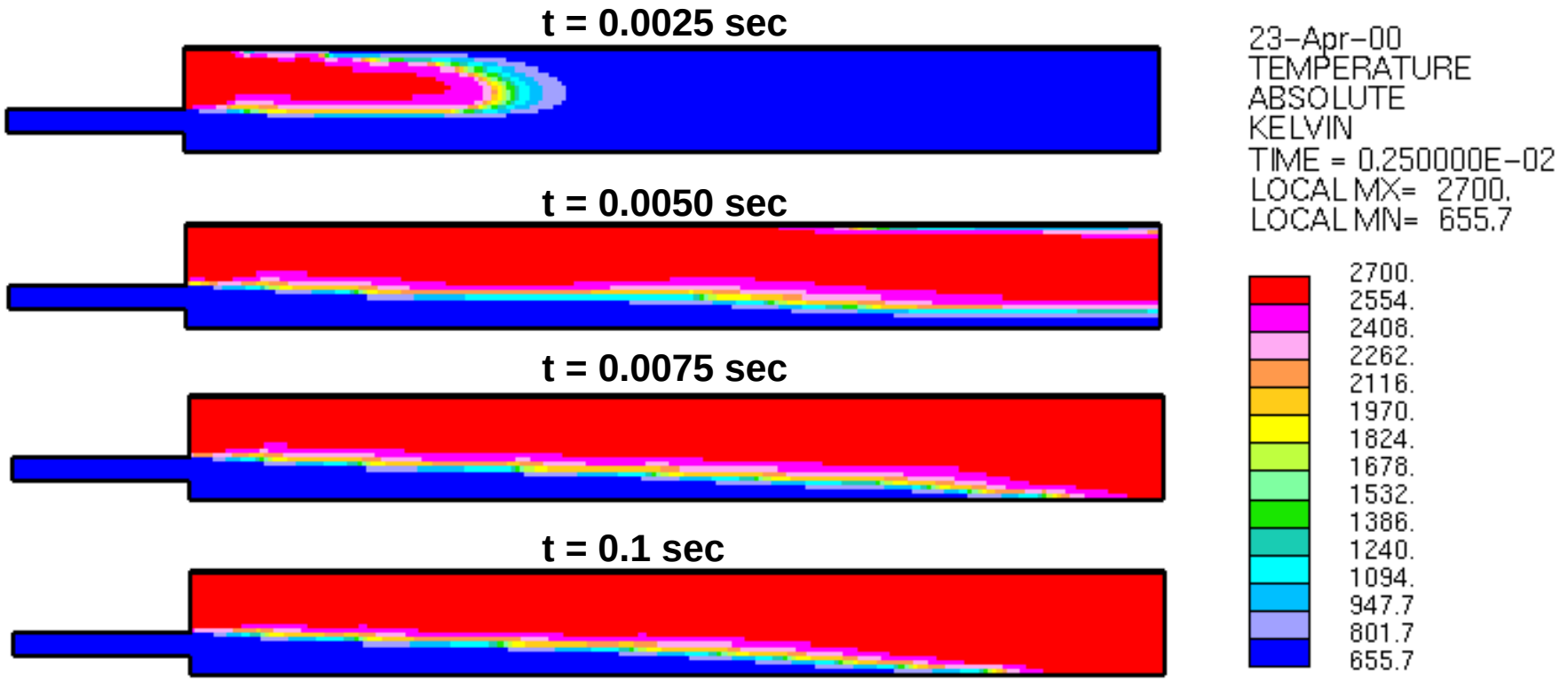
CHEMKIN Reaction Mechanism

```
ELEMENTS
  C H O N
END
SPECIES
  C2H4 O2 H2O N2 CO2 H2 O H OH CO
END
REACTIONS
     H +  H +  M =    H2 +   M
     O + H2     =    OH +   H
     H + O2     =    OH +   O
     H + OH +  M =   H2O +   M
    H2 + OH     =   H2O +   H
    CO +  O +  M =   CO2 +   M
    CO + OH     =   CO2 +   H
  C2H4 + O2     = 2 CO  + 2 H2
END
```

REACTION DESIGN

Upon ignition, temperature profile is established quickly

Temperature profiles



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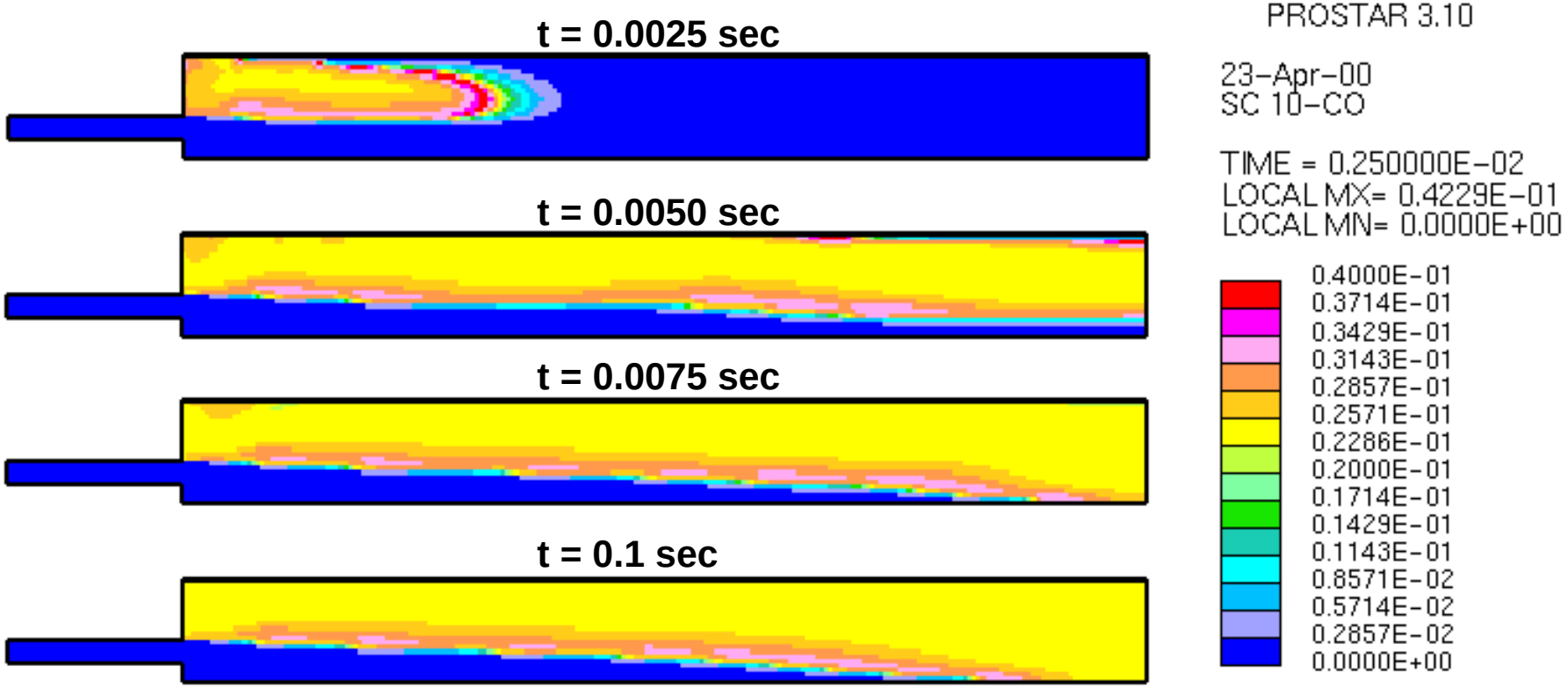
Evolution of products and radicals are closely coupled to the temperature

Carbon Monoxide Profiles



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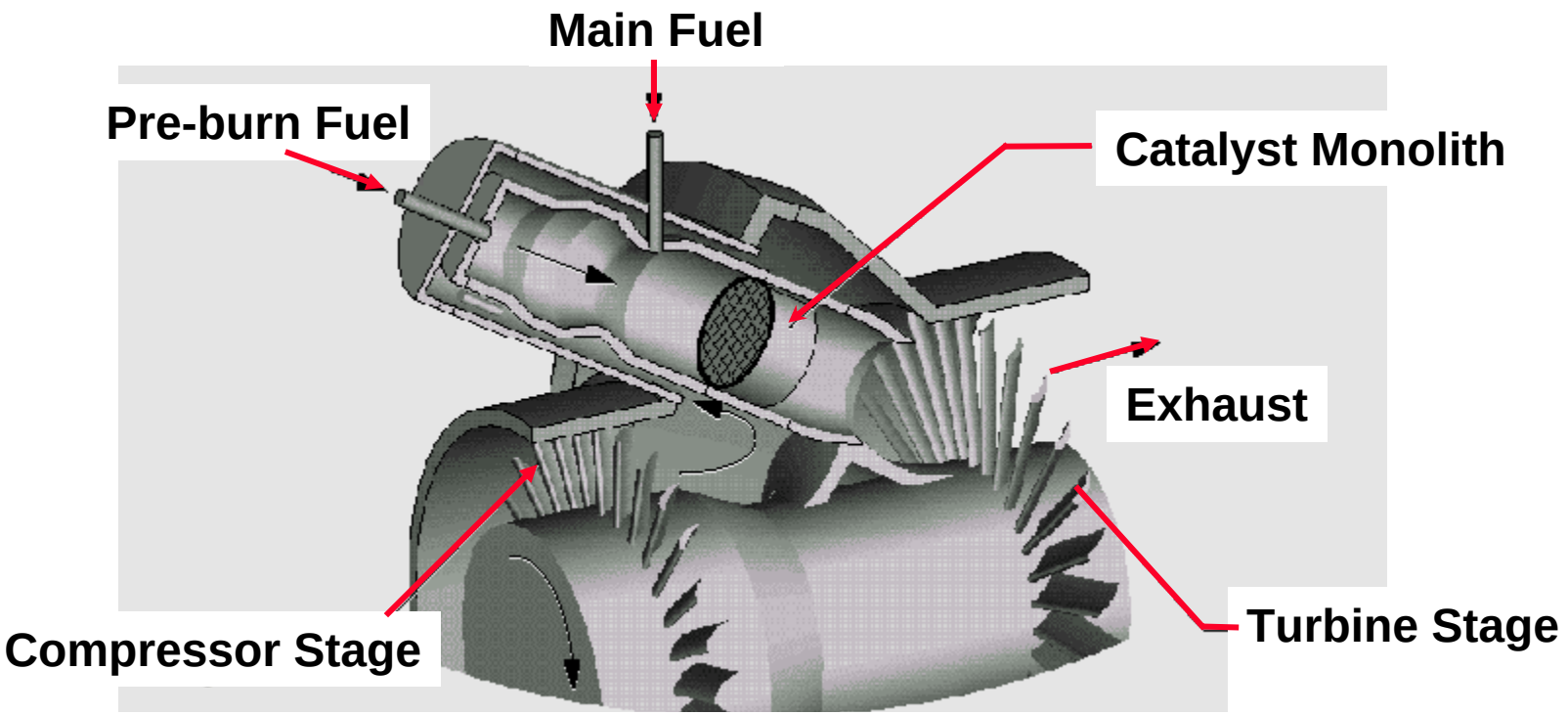
We will continue to refine the solver to maximize efficiency and robustness

- Target is 10X speed-up from initial implementation
- Minimize requirement for “smart” initial guesses by user
- Test on a wide range of combustion problems under turbulent, transient conditions

Our surface-chemistry module will target simulation of catalytic combustion in turbines

The Challenge: Improve efficiency and reduce pollutant emissions (NO_x)



Main features of GE and Allison Systems Designs

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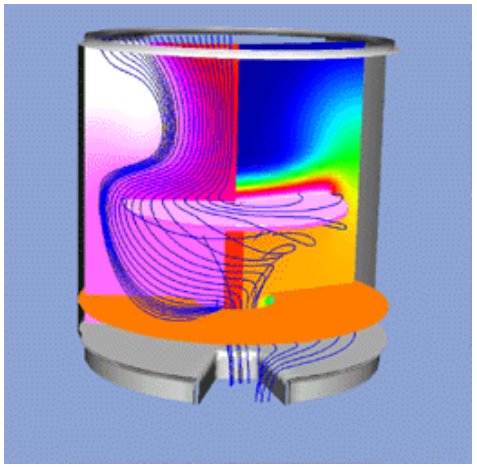
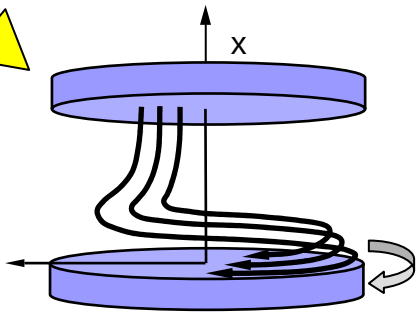
Our partnerships with CFD Companies enable a hierarchical modeling approach



Full 3-D CFD Simulation

- Common chemistry data descriptions
- From mechanism development to industry application

Geometric Complexity



1-D Model
(Similarity Transformation)

Chemistry Complexity

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The CHEMKIN Collection – Release 3.5

Application	Problem Solving Capability
AURORA	Well stirred plasma/thermal reactors with gas and surface reactions
CRESLAF	Laminar, boundary layer flows in cylindrical or planar channels
EQUIL	Chemical equilibrium of an ideal gas mixture or solution
OPPDIF	Diffusion flame between opposing nozzles
PLUG	Plug flow reactor with gas and surface reactions
PREMIX	Steady, one-dimensional laminar and pre-mixed flames
SENKIN	Transient analysis of homogeneous gas-phase chemistry
SHOCK	Chemical dynamics behind incident and reflect shock waves
SPIN	Rotating disk/stagnation flow chemical vapor deposition reactors
SURFTHERM	Analysis of thermochemical/kinetic data in reaction mechanisms

Plus: CHEMKIN Utilities and solvers that serve as building blocks for other applications

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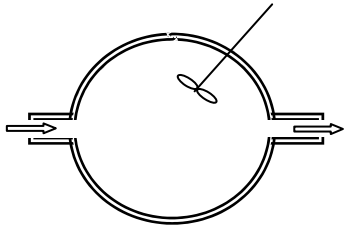
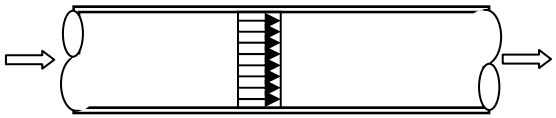
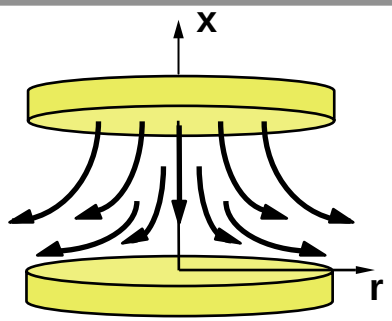
Applications Represent Different Geometries



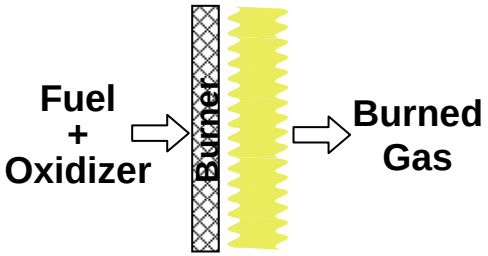
AURORA



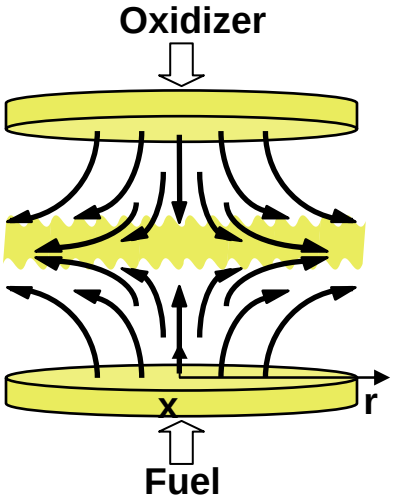
PLUG



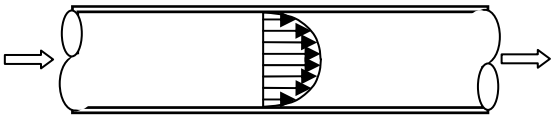
SPIN



PREMIX



OPPDIF



CRESLAF

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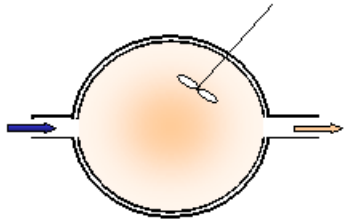
CHEMKIN allows “mix and match” of Applications and chemistry systems

Chemistry Mechanisms

H_2/Air

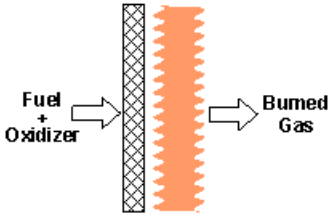
CH_4/O_2

$C_2H_2/O_2/Ar$



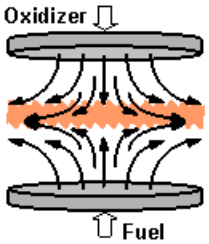
Perfectly Stirred Reactor

AURORA



Premixed Laminar Flame

PREMIX



Opposed-flow Diffusion Flame

OPPDIF

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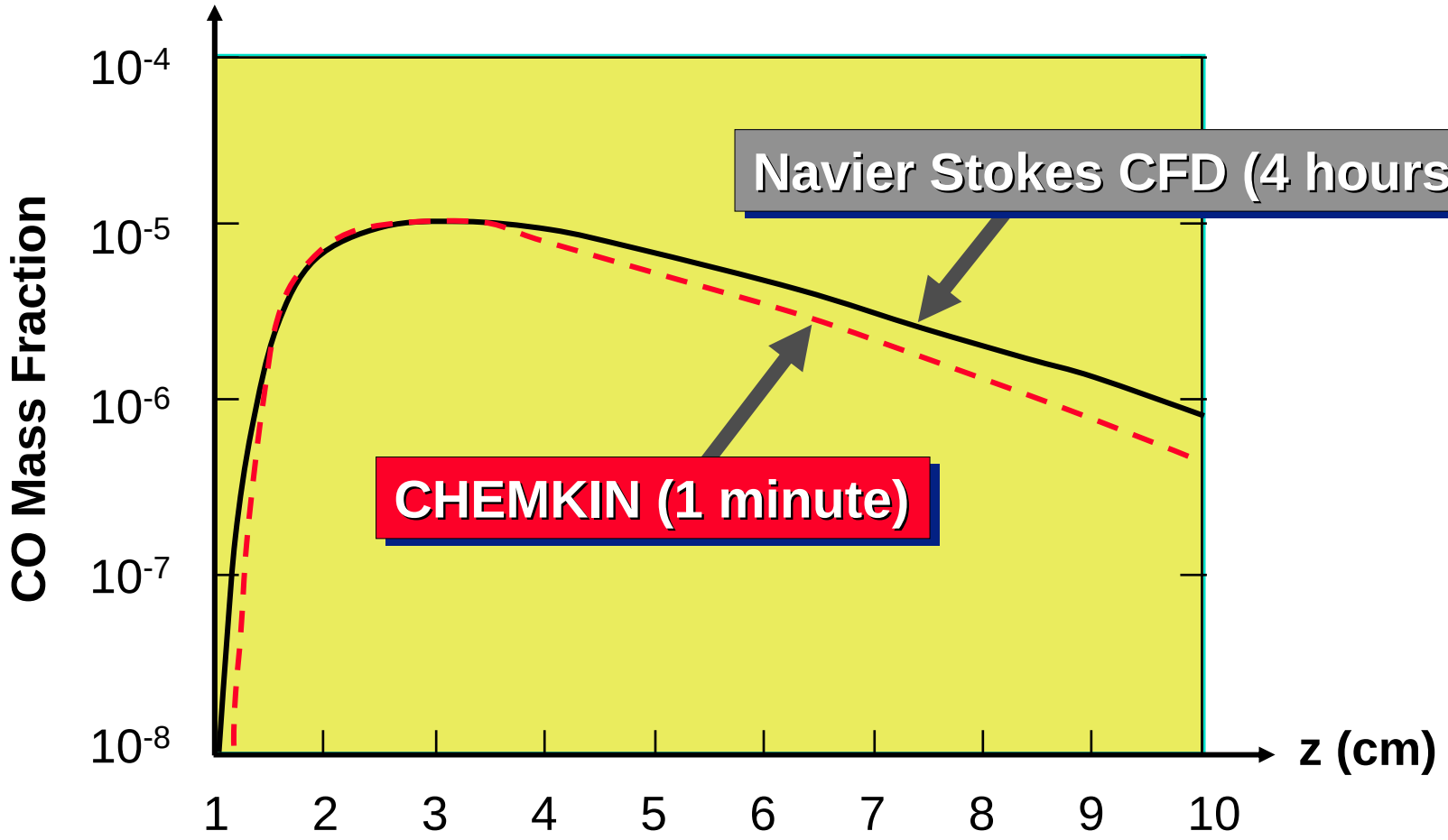
Choosing the right level of model for the right problem is an important step

Simulation results for catalytic combustion in radially symmetric tube



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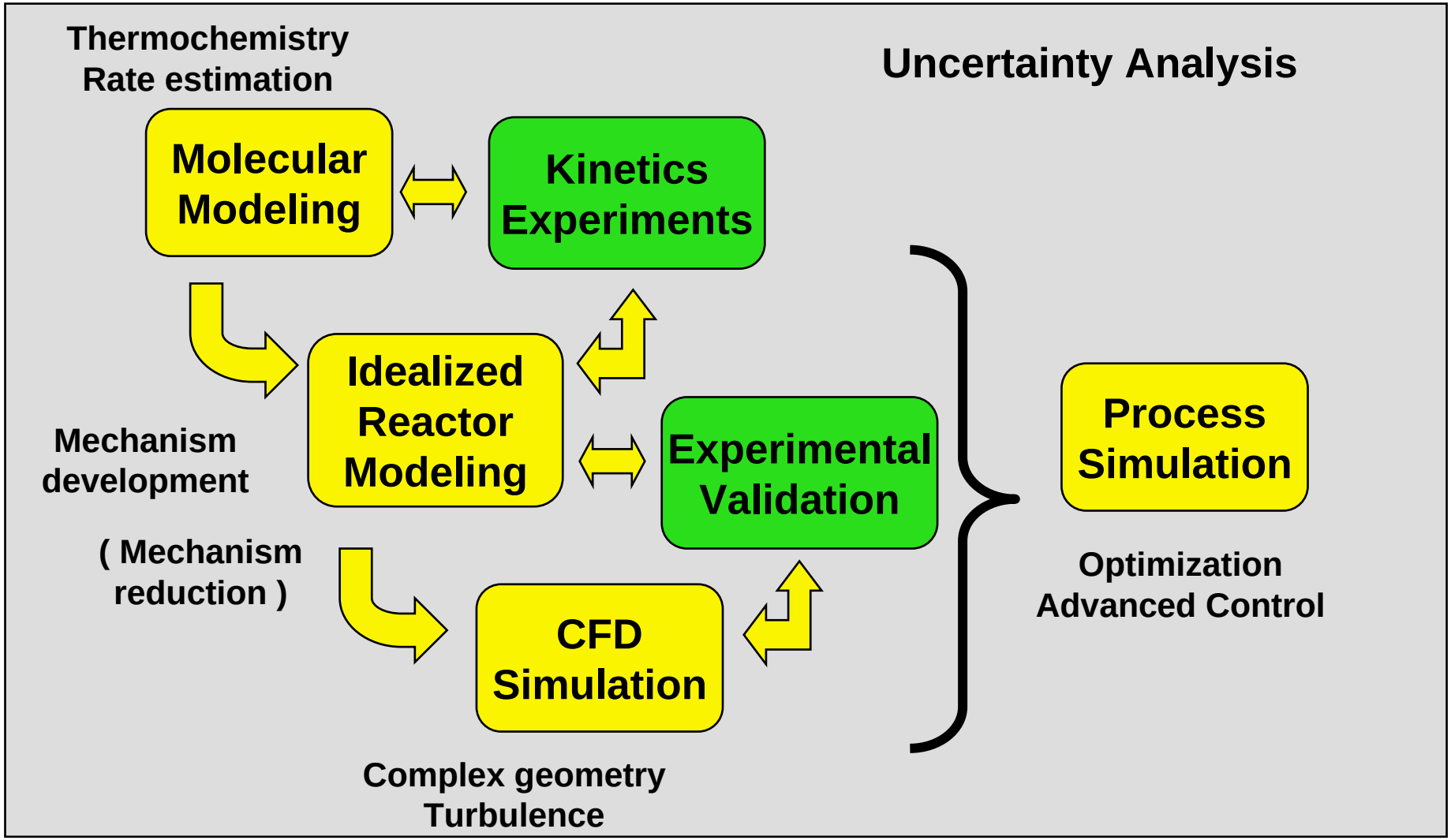

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CONCLUSIONS AND KEY MESSAGES

1. There is a growing need for integration of flow models with detailed chemical and physical phenomena.

2. Collaboration between Reaction Design and Adapco/CD will result in new capabilities that meet these needs.

RD
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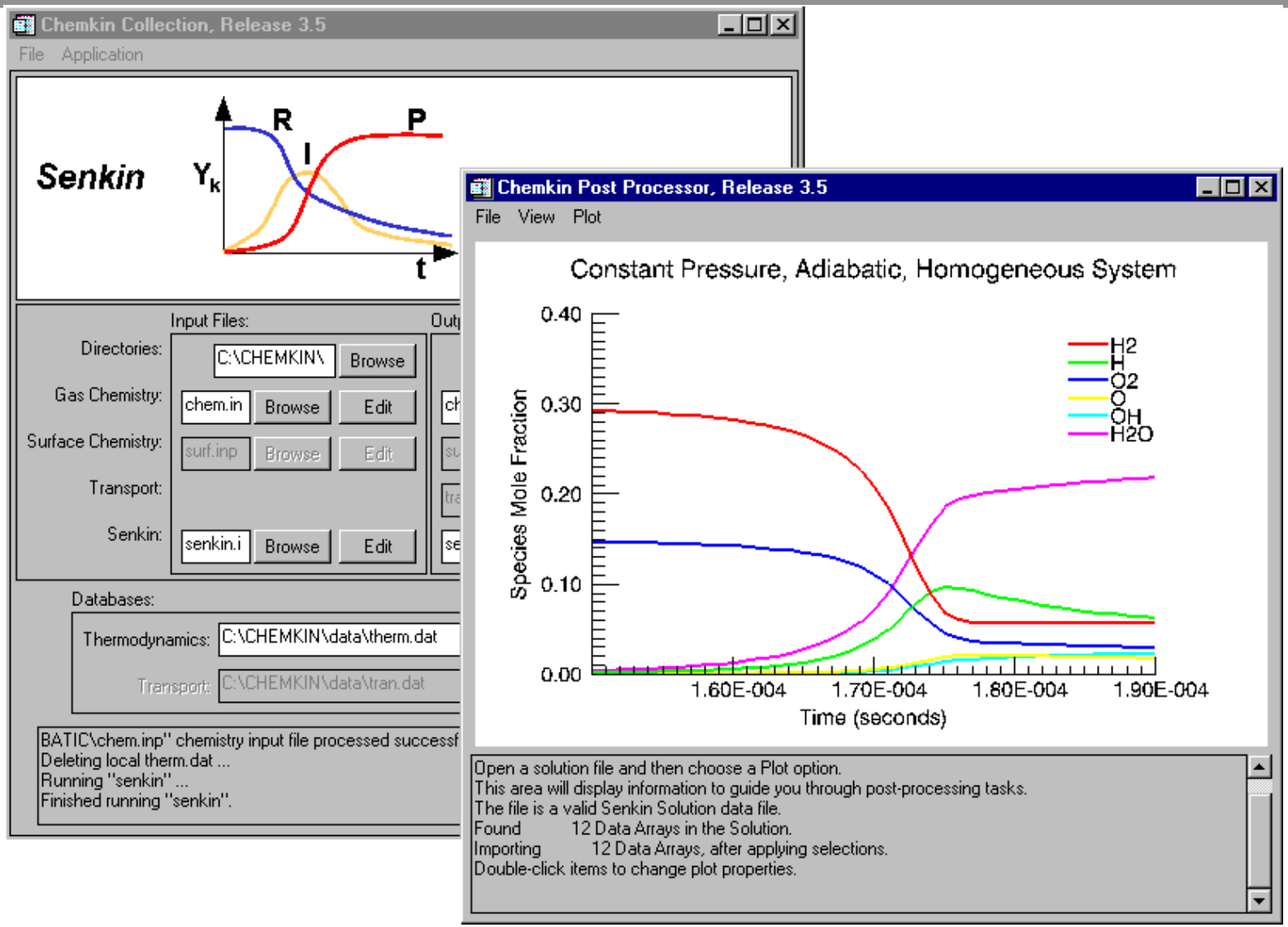
Introduction to CHEMKIN 3.5 Software



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Why RD CHEMKIN vs. "free" CHEMKIN II?

- Technical Support for all users.
- Up-to-date Documentation
  - indexed and available electronically
  - New *Getting Started* manual.
- Maintenance, updates, bug fixes, quality control.
- Many new features and Applications!
  - Heterogeneous gas-solid reactions (SURFACE CHEMKIN)
  - Multiple material Gas-Surface mechanisms
  - Plasma modeling (AURORA)
  - Opposed-flow diffusion flame model (OPPDIF)
  - Plug-flow model (PLUG)
  - Global reactions (non-stoichiometric reaction orders and non-integer stoichiometry)
  - Improved performance and algorithms
  - Available on PCs

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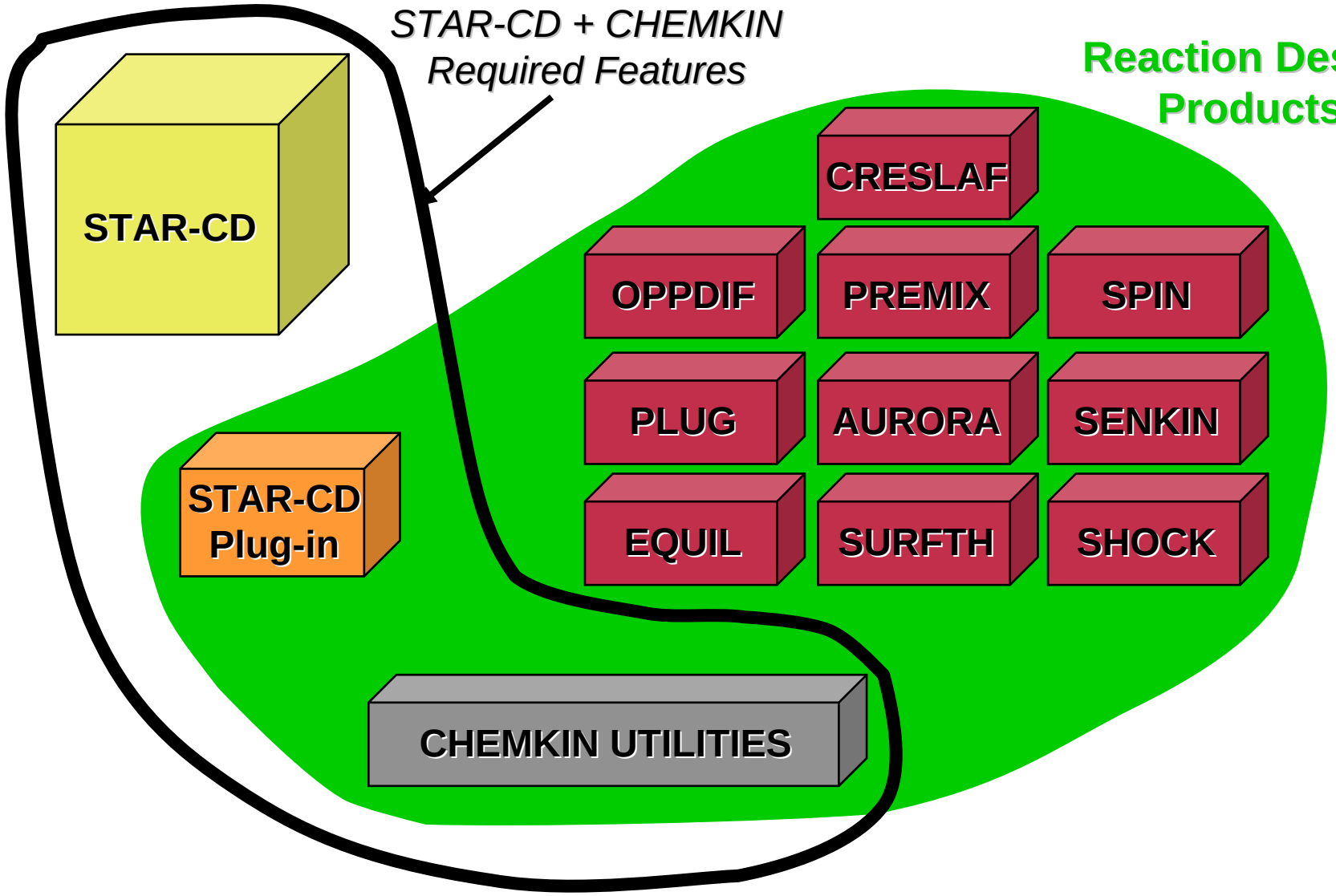
STAR-CD + CHEMKIN builds on existing modules to provide new capabilities



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