NSF Workshop on Cyber-based Combustion Science:

RIOT & a vision for predictive modeling of combustion

Prof. William H. Green
MIT Dept. of Chem. Eng.
whgreen@mit.edu

What is RIOT?

- RIOT = “Range Identification & Optimization Tool”
- Software for constructing reduced chemical kinetic models.
- Helps put large chemical mechanisms into reacting-flow simulations.
- Unique feature - identifies “valid range”
  - reaction conditions over which the reduced model is guaranteed to match the full model within a tolerance.
- Made available on the Web through the CMCS Portal http://www.cmcs.org.
- Who built RIOT: Luwi Oluwole, Binita Bhattacharjee, and Karen Schuchardt

My Workspace | Active Tables Developers | CMCS Demonstrations | (more) | RIOT Dev

RIOT Dev : Riot

RIOT - Range Identification and Optimization Tool

Start Over **Previous Results** **Show Job Queue** **Help**

RIOT Setup

Title: Riot

Task: I want to: Reduce the model

Model Output: I want: One Model

Reaction Conditions

1 #1, P=1 atm T=394 K
2 #126, P=42.5 atm T=1387 K
3 #288, P=84.4 atm T=2098 K
4 #384, P=4.8 atm T=1100 K

Specify... Remove

Points selected

Model Reduction Parameters (all models) : Edit...

Temp tolerances: atol(K/s) = 1000.0, rtol = 0.0010
Global species tolerances: atol(1/s) = 500.0, rtol = 0.0010
0 of 2539 Reactions Fixed

Submit Request | Submit Sync Request

! Default tolerances set for demo purposes. Adjust for accuracy requirements.

Working dir: /sam/files/projects/RIOT_Dev/n-heptane/ 561 Species 2539 Reactions

powered by Chef SCIENTIFIC ANNOTATION MIDDLEWARE Jetspeed

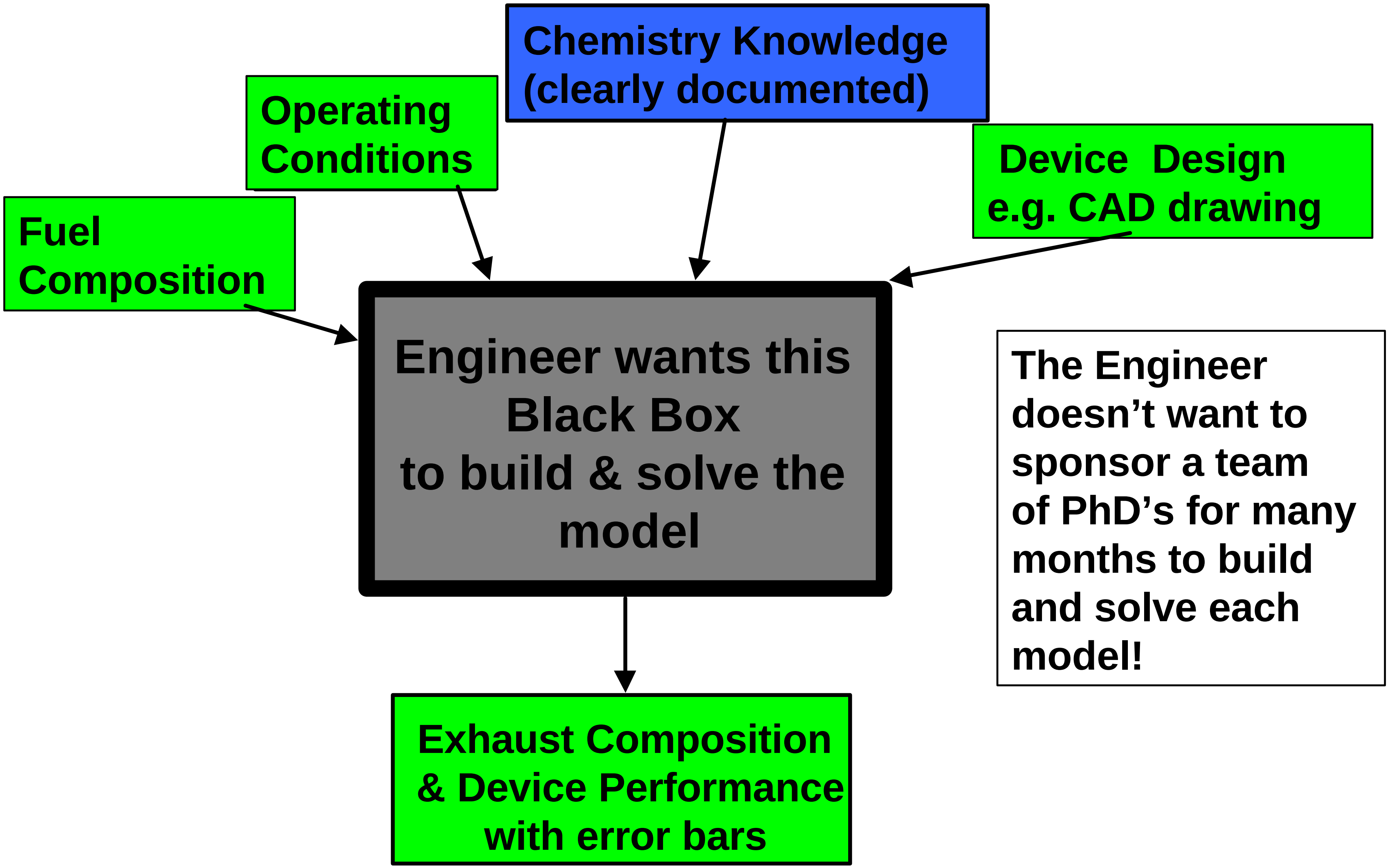
CMCS v2.01 | SAM v1.1.8 | CHEF v1.1.01 [build #307231] | Jetspeed v1.4b2[cvs08oct2002p]

Tools like RIOT are not enough to make Combustion Science “Cyber-Based”

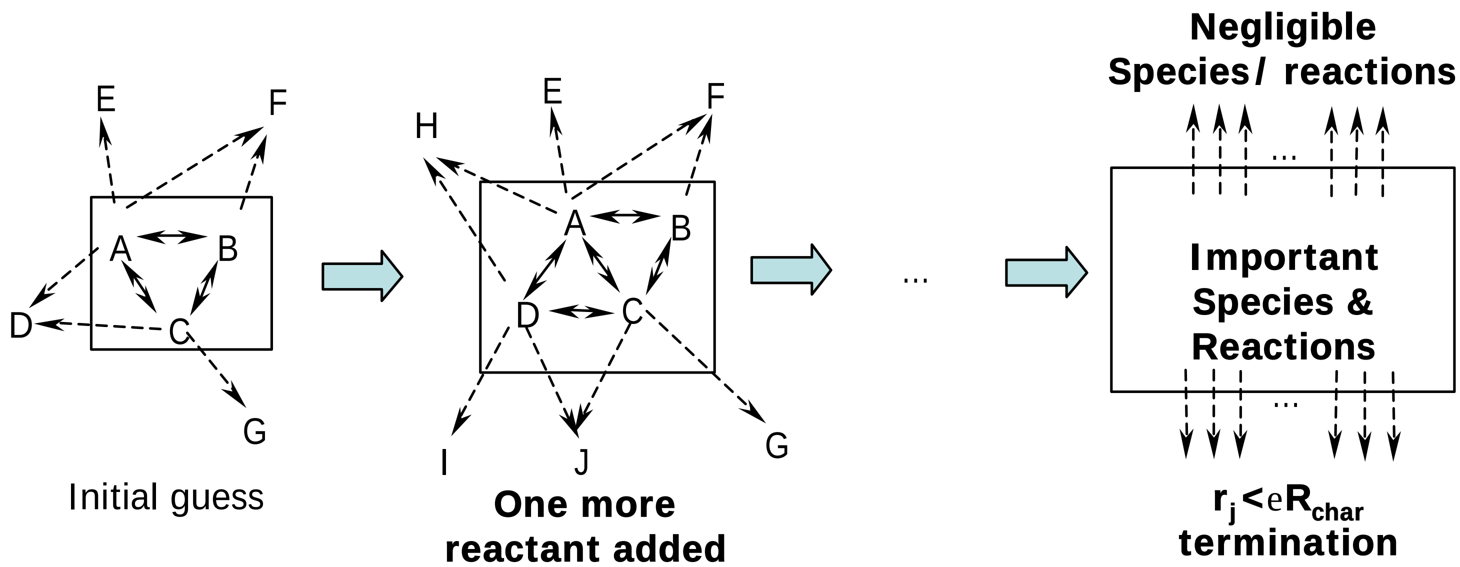
- **RIOT is a nice tool:**
  - used in HCCI engine simulations, laminar flame simulations
  - Free, easy to access, nice interface, automated
- **But…RIOT demands a lot from user:**
  - An accurate large “full” reaction mechanism for fuel of interest.
  - Access to suitable reacting-flow software
    - that can solve the problem of interest in reasonable time
    - that can use RIOT’s reduced models with valid ranges
  - Consistent uncertainty/error analysis throughout
    - otherwise, what rationale for RIOT error tolerance?

User needs access to <u>full</u> capability: then combustion science can really become “cyber-based”.

What an Engineer *Really* Wants



Which Species & Rxns Belong in Model? Rate-Based Model Construction



Iteratively add reactions/species until all the reactions leading to new species are negligible:

all minor species rates < ε·||major species rates||

Note: model structure depends on reaction conditions & rate estimates

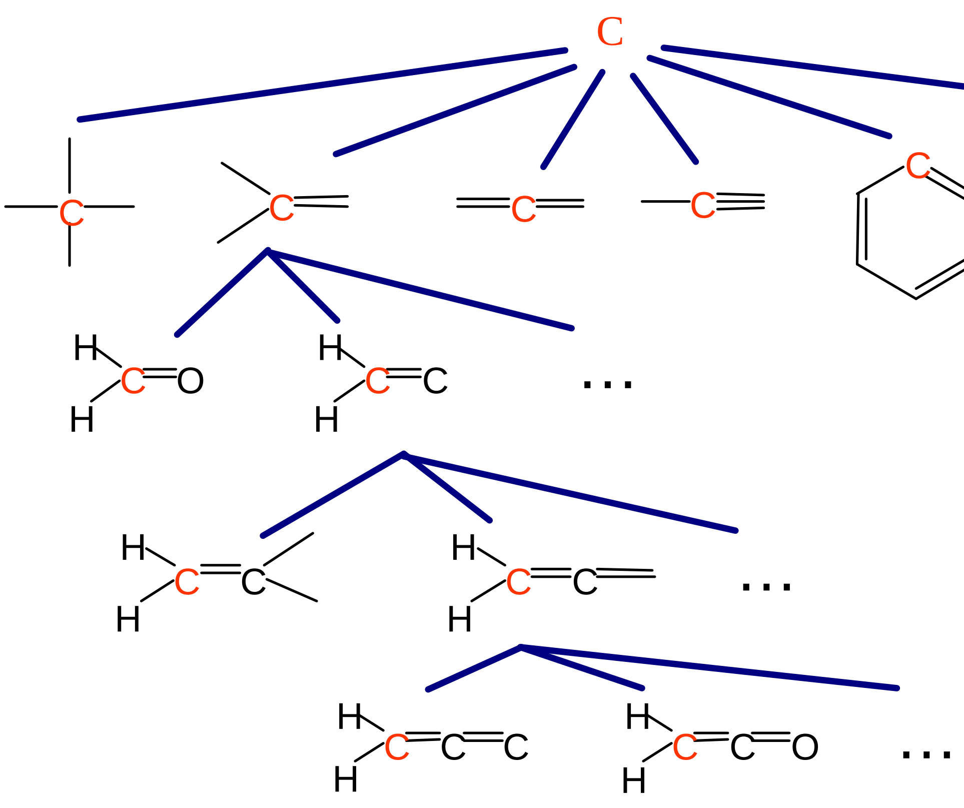
See Susnow *et al.*, *J. Phys.Chem. A* (1997)

The Model-Construction Algorithm Requires the Computer to…

- Identify Every Way Reactant X can react with other species in the model {A,B,C…}
- Estimate rate constants k(T,P) for all those reactions.
- Estimate the reverse rate constants, i.e. estimate $\Delta G_f(T)$ for every important species.
- Can look up <u>some</u> of the reactions, rate constants, and thermo, but <u>many</u> reactions, rates, thermo have never been measured.

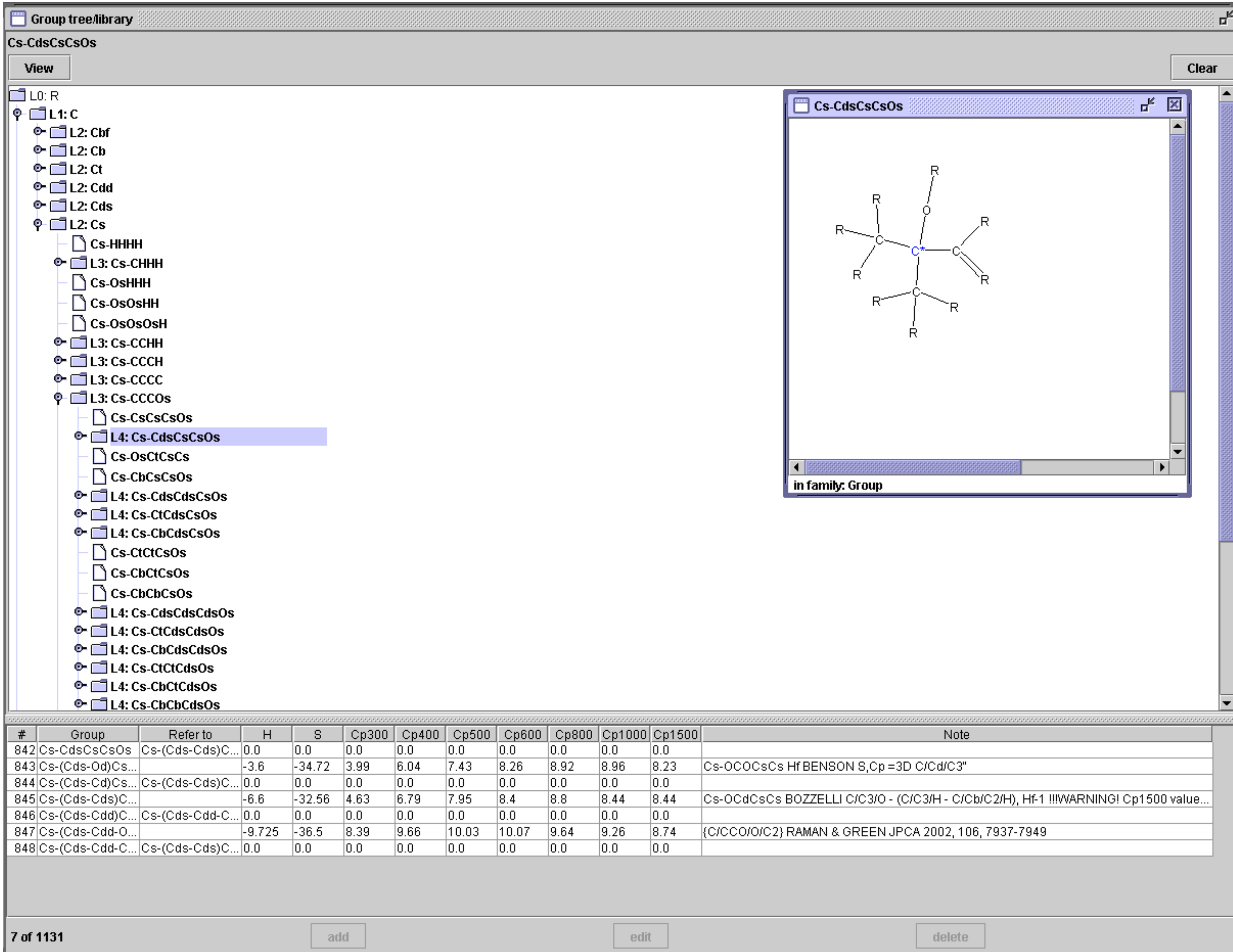
Documenting the Chemistry Details in an Unambiguous, Extensible Way

Functional Group Tree



- **Quick search**
- **Human-Readable**
- **Easy to update**
- **Easy to extend (new leafs)**
- **~700 current tree leafs for thermo group values, from quantum calcs & expt.**

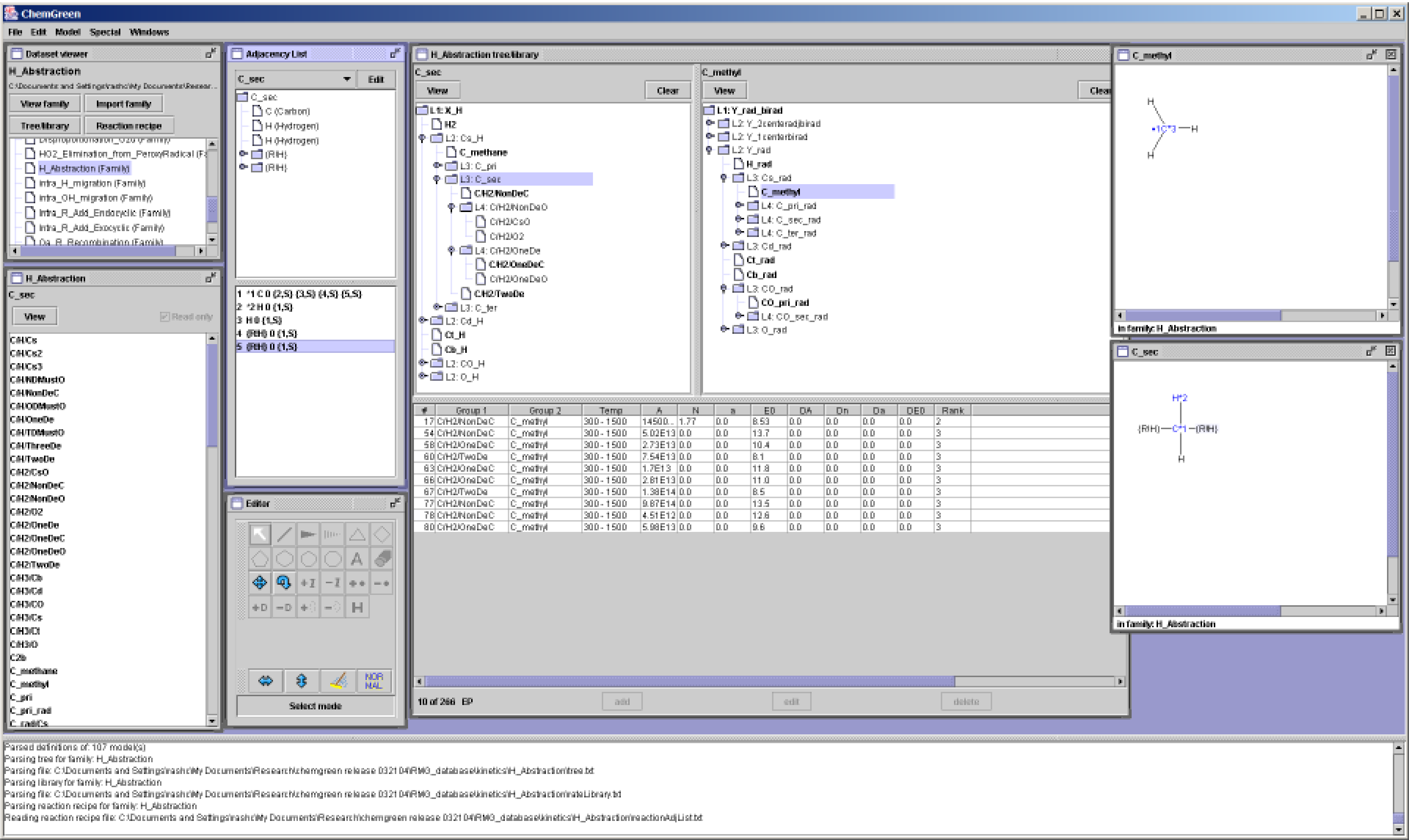
Functional Group Tree Database for Thermo



#	Group	Refer to	H	S	Cp300	Cp400	Cp500	Cp600	Cp800	Cp1000	Cp1500	Note
842	Cs-CdsCsCsOs	Cs-(Cds-Cds)C...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
843	Cs-(Cds-Od)Cs...		-3.6	-34.72	3.99	6.04	7.43	8.26	8.92	8.96	8.23	Cs-OCOCsCs Hf BENSON S,Cp =3D C/Cd/C3"
844	Cs-(Cds-Cd)Cs...	Cs-(Cds-Cds)C...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
845	Cs-(Cds-Cds)C...		-6.6	-32.56	4.63	6.79	7.95	8.4	8.8	8.44	8.44	Cs-OCdCsCs BOZZELLI C/C3/O - (C/C3/H - C/Cb/C2/H), Hf-1 !!!WARNING! Cp1500 value...
846	Cs-(Cds-Cdd)C...	Cs-(Cds-Cdd-C...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
847	Cs-(Cds-Cdd-O...		-9.725	-36.5	8.39	9.66	10.03	10.07	9.64	9.26	8.74	{C/CCO/O/C2} RAMAN & GREEN JPCA 2002, 106, 7937-7949
848	Cs-(Cds-Cdd-C...	Cs-(Cds-Cds)C...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

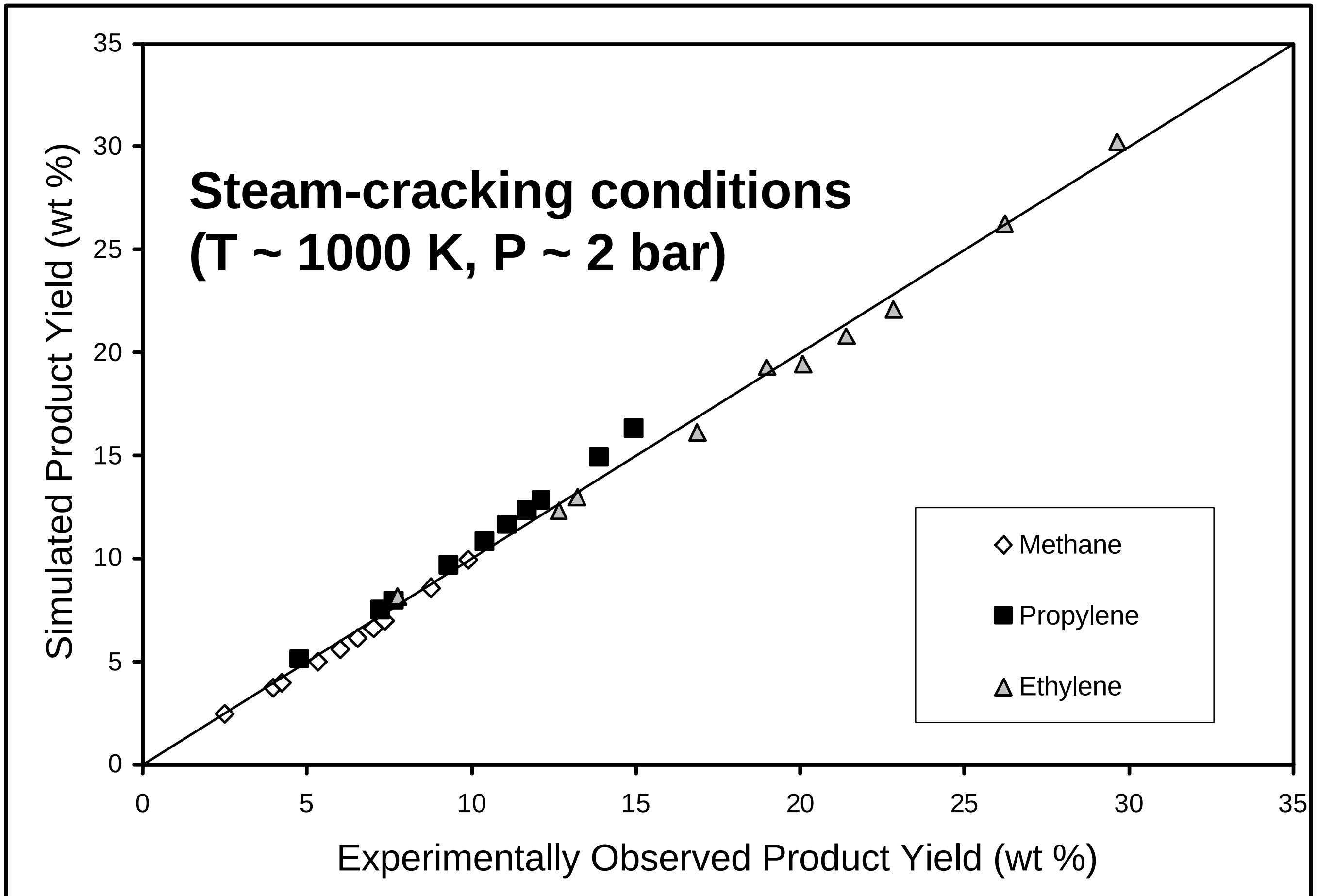
Functional Group Trees for Rate Estimates

Reacting group A with different kind of group B, different trees. Sometimes group C…



Does this really work? Are computer-generated models accurate? Don't you need a human touch (or tweak)?

RMG-Generated Model for n-Hexane Pyrolysis

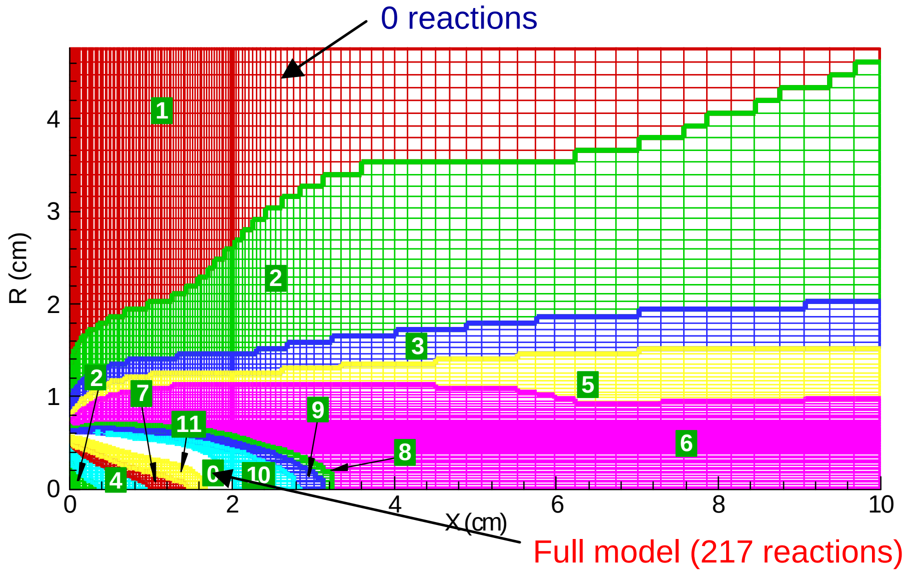


K. van Geem, *et al.* (AIChE J 2005)

How to Solve Multidimensional Reacting Flows with large computer-generated chemistry models?

Often cannot solve the full set of equations on full mesh…

- The Adaptive Chemistry concept
  - Chemistry depends on conditions, so…use several reduced chemistry models, each where it is locally-valid.
  - Appropriate reduced chemistry models selected from a pre-constructed library.



- ✓ **Method shown to speed up simulations (~4x in test cases)**
- ✓ **Automated method developed for obtaining reduced models**

Challenge:

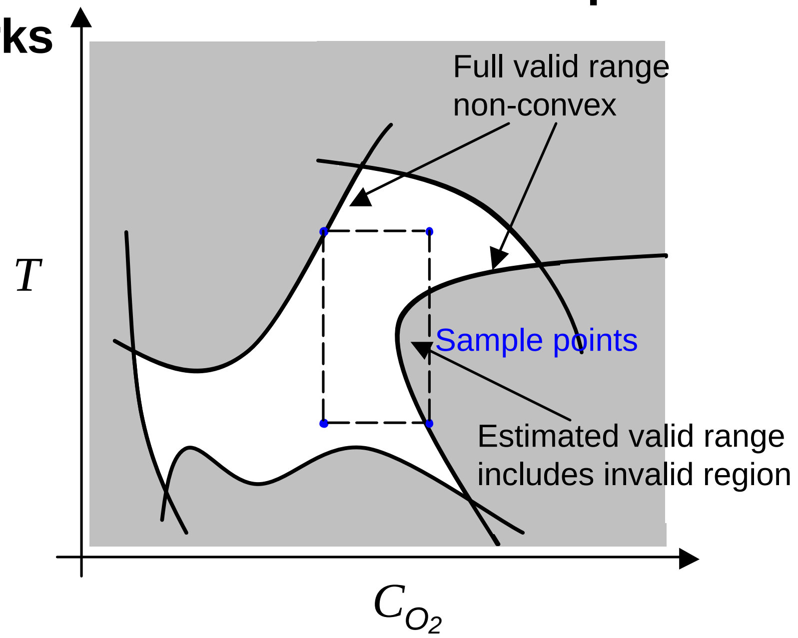
Guarantee accuracy of Adaptive Chemistry solution without ever running full chemistry problem

The Valid Range of a Reduced Chemistry Model

Model is "valid" at (C,T) where $|S_{reduced}(\underline{C},T)-S_{full}(\underline{C},T)| < tol$

Most reduced models are only known to be valid at individual points (C,T)

CFD calculation assumes each reduced model valid over a continuous range of conditions F. But just because model works at certain points f=(C,T) in F does not guarantee it works at every point in range: *non-convex!*



RIOT gives reduced models with guaranteed-valid ranges: just right for Adaptive Chemistry!

Oluwole et al. *Combust. Flame* (2006)

Controlling the reduced-model error in steady-state CFD

- Conservation equations: $F_k(\underline{f}) = \frac{\partial f_k}{\partial t} = T_k(\underline{f}) + S_k(\underline{f})$

  T = transport terms

  S = chemistry terms

- Want to solve full model problem to steady-state $\underline{f}_{ss}^{\text{full}}$ such that steady state residuals $\left|F_k^{\text{full}}(\underline{f}_{ss}^{\text{full}})\right| \le d_k^{\text{full}}$ ...but we can't afford it

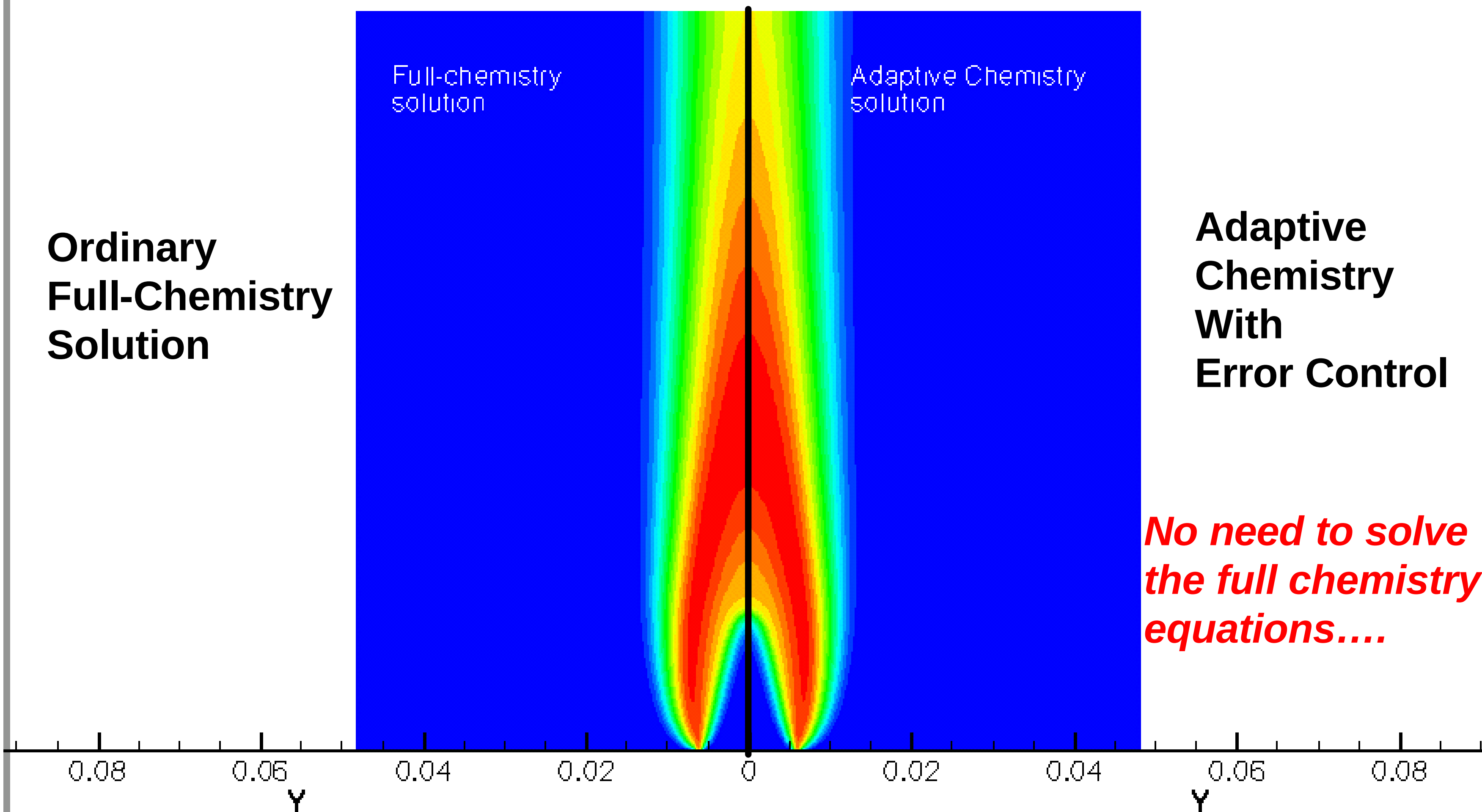
- Instead, solve Adaptive Chemistry problem (using reduced models) to steady-state $\underline{f}_{ss}^{\text{red}}$ such that $\left|F_k^{\text{red}}(\underline{f}_{ss}^{\text{red}})\right| \le d_k^{\text{red}}$
- **If we craftily set model reduction error tolerances so we are sure**

  $|S_{reduced}(\underline{C},T)-S_{full}(\underline{C},T)| <$ tol at $\underline{f}_{ss}^{\text{red}}$ and set $d^{red} < d^{full}$ - tol

  We can guarantee that we'll solve the full problem: $\left|F_k^{\text{full}}(\underline{f}_{ss}^{\text{red}})\right| \le d_k^{\text{full}}$

Error Control Works As Promised

Predicted Temperature Fields for Partially Premixed CH_4 Flame



Ordinary Full-Chemistry Solution

Adaptive Chemistry With Error Control

No need to solve the full chemistry equations….

A vision for Cyber-Based Combustion Science