4th Fuels Research Review
September 20, 2011

PrIMe Update: Workflow 2.0 and Automated UQ-Predictive Modeling of Hydrogen Combustion

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Collaborators

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-Drs. T. Russi, D. Yeates, X. You, F. Lei

-W.M. Speight, M. Gutkin

Supported by

-NSF Chemistry Division; Cyber-infrastructure

-AFOSR, Siemens, CITRIS

Berkeley
University of California

http://primekinetics.org

PrIMe

Process Informatics Model

Infrastructure for UQ-predictive modeling

- Data sharing
- App sharing
- Automation

PrIMe
Process Informatics Model

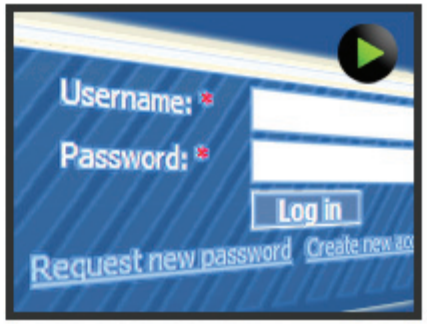
Username: *
Password: *
Log in
Request new password Create new account

Home Announcements

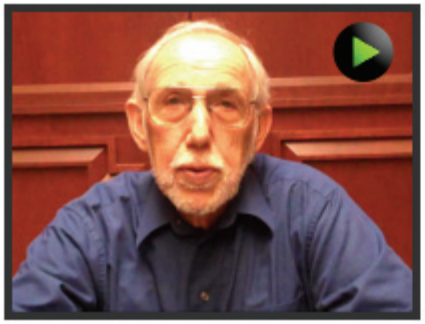
Welcome to PrIMe

What can PrIMe do? Make predictions

How to Register and Log into PrIMe



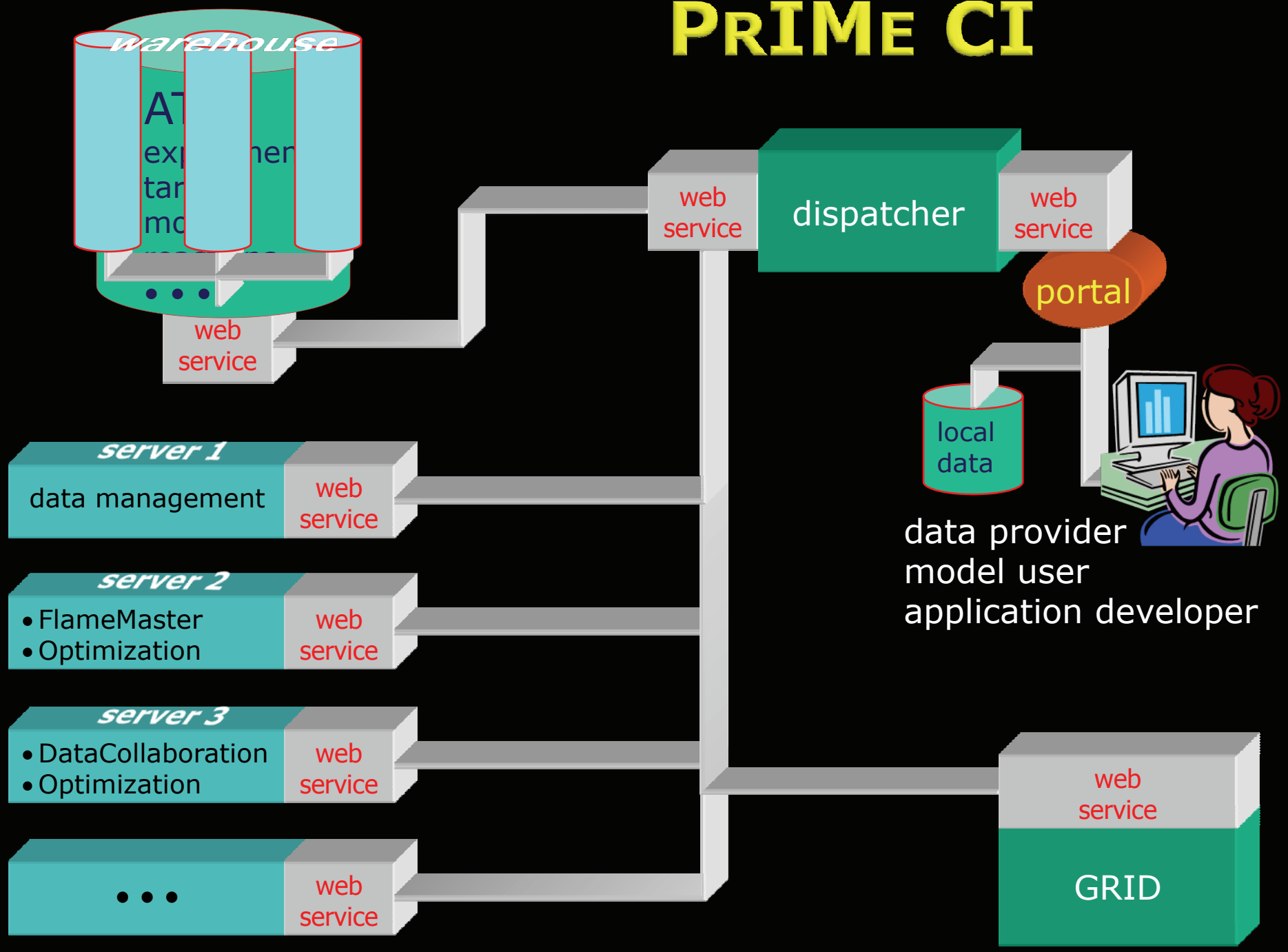
David Golden speaks about PrIMe



More information about PrIMe

» Read more about PrIMe

PRIME CI


warehouse
web service
dispatcher
web service
portal
local data
data provider
model user
application developer
server 1
data management
web service
server 2
• FlameMaster
• Optimization
web service
server 3
• DataCollaboration
• Optimization
web service
• • •
web service
web service
GRID

OUTLINE

- Present status of PrIMe Infrastructure
- New major developments: Workflow and Portal
- Instrumental Model: ALS
- Automation: H_2-O_2 ignition

Current status: Data Warehouse

• bibliography (refs)	~20,000
• chemical elements	
• chemical species	~10,000
• chemical reactions	~15,000
• experiments	> 400
• dataAttributes (targets)	> 100
• models (GRI-Mech 3.0 and H_2-O_2)	2
• datasets	2
• optimizationVariables	> 100

```
! GRI-Mech Version 3.0 7/30/99  CHEMKIN-II format
! See README30 file at anonymous FTP site unix.sri.com, directory gri;
! WorldWideWeb home page http://www.me.berkeley.edu/gri_mech/ or
! through http://www.gri.org , under 'Basic  Research',
! for additional information, contacts, and disclaimer
ELEMENTS
O  H  C  N  AR
END
SPECIES
H2      H       O       O2      OH      H2O     HO2     H2O2
C       CH      CH2     CH2(S)  CH3     CH4     CO      CO2
HCO     CH2O    CH2OH   CH3O    CH3OH   C2H     C2H2    C2H3
C2H4    C2H5    C2H6    HCCO    CH2CO   HCCOH   N       NH
NH2     NH3     NNH     NO      NO2     N2O     HNO     CN
HCN     H2CN    HCNN    HCNO    HOCN    HNCO    NCO     N2
AR      C3H7    C3H8    CH2CHO  CH3CHO
END
!THERMO
! Insert GRI-Mech thermodynamics here or use in default file
!END
REACTIONS
2O+M<=>O2+M                             1.200E+17   -1.000        .00
H2/ 2.40/ H2O/15.40/ CH4/ 2.00/ CO/ 1.75/ CO2/ 3.60/ C2H6/ 3.00/ AR/  .83/
O+H+M<=>OH+M                            5.000E+17   -1.000        .00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+H2<=>H+OH                             3.870E+04    2.700    6260.00
O+HO2<=>OH+O2                           2.000E+13     .000        .00
O+H2O2<=>OH+HO2                         9.630E+06    2.000    4000.00
O+CH<=>H+CO                             5.700E+13     .000        .00
O+CH2<=>H+HCO                           8.000E+13     .000        .00
O+CH2(S)<=>H2+CO                        1.500E+13     .000        .00
O+CH2(S)<=>H+HCO                        1.500E+13     .000        .00
O+CH3<=>H+CH2O                          5.060E+13     .000        .00
O+CH4<=>OH+CH3                          1.020E+09    1.500    8600.00
O+CO(+M)<=>CO2(+M)                      1.800E+10     .000    2385.00
   LOW/ 6.020E+14     .000    3000.00/
H2/2.00/ O2/6.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/3.50/ C2H6/3.00/ AR/ .50/
O+HCO<=>OH+CO                           3.000E+13     .000        .00
```

GRI-Mech 3.0


```
<chemicalModel primeID="m00000003">
 <copyright>©primekinetics.org 2006</copyright>
 <preferredKey group="prime">GRI-Mech 3.0</preferredKey>
 <bibliographyLink preferredKey="Smith et al., 1999." primeID="b00014718"/>

<speciesSet>
   <speciesLink preferredKey="Ar" primeID="s00000049">
      <thermodynamicDataLink preferredKey="120186" primeID="thp00000001"/>
   </speciesLink>
  <speciesLink preferredKey="H" primeID="s00009800">
     <thermodynamicDataLink preferredKey="L 7/88" primeID="thp00000001"/>
   </speciesLink>
 </speciesSet>

<reactionSet>
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     <reactionRateLink preferredKey="2O + CO = O2 + CO" primeID="rk00000019"/>
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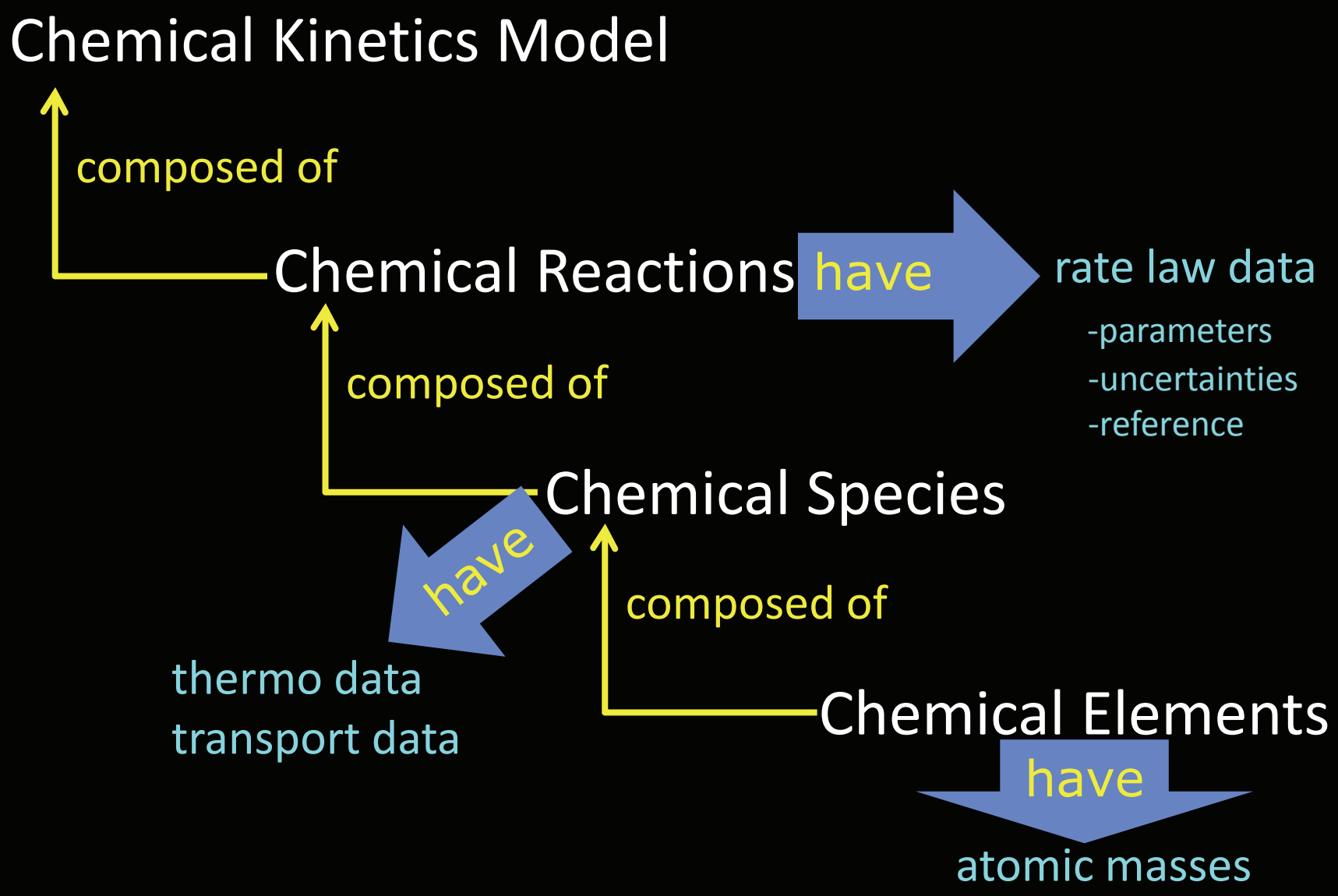
• • •

PrIMe Data Model



```
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    <reactionRateLink preferredKey="O + H2 = H + OH" primeID="rk00000005"/>
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    <speciesLink preferredKey="H"   primeID="s00009800">1</speciesLink>
    <speciesLink preferredKey="H2"  primeID="s00009809">−1</speciesLink>
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    <reactionRateLink preferredKey="O + H2 = H + OH" primeID="rk00000005"/>
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warehouse.primekinetics.org - /depository/reactions/data/r00012186/

[To Parent Directory]

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      </parameter>
    </expression>
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</reactionRate>
```

```
<reactionLink preferredKey="O + H2 = H + OH" reversible="true" primeID="r00012186">
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```

warehouse.primekinetics.org - /depository/reactions/data/r00012186/

```
[To Parent Directory]
      Monday, August 23, 2010   9:00 PM        <dir> _attic
    Tuesday, January 09, 2007   7:16 PM          553 rk00000000.xml
 Wednesday, February 03, 2010   7:47 PM         1186 rk00000001.xml
 Wednesday, February 03, 2010   7:47 PM         1090 rk00000002.xml
 Wednesday, February 03, 2010   7:47 PM         1191 rk00000003.xml
```

```
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  </rateCoefficient>
</reactionRate>
```

PrIMe Data Model: experiments

Experimental Record

- reference
- apparatus
- conditions
- observations
  - inner: XML
  - remote: HDF5, …
- uncertainties
- additional items
  - links, docs, …
  - video files, …

dataAttribute (target)

a specific feature extracted for modeling:

- peak value
- peak location
- induction time
- ratio of peaks

(from multiple experiments)

…

instrumentalModel

PrIMe Data Model: dataset

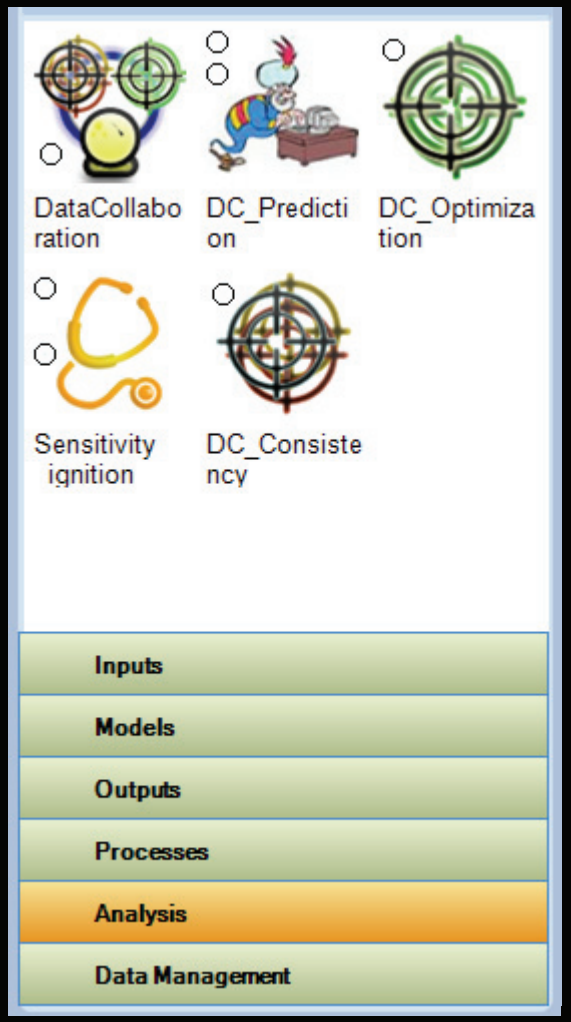
targets + model + uncertainties = dataset

For the purposes of

- comparison among data and models
- model optimization
- **uncertainty quantification**
  - UQ-predictive modeling
  - identification of needed effort
  - what-if scenarios, …

PrIMe Infrastructure: Apps

- data management
  - search, submission, retrieval
  - creation/appending of a dataset
- process simulation
  - 0-D kinetics (plug-flow, ignition)
- system analysis
  - sensitivity
  - response surfaces
  - model optimization
  - uncertainty
  - dataset consistency
  - UQ prediction



PRIME CI: WORKFLOW

- platform for / user interface to
  - data management and sharing
  - apps sharing
  - simulation and analysis
  - collaboration
- linking everything with everything
  - data, apps, and users
- automation of all tasks
  - data management
  - simulation/analysis/prediction

PrIMe CI: Workflow

- architecture
  - cloud-based
  - browser-based
  - composed of components (apps, database, …)
  - graphical user interface for creation of projects from components
  - runs components (apps) on client (user) machine
- supports components written in
  - Matlab and C# (running on a client desktop)
  - any language (running on a client server)
- supports external access via web services

PrIMe CI: Workflow

- major upgrade to version 2.0
  - simplified installation
  - speedup loading and operation
  - wider variety of platforms
  - *Search* and *Submit* components are rewritten in C#

    and thus can be used without Matlab;

    PrIMe users can submit/retrieve data entirely on their own
  - redesign of component uploading

    users designated as Developers can submit their own components entirely on their own

PrIMe CI: Portal

- a unified user access to all PrIMe features
- control of user-access privileges / roles
- support of user collaboration
  - autonomous Work Groups (unlimited number of)
  - conference “proceedings” (Soot Workshop 2007)
  - discussion forums
- PrIMe Data Model description
- (Video) tutorials and demos
- built on Drupal; updated to new version

PrIMe
Process Informatics Model

Username:
mfrenklach
Log out

Home ▽ Announcements PrIMe Data ▽

mfrenklach

- ⊞ Case Tracker
- ⊞ Create content
- PrIMe Workflow
- Switch to test user
- My account
- ⊞ Administer

other

- Work Groups
- Membership Statistics
- Group Leaders Manual

Home

Home Page

View | Edit | Outline | Track

GROUPS

- Soot
- Management
- PrIMe Team
- SERDP
- MURI
- Portal Development
- ReactionDesign

Lost or Confused?

We have **tutorials** to help! Take a look at our tutorial categories below:

Getting Started
What can I do?, Installing the PWA (PrIMe Workflow Application)...

Data Management
Introduction, Searching for Data, Submitting Data...

Analysis
What is the PWA?, Using the PWA, Data Collaboration...

Collaboration
Introduction, Joining Work Groups...

Examples of Analysis
Shock-tube Ignition Simulation, Predicting H2-O2 Ignition...

» Add new comment | 4650 reads

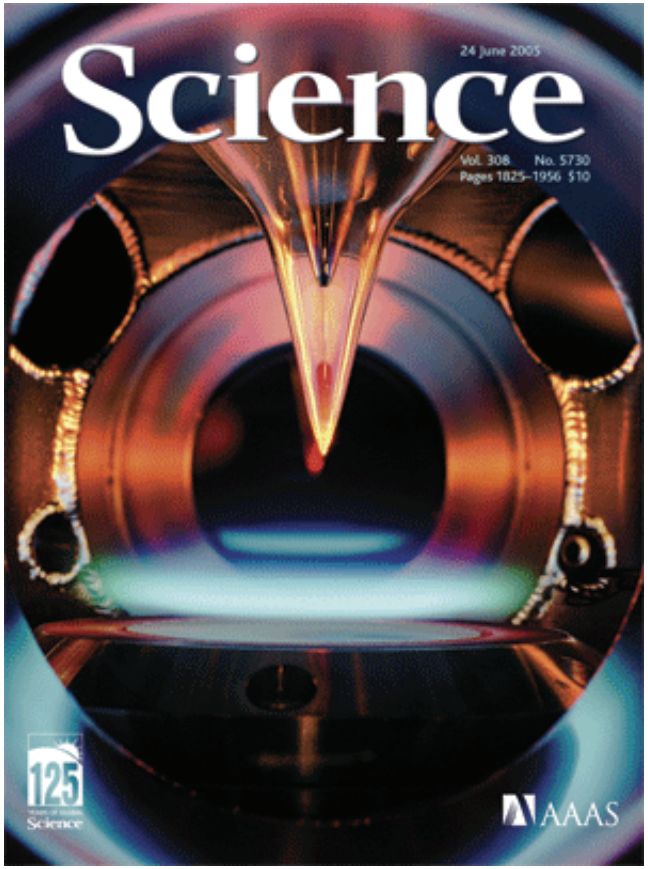
Examples of PrIMe applications

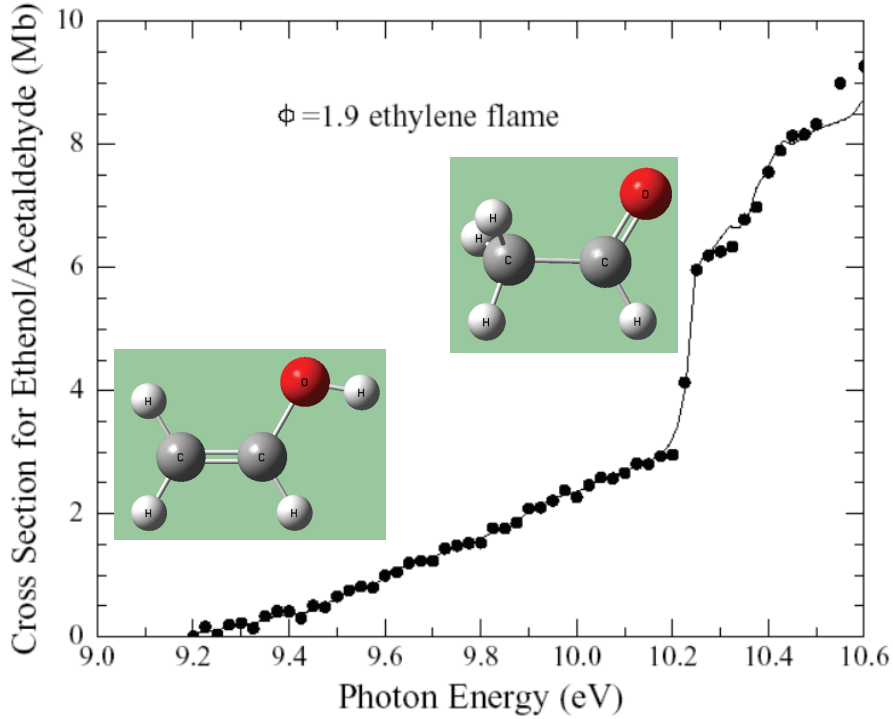
Instrumental Model

from Yeates, Li, Westmoreland, Russi, Packard, Frenklach,
7th U.S. National Combustion Meeting, March, 2011

Advanced Light Source, LBNL: Flame-Sampling MBMS Apparatus

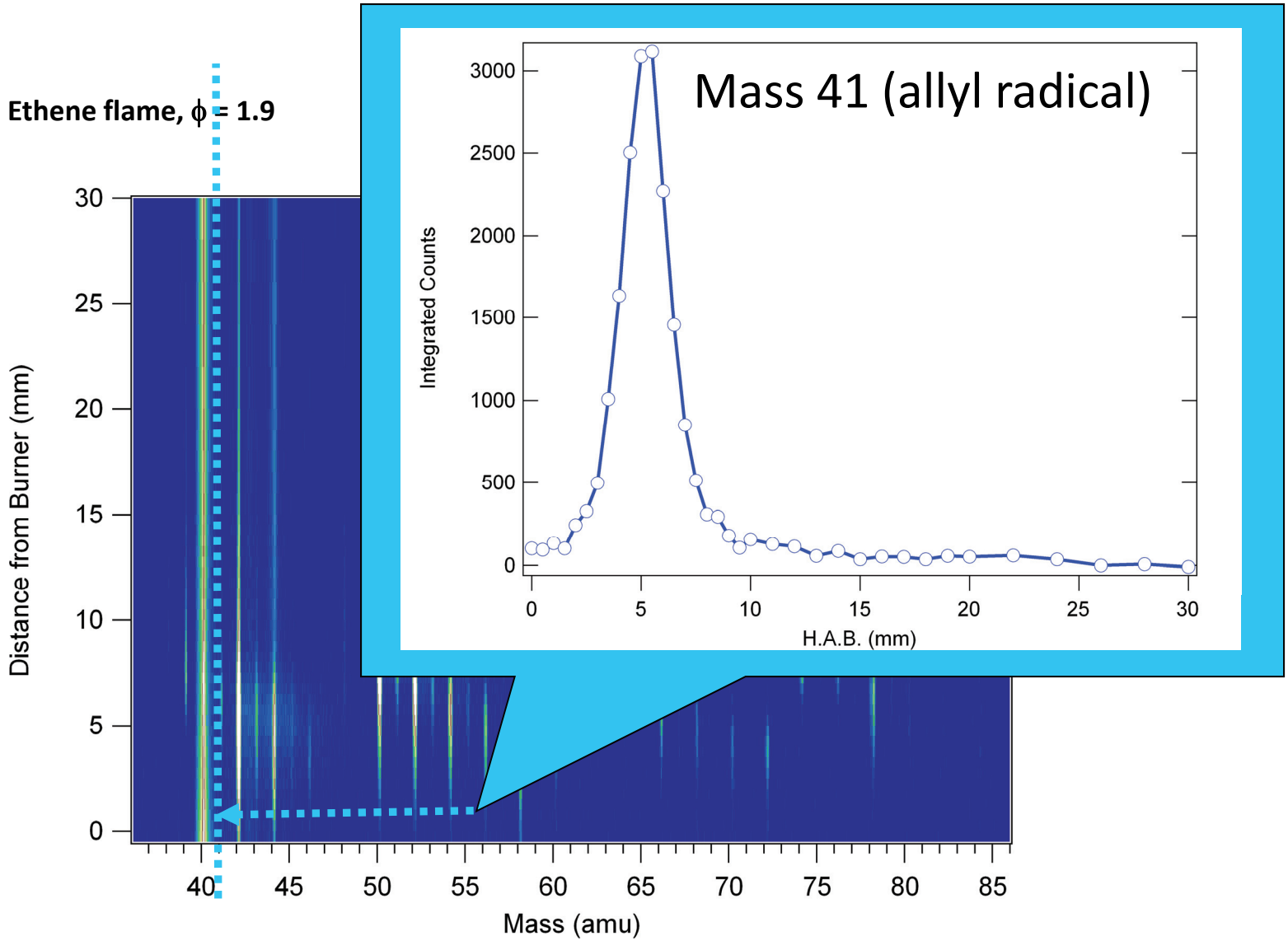
Identify species using mass and ionization threshhold.





Line is fit of pure-species cross sections for split:
0.37±0.05 ethenol and 0.63±0.05 acetaldehyde

For composition profiles, measure spectrum at each position.



To obtain mole fractions, need calibrations and corrections.

- Subtract isotopic contributions (e.g., $^{13}CH_3$ from $^{12}CH_4$).

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- Measure, look up, or estimate ionization cross-sections:

$$\frac{x_i}{x_{ref}} = \frac{I_i}{I_{ref}} \times \frac{(\text{cross section})_i}{(\text{cross section})_{ref}}$$

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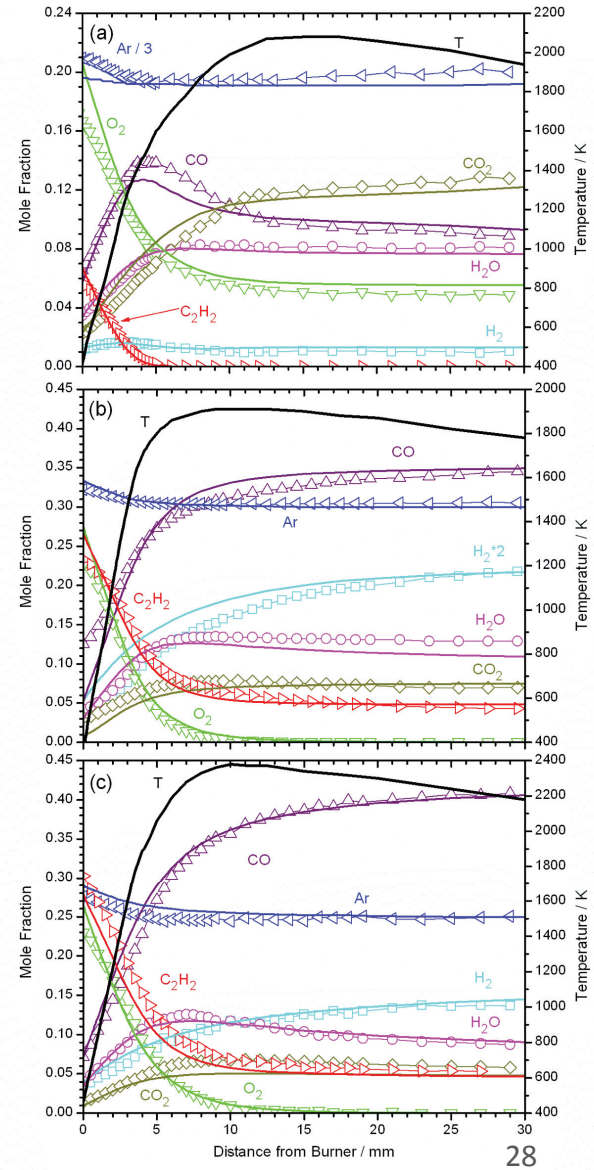
$$\frac{x_i}{x_{ref}} = \frac{I_i}{I_{ref}} \times \frac{(\text{cross section})_i}{(\text{cross section})_{ref}}$$

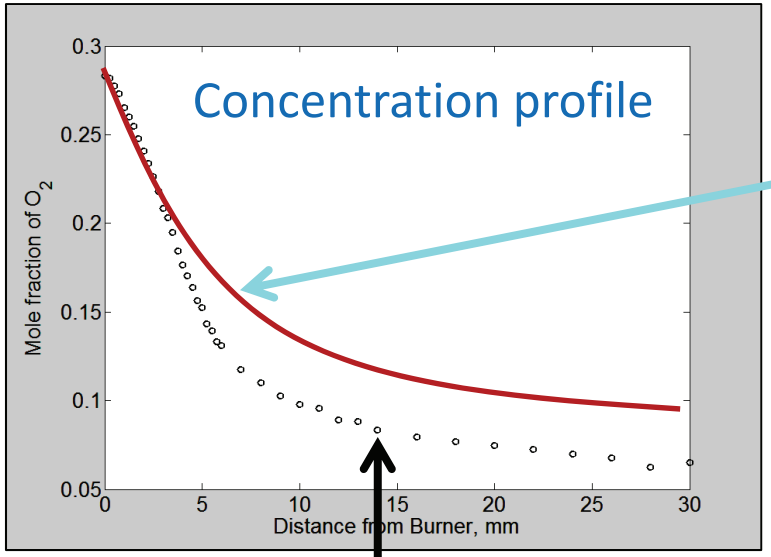
- Direct calibration of CO/CO_2.
- Infer x_{fuel}/x_{Ar} and x_{O2}/x_{Ar} from feed composition and x_{H2O}/x_{Ar} from post-flame H balance.
- Infer x_{Ar} and thus all x_i from mole-fraction ratios:

$$\frac{x_1 + x_2 + \ldots + x_{Ar}}{x_{Ar}} = \frac{1}{x_{Ar}} \qquad = \sum_{i \neq Ar} \frac{x_i}{x_{Ar}} + 1$$

- There are parametric uncertainties and stochastic signal noise.



Summarize this analysis conceptually:



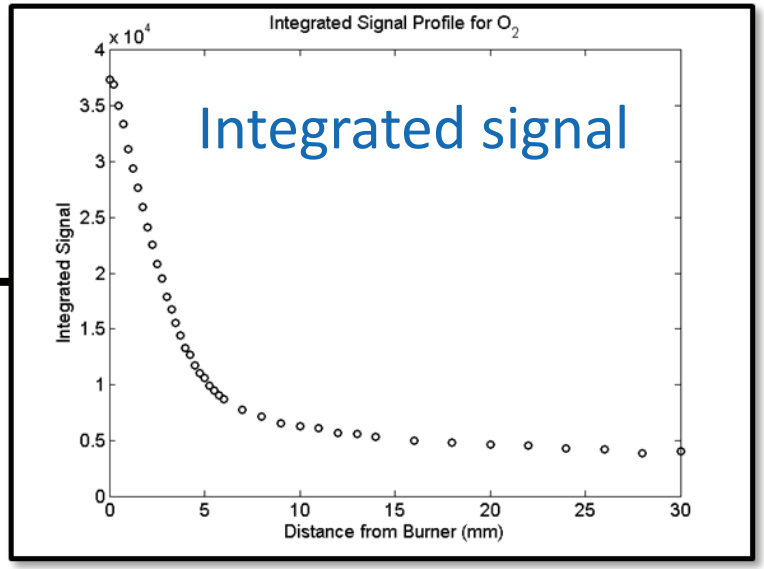
Model

Data Analysis

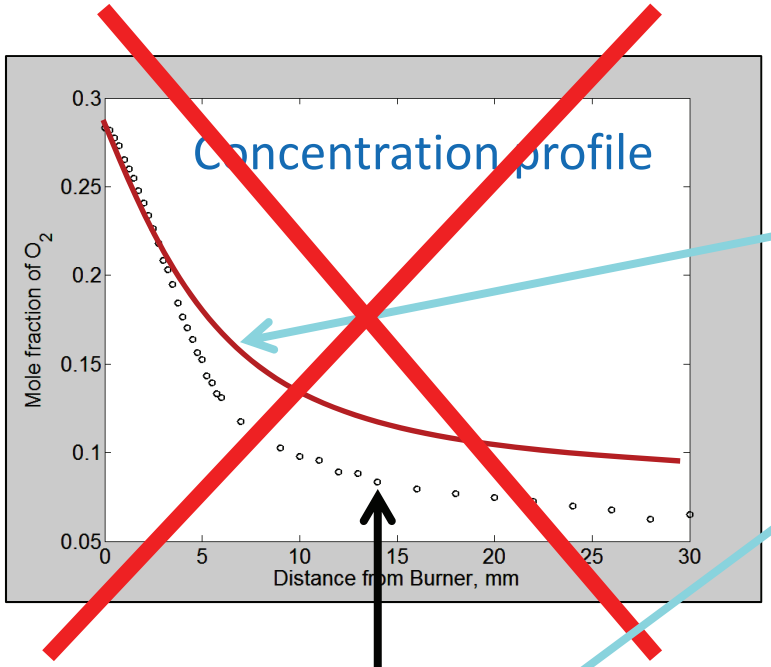
$$y = f(x,c)$$

Calibration, c

Assumptions



Instead, incorporate uncertainties using Instrumental Model:



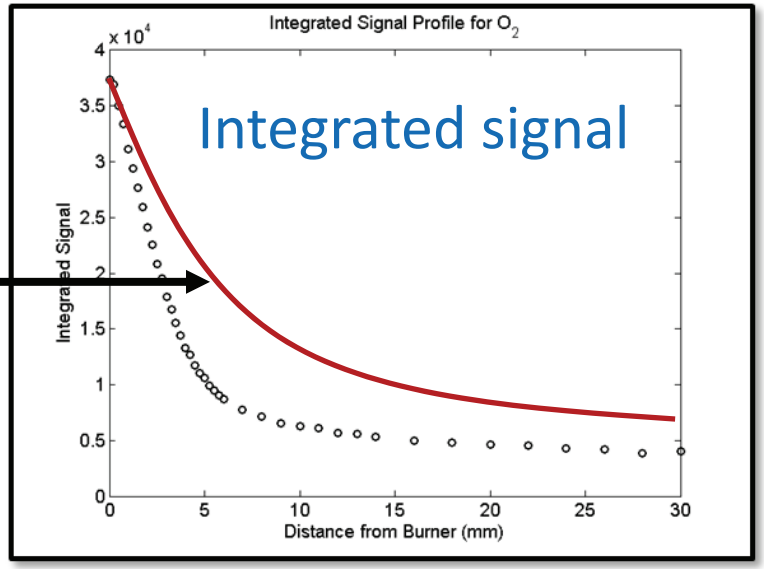
Model

Data Analysis

$y = f(x,c)$

Calibration, c

Assumptions



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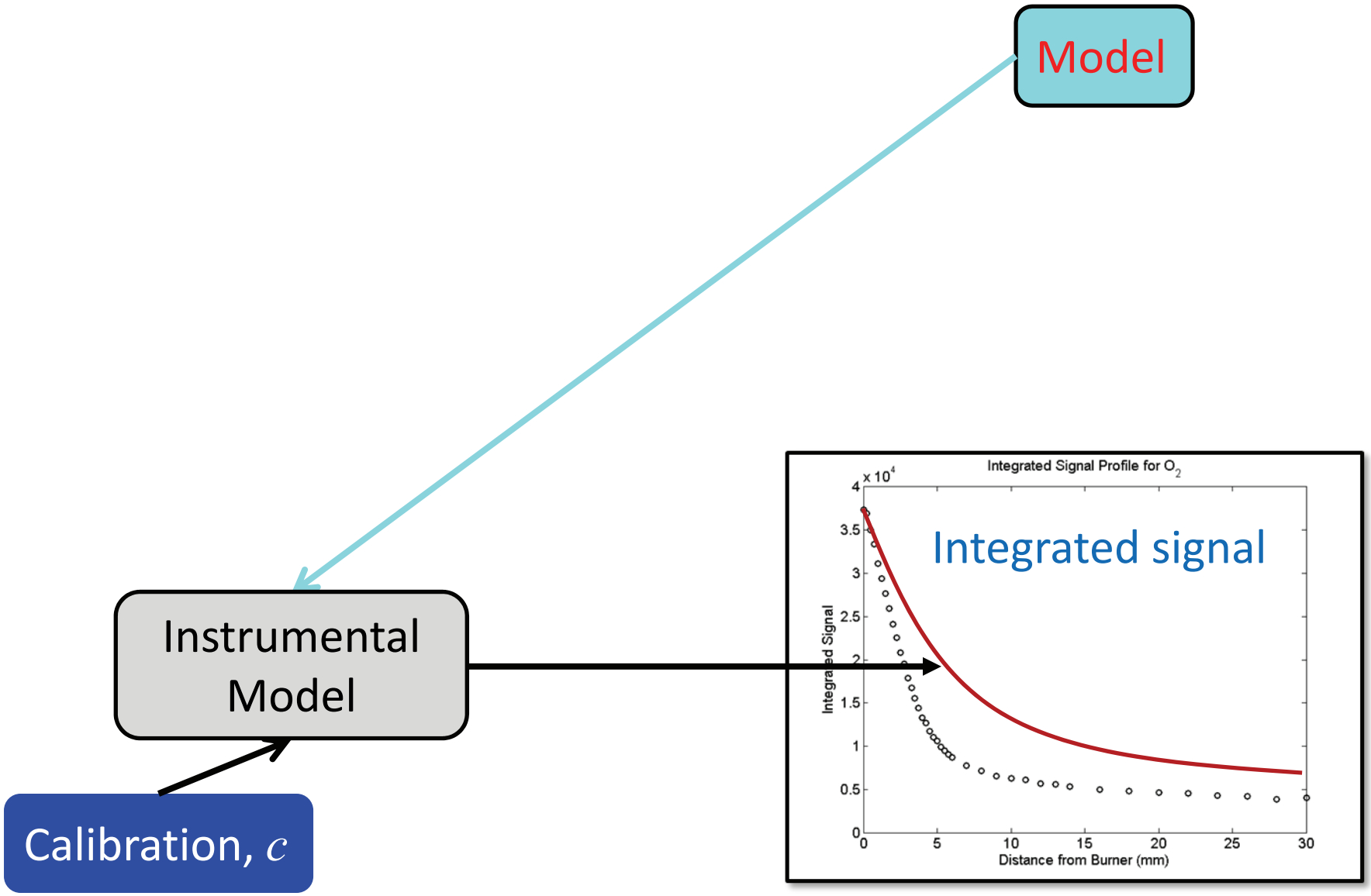
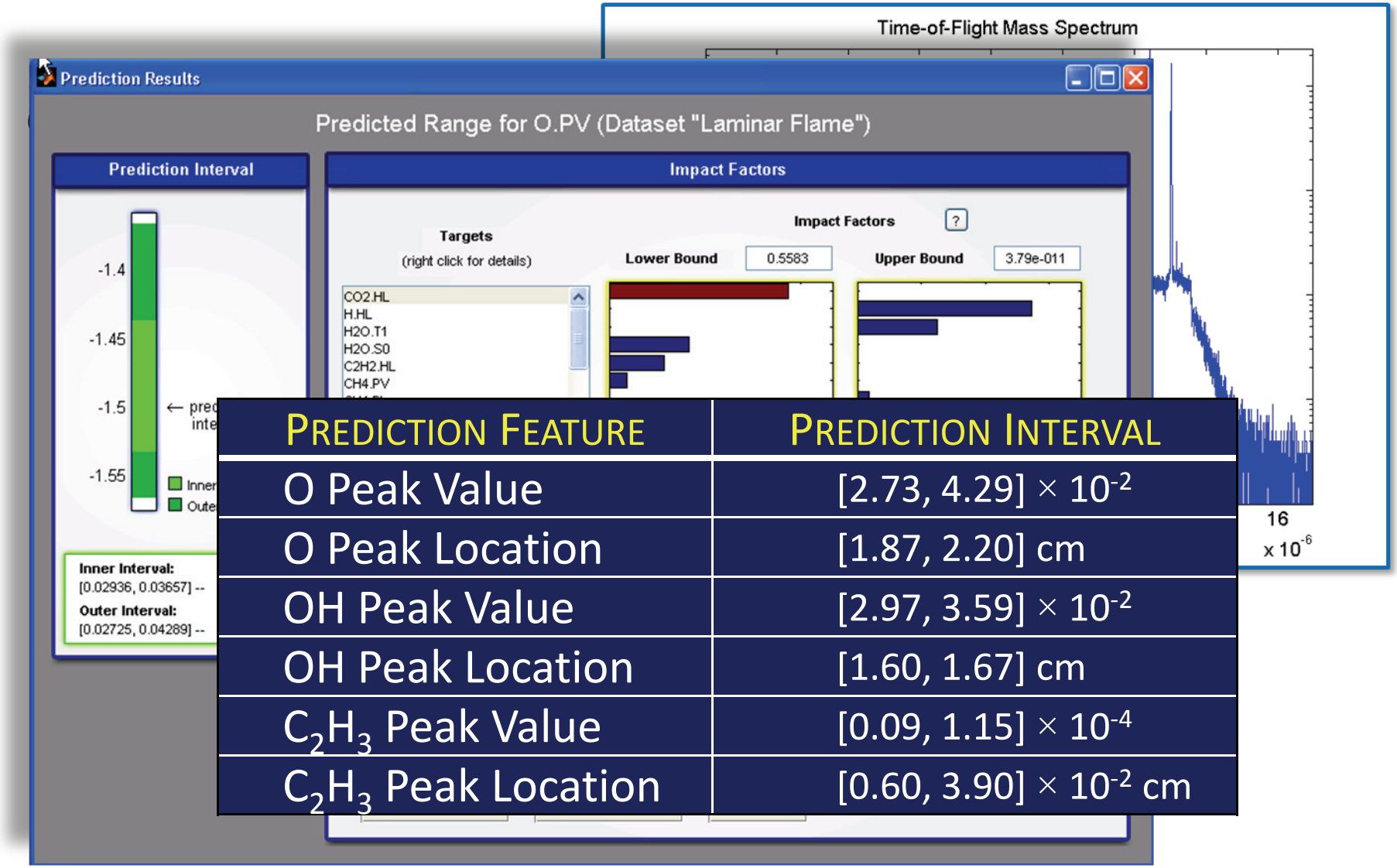


Thus, assess uncertainties such as peak location and value.

IM complements Reaction Path Analysis of (only) the model.



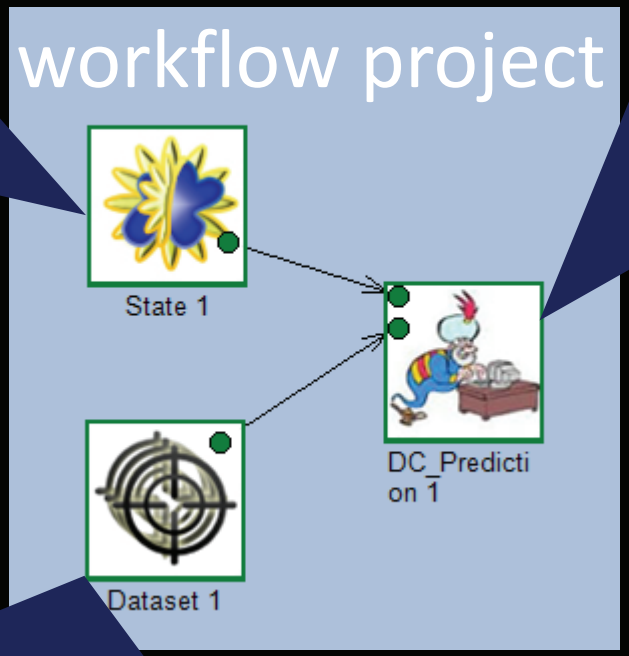
Prediction Feature	Prediction Interval
O Peak Value	$[2.73, 4.29] \times 10^{-2}$
O Peak Location	[1.87, 2.20] cm
OH Peak Value	$[2.97, 3.59] \times 10^{-2}$
OH Peak Location	[1.60, 1.67] cm
C_2H_3 Peak Value	$[0.09, 1.15] \times 10^{-4}$
C_2H_3 Peak Location	$[0.60, 3.90] \times 10^{-2}$ cm

Automation with PrIMe

Automated H_2-O_2 System

- Detailed Model
  - 21 elementary reactions
- Dataset
  - 12 Targets
    - 8 shock-tube ignition times
    - 4 flow-reactor conversions
- All documented/archived in PrIMe Data Warehouse

user specifies conditions of interest



workflow component performs:

- retrieves the pertinent kinetics model (via link in the dataset)
- performs simulations on the fly for the conditions specified and builds a new surrogate model
- performs UQ-DC analysis combining the new surrogate model with the archived ones and the rest of the pertinent data
- reports results

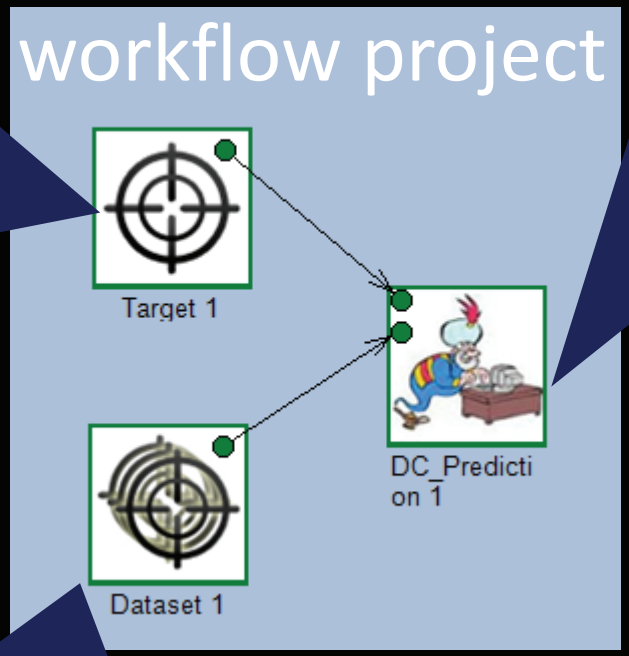
workflow component retrieves archived data: a set of relevant targets

target values and their uncertainty ranges

surrogate models developed for relevant targets

active variables and their uncertainty ranges

user specifies a *new target* (submitted to the Data Warehouse previously)



workflow component performs:

- retrieves the pertinent kinetics model (via link in the dataset)
- performs simulations on the fly for the ***new target*** and builds a new surrogate model
- performs UQ-DC analysis combining the new surrogate model with the archived ones and the rest of the pertinent data
- reports results
- adds the new target data to the dataset and archives in Warehouse

workflow component retrieves archived data: a set of relevant targets

target values and their uncertainty ranges

surrogate models developed for relevant targets

active variables and their uncertainty ranges

enrichment

Concluding Remarks

- PrIMe Data Models are suitably mature and current PrIMe Infrastructure is sufficiently stable to serve as initial platform for the "Combustion CI"
  - Everybody will work then with the same data
  - User-assembled information-based collaboration (a la Facebook)
  - Democratization of Science
- It is not a zero-activation-energy entry, but can be easily mastered (e.g., tutorial sessions)
- Suggest H_2-O_2 as a "test-bed" for the immediate communal activity