NIST, September 10, 2008

# A New Platform for Predictive Modeling: PrIMe


Michael Frenklach
Zoran Djurisic
Michael Gutkin



*Supported by:*

*NSF Chemistry Division (Cyber-infrastructure)*

***AFOSR (MACCCR)***

*SERDP*


Berkeley
University of California

# What's New with PrIMe

- PrIMe Portal – true 24/7 service; new features
- 2 new PrIMe Work Groups: SERDP, MURI / *private* mode
- "C0-C2" PWG is active – NSF-EVO project
- total registered members: >180
- Data Depository
  - species records were cleaned: joint MIT-UCB efforts
  - new species data are being developed (geometries, frequencies,…): MIT+Stanford
  - next: cleaning reaction records
- new components of Data Model
  - *Targets* – features of experiments to match / model training
  - *Instrumental* model – separation of experimental facts from experimenters' opinions/assumption
  - next: Optimization variables
- PrIMe Workflow – new paradigm of data/codes sharing

# What does it mean:

## "To Archive Data"

# PrIMe Data Model

- One copy per number
- Complete documentation
  - who, when, what
  - uncertainty
- Extendable and expandable
- Zero-error fetching
- Facts vs opinions

# PrIMe Data Model

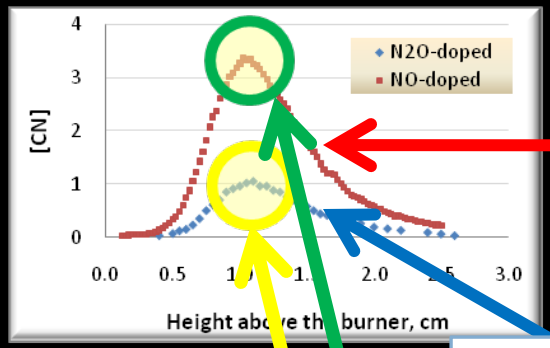
- Bibliography
- Chemical Elements
- Species
- Reactions
- Models
- Experiments
- Targets
- Instrumental models

# 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>
  <reactionLink preferredKey="O + O = O2" reversible="true" primeID="r00013869">
    <reactionRateLink preferredKey="2O + M = O2 + M" primeID="rk00000015"/>
    <reactionRateLink preferredKey="2O + H2 = O2 + H2" primeID="rk00000016"/>
    <reactionRateLink preferredKey="2O + H2O = O2 + H2O" primeID="rk00000017"/>
    <reactionRateLink preferredKey="2O + CH4 = O2 + CH4" primeID="rk00000018"/>
    <reactionRateLink preferredKey="2O + CO = O2 + CO" primeID="rk00000019"/>
    <reactionRateLink preferredKey="2O + CO2 = O2 + CO2" primeID="rk00000020"/>
    <reactionRateLink preferredKey="2O + C2H6 = O2 + C2H6" primeID="rk00000021"/>
    <reactionRateLink preferredKey="2O + Ar = O2 + Ar" primeID="rk00000022"/>
  </reactionLink>
  <reactionLink preferredKey="O + H2 = H + OH" reversible="true" primeID="r00012186">
     <reactionRateLink preferredKey="O + H2 = H + OH" primeID="rk00000005"/>
  </reactionLink>
  <reactionLink preferredKey="O + HO2 = OH + O2" reversible="true" primeID="r00012138">
    <reactionRateLink preferredKey="O + HO2 = OH + O2" primeID="rk00000002"/>
  </reactionLink>
</reactionSet>

</chemicalModel>
```

# What does it mean:

"To Compare Models and Data"




```
<experiment primeID="x00000031">

<experiment primeID="x00000033">
 <bibliographyLink preferredKey="Miller, J.A. 1985" primeID="b00006746"/>
 <apparatus>
   <kind>flame</kind>
   <mode>laminar</mode>
```

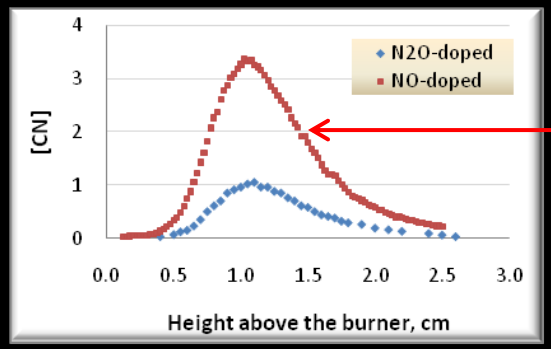
```
<target primeID="t00000074">

 <propertyLink id="x" experimentPrimeID="x00000031" dataGroupID="dg1" propertyID="x1"/>
 <propertyLink id="[CN]NO" experimentPrimeID="x00000031" dataGroupID="dg1" propertyID="x2"/>
 <propertyLink id="x" experimentPrimeID="x00000033" dataGroupID="dg1" propertyID="x1"/>
 <propertyLink id="[CN]N2O" experimentPrimeID="x00000033" dataGroupID="dg1" propertyID="x2"/>

 <feature id="[CN]N2Opeak">
   <indicator id="x" propertyID="t" transformation="1"/>
   <observable id="[CN]" propertyID="[CN]N2O" transformation="1"/>
   <method type="peak">
      <methodParameter name="type">least-squares fit</methodParameter>
     <methodParameter name="order">3</methodParameter>
   </method>
 </feature>

 <feature id="[CN]NOpeak">
   <indicator id="x" propertyID="t" transformation="1"/>
   <observable id="[CN]" propertyID="[CN]NO" transformation="1"/>
   <method type="peak">
      <methodParameter name="type">least-squares fit</methodParameter>
      <methodParameter name="order">3</methodParameter>
   </method>
 </feature>

 <targetValue>
   <indicator id="[CN]NO" featureID="[CN]NOpeak" propertyID="[CN]" transformation="1">
      <property name="composition" units="ppm" label="[CN]NO" description="peak CN fraction in the NO-doped  flame"/>
    </indicator>
   <indicator id="[CN]N2O" featureID="[CN]N2Opeak" propertyID="[CN]" transformation="1">
      <property name="composition" units="ppm" label="[CN]N2O" description="peak CH fraction in the N2O-doped flame"/>
   </indicator>
   <observable id="CN peak ratio" featureID="" propertyID="" transformation="1">
      <property name="composition" units="dimensionless" label="peak [CN] ratio" description="ratio of peak [CN] in NO- and N2O-doped flame">
         <value>2.9</value>
      </property>
    </observable>
   <method type="custom">
      <customMethod type="simple eval">[CN]NO/[CN]N2O</customMethod>
   </method>
 </targetValue>
```

TARGET:
their ratio

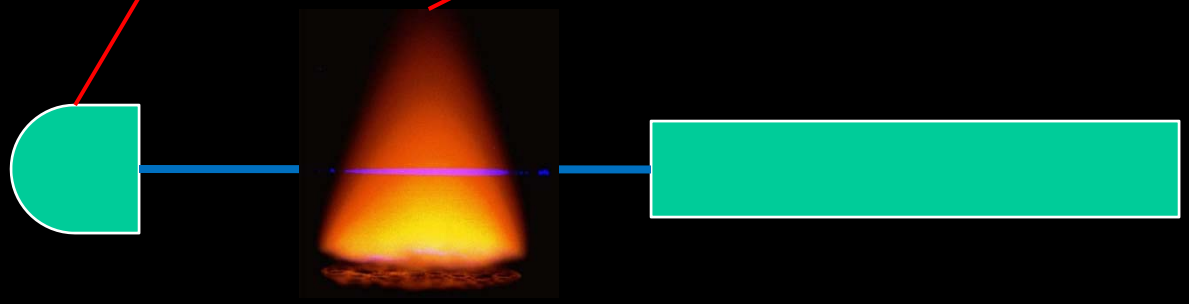
# What does it mean:

# "Experimental Data"

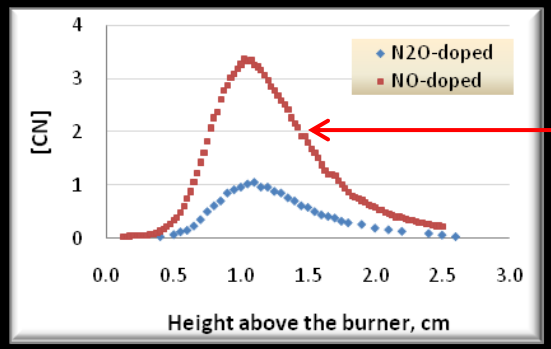
# PrIMe Data Model: Instrumental Model



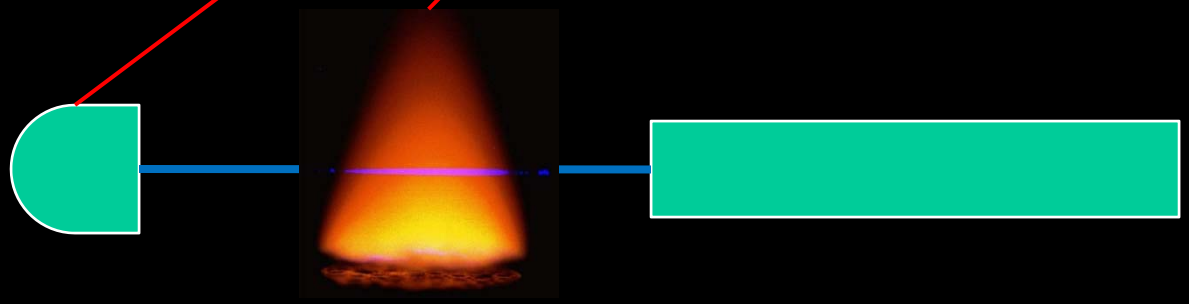

$$\frac{I}{I_0} = e^{-\varepsilon[\mathrm{CN}]L}$$



# PrIMe Data Model: Instrumental Model




```
<instrumentalModel primeID="i00000001">

  <preferredKey Beer-Lambert Law</preferredKey>
  <keywords>laser absorption</keywords>

  <expression type="MathML" implicit="true">
    <math>
      <apply>
        <eq/>
        <ci>C</ci>
        <apply>
          <divide/>
          <apply>
            <ln/>
            <apply>
              <divide/>
              <apply>
                <minus/>
                <ci>V_inf</ci>
                <ci>V</ci>
              </apply>
              <apply>
                <ci>V_inf</ci>
                <ci>V_0</ci>
```



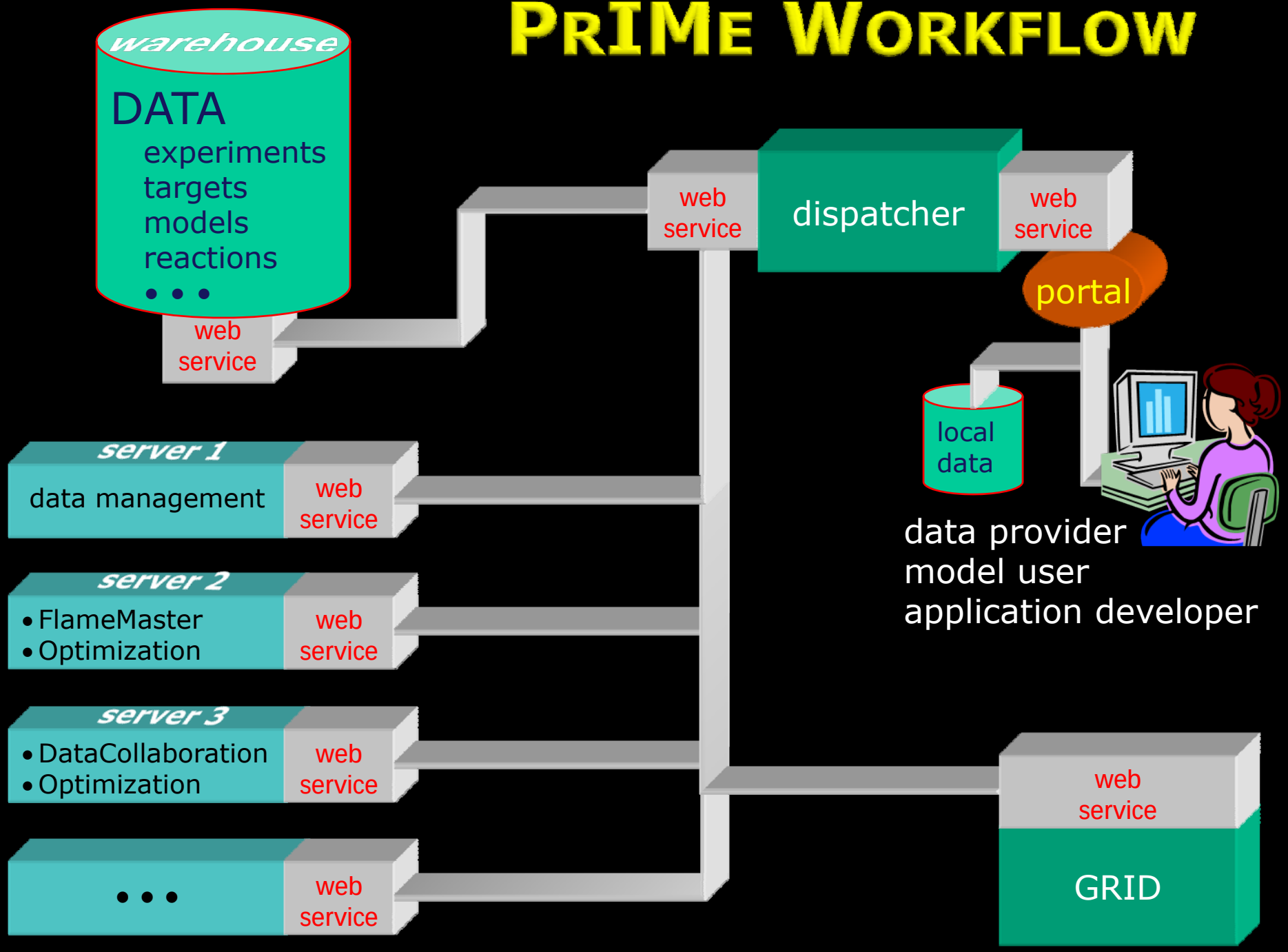
# What does it mean:

"AUTOMATE MODEL BUILDING"

# PrIMe Workflow

- Collect and curate data
- Share data
- Link data to applications
- Share applications

# PrIMe Workflow



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## About PrIMe

PrIMe—Process Informatics Model—is a new approach for developin mical reaction systems that is based on the scientific collaboratory pa takes full advantage of existing and developing cyber infrastructure. The primary goals of PrIMe are collecting and storing data, validating the data and uncertainties, and assembling the data into predictive models with quantified uncertainties to meet specific user requirements. The principal components of PrIM data Depository, which is a repository of data provided by the community, a data Library for storage of evaluated data, and a set of computer-based tools to proce to assemble data into predictive models. Two guiding principles of PrIMe are: open membership—a qualified individual or industrial organization can register to partic project; and open source—all submitted data, tools and models will be in the public domain.

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http://primekinetics.org/data_model

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3.2.1. *Species Collection*. The following figure is a schematic diagram of the PrIMe Warehouse **species** collection.

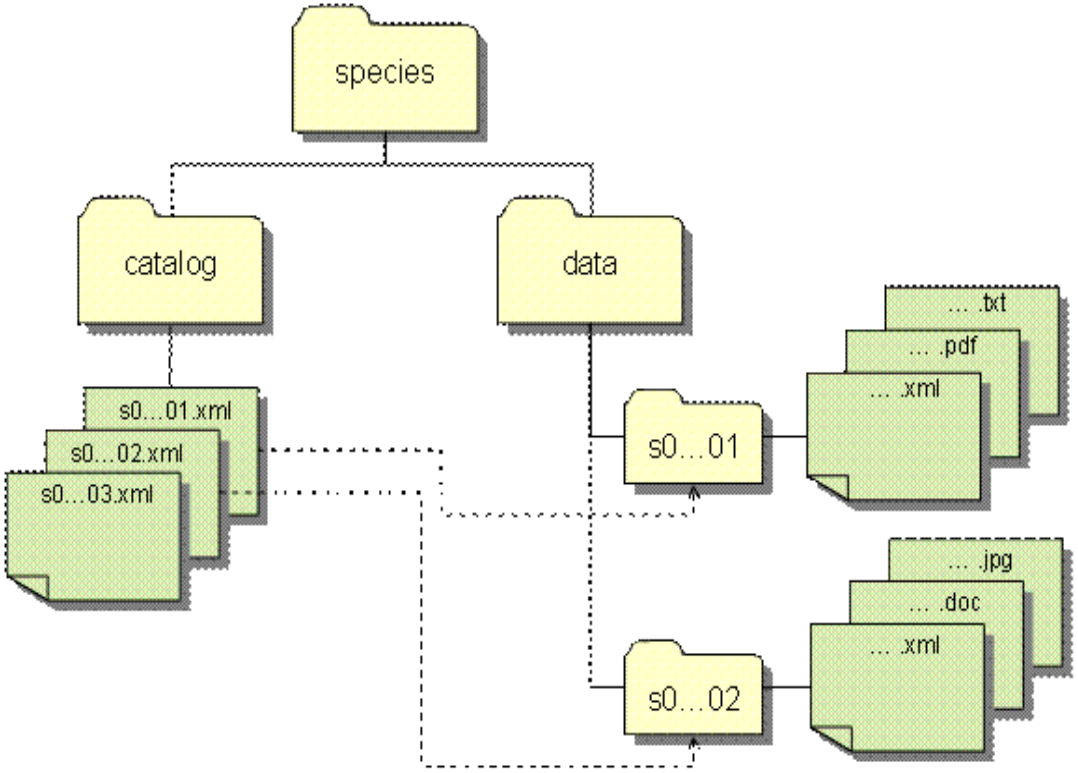


Figure 1. A schematic diagram of the PrIMe Warehouse **species** collection

The **catalog** files are named starting with the letter **s** followed with the 8-digit number, and this is the PrIMe species **primeID** (like **s00000001** or **s00001234**). The same **primeID** is used to name the corresponding subdirectories of **species/data**. These subdirectories contain data files, which can be of any type, as illustrated in the diagram.

**3.3. Data Definition Files.** The XML files of the catalog collections and of some data subdirectories will be validated against *schemas*. XML schemas express shared vocabularies and allow machines to carry out rules made by people. They provide a means for defining the structure, content and semantics of XML documents in more detail.Â  Passing XML validation means that the submitted/created XML documents adhere to the scientific rules set by the PrIMe community.

## 4. REFERENCES

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http://primekinetics.org/prime_data_warehouse

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# warehouse.primekinetics.org - /depository/

[To Parent Directory]

| | | |
|---|---|---|
| Thursday, October 05, 2006 4:06 PM | <dir> | bibliography |
| Thursday, October 05, 2006 4:06 PM | <dir> | elements |
| Thursday, October 05, 2006 4:06 PM | <dir> | experiments |
| Monday, February 26, 2007 12:18 PM | <dir> | incoming |
| Thursday, October 05, 2006 4:06 PM | <dir> | models |
| Thursday, October 05, 2006 4:00 PM | <dir> | reactions |
| Thursday, October 05, 2006 3:38 PM | <dir> | species |
| Thursday, October 05, 2006 3:37 PM | <dir> | targets |

[To Parent Directory]

| | | |
|---|---|---|
| Tuesday, February 20, 2007 3:34 PM | <dir> | catalog |
| Thursday, October 05, 2006 4:06 PM | <dir> | data |

| | | | |
|---|---|---|---|
| 4:47 PM | 2238 | x00000001.xml |
| Friday, February 02, 2007 4:47 PM | 3047 | x00000002.xml |
| ry 02, 2007 4:47 PM | 71957 | x00000003.xml |
| ry 02, 2007 4:47 PM | 75579 | x00000004.xml |
| ry 02, 2007 4:47 PM | 2610 | x00000005.xml |
| ry 02, 2007 4:47 PM | 117357 | x00000006.xml |
| ry 02, 2007 4:47 PM | 109925 | x00000007.xml |
| ry 02, 2007 4:47 PM | 1695 | x00000008.xml |
| ry 02, 2007 4:47 PM | 1852 | x00000009.xml |
| ry 02, 2007 4:47 PM | 1759 | x00000010.xml |
| ry 02, 2007 4:47 PM | 1759 | x00000011.xml |
| Friday, February 02, 2007 4:47 PM | 1759 | x00000012.xml |
| Friday, February 02, 2007 4:47 PM | 1931 | x00000013.xml |
| Friday, February 02, 2007 4:47 PM | 1931 | x00000014.xml |
| Friday, February 02, 2007 4:47 PM | 1924 | x00000015.xml |
| Friday, February 02, 2007 4:47 PM | 1929 | x00000016.xml |
| Friday, February 02, 2007 4:47 PM | 1923 | x00000017.xml |
| Friday, February 02, 2007 4:47 PM | 1924 | x00000018.xml |
| Friday, February 02, 2007 4:47 PM | 1923 | x00000019.xml |
| Friday, February 02, 2007 4:47 PM | 2718 | x00000020.xml |
| Friday, February 02, 2007 4:47 PM | 1923 | x00000021.xml |
| Friday, February 02, 2007 4:47 PM | 2385 | x00000022.xml |
| Friday, February 02, 2007 4:47 PM | 2383 | x00000023.xml |
| Friday, February 02, 2007 4:47 PM | 2383 | x00000024.xml |
| Friday, February 02, 2007 4:47 PM | 2383 | x00000025.xml |
| Friday, February 02, 2007 4:47 PM | 2387 | x00000026.xml |
| Friday, February 02, 2007 4:47 PM | 4641 | x00000027.xml |
| Friday, February 02, 2007 4:47 PM | 2101 | x00000028.xml |

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## CONTACT INFORMATION

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**Phone Number**
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**Homepage**
http://www.me.berkeley.edu/faculty/frenklach

## PERSONAL INFORMATION

**Last Name**
Frenklach

**First Name**
Michael

**Company/Institution**
University of California at Berkeley

## HISTORY

**Member for**
2 years 18 weeks

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PrIMe Workflow App.
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PWA Installation

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# SERDP

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## SERDP BOOK

Submitted by Med Colket on April 16, 2007 - 11:34am.

Welcome to the SERDP Book

- AFRL Team
- Mechanisms
- Sandia Team
- Stanford team
- Univ of Illinois, Chicago team
- Univ of Utah team

AFR

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» 515 reads

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my group: feed page
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Submitted by Med Colket on May 29, 2008 - 11:19am.

Enter reports, publications, presentations

- AFRL SERDP reports
- AFRL team presentations
- AFRL team publications
- AFRL team results

‹ SERDP Book up AFRL SERD

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    - AF Quarterly Jan - Mar 07
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Submitted by Med Colket on May 29, 2008 - 5:29pm.

Folder for Quarterly, Annual reports

| Attachment | Size |
|---|---|
| 1st Qrt Oct-Dec 07.doc | 121 KB |

- 3rd Quarterly Report April - June 2008
- AF Quarterly Jan - Mar 07

‹ AFRL Team up 3rd Quarterly Report April - Ju

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  - PrIMe Workflow App.
  - Component Uploader
  - PWA Installation
- Switch to test user
- My account
- Administer

other

- Work Groups
- Membership Statistics
- Group Leaders Manual

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| Name | Subscribers | Description |
|---|---|---|
| Burner-stabilized premixed flames | 22 | Burner-stabilized premixed flames |
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| C3-C4 | 39 | C3-C4 hydrocarbon pyrolysis and oxidation |
| C5-C16 | 35 | C5-C16 hydrocarbon pyrolysis and oxidation |
| C6 + aromatics | 20 | C6 + aromatic hydrocarbon pyrolysis and oxidation |
| Cyber-numerics | 26 | Cyber-numerics |
| Diffusion flames | 22 | Diffusion flames |
| Flow reactors | 2 | Flow reactors |
| Industrial | 1 | Industrial |
| Laminar premixed flames | 32 | Laminar premixed flames (global properties) |
| N | 7 | Nitrogen containing |
| P-dependence | 15 | Pressure dependence of reactions |
| Portal Development | 5 | Portal Development |
| Quantum chemistry | 2 | Quantum chemistry |
| Shock tubes | 27 | Shock tubes |
| Soot | 54 | Soot |
| Spectroscopy | 4 | Spectroscopy |
| Stirred reactors | 7 | Stirred reactors |
| Thermo | 33 | Thermodynamic data |
| Transport | 11 | Transport data |
| TST | 9 | Transition-State theory |
| Turbulent flames | 1 | Turbulent flames |

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all posts: feed page

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## C0-C2 BOOK

Submitted by administrator on May 12, 2006 - 3:47pm.

Welcome to the first page of **C0-C2** Book. Click on the links below to contribute to the various discussions.

- Discussion of organization and procedures
- Kinetics sub-area divisions discussion
- Notices of interest
- REACTIONS
- Voting page

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PrIMe Workflow Application

Workflow

**Recent Projects**

myProject1
USCserverTest

**Getting Started**

New Project
Sample Project
How do I?
Help

**PrIMe Workflow**

## Start: create a new project

- go to "New Project"
- create a network by dragging and connecting the appropriate objects (i.e., Target from Targets, PlugFlow from Processes, etc)
- save the network giving it a distinct name
- execute the network by clicking 'Run'

## Execute saved project

- go to "Open"
- double-click a previously saved project
- execute the network by clicking 'Run

## Collaborating

- check the "Public" box

PrIMe Workflow Application

Workflow

Save | Save as | Run | Node status

**Process Elements**

Input

SetOfTargets

State

Target

**Inputs**

**Models**

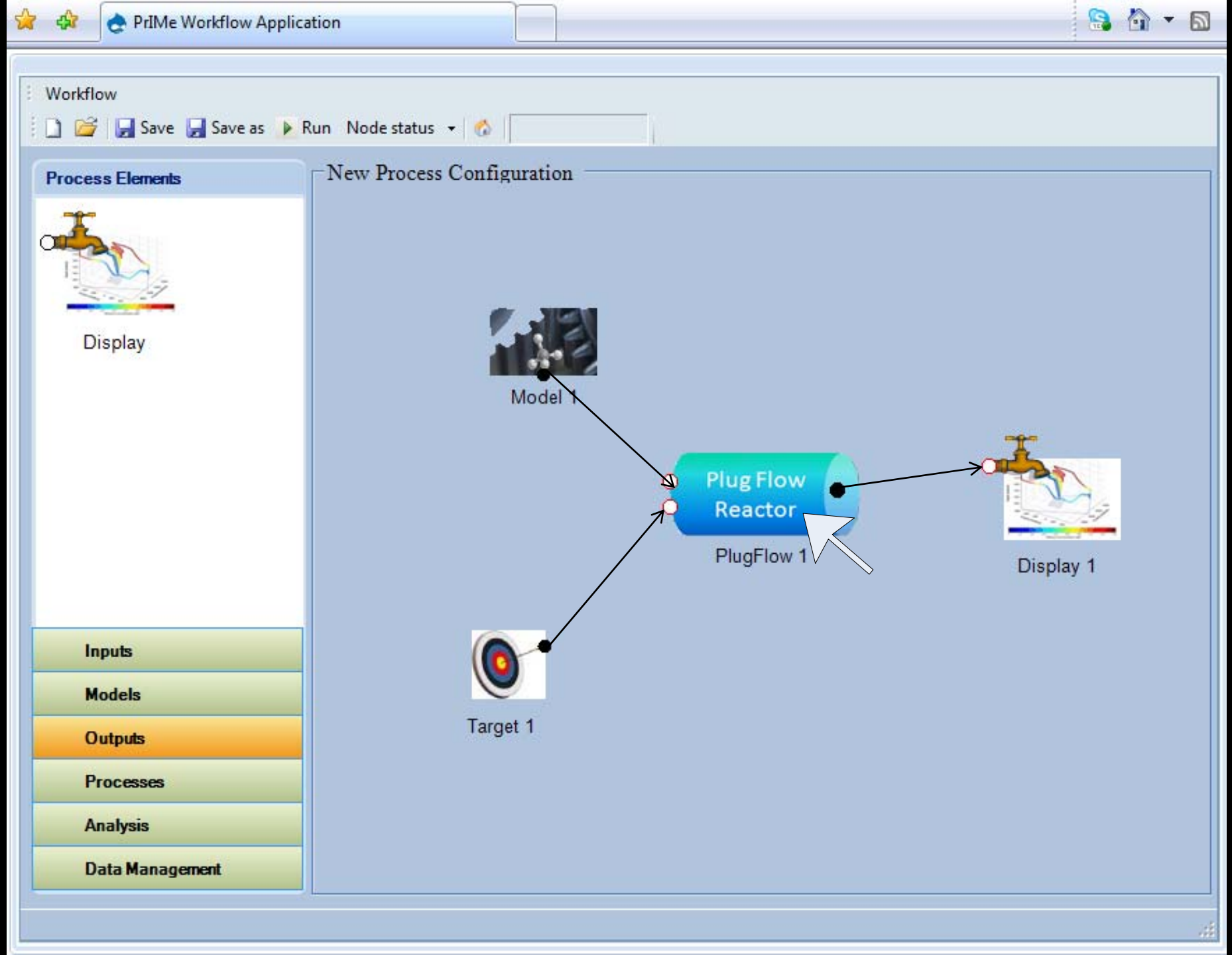
**Outputs**

**Processes**

**Analysis**

**Data Management**

New Process Configuration

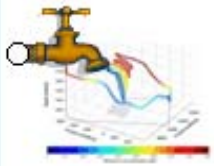

PrIMe Workflow Application
Workflow
Save
Save as
Run
Node status
Process Elements
Display
New Process Configuration
Model 1
Plug Flow Reactor
PlugFlow 1
Display 1
Target 1
Inputs
Models
Outputs
Processes
Analysis
Data Management

PrIMe Workflow Application

Workflow

Save | Save as | Run | Node status

**Process Elements**



Display

**Inputs**

**Models**

**Outputs**

**Processes**

**Analysis**

**Data Management**

New Proces

PlugFlow properties

Properties | About

| | |
|---|---|
| **attributes** | |
| Energy Control | **adiabatic** |
| Numerical Code | ReactionLab |
| Process | FlameMaster |
| Residence time (msec) | **1.6** |
| **general** | |
| Name | **PlugFlow 1** |

**Numerical Code**
Code Specification
Matlab application
http://reactionlab.sourceforge.net/

OK | Cancel | Run

PrIMe Workflow Application

Workflow

Save | Save as | Run | Node status

Process Elements

Display

Inputs

Models

Outputs

Processes

Analysis

Data Management

New Process C

PlugFlow properties

Properties | About

Save workflow project

Title: myProject1

Summary

Author

Status

Created 2008-09-05 08:45

Submitted 2008-09-05 08:45

Public | Share

Save | Cancel

Matlab application
http://reactionlab.sourceforge.net/

OK | Cancel | Run

PrIMe Workflow Application

Workflow

Save | Save as | Run | Node status

Process Elements

Display

Inputs

Models

Outputs

Processes

Analysis

Data Management

New Process C

PlugFlow properties

Properties | About

Save workflow project

Title: myProject1

Summary

Author

Created 2008-09-05 08:45

Public | Share | Save | Cancel

Share project

Users to share with

- abf123
- adityaj
- adityajami
- admin
- administrator
- aer0201
- alx
- amdean
- ammebel
- andrea.danna
- AndreiStarikovskii
- Andy Packard
- ansayre
- arazsarchami
- arvmenon
- ashutoshgupta
- baukalc
- Ben Akih

Share | Cancel

Matlab application
http://reactionlab.sourceforge.net/

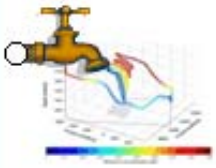
OK | Cancel | Run

PrIMe Workflow Application

Workflow

Save | Save as | Run | Node status

**Process Elements**



Display

- Inputs
- Models
- Outputs
- Processes
- Analysis
- Data Management

New Process Configuration

PrIMe Depository - search for target

Search: modeling targets | Find

where: any field | contains | ignition

any field | contains

Search results (13 hits): | Show details

/depository/targets/catalog/t00000001.xml
/depository/targets/catalog/t00000002.xml
/depository/targets/catalog/t00000003.xml
/depository/targets/catalog/t00000004.xml
/depository/targets/catalog/t00000005.xml
/depository/targets/catalog/t00000006.xml
/depository/targets/catalog/t00000007.xml
/depository/targets/catalog/t00000008.xml
/depository/targets/catalog/t00000009.xml
/depository/targets/catalog/t00000010.xml
/depository/targets/catalog/t00000011.xml

primeTarget: GRI-Mech 3.0 - IG.1a

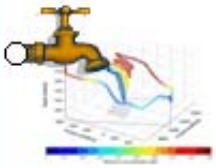
upload | View / Edit | Close

PrIMe Workflow Application

Workflow

Save | Save as | Run | Node status

**Process Elements**



Display

**Inputs**

**Models**

**Outputs**

**Processes**

**Analysis**

**Data Management**

## New Process Configuration

PrIMe Depository - search for model

Search: models | Find

where: any field | contains | gri

any field | contains

Search results (1 hits): Show details

/depository/models/catalog/m00000003.xml

primeModel
:
GRI-Mech 3.0
--
Smith et al., 1999.

upload | View / Edit | Close

PrIMe Workflow Application

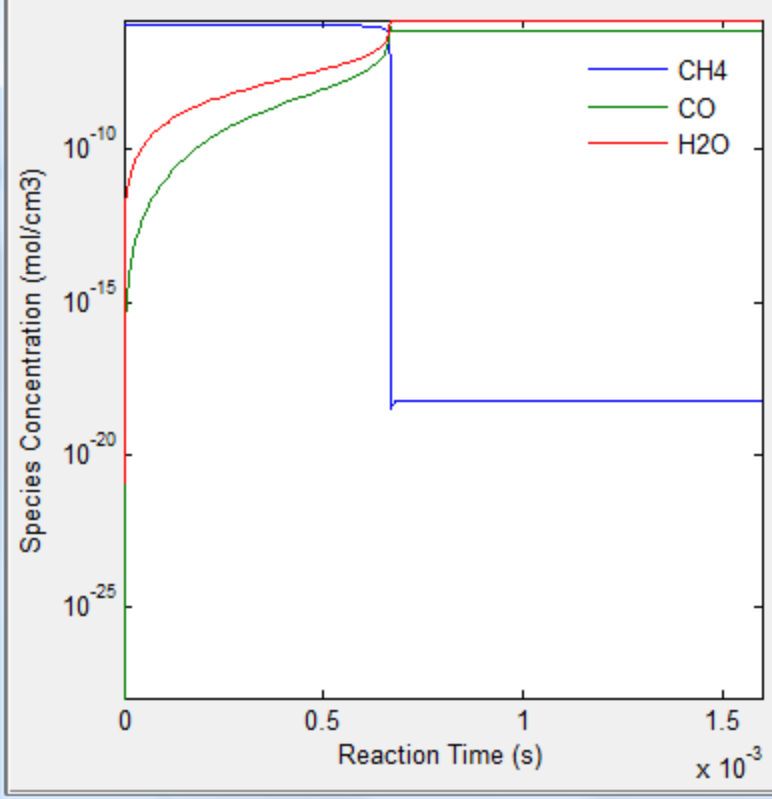
Workflow

Save | Save as | Run | Node status

Process Elements | myProject1

GRI-Mech 3.0 (adiabatic, V = const) Species Composition

File | Plot | Data




C3H7
C3H8
CH
CH2
CH2(S)
CH2CHO
CH2CO
CH2O
CH2OH
CH3
CH3CHO
CH3O
CH3OH
CH4
CN
CO
CO2
H
H2
H2CN
H2O
H2O2
HCCO
HCCOH
HCN
HCNN
HCNO
HCO
HNCO
HNO
HO2
HOCN

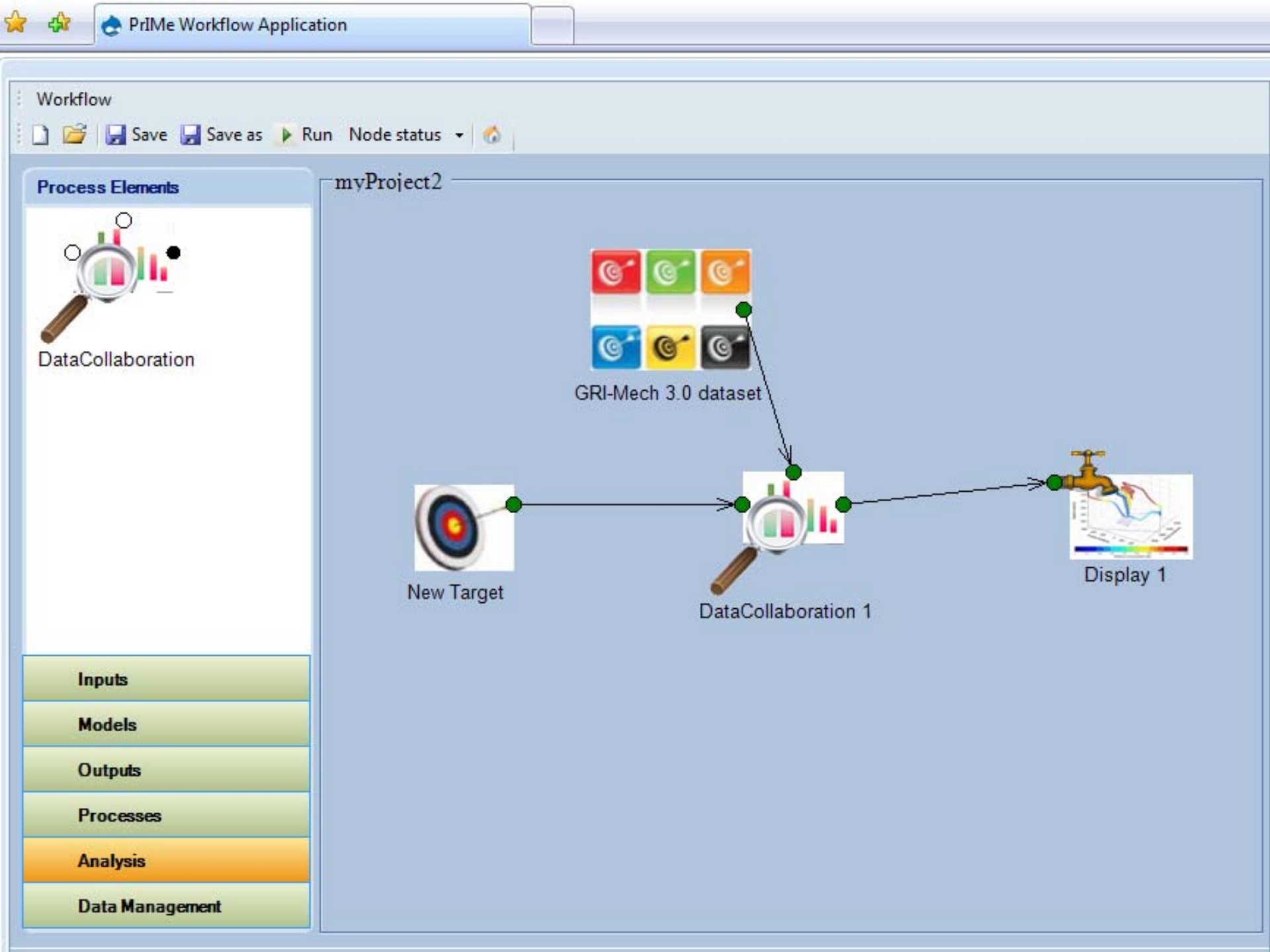
PFR (adiabatic, V = const)

View | Format

| | | |
|---|---|---|
| Temperature | 3137.7 | K |
| Pressure | 3.98 | atm |
| Total Conc | 1.55e-005 | mol/cm3 |
| Reaction Time | 1.6 | msec |

| Species | Mole Fraction | Rate (mol/cm3 s) |
|---|---|---|
| Ar | 6.77e-001 | 0.00e+000 |
| C | 1.38e-011 | -8.76e-020 |
| C2H | 3.25e-017 | -2.18e-025 |
| C2H2 | 2.08e-016 | 7.33e-025 |
| C2H3 | 2.20e-020 | 9.11e-028 |
| C2H4 | 2.40e-021 | -8.65e-028 |
| C2H5 | 2.24e-025 | 1.29e-027 |
| C2H6 | 3.68e-027 | 1.65e-029 |
| C3H7 | 0.00e+000 | 1.58e-027 |
| C3H8 | 0.00e+000 | 2.81e-026 |
| CH | 1.54e-012 | -1.97e-020 |
| CH2 | 8.14e-013 | 4.69e-021 |
| CH2(S) | 8.41e-014 | -3.57e-022 |
| CH2CHO | 4.75e-020 | 3.56e-025 |
| CH2CO | 9.70e-016 | 4.68e-025 |
| CH2O | 2.14e-009 | 1.37e-019 |
| CH2OH | 1.51e-013 | -8.33e-024 |
| CH3 | 4.55e-013 | 5.17e-022 |
| CH3CHO | 8.33e-022 | -7.28e-025 |
| CH3O | 3.95e-015 | -1.53e-023 |
| CH3OH | 3.32e-015 | 2.46e-023 |
| CH4 | 3.90e-014 | 1.83e-022 |
| CN | 0.00e+000 | -6.05e-028 |
| CO | 5.23e-002 | -7.41e-013 |
| CO2 | 3.25e-002 | 7.41e-013 |

Data Management

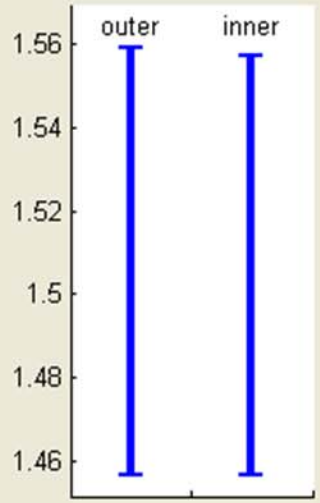

PrIMe Workflow Application
Workflow
Save
Save as
Run
Node status
Process Elements
DataCollaboration
Inputs
Models
Outputs
Processes
Analysis
Data Management
myProject2
GRI-Mech 3.0 dataset
New Target
DataCollaboration 1
Display 1

PrIMe Workflow Application

PredictionViewer

# Interval Prediction for Model co psu from Dataset GRIMech 3

## Prediction Interval




Inner Int. [1.457, 1.557]

Outer Int. [1.457, 1.559]

Analysis found feasible parameter values at which the model produces the endpoints of the inner interval.

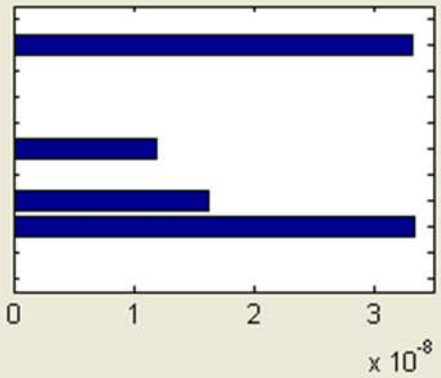
Constrained by the dataset, the model does not take values outside the outer interval.

## Constraint Multipliers

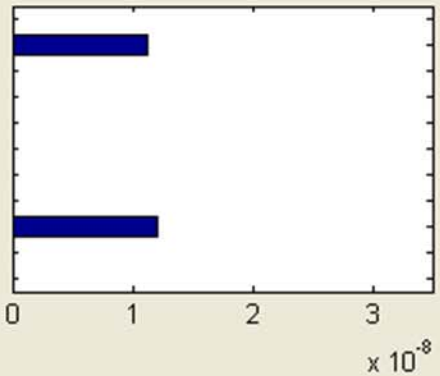
GRIMech 3 targets
(double-click for details)

t_[CO]max/2 (bch2o.t1): Hidaka et al C
t_[CO]max/2 (bch2o.t2): Hidaka et al C
t_[CO]max/2 (bch2o.t3): Hidaka et al C
t_[CO]max/2 (bco.t1): UCB CH2O-Ar=
t_[CO]max/2 (bco.t2): UCB CH2O-Ar=
t_[CO]max/2 (bco.t3): UCB CH2O-O2-
t_[CO]max/2 (bco.t4): UCB CH2O-O2-
t_[CO]max/2 (bco.t5): UCB CH2O-O2-
t_[CO]max/2 (bco.t6): UCB CH2O-O2-
t_[CO]max/2 (bco.t7): UCB CH2O-O2-
[CH] & [NO] max (ch.st): Stanford Woil

Multipliers (LB)

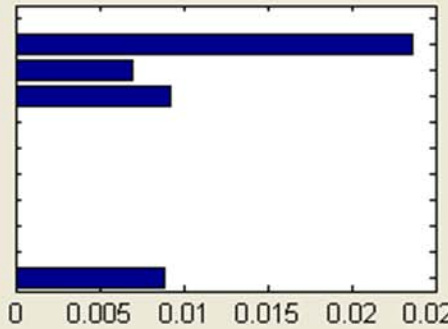


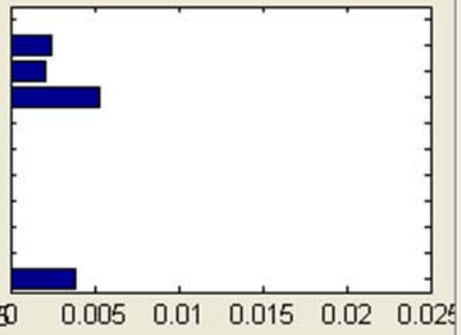

Multipliers (UB)




GRIMech 3 parameters
(double-click for details)

96
97
98
99
101
116
121
125
126
129
135




## Multipliers

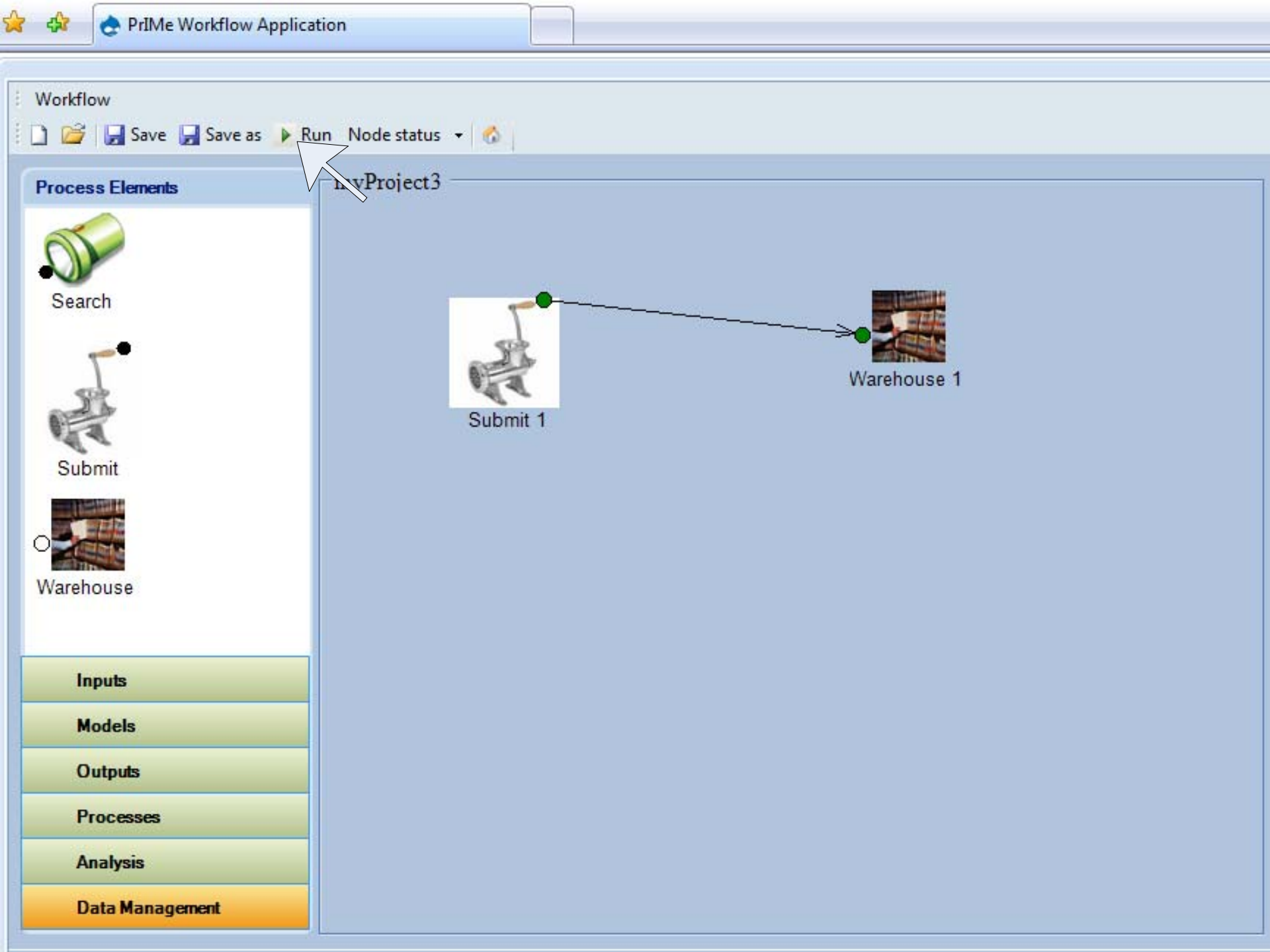
| | LB | UE |
|---|---|---|
| Selected Target | 0 | 0 |
| Selected parameter | 0 | 0 |

- (•) Dataset Order
- ( ) Sort Right Panel
- ( ) Sort Left Panel

## Navigation

Prev.

Next


PrIMe Workflow Application
Workflow
Save
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Submit
Warehouse
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Analysis
Data Management
MyProject3
Submit 1
Warehouse 1

PrIMe Workflow Application

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Process Elements

myProject3

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Submit

Warehouse

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Data Management

Submit to Warehouse

# Submit Data to PrIMe Warehouse

Bibliography (EndNote) help

Experimental Data help

Reaction Rate Coefficient help

Other help

PrIMe Experiment - x00000001

File Edit Help

Apparatus | Conditions | Data | References | Attachments

Experimental setup

Apparatus type: -- choose apparatus type --

Apparatus properties

| | Label | Value | Uncertainty | Units | Description |
|---|---|---|---|---|---|
| 1 | | | | | |

Add... Edit... Remove

Submit to PrIMe Cancel

PrIMe Workflow Application

Workflow

Save | Save as | Run | Node status

Process Elements

Plug Flow Reactor

PlugFlow

USC

USC

Inputs

Models

Outputs

Processes

Analysis

Data Management

New Process Configurati

USC

USC properties

Properties | About

| | |
|---|---|
| **general** | |
| Name | USC 1 |
| **Misc** | |
| delay | 12875 |
| first | H2 |
| firstN | 3 |
| fourth | OH |
| n1 | 1200 |
| n2 | 1 |
| n3 | 1 |
| n4 | 1000 |
| second | O2 |
| secondN | 3 |
| third | N2 |
| thirdN | 5 |

**delay**

OK | Cancel | Execute

# mfrenklach

View | Edit | Track | Contact

## GROUPS

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

## CONTACT INFORMATION

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**Phone Number**
(510) 643-1676

**Homepage**
http://www.me.berkeley.edu/faculty/frenklach

## PERSONAL INFORMATION

**Last Name**
Frenklach

**First Name**
Michael

**Company/Institution**
University of California at Berkeley

## HISTORY

**Member for**
2 years 18 weeks

PrIMe Component Uploader

Resources | Components | Shapes editor

Local files

Remote files

- analysis.gif
- input.GIF
- interrogate3.jpg
- interrogate4.gif
- model.GIF
- output.GIF
- pfr.gif
- search.gif
- state.jpg
- submit2.jpg
- target.gif
- target2.jpg
- targets_80.gif
- USC.gif
- warehouse.jpg

Preview

Add | Remove | Upload | Remove from server

Manager.dll, Version 1.0.0.119 Built:30.08.2008 15:19:32,81

PrIMe Component Uploader

Resources | Components | Shapes editor

Revision: 70

Description

Original shapes

Save | Test | Revision manager

Shapes structure

- Shape groups
  - Inputs
  - Models
  - Outputs
  - Processes
    - Shapes
      - PlugFlow
      - USC
        - Layout
        - Inputs
        - Outputs
        - Properties
          - Floats
          - Integers
          - Booleans
          - Execution DLL
          - Remote server
            - USC
          - Lists
            - first
            - second
            - third
            - fourth
  - Analysis

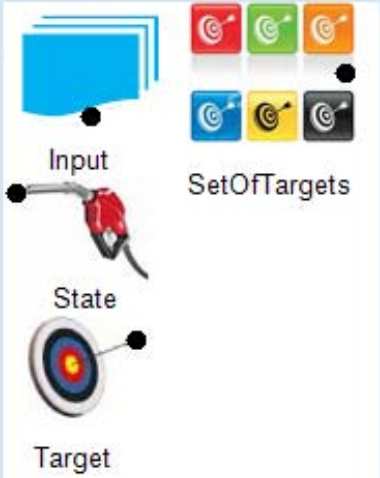
Delete | Add

Properties

| Misc | |
|---|---|
| Description | USC server |
| Host | 72.167.141.95 |
| Name | USC |
| Port | 9080 |

Name

Preview




Inputs
Models
Outputs
Processes
Analysis
Data Management

Manager.dll, Version 1.0.0.119 Built:30.08.2008 15:19:32,81

# mfrenklach

View | Edit | Track | Contact

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Frenklach

**First Name**
Michael

**Company/Institution**
University of California at Berkeley

## HISTORY

**Member for**
2 years 18 weeks

# PWA Installation

View Edit Outline Track

Note: The present version of the PrIMe Workflow Application (PWA) is implemented only for the Microsoft platform: Windows and Internet Explorer

**Adjusting .Net Security Settings**
PWA requires certain security configuration settings to work properly within Internet Explorer. These settings apply only to components received from **Primekinetics.org** web server, and do not relax security measures for any other server.
Run following script to relax security setting for PWA application: run .NET Security Script

**Install MatLab Run-Time library**
PWA requires MatLab Run-Time library to be installed on your computer to function properly.
To install MatLab run-time click following link "MatLab Installer"

**PWA Installation Diagnostics Utility**
This utility is designed to help you to examine the configuration of your workstation as needed for working with the PrIMe Workflow. To start, click the link below. When asked, save the file to your workstation and execute it. If you use Vista, right-click the icon of that application and select "Run as administrator". Running this test unitility, will open a window. Click the upper-left button "test". The configuraion report will be appear. The report contains three sections: .NET configuraion, MatLab configuration, firewall issues and list of errors. You may submit the report by clicking the upper-right button "send report" and fill in your PrIMe userid and an optional message in the corresponding boxes of the form. Start Diagnostics Utility

» Add new comment | 98 reads


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# Future Plans

- Continue community engagement
  - data submission / analysis
  - application "submission"
  - education
  - mirror site in EU
- Complete Data Model (NSF)
  - targets, instrumental
  - optimization variables
- Workflow interface ($$?)
- Model development

# Issues/Needs

- Home for PrIMe Data Warehouse
  - oversight but not possession
  - new job: data-record admission
- Computer hardware
  - storage: data, Work-Group docs
  - running applications
- Professional-level programming