Appendix A. Supporting Information

Table SI Species thermodynamics data: enthalpy of formation, ΔH_f^0 in kcal mol⁻¹ at 298.15 K; entropy S^0 in cal mol⁻¹K⁻¹ at 298.15 K; and specific heat, c_p in cal mol⁻¹K⁻¹ at a number of temperatures in Kelvin

Species	ΔH_f^0 (298)	$S^0(298)$	$c_{\rm p}(300)$	$c_{\rm p}(800)$	$c_{\rm p}(1000)$	$c_{\rm p}(1500)$	$c_{\rm p}(2000)$	$c_{\rm p}(2500)$
N_2	0.000	45.792	6.961	7.512	7.811	8.309	8.606	8.772
Ar	0.000	37.006	4.968	4.968	4.968	4.968	4.968	4.968
Н	52.102	27.416	4.968	4.968	4.968	4.968	4.968	4.968
H_2	0.000	31.229	6.895	7.078	7.209	7.734	8.173	8.541
O	59.554	38.491	5.234	5.016	5.001	4.983	4.976	4.984
O_2	0.000	49.028	7.024	8.066	8.337	8.725	9.048	9.321
OH	8.915	43.910	7.141	7.150	7.336	7.885	8.297	8.609
HO_2	2.939	54.753	8.348	10.771	11.380	12.483	13.330	13.954
H_2O	-57.797	45.127	8.030	9.257	9.870	11.313	12.351	13.081
H_2O_2	-32.475	56.051	10.154	13.990	14.947	16.592	17.678	18.381

Table SII. Values of the active variables of the trial, x_0 , and optimized, x_{opt} , reaction models

	Reactions	x_0	x_{opt}
1	$H+O_2=O+OH$	0	0.79
2	$O+H_2=H+OH$	-0.01	-0.01
3	$OH+H_2=H+H_2O$	0	-0.95
4	$OH+OH=O+H_2O$	-0.01	-0.01
5	$H+H+M=H_2+M$	0	0
	$H+H+H_2=H_2+H_2$		
	$H+H+H_2O=H_2+H_2O$		
6	$O+O+M=O_2+M$	0	0
7	O+H+M=OH+M	0	0
8	$H+OH+M=H_2O+M$	0	0
9	$H+O_2+M=HO_2+M$	0	0
	$H+O_2=HO_2$		
10	$H+HO_2=O+H_2O$	0	0
11	$H+HO_2=H_2+O_2$	0	0
12	H+HO ₂ =OH+OH	0.07	-0.39
13	$O+HO_2=OH+O_2$	0	0
14	$OH+HO_2=H_2O+O_2$	0	0
15	$HO_2 + HO_2 = H_2O_2 + O_2$	0	0
	$HO_2 + HO_2 = H_2O_2 + O_2$		0
16	$OH+OH+M=H_2O_2+M$	-0.4	-0.88
	$OH+OH=H_2O_2$		
17	$H+H_2O_2=H_2O+OH$	0	0
18	$H+H_2O_2=HO_2+H_2$	0	-0.56
19	$O+H_2O_2=HO_2+OH$	0	0
20	$OH+H_2O_2=H_2O+HO_2$	0	0
	$OH + H_2O_2 = H_2O + HO_2$	0	0
21	$O+OH+M=HO_2+M$	-0.1	-0.1

```
<dataAttribute xmlns:xml="http://www.w3.org/XML/1998/namespace" xmlns="http://purl.org/NET/prime/"</pre>
  dataAttribute ximis:xim= http://www.w3.org/xMr.f998/hdmespace ximis= http://pun.org/xeixmlsxxsi="http://www.w3.org/2001/XMLSchema-instance" type="target" primeID="a00000092" xsi:schemaLocation="http://punl.org/NET/prime/http://warehouse.primekinetics.org/schema/dataAttribute.xsd">
copyright>@primekinetics.org 2010</copyright>
corgin type="primeID">b00018626</orgin>
   cpreferredKey group="prime">IG.H2.2a</preferredKey>
cpropertyLink dataGroupID="dg1" experimentPrimeID="x00000357" id="T" propertyID="x1"/>
cpropertyLink dataGroupID="dg1" experimentPrimeID="x00000357" id="T" propertyID="x2"/>
cpropertyLink dataGroupID="dg1" experimentPrimeID="x00000357" id="t_ign" propertyID="x3"/>
cfeature id="log(t_ign)-1/T" type="ignitionDelayAt">
cindicator id="1/T" propertyID="T" transformation="inverse"/>
cindicator id="1/T" propertyID="T" transformation="inverse"/>
condicator id="P" propertyID="P" transformation="1"/>
condicator id="log(t_ign)" propertyID="t_ign" transformation="log10"/>
ciffaatures
   <dataAttributeValue type="derived">
   <value>1033</value>
       </property>
</indicator>
      cobservable featureID='log(t_ign)-1/T" id="t_ign" propertyID='log(t_ign)" transformation="10^">
- cproperty name="time" units="µs" label='t_ign" description="ignition delay">
             <value>238</value>
      /property>
- <bounds kind="relative" source="b00018626">
            <upper id="ub">2.5225</upper:
<lower id="lb">0.1696</lower>
          </bounds>
    </dataAttributeValue>
   <additionalDataItem itemType="text" description="dataAttribute description" MIME=" "> Ignition delay of 0.2H2-0.102-0.7Ar mixture at 1033 K, 0.518 atm </additionalDataItem>
```

Figure S1. An example of a *dataAttribute* XML file.

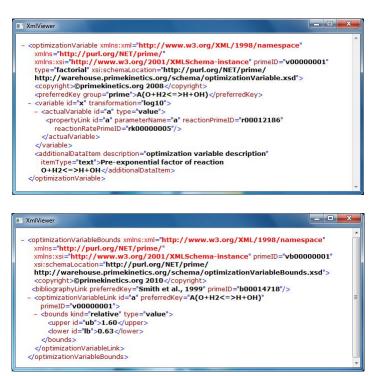


Figure S2. An examples of *optimizationVariable* and *optimizationVariableBounds* XML files.

```
<surrogateModel xmlns:xml="http://www.w3.org/XML/1998/namespace" xmlns="http://purl.org/NET/prime/'
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" primeID="sm00000001" type="quadratic"
xsi:schemal.ocation="http://purl.org/NET/prime/
http://warehouse.primekinetics.org/schema/surrogateModel.xsd">
<copyright>@primekinetics.org 2010</copyright></copyright></copyright></cr>
 <optimizationVariables>
   <optimizationVariableLink boundsPrimeID="vb00000001" id="1" preferredKey="A(O2 + H <=> OH + O)"
      primeID="v00000014"/>
   <optimizationVariableLink boundsPrimeID="vb000000001" id="2" preferredKey="A(H2 + O <=> OH + H)"
   primeID="v00000001"/>
coptimizationVariableLink boundsPrimeID="vb00000001" id="3" preferredKey="A(HO2 + H <=> H2 + O2)"
      primeID="v00000132"/>
   <optimizationVariableLink boundsPrimeID="vb00000001" id="4" preferredKey="A(H2 + OH <=> H2O + H)"
      primeID="v00000033"/>
   <optimizationVariableLink boundsPrimeID="vb000000001" id="5" preferredKey="A(O + H2O2 <=> OH + HO2)"
      primeID="v00000126"/>
                          Link boundsPrimeID="vb00000001" id="6" preferredKey="A(OH + H <=> H2O)"
      primeID="v00000120"/>
   <optimizationVariableLink boundsPrimeID="yb00000001" id="7" preferredKey="A(O2 + H <=> HO2)"
   primeID="v00000118"/>
<optimizationVariableLink boundsPrimeID="vb00000001" id="8" preferredKey="A(O + O <=> O2)"
      primeID="v00000128"/>
      optimizationVariableLink boundsPrimeID="vb00000001" id="9" preferredKey="A(H + O <=> OH)"
   primeID="v00000129"/>

coptimizationVariableLink boundsPrimeID="vb00000001" id="10" preferredKey="A(2 H <=> H2)"

      primeID="v00000119"/>
   <optimizationVariableLink bo
primeID="v00000133"/>
                          Link boundsPrimeID="vb00000001" id="11" preferredKey="A(O + OH <=> HO2)"
  </optimizationVariables>
   <coefficient>
  - <variables>
      cvariablet ink>0/variablet ink>
       <variableLink>0</variableLink>
    </variables>
    <value>2.53610742
```

Figure S3. An example of a *surrogateModel* XML file.

```
XmlViewer
      <chemicalModel xmlns:xml="http://www.w3.org/XML/1998/namespace" xmlns="http://purl.org/NET/prime/"</pre>
             xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" primeID="m00000004
             xsi:schemal.ocation="http://purl.org/NET/prime/ http://warehouse.primekinetics.org/schema/model.xsd">
<copyright>@primekinetics.org 2009-2010</copyright>
          <speciesSet>
                <speciesLink preferredKey="Ar" primeID="s00000049">
<thermodynamicDataLink preferredKey="L 6/88" primeID="thp00000002"/>
                 </speciest ink>
                 <speciesLink preferredKey="N2" primeID="s00010231">
             + <speciesLink preferredKey="H" primeID="s00009800"
              cspeciesLink preferredKey="H" primeID="s00009800">
cspeciesLink preferredKey="H2" primeID="s00009809">
cspeciesLink preferredKey="O" primeID="s00010285">
cspeciesLink preferredKey="O" primeID="s00010295">
cspeciesLink preferredKey="O" primeID="s00010102">
cspeciesLink preferredKey="H2" primeID="s00010102">
cspeciesLink preferredKey="H2" primeID="s00010103">
cspeciesLink preferredKey="H20" primeID="s0001013">
cspeciesLink preferredKey="H202" primeID="s00009881">
cspeciesLink preferredKey="H202" primeID="s00009882">
cspeciesL
           </speciesSet>
<reactionSet>
            - <reactionLink preferredKey="0 + 0 = 02" reversible="true" primeID="r00013869">
                     <reactionRateLink preferredKey="20 = 02" primeID="rk00000026"/:
                 </reactionLink>
             + <reactionLink preferredKey="O + H = OH" reversible="true" primeID="r00012023">
             + <reactionLink preferredKey="0 + H2 = H + OH" reversible="true" primeID="r00012186":
            + <reactionLink preferredKey="0 + H02 = OH + O2" reversible="true" primeID="r00012138">
+ <reactionLink preferredKey="0 + H202 = OH + H02" reversible="true" primeID="r00015825">
+ <reactionLink preferredKey="H + O2 = H02" reversible="true" primeID="r00011821">
                <reactionLink preferredKey="H + O2 = O + OH" reversible="true" primeID="r00012255">
<reactionLink preferredKey="H + H = H2" reversible="true" primeID="r0009454">
                <reactionLink preferredKey="H + OH = H20" reversible="true" primeID="r00013764">
<reactionLink preferredKey="H + H02 = O + H20" reversible="true" primeID="r00013804">
                <reactionLink preferredKey="H + HO2 = O2 + H2" reversible="true" primeID="r00009509">
                reactionLink preferredKey="H + H02 = OH + OH" reversible="true" primeID="r00009484":

<reactionLink preferredKey="H + H202 = H02 + H2" reversible="true" primeID="r00009484":
             + <reactionLink preferredKey="H + H2O2 = OH + H2O" reversible="true" primeID="r00013701">
```

Figure S4. An example of a *chemicalModel XML* file.

```
- <dataset xmlns:xml="http://www.w3.org/xML/1998/namespace"
xmlns:xsi="http://www.w3.org/x01/XML/schema-instance" primeID="d00000002"
xsi:schemaLocation="http://purl.org/NET/prime/
http://warehouse.primekinetics.org/schema/dataset.xsd">
<copyright>©primekinetics.org/schema/dataset.xsd">
<copyright>©primetD="b00018992"/>
<compateModelLink preferredKey="IG.H2.2a" primeID="sm00000001"/>
<copyright>©primetics.org/schema/dataset.ymlogateModelLink preferredKey="IG.H2.1a" primeID="sm00000005"/>
<copyright>©primetics.org/schema/dataset.ymlogateModelLink preferredKey="IG.H2.4a" primeID="sm00000006"/>
<copyright>©primetics.org/schema/dataset.ymlogateModelLink preferredKey="IG.H2.3a" primeID="sm000000009"/>
<copyright>©primetics.org/schema/dataset.ymlogateModelLink preferredKey="PrIMe H2 1.0 - flw4" primeID="sm0000001"/>
<surrogateModelLink preferredKey="PrIMe H2 1.0 - flw3" primeID="sm0000001"/>
<surrogateModelLink preferredKey="PrIMe H2 1.0 -
```

Figure S5. An example of a dataset XML file.

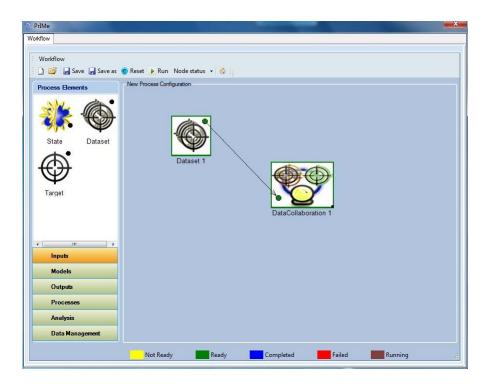


Figure S6. A snapshot of the PrIMe Workflow Application.

♠ PrIMe	Depository - search			_ D X			
Search	dataAttribute •			Find			
Where	any field ▼	contains ▼	a00000092	•			
	any field ▼	contains *					
	arch results (1 hits): pository/dataattributes/catalog/	a00000092.xml		Show details			
	,,,						
dataAttribute: IG.H2.2a dataAttribute description: Ignition delay of 0.2H2-0.1O2-0.7Ar mixture at 1033 K, 0.518 atm							
			Load	ew Xml Close			

Figure S7. A snapshot of the PrIMe Search-component window.

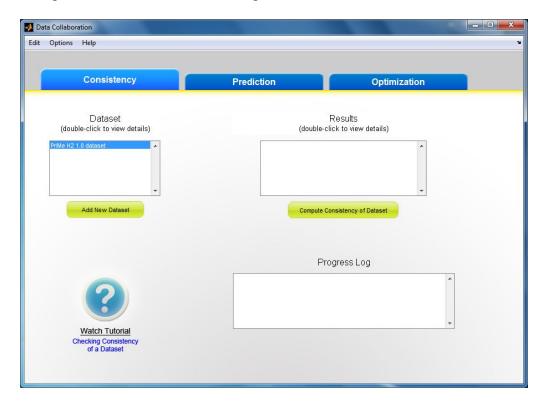


Figure S8. A snapshot of the DataCollaboration window.

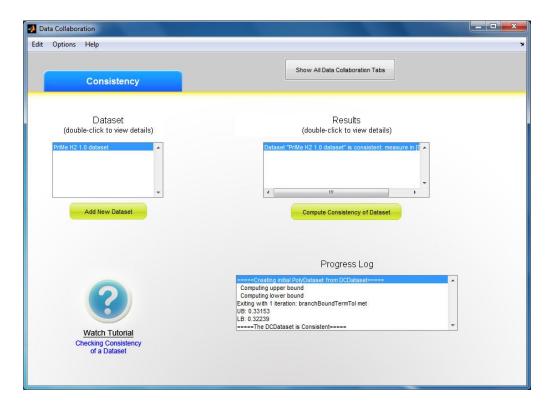


Figure S9. A snapshot of the DataCollaboration window initiating the Consistency analysis.

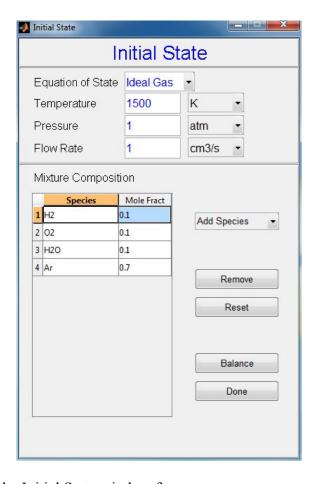


Figure S10. A snapshot of the Initial State window form.

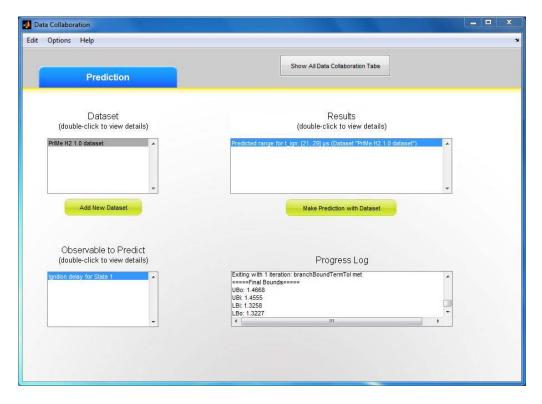


Figure S11. A snapshot of the DataCollaboration window initiating Prediction.

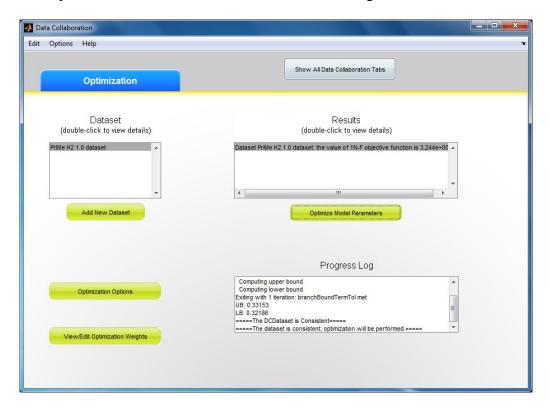


Figure S12. A snapshot of the DataCollaboration window initiating Model Optimization.

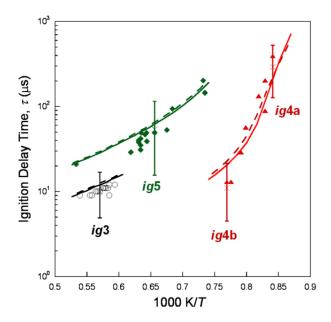


Figure S13. Ignition delay times for the $H_2/O_2/Ar$ mixtures: 0.5% $H_2 - 0.25\%$ O_2 , 33 atm; \triangle 2% $H_2 - 1\%$ O_2 , 33 atm; \triangle 0.1% $H_2 - 0.05\%$ O_2 , 64 atm; -- trial model; — optimized model; × experimental targets with error bars.

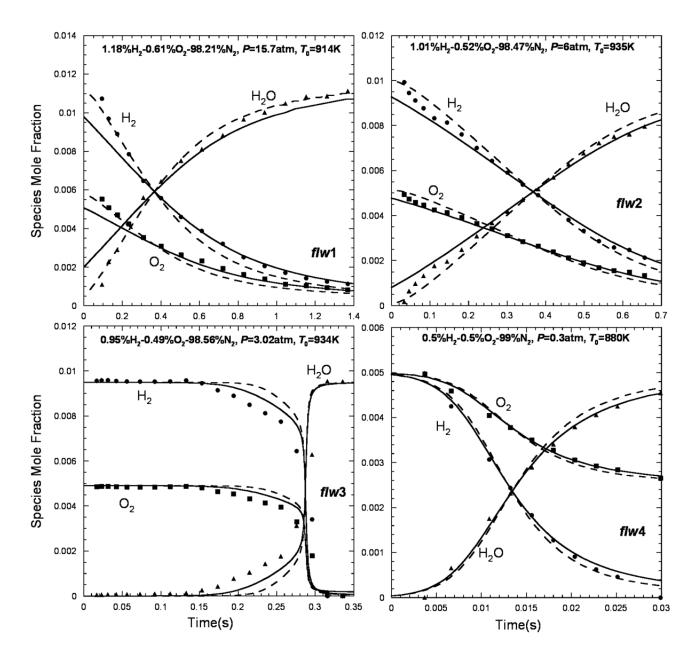


Figure S14. Experimental (symbols) and computed (lines) species mole fractions of hydrogen oxidation in a flow reactor. Solid lines: optimized model; dashed lines: trial model.