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^{-1}K^{-1}at 298.15 K; and specific heat, c_p in cal mol^{-1}K^{-1} at a number of temperatures in Kelvin

Species	ΔH_f^0(298)	S^0(298)	c_p(300)	c_p(800)	c_p(1000)	c_p(1500)	c_p(2000)	c_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
H	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

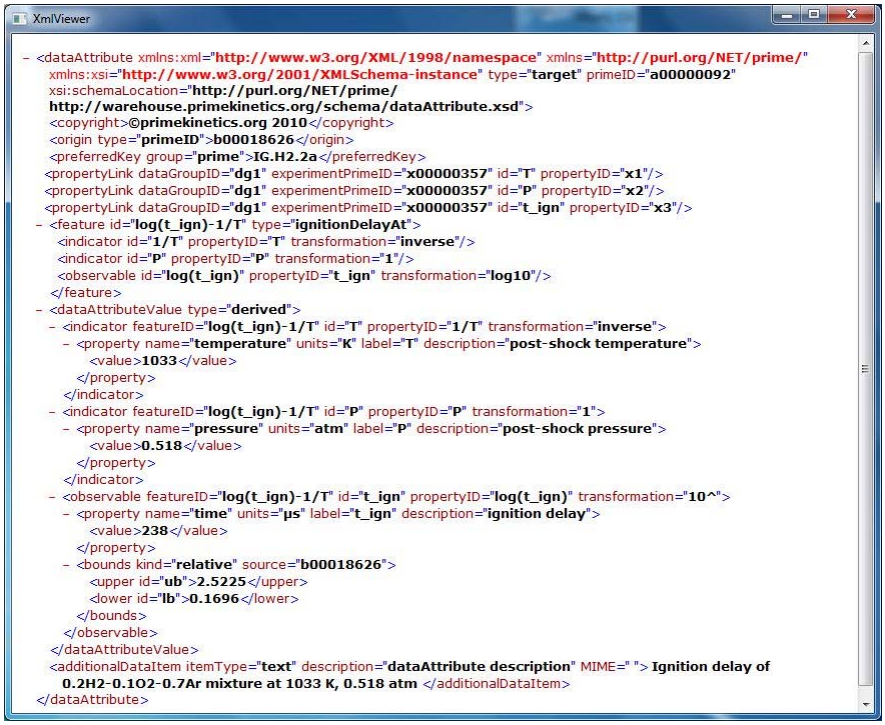
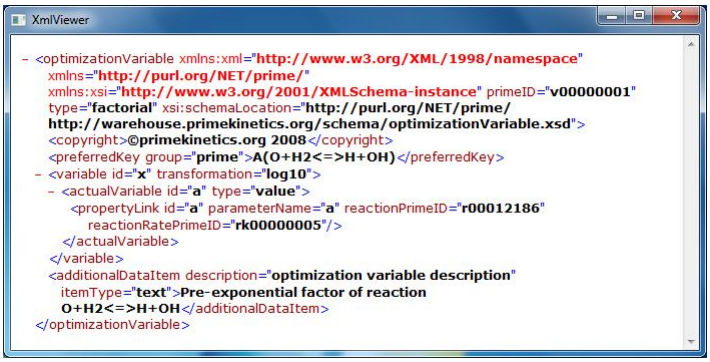


Figure S1. An example of a *dataAttribute* XML file.



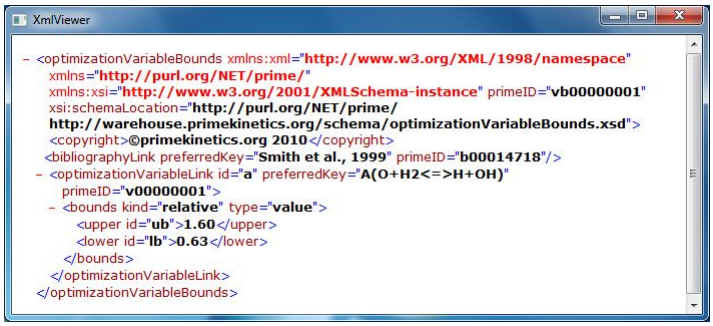


Figure S2. An examples of *optimizationVariable* and *optimizationVariableBounds* XML files.

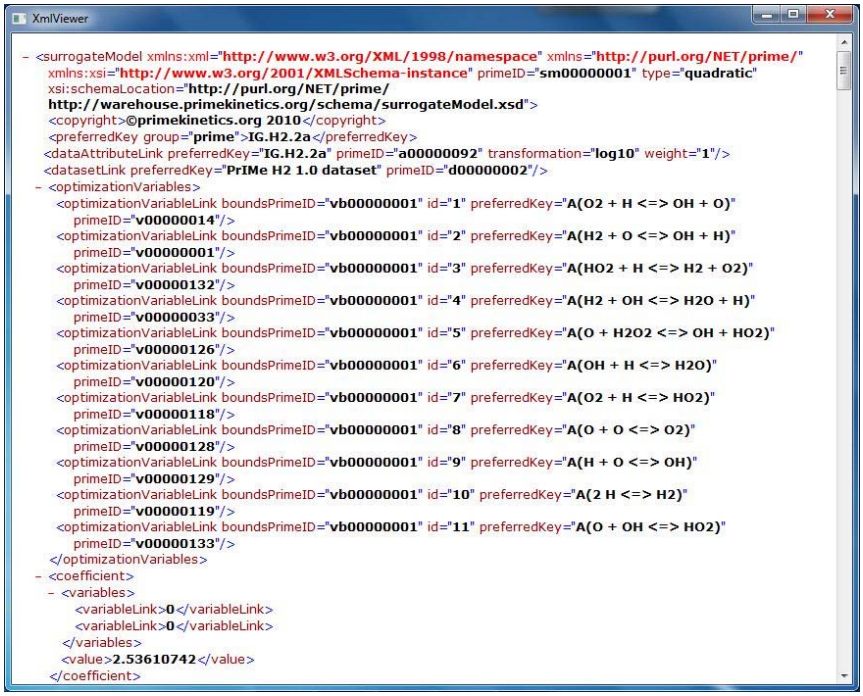


Figure S3. An example of a *surrogateModel* XML file.

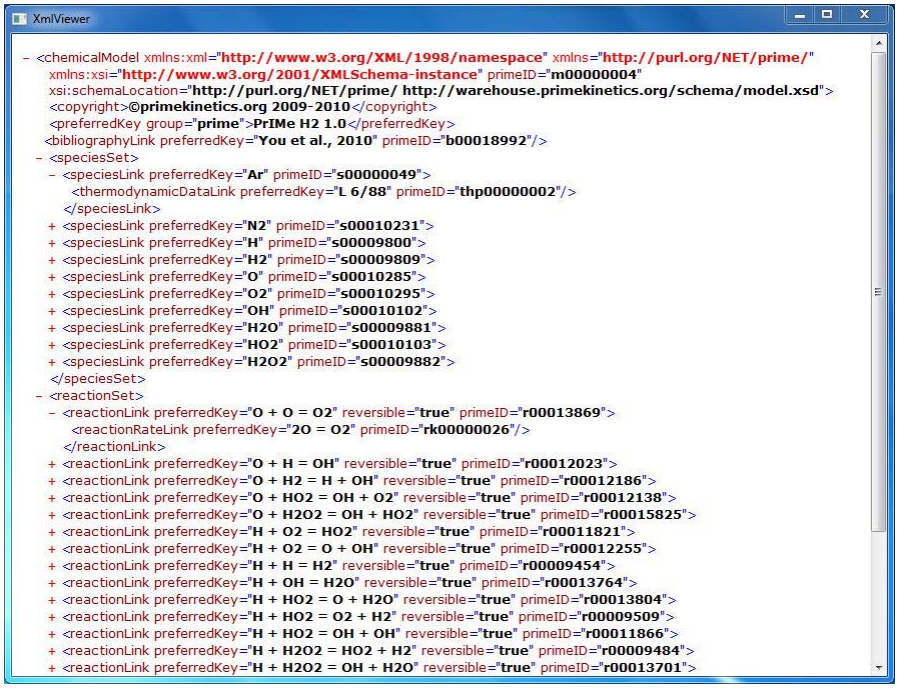


Figure S4. An example of a *chemicalModel* XML file.

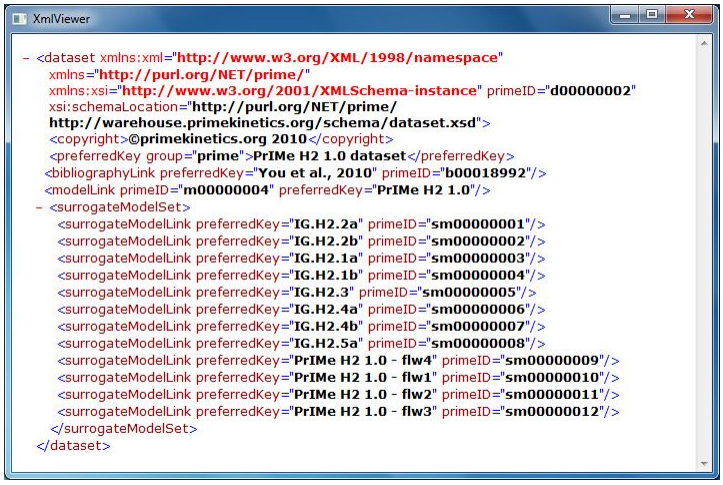


Figure S5. An example of a *dataset* XML file.

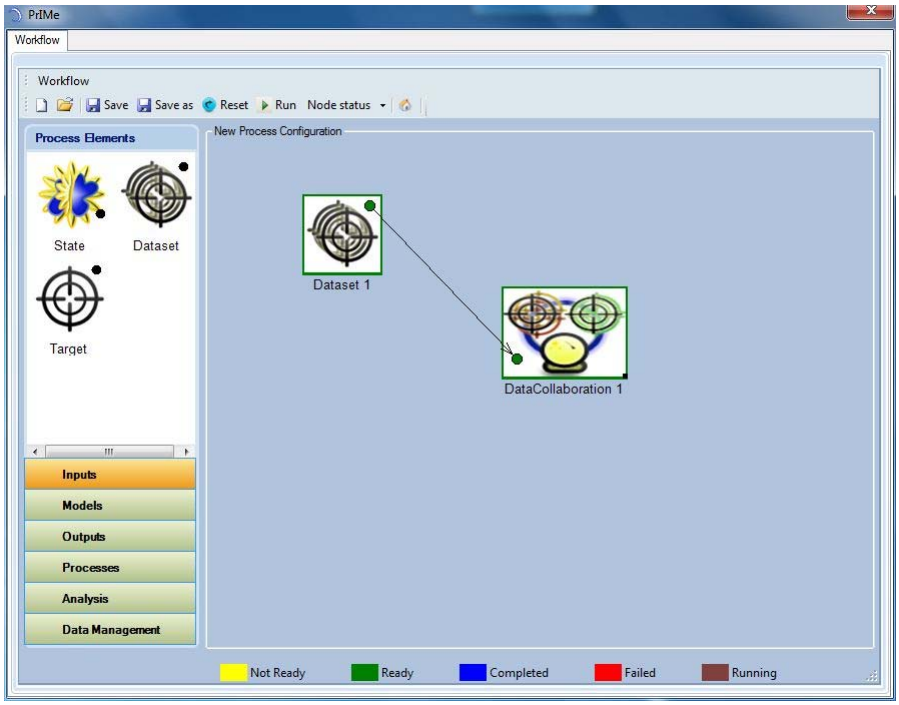


Figure S6. A snapshot of the PrIMe Workflow Application.

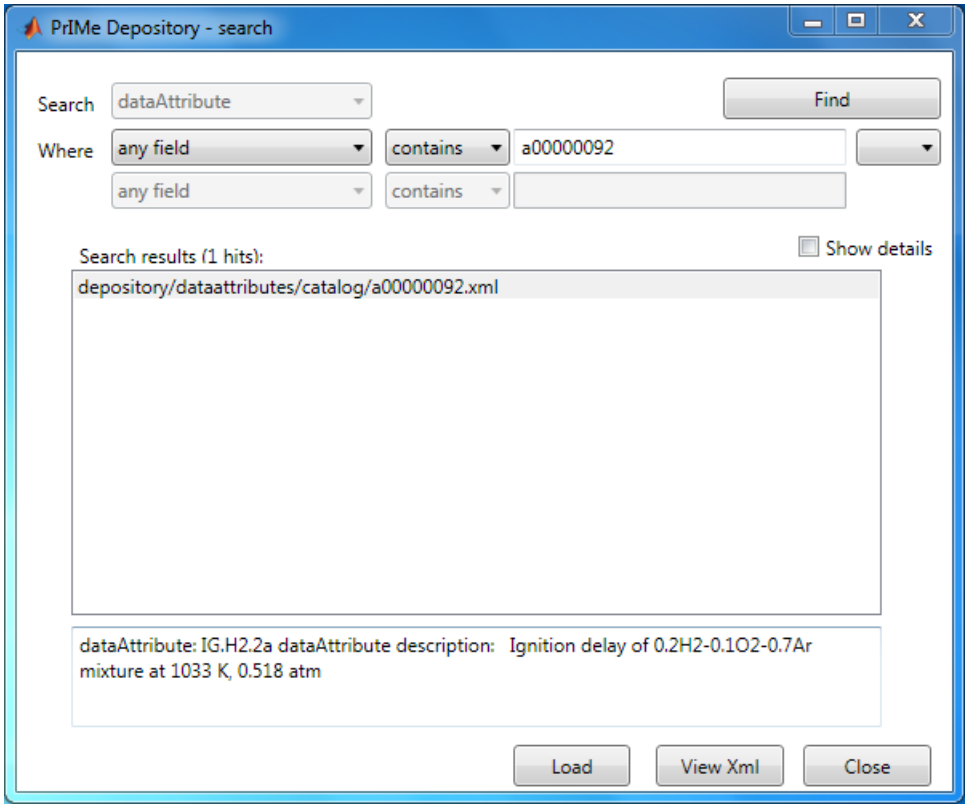


Figure S7. A snapshot of the PrIMe Search-component window.

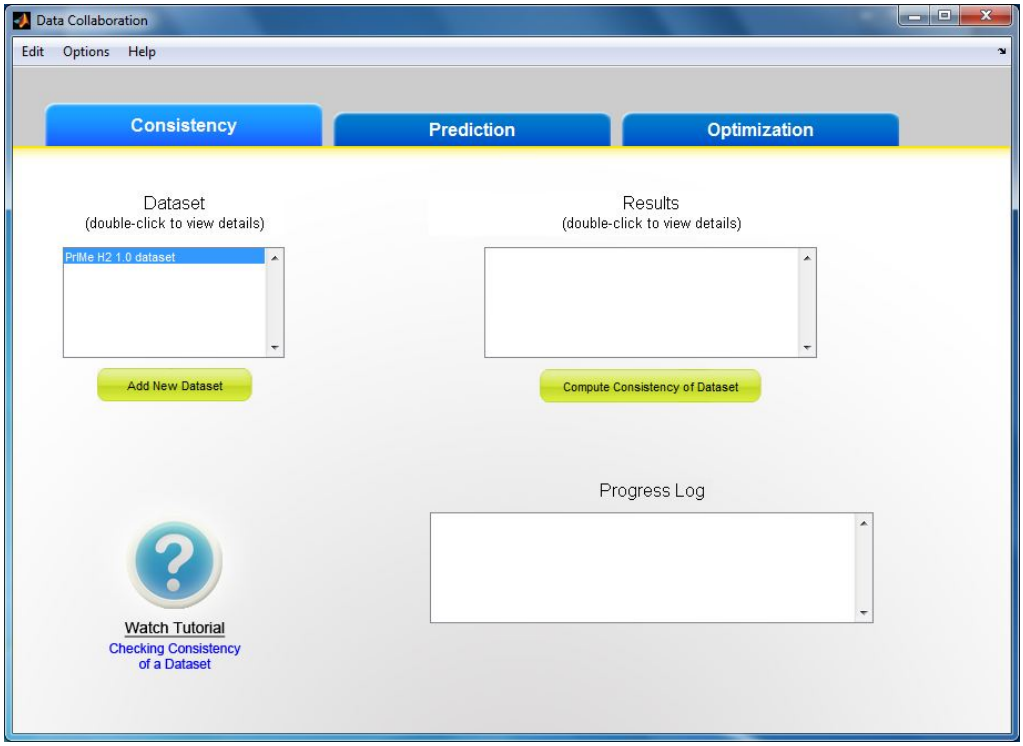


Figure S8. A snapshot of the DataCollaboration window.

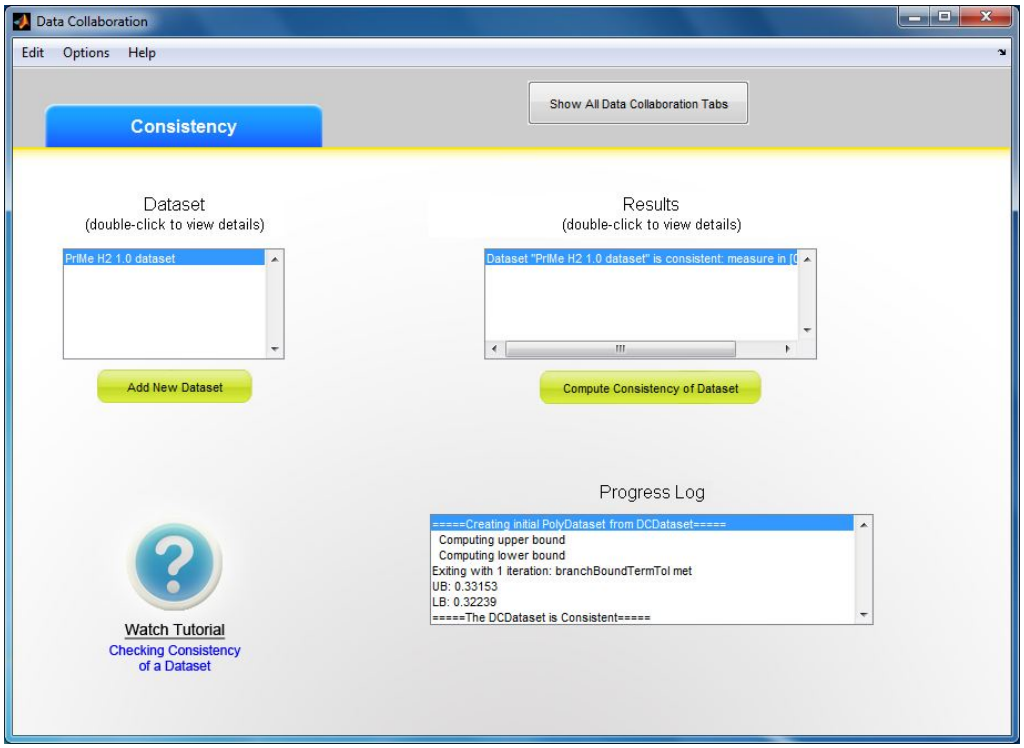


Figure S9. A snapshot of the DataCollaboration window initiating the Consistency analysis.

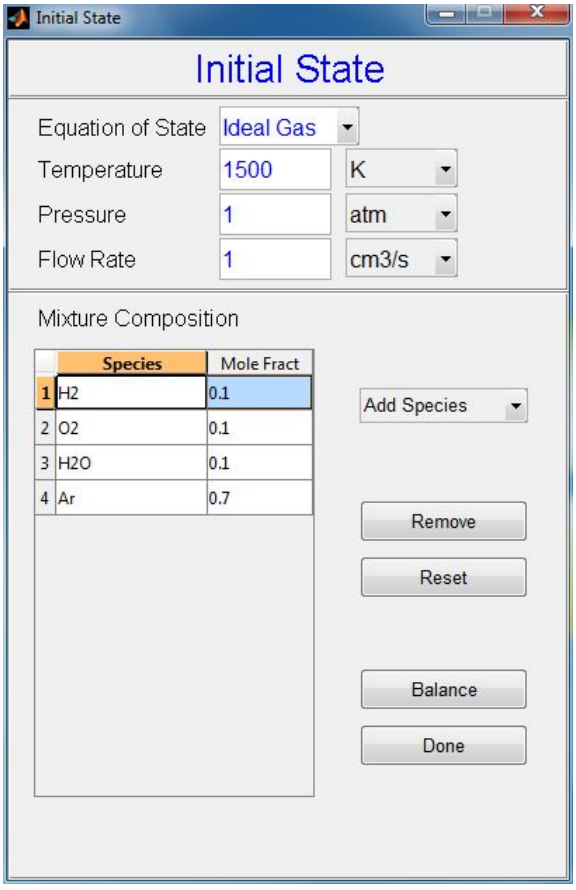


Figure S10. A snapshot of the Initial State window form.

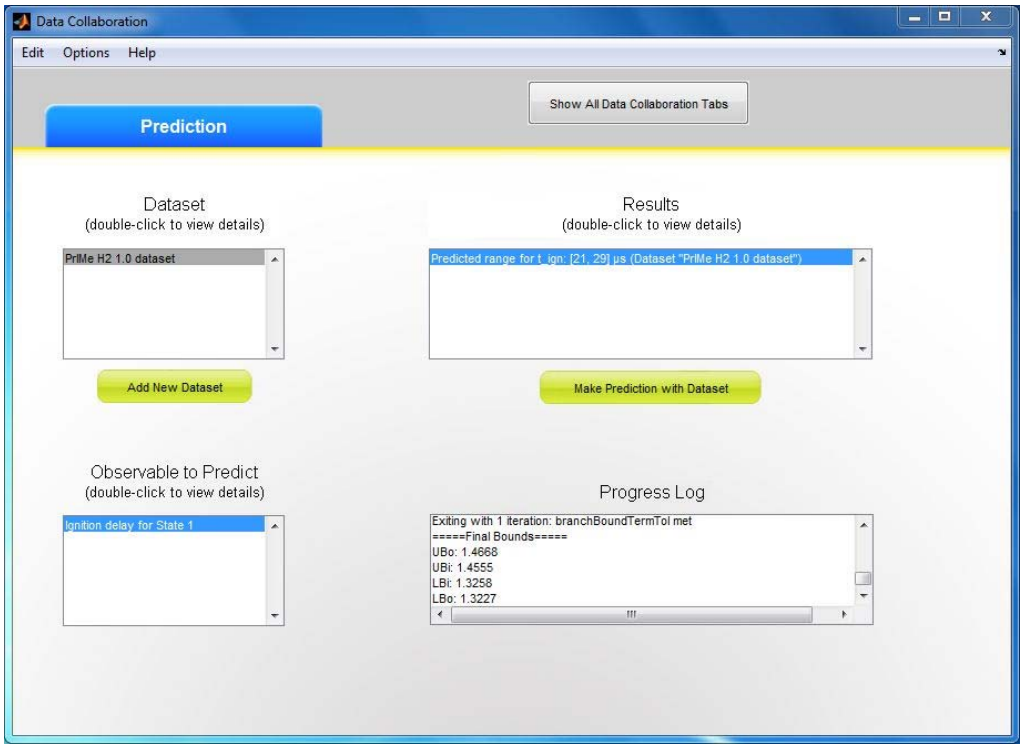


Figure S11. A snapshot of the DataCollaboration window initiating Prediction.

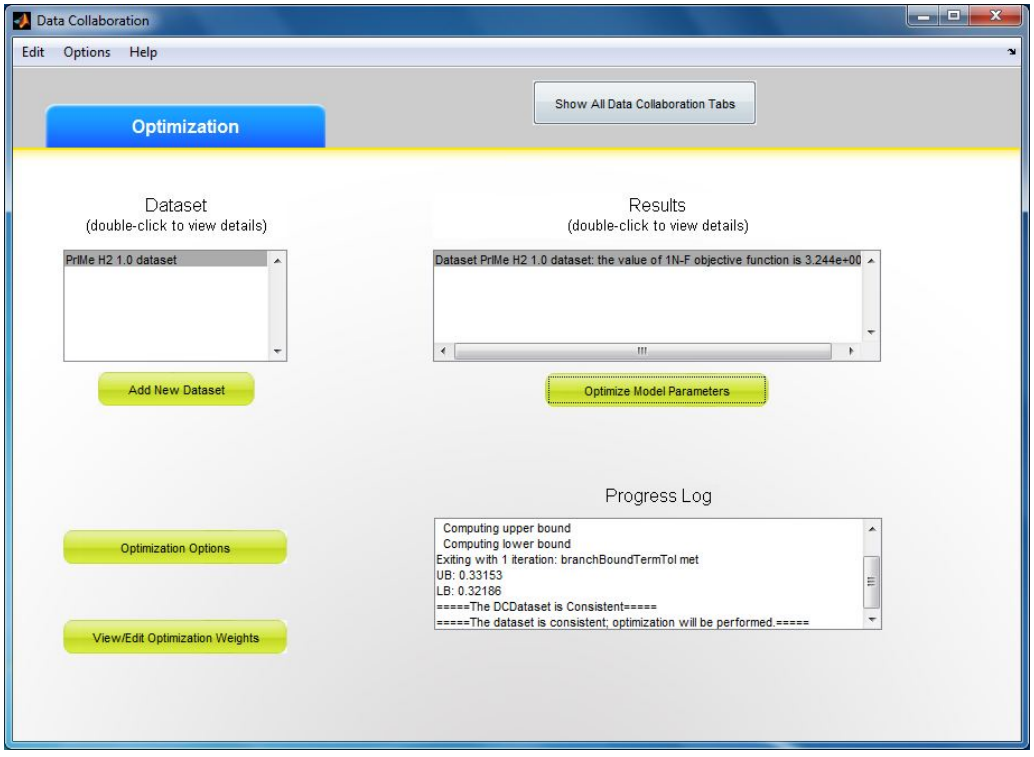


Figure S12. A snapshot of the DataCollaboration window initiating Model Optimization.

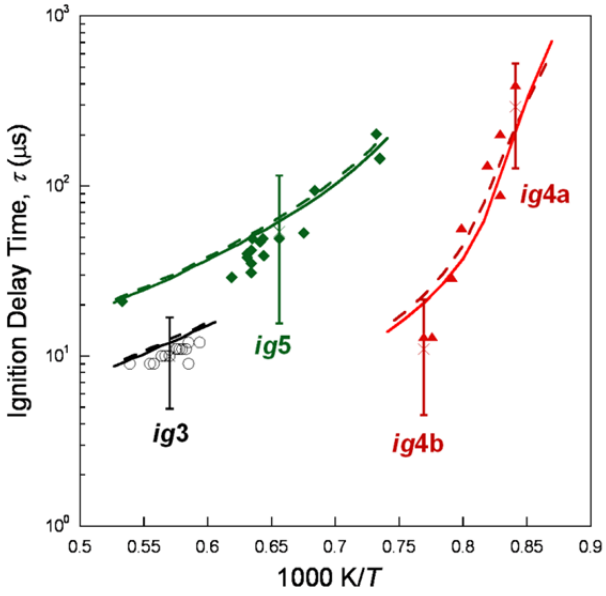


Figure S13. Ignition delay times for the H_2/O_2/Ar mixtures: ○ 0.5% H_2 – 0.25% O_2, 33 atm; ▲ 2% H_2 – 1% O_2, 33 atm; ♦ 0.1% H_2 – 0.05% O_2, 64 atm; − − − trial model; — optimized model; × experimental targets with error bars.

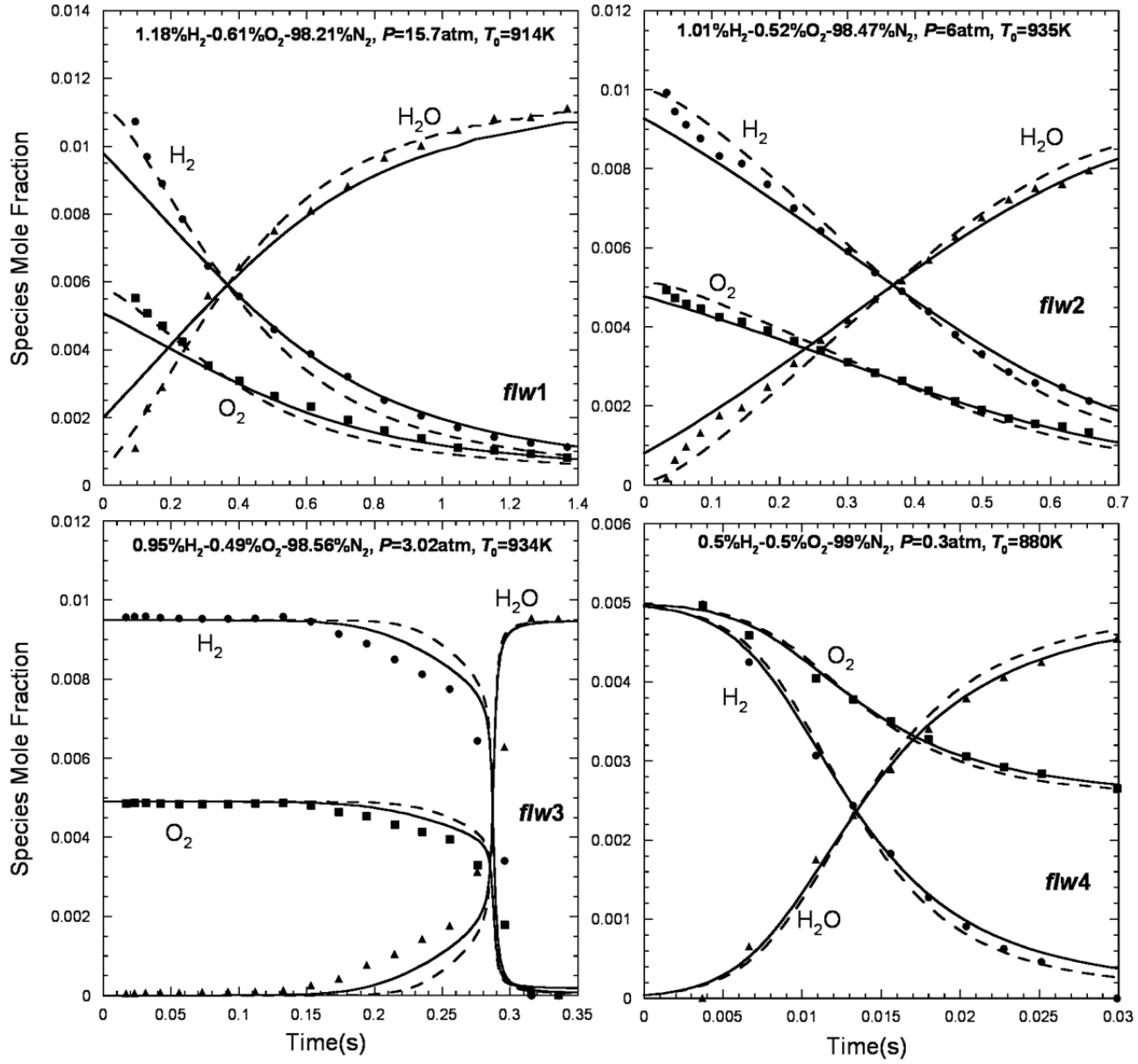


Figure S14. Experimental (symbols) and computed (lines) species mole fractions of hydrogen oxidation in a flow reactor. Solid lines: optimized model; dashed lines: trial model.