Experiment 1
n-Heptane shock tube ignition delay

```
<reactingFlow >
 <description title="n-Heptane shock tube ignition delay">
  <configuration>
    <keyword> shock-tube  </keyword>
  </configuration>
  <species>
    <molecule  name="n-heptane"  href="./n-heptane.xml"  />
  </species>
  <parameter name="fuel-air-equivalence-ratio" >
     1<units unit="dimensionless" />
  </parameter>
  <parameter name="ignition -delay" format="double">
     12.45<units unit="ms" />
  </parameter>
 </reactingFlow  >
```

Translate to Model Format

```
#FlameMaster input
Flame is IsochoricReactor
Phi = 1.0
Fuel is n-C7H16
Pressure = 13.6e5
etc.
```

Translate to Model Format

```
!Input file for
!Chemkin SHOCK
FUEL  NC7H16   0.05
PRES  13.6
etc.
```

Experiment 2
n-Heptane premixed flame

```
<reactingFlow >
 <description title="n-Heptane premixed flame">
  <configuration>
    <keyword> unstrained-premixed-flame  </keyword>
  </configuration>
  <species>
    <molecule  name="n-heptane"  href="./n-heptane.xml"  />
  </species>
  <parameter name="fuel-air-equivalence-ratio" >
     1<units unit="dimensionless" />
  </parameter>
  <parameter name="burning-velocity" format="double">
     37.45<units unit="cm/s" />
  </parameter>
 </reactingFlow  >
```

Translate to Model Format

```
#FlameMaster input
Flame is
    UnstretchedPremixed
Phi = 1.0
Fuel is n-C7H16
Pressure = 1.0e5
etc.
```

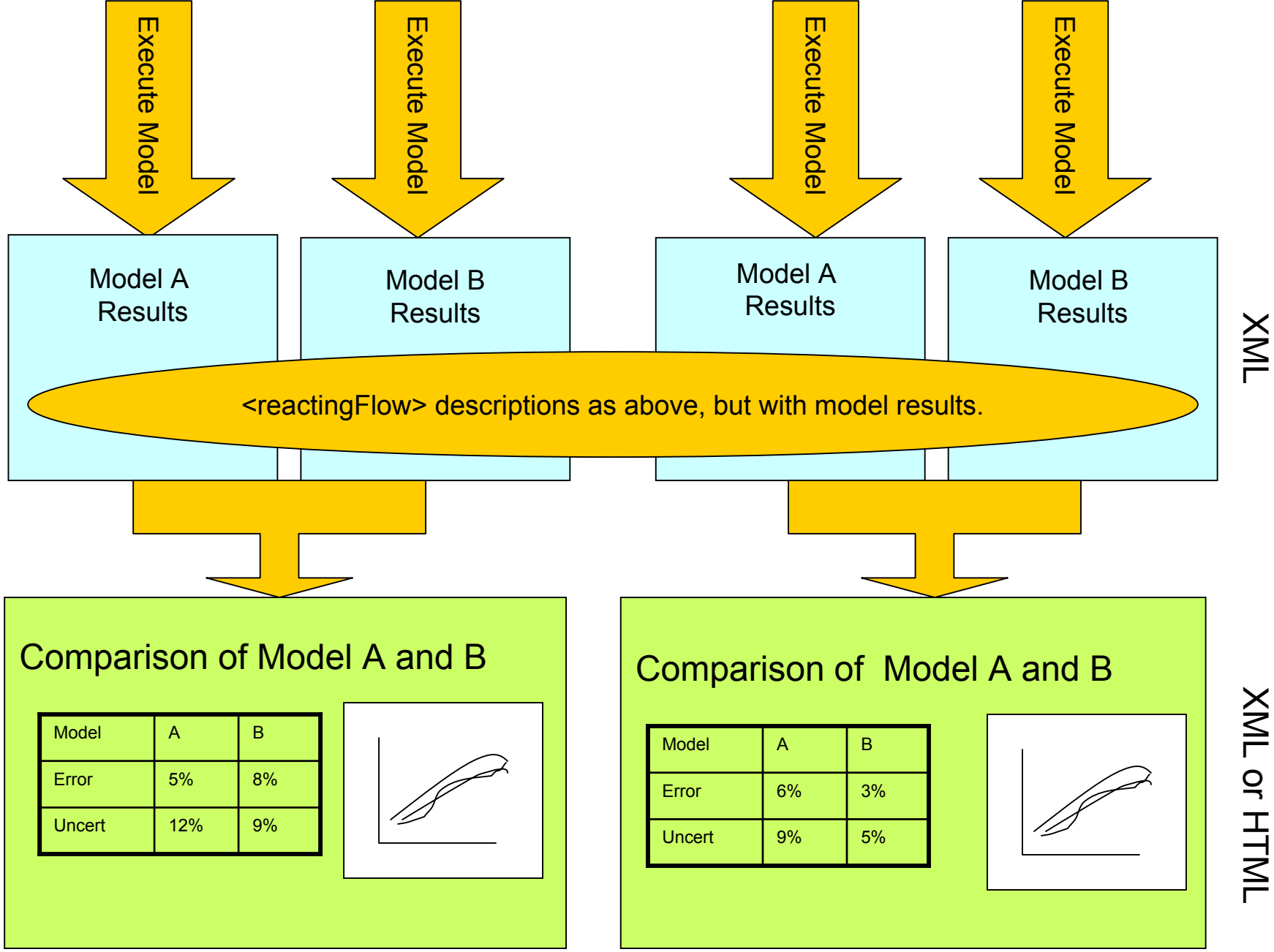
Translate to Model Format

```
!Input file for
!Chemkin PREMIX
FUEL  NC7H16   0.05
PRES  13.6
etc.
```

XML

XSLT

Native Formats


Execute Model
Execute Model
Execute Model
Execute Model
Model A Results
Model B Results
Model A Results
Model B Results
XML
<reactingFlow> descriptions as above, but with model results.
Comparison of Model A and B
Model | A | B
Error | 5% | 8%
Uncert | 12% | 9%
Comparison of Model A and B
Model | A | B
Error | 6% | 3%
Uncert | 9% | 5%
XML or HTML

Model A Summary and Pedigree

Summary

Expt.	1	2
Error	5%	6%
Uncert.	12%	9%

Link to results:
Experiment 1: n-Heptane shock tube ignition delay
Experiment 2: n-Heptane premixed flame

Link to code: FlameMaster
Link to model: nHeptane1.xml
Publication: Hewson et al, Journal of Irreproducible Results, 2002.

Model B Summary and Pedigree

Summary

Expt.	1	2
Error	8%	3%
Uncert.	9%	5%

Link to results:
Experiment 1: n-Heptane shock tube ignition delay
Experiment 2: n-Heptane premixed flame

Link to code: Chemkin
Link to model: heptane2002.xml
Publication: Pitz et al, Very Reputable Journal, 2000.

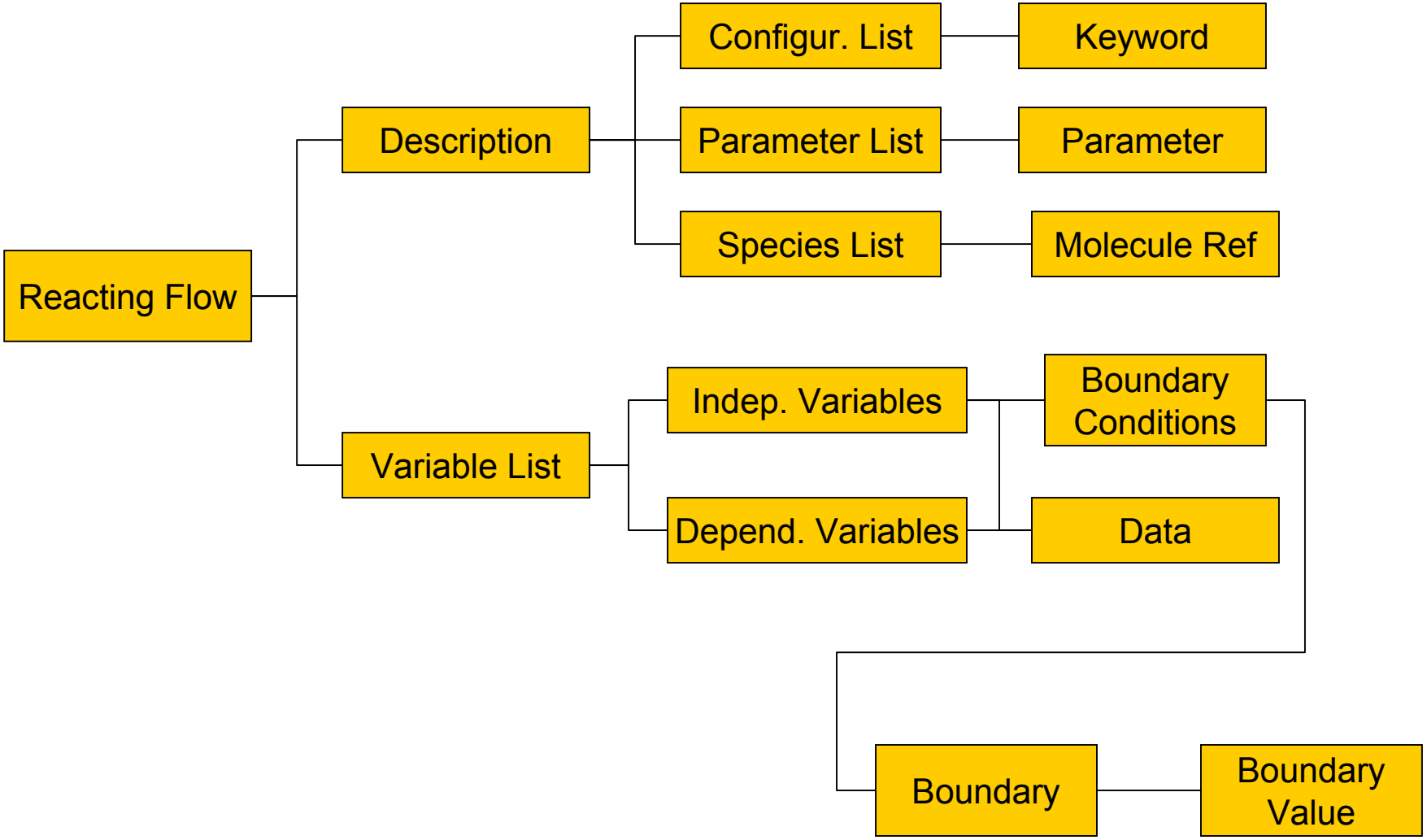
XML or HTML

- Each experiment-model comparison (or model-model comparison, etc.) represents a single parallelizable path.
- For complex models, multiply the number of parallel paths by 10's, 100's or 1000's.

Sample Application
Model Validation

- *General definition of a* **Model**: Set of rules for transforming inputs into outputs.
- **Models** reproduce observable phenomena.
- **Models** are validated using experimental data.
- **Complex models** may require extensive validation and verification.
  - *Many people may contribute* to such validation.
  - Creation of model inputs and comparison of output is *error prone.*
  - Chemical mechanisms are one model type where 100's or 1000's of validation tests are desired.

What might CMCS add to model validation?

- **Common data formats** provide a single point of translation.
  - Translate in and out of one format rather than many formats.
- CMCS facilitates automatic creation of input files, execution of models and documentation of results. Enables **automation of validation** process.
- CMCS **Pedigree** links methods, models and data sets.
- Translation into **HTML** for discussion with remote colleagues is relatively easy.

Reacting Flow Data Model