Encoding combustion experimental data

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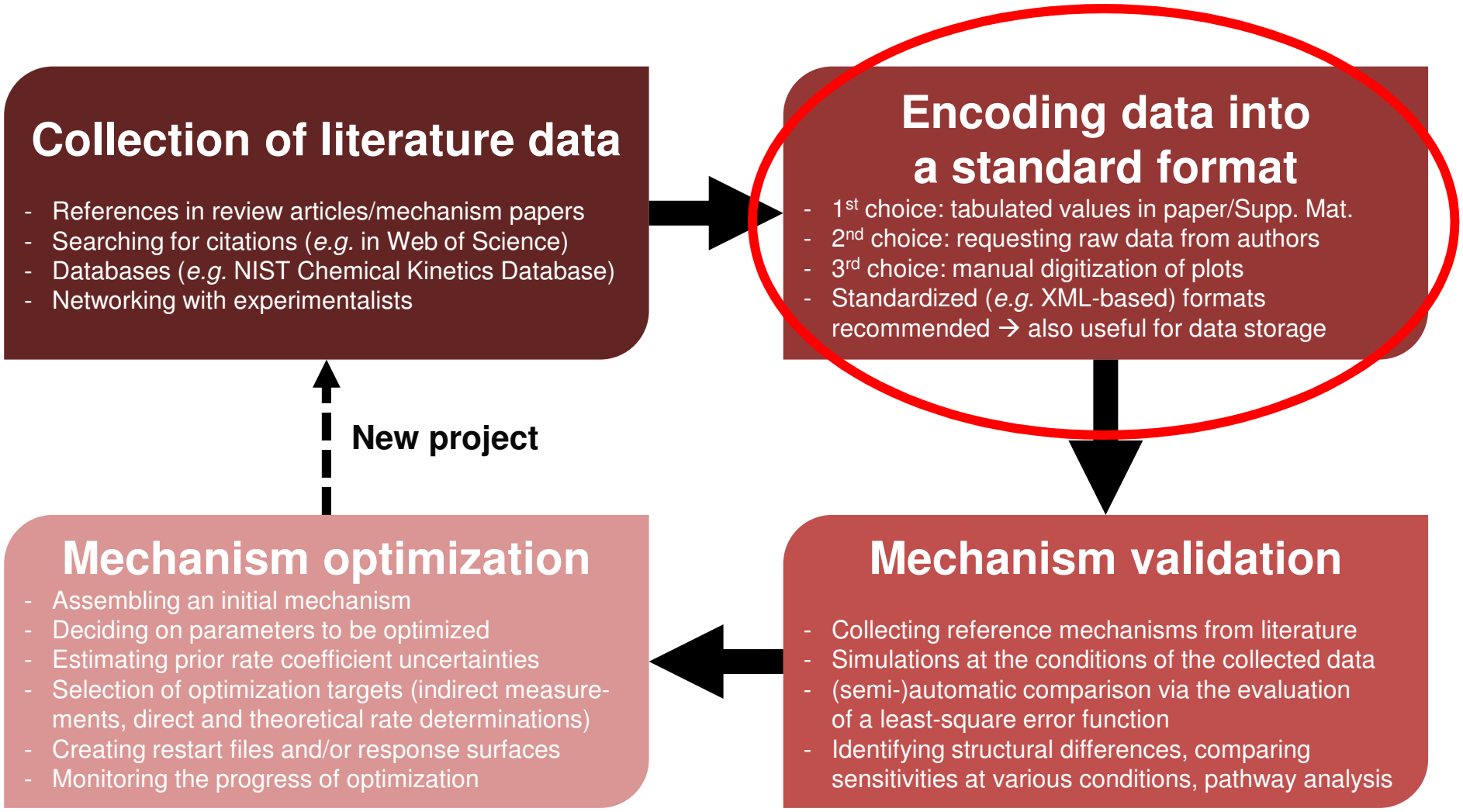
General workflow



Standardization of data

Problem

- Lots of groups, lots of data, lots of internal formats
- Experimental data are published – not always complete
- Raw data are eventually discarded or no one understands them anymore

Standardization

- Data will be always understood
- Easier for computer codes to process

ReSpecTh experimental dataformat

- Directly based on the PrIMe experimental data format
- Detailed specification available
  - How to specify experimental conditions and results
  - What must be specified to completely characterize an experiment
- XML format files
  - Easy and fast to process with programs
  - Naturally extendible

Experiment types

The available experiment types cover typical fundamental combustion experiments

- Ignition delay measurement
- Laminar flame speed measurement
- Outlet concentration measurement
- Concentration time profile measurement
- Jet stirred reactor measurement
- Burner stabilized flame speciation measurement ← **Simulations not hanlded yet**
- Direct rate coefficient determination
  - Experiment or theory

Creating ReSpecTh XML files

Optima++ has a TXT_TO_XML function that can be used to convert, easily understandable text files into ReSpecTh XMLs – see examples/xmlForms in release package

Contents

- `Author:` - Who made the file
- `Specification version:` - Currently is always 1.0
- `Source reference:` - Bibliographic source of experiments
- `Common experimental conditions:`
  - Constants in dataset (always conditions)
- `Varied experimental conditions and measured results:`
  - Variables in dataset (conditions or results)

Specifying properties

The common or varied experimental conditions/results must contain lines that specify the physical properties

Examples:

```
Type: pressure  Value: 1 Unit:atm
```

Common experimental condition
- **Type**
- **Value**
- **Unit**

```
Type:composition    Species: H2   Unit: mole fraction   Value:0.005
```

Composition/concentration types must have the species name given

```
Type:ignition delay    Unit: us   ID: x2
```

Varied experimental condition/result
- **Type**
- **ID**
- **Unit**

Specifying data points

The varied experimental conditions have ID-s, but no values. The values are given for each point after „Varied values:”, in columns marked with the ID-s given beforehand

```
Varied experimental conditions and measured results:
Type:  temperature     Unit: K    ID: x1
Type:ignition delay    Unit: us   ID: x2

Varied values:
x1          x2
1684        12
1709        9
1709        12
1715        11
1724        11
1730        11
```

Ignition delay measurement

Examples: ignitionExample; RCMExample

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C/V	The temperature behind the reflected shock wave in a shock tube experiment. For an RCM experiment this can be the temperature before the start of the compression, or the temperature at the end of compression, depending on the accompanying volume-time history.
pressure	C/V	The pressure behind the reflected shock wave in a shock tube experiment. For an RCM experiment this can be the pressure before the start of the compression, or the pressure at the end of compression, depending on the accompanying volume-time history.
composition	C/V	The composition of the reaction mixture, given in mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.
ignition delay	V	The measured ignition delay. For an RCM experiment the delay should be given compared to the end of compression, even if a volume-time history is available from the beginning of compression.

Ignition delay measurement

- Ignition delay definition
  - Often very different ignition delays can calculated based on different definitions
  - Can define target – pressure, temperature, or species
  - Can define feature – max, d/dt max, baseline intercepts, etc.
- Volume-time histories
  - RCM experiments need a volume-time profile to simulate the compression stroke
  - Pressure rise in shock-tubes can also be simulated with such profiles

Laminar flame speed measurement

Example: laminarFlameExample

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C/V	Unburned gas temperature.
pressure	C/V	Inlet gas pressure.
composition	C/V	The composition of the reaction mixture, given in mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.
flame speed	V	The measured laminar flame speed.

Concentration time profile measurement

Example: concentrationProfileExample

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C	Inlet gas temperature.
pressure	C	Inlet gas pressure.
composition	C	The composition of the reaction mixture, given in mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.
time	V	The time values at which concentrations were measured.
composition	V	The measured species mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.

Concentration time profile measurement

- Time shifting of the simulations to match with experimental results is often used

- Time shifting can be defined which will be automatically applied to simulations
  - Can define target – using a species name
  - Can define feature – half depletion, inflexion, etc.

Outlet concentration measurement

Example: outletConcentrationExample

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C/V	Inlet gas temperature.
pressure	C/V	Inlet gas pressure.
residence time	C/V	Residence time of the reactive mixture in the reactor.
composition	C	The composition of the reaction mixture, given in mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.
composition	V	The measured species mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.

Jet stirred reactor experiments

Example: JSRExample

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C/V	Inlet gas temperature.
pressure	C/V	Inlet gas pressure.
residence time	C/V	Residence time of the reactive mixture in the reactor.
volume	C/V	Volume of the reactor
composition	C	The composition of the reaction mixture, given in mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.
composition	V	The measured species mole fractions. A separate **property** element has to be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.

Direct rate coefficient determinations

Example: directRateDeterminationExample

- Define reaction
  - Reaction string
  - Order
  - Bulkgas

Mandatory properties		
Property	**C/V**	**Notes**
temperature	C/V	Temperature at which the rate coefficient was measured.
rate coefficient	V	Inlet gas pressure.

Allowed properties		
Property	**C/V**	**Notes**
pressure	C/V	Pressure at which the rate coefficient was measured. This is only relevant for pressure dependent reactions, but can be defined in any case.
composition	C/V	The gas composition in which the rate coefficient was measured.