# ReSpecTh Kinetics Data Format Specification

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# Contents

# ReSpecTh Kinetics Data Format Specification

The ReSpecTh Kinetics Data Format Specification is a set of specifications for an unambiguous definition and storage of combustion experiments and gas kinetics rate coefficient determinations. It uses an XML-type data format to provide a flexible way of data representation and allow for easy extension of the format specification.

The ReSpecTh Kinetics Data Format Specification (RKD format for short in this document) is directly based on the PrIMe Experimental Data Format (http://primekinetics.org/), and most of the specification is directly derived from the XML elements and attributes defined in PrIMe. Note that the PrIMe Experimental Data Format does not specify in detail how the data should be interpreted and what is required to describe an experiment completely.

The RKD format, as defined in this document, is unambiguous; therefore, the corresponding data can be well interpreted by computer codes. Specification of the RKD format also extends the PrIMe format with certain elements (e.g. ignition type definition). Consequently, the PrIMe experimental format files are not correct RKD format files. However, any PrIMe experimental data file can be easily converted to RKD format.

An XML file adhering to the RKD format specification should contain all information required for the proper simulation of an experiment using any simulation software package, which supports the given experiment type. The main XML file should contain reported values and estimated/calculated properties. Additional information needed by certain simulation or plotting codes should not appear in the main XML that describes the experiment. Such information may be stored in an additional XML file named "*[xmlname]*_info.xml", where *[xmlname]* is the name of the main XML file.

The RKD format specification provides a set of instructions for the interpretation of XML files. It defines XML elements and attributes, and how they must be interpreted within the ReSpecTh Kinetics Data Format Specification and what types of elements must occur within an XML file to be considered a complete data file. Non-necessary elements in a data file can be ignored. Also, further XML nodes can be present in the file, which will not be interpreted within the RKD format specification but can be used to store auxiliary information.

In the past it was possible to request DOI identifiers for the XML files for free (in addition to the DOI identifier belonging to a publication), thus some of the early XML files have a DOI. DOI identifiers have a cost now, thus all recent XML files have no DOI. Please, contact the authors of this format specification if you would like to request DOIs for the files you create.

# Versioning

The versioning of the RKD format is assigned according to the following guidelines:

- A major and minor version numbers will be assigned to all releases of the RKD format, which will be represented by the “major.minor” format, e.g. “1.5” for major 1, minor version “5”.
- If an update to the RKD format does not invalidate any file created based on the previous release, the minor version will be incremented, and the major version will be unchanged. Such an update could mean the following change: “v1.5” → “v1.6”
- If an update to the RKD format invalidates any file created based on the previous release, the major version will be incremented, and the minor version will be assigned zero. Such an update could mean the following change: “v1.6” → “v2.0”
- For each release of the RKD format, a new documentation version will be released. When the documentation is updated, but no changes are made to the specification itself (e.g., typos are corrected, or examples are added to the present documentation), the release date of the documentation will be altered.

## Elements of XML files

The ReSpecTh Kinetics Data Format is an XML-based format. The present document follows the terminology defined by the Document Object Model (DOM) when discussing the XML format, such as “element”, “attribute” and “node”. For further reference, see http://www.w3.org/DOM/.

All data are stored in XML elements, as well as the attributes and text nodes of these elements. This section describes what types of elements are defined within the ReSpecTh Kinetics Data Format Specification and how they are to be interpreted. **Element names** are in bold, and *attribute names* are in italics.

Four categories of data are defined: mandatory, optional, non-handled, and forbidden.

- Mandatory (M) elements and attributes are required to make the file a valid ReSpecTh Kinetics file.
- Optional (O) elements and attributes are part of the ReSpecTh Kinetics format and are to be interpreted, but their presence is not necessary for the validity (i.e., completeness) of the ReSpecTh Kinetics file. If they are present, then they are used either for defining the simulation (effective volume profile in RCM experiments) or for plotting the results (e.g. compressed pressure in RCM experiments).
- Non-handled (N) data are not interpreted within the ReSpecTh Kinetics format. Every XML element, attribute, or other feature not described within this document falls into this category. Also, the elements described in the present specification outside their defined context fall into this category. Non-handled data can be present in a ReSpecTh Kinetics file without invalidating it. Non-handled data usually provide information that is not needed to simulate the experiment, but the authors of the XML considered it relevant to include it as auxiliary information about the experiment.
- Forbidden (F): data which invalidates the xml file. For example, rate coefficients and branching ratios cannot be included in the same XML file. Codes which process the XML file should report an error in this case.

This section defines the elements of the ReSpecTh Data Format Specification. For each element, its parent, valid children and attributes, and the interpretation of a text content node are defined. Two slightly different schemes describe indirect (ignition delay time, laminar burning velocity, concentration) and direct (rate coefficient) measurements. The differences are the name of the root element and what elements are considered mandatory. In the description of child elements of the root element, the mandatory/optional/non-handled/forbidden state (M/O/N/F) is given independently for both direct and indirect measurements.

The elements are listed in tables using the following structure:

<table>
<tr><td colspan="2">element<br>The name of the element</td><td>experiment – M/O/N/F<br>The M/O/N/F state of the element if it is used in XML files with experiment root element (indirect measurements)</td><td>kdetermination – M/O/N/F<br>The M/O/N/F state of the element if it is used in XML files with kdetermination root element (direct measurements)</td></tr>
<tr><td>Child of</td><td>list of parent nodes with M/O/N/F state</td><td>Children</td><td>list of child elements with M/O/N/F state</td></tr>
<tr><td>Attributes</td><td>list of possible attributes with M/O/N/F state</td><td>Text content</td><td>textual information of the element (e.g., the text between the opening and closing tags)</td></tr>
<tr><td colspan="4">Description<br>A detailed description of the element.</td></tr>
</table>

## *Root elements*

Each ReSpecTh Kinetics file must have a single root element with the name **experiment** if the file describes an indirect experiment; **kdetermination** in the case of measured reaction rate coefficients ("direct measurement") or theoretically determined rate coefficients; or **xmlinfo** if the XML file contains information that is not required for the description of an experiment but may be needed for simulations or further data processing.

.

| **experiment** | | experiment – M | kdetermination – N |
|---|---|---|---|
| **Child of** | None | **Children** | **- fileAuthor** – M<br>**- fileDOI** – O<br>**- fileVersion** – O<br>**- ReSpecThVersion** – M<br>**- bibliographyLink** – M<br>**- experimentType** – M<br>**- apparatus** – O<br>**- commonProperties** – O<br>**- dataGroup** – M<br>**- ignitionType** – M/N; see element def.<br>**- timeshift** – O/N; see element def.<br>**- comment** – O |
| **Attributes** | None | **Text content** | None |
| **Description**<br>Root element to describe an indirect experiment. Possible types of indirect experiments are measurements of ignition delay times, laminar burning velocities, concentration profiles, stationary and outlet concentrations measured as a function of time, distance, or varying experimental conditions (e.g., reactor temperature). | | | |

| **kdetermination** | | experiment – N | kdetermination – M |
|---|---|---|---|
| **Child of** | None | **Children** | - **fileAuthor** – M<br>- **fileDOI** – O<br>- **fileVersion** – O<br>- **ReSpecThVersion** – M<br>- **reaction** – M<br>- **bibliographyLink** – M<br>- **apparatus** – O/N<br>- **commonProperties** – O<br>- **dataGroup** – M<br>- **method** – O<br>- **comment** – O |
| **Attributes** | None | **Text content** | None |
| **Description**<br>Root element to describe a direct experiment (i.e., a measurement of a reaction rate coefficient) or a theoretical rate determination. | | | |

| **xmlinfo** | | experiment – O | kdetermination – O |
|---|---|---|---|
| **Child of** | None | **Children** | - **fileAuthor** – M<br>- **referenceFileDOI** – O<br>- **referenceXMLFile** – M<br>- **fileVersion** – O<br>- **ReSpecThVersion** – M<br>- **plottingInfo** – O<br>- **modelingInfo** – O<br>- **keywords** – O<br>- **comment** – O |
| **Attributes** | None | **Text content** | None |
| **Description**<br>The root element for an additional XML file containing information that is not required to describe an experiment but may be needed for simulations or further data processing.<br>Note that this root element should only appear in a separate file, the additional XML file named "*[xmlname]*_info.xml", where *[xmlname]* is the name of the main XML file. | | | |

## *Common data elements*

| **fileAuthor** | | experiment – M | kdetermination – M |
|---|---|---|---|
| **Child of** | **- experiment**<br>**- kdetermination**<br>**- xmlinfo** | **Children** | None |
| **Attributes** | None | **Text content** | author of the file as a string – M |
| **Description**<br>The **fileAuthor** element contains the author of the file (not the data) as the value of the element. | | | |

| **fileVersion** | | experiment – O | kdetermination – O |
|---|---|---|---|
| **Child of** | **- experiment**<br>**- kdetermination**<br>**- xmlinfo** | **Children** | **- major** – O<br>**- minor** – O |
| **Attributes** | None | **Text content** | None |
| **Description**<br>The **fileVersion** element can be used to track the revisions of a file. While it is not mandatory, it is recommended for users to use the **fileVersion** element for this purpose. Two child elements, **major** and **minor** are also provided, to track the major and minor file versions.<br>A version tracking system for the individual files within the RKD format, as each user might have different preferences.<br>It is recommended to add a **comment** to describe the changes of a file between two file versions. | | | |

| **ReSpecThVersion** | | experiment – M | kdetermination – M |
|---|---|---|---|
| **Child of** | **- experiment**<br>**- kdetermination**<br>**- xmlinfo** | **Children** | **- major** – M<br>**- minor** – M |
| **Attributes** | None | **Text content** | None |
| **Description**<br>The **ReSpecThVersion** element defines which version of the ReSpecTh Kinetics Data Format Specification a file adheres to. It has two child elements, **major** and **minor**, containing the major and minor version numbers as text nodes, respectively. | | | |

| **firstPublicationDate** | | experiment – O | | kdetermination – O |
|---|---|---|---|---|
| **Child of** | **- experiment**<br>**- kdetermination**<br>**- xmlinfo** | **Children** | None | |
| **Attributes** | None | **Text content** | date in YYYY-MM-DD format – M | |
| **Description**<br>The date when the RKD file was first made publicly available using date format YYYY-MM-DD. | | | | |

| **lastModificationDate** | | experiment – O | | kdetermination – O |
|---|---|---|---|---|
| **Child of** | **- experiment**<br>**- kdetermination**<br>**- xmlinfo** | **Children** | None | |
| **Attributes** | None | **Text content** | date in YYYY-MM-DD format – M | |
| **Description**<br>The date when the file was created, or when either the fileVersion or the ReSpecThVersion was changed, using date format YYYY-MM-DD. | | | | |

## *Specific data elements of root elements* experiment *and* kdetermination

| **fileDOI** | | experiment – O | kdetermination – O |
|---|---|---|---|
| **Child of** | **- experiment**<br>**- kdetermination** | **Children** | None |
| **Attributes** | None | **Text content** | DOI of the file as a string – O |
| **Description**<br>The **fileDOI** element can be used to specify a unique digital object identifier (DOI) that belongs to the dataset. Please get in touch with the authors of this format specification if you would like to request DOIs for the files you create. Do not add prefixes such as "http://dx.doi.org/" to the **fileDOI**. | | | |

| **bibliographyLink** | | experiment – M | kdetermination – M |
|---|---|---|---|
| **Child of** | **- experiment**<br>**- kdetermination** | **Children** | **- description** – M<br>**- referenceDOI** – O<br>**- location** – O<br>**- table** – O<br>**- figure** – O<br>**- details** – O |
| **Attributes** | None | **Text content** | None |
| **Description**<br>The **bibliographyLink** element contains the bibliographic reference to the source of the experimental data. An unformatted string must be defined in the child element **description**. This may include the name of the authors of the corresponding publication, journal name, page numbers, etc.<br>The RKD format specification can be used to encode own unpublished measurements. In this case, we suggest providing a meaningful description of the measured data series in the child element **description**.<br>Adding the DOI of the corresponding publication in the child element **referenceDOI** is strongly recommended for easier backtracking of the data found in the XML file. Do not add prefixes such as "http://dx.doi.org/" to the **referenceDOI**. The hexadecimal URL (%) encoding can be used if the DOI contains special characters. The hexadecimal encoding is mandatory for characters "<", ">" and "%". If the character "<" appears in the DOI, replace it with "%3C", if the character ">" appears in the DOI, replace it with "%3E" and the "%" character in the DOI must be replaced with "%25" (see https://www.doi.org/doi_handbook/2_Numbering.html#2.5.2.4 for details).<br>Additional child elements may help the users of XML files to locate the data in the corresponding publication: **location** (e.g., "Main article" or "Supplementary Material"), table (e.g., "Table 1, high-pressure series"), and figure (e.g., "Figure 2, blue circle"). | | | |

Suppose data occurs at multiple places within the same paper (e.g., in a summary table and a figure). In that case, we suggest to include both information in the **bibliographyLink**, but indicate the sources which were NOT used for the creation of the XML file (e.g. "Figure 2 (not used)").
Literature details using standard BibTeX fields can be given in child element **details**.

| **- details** | | experiment – O | kdetermination – O |
|---|---|---|---|
| **Child of** | **- bibliographyLink** | **Children** | **- any standard BibTeX field listed below** – O |
| **Attributes** | None | **Text content** | None |

**Description**

The **details** element contains a detailed bibliography for the reference document described in the **description** element of **bibligraphyLink** using standard BibTeX fields:

**address**
: Usually, it is the address of the **publisher** or other type of institution. For major publishing houses, van Leunen recommends omitting the information entirely. For small publishers, on the other hand, you can help the reader by giving the complete address.

**author**
: The name(s) of the author(s) in the format described in the LaTeX book.

**booktitle**
: Title of a book, part of which is being cited. See the LaTeX book for how to type titles. For book entries, use the **title** field instead.

**chapter**
: A chapter (or section or whatever) number.

**edition**
: The edition of a book--for example, "Second". This should be an ordinal number and have the first letter capitalized, as shown here; the standard styles will convert it to lower case when necessary.

**editor**
: Name(s) of the editor(s), type as indicated in the LaTeX book. If there is also an **author** field, then the **editor** field gives the editor of the book or collection in which the reference appears.

**institution**
: The sponsoring institution of a technical report.

**journal**
: A journal name. Abbreviations are provided for many journals; see the *Local Guide*.

**month**
: The month in which the work was published or, for an unpublished work, in which it was written. It would be best to use the standard three-letter abbreviation, as Appendix B.1.3 of the LaTeX book described.

**number**
: The number of a journal, magazine, technical report, or work in a series. An issue of a journal or magazine is usually identified by its volume and number; the organization

that issues a technical report usually gives it a number, and sometimes, books are assigned numbers in a named series.

**organization**

The organization that sponsors a conference or that publishes a manual.

**pages**

One or more page numbers, or range of numbers, such as 42-111 or 7,41,73-97 or 43+ (the "+" in this last example indicates pages following that don't form a simple range). The standard styles convert a single dash (as in 7-33) to the en dash used in TeX to denote number ranges (as in 7--33) to make it easier to maintain Scribe-compatible databases.

**publisher**

The publisher's name.

**school**

The name of the school where a thesis was written.

**series**

The name of a series or set of books. When citing an entire book, the title field gives its title, and an optional **series** field shows the name of a series or multi-volume set in which the book is published.

**title**

The work's title is typed as explained in the LaTeX book.

**type**

The type of a technical report, for example "Research Note".

**volume**

The volume of a journal or multivolume book.

**year**

The year of publication or, for an unpublished work, the year it was written. Generally, it should consist of four numerals, such as 1984, although the standard styles can handle any **year,** whose last four nonpunctuation characters are numerals, such as "(about 1984)".

(source: https://www.openoffice.org/bibliographic/bibtex-defs.html)

| **experimentType** | | experiment – M | kdetermination – N |
|---|---|---|---|
| **Child of** | - **experiment** | **Children** | None |
| **Attributes** | None | **Text content** | experiment type as a string |
| **Description**<br>The **experimentType** element defines the experiment type for indirect experiments. The possible values are the following:<br>- ignition delay measurement<br>- laminar burning velocity measurement<br>- outlet concentration measurement<br>- concentration time profile measurement<br>- jet stirred reactor measurement<br>- burner stabilized flame speciation measurement<br>- burner-stabilized stagnation flame concentration measurement<br>- micro flow reactor concentration profile measurement | | | |

| **apparatus** | | experiment – O | kdetermination – O/N |
|---|---|---|---|
| **Child of** | - **experiment**<br>- **kdetermination** | **Children** | - **kind** – O<br>- **mode** – O (multiple instances possible)<br>- **type** – O |
| **Attributes** | None | **Text content** | None |
| **Description**<br>The **apparatus** element contains the apparatus type as the Text content node of the child element kind and the operation mode as the Text content node of the **mode** child element(s).<br>The **apparatus** element provides additional information about the experimental apparatus used for experiments described in a file (either indirect experiments with the root element **experiment** or indirect measurements with the root element **kdetermination**).<br>For jet-stirred reactor measurements, the isothermal or adiabatic nature of the reactor can be specified as the Text content node of the **type** child element. | | | |

| **method** | | experiment – N | kdetermination – O |
|---|---|---|---|
| **Child of** | - **kdetermination** | **Children** | None |
| **Attributes** | None | **Text content** | Name of the method as a string – O |
| **Description** | | | |

The **method** element can be used to describe the experimental method that was used in a direct measurement (e.g., "laser photolysis, laser-induced fluorescence") or the method used in a theoretical determination study (e.g., "VTST").

| **commonProperties** | | experiment – O | kdetermination – O |
|---|---|---|---|
| **Child of** | - **experiment**<br>- **kdetermination** | **Children** | - **property** – O |
| **Attributes** | None | **Text content** | None |

**Description**

The **commonProperties** element contains **property** elements describing the common physical properties across all experiments within the file. These are usually the boundary or the initial conditions for an experimental dataset, e.g., residence time in jet-stirred reactors, the initial gas composition for a flow reactor experiment or auxiliary data required for a complete experiment description (e.g., rate of pressure rise in a shock tube).

The values of the properties are stored within **property** elements.

It should be noted that a **commonProperties** element is not mandatory, as it is possible that all experimental conditions were varied within the dataset that is described in a single file, and none was kept constant. This is, however, not very likely, and files will typically contain this element.

| **dataGroup** | | experiment – M | kdetermination – M |
|---|---|---|---|
| **Child of** | - **experiment**<br>- **kdetermination** | **Children** | - **property** – M<br>- **dataPoint** – M |
| **Attributes** | - *id* – M<br>- *label* – O<br>- *dataPointLink* – M/N, see below | **Text content** | None |

**Description**

The **dataGroup** element contains **property** elements describing the physical properties that are varied across the experiments within the file if multiple experiments are recorded in the file or change within one experiment if the data file describes multiple measurements made during a single experiment.

These properties can be varied boundary/initial conditions or temporal/spatial coordinates (e.g., the temperature in a series of ignition delay measurements), the independent variable within a single experiment (e.g., reaction time in a flow reactor, position coordinates where the concentration profile measured in a micro flow reactor), and the respective experimental results (ignition delays, concentrations, laminar burning velocities).

It also contains the corresponding data in the **dataPoint** elements. For the details of the data storage, see the description of **dataPoint**.

The *id* attribute is mandatory for the **dataGroup** element. The *id* attributes of data groups usually follow the progression "**dg1**", "**dg2**", but can have any other name.

The *label* attribute may contain a string describing the type of data grouped in a dataGroup. This can be useful, e.g., to distinguish a dataGroup with the properties volume and time from the primary one containing the measured data.

A data point link must be provided via the dataPointLink attribute if the non-primary dataGroup contains a pressure-time, volume-time, or temperature-time history. If you want to link one profile to each datapoint use "all". If it shall only be used for selected points of the primary **dataGroup**, the value of this attribute should be specified e.g. as "1" for the 1st point in order of occurrence. Multiple links may be used. In this case, all linked data points must be separated with a semicolon, e.g. "1;2;5;6;" for the value of the *dataPointLink* attribute.

| **comment** | | experiment – O | kdetermination – O |
|---|---|---|---|
| **Child of** | - **experiment**<br>- **kdetermination** | **Children** | None |
| **Attributes** | None | **Text content** | Comment as a string – O |

**Description**

The **comment** element can provide information necessary for a complete understanding of the nature or origin of the data described in the XML file (e.g. if parts of the data are taken from another source). It may also provide information about estimating or calculating specific properties (e.g., the oxidizer composition used to calculate mole fractions from the equivalence ratio).

| **ignitionType** | | experiment – M/N; see below | kdetermination – N |
|---|---|---|---|
| **Child of** | - **experiment** | **Children** | None |
| **Attributes** | - *target* – M<br>- *type* – M<br>- *amount* – O<br>- *units* – O | **Text content** | None |

**Description**

An **ignitionType** element describes how the ignition delay was defined in an ignition delay measurement file. It is mandatory in such a file and non-handled otherwise.

The attribute *target* defines the physical property on which the ignition delay definition is based. This can be pressure, temperature, or the concentration of a species. These are to be denoted by "p", "T", and the name of the species (e.g. OH), respectively. If the ignition delay is defined based on multiple physical properties, e.g., the product of the CO and $O_2$ mole fractions, the *target* attribute should contain all names separated by semicolons.

The attribute *type* defines which feature of the measured physical property is considered for the ignition delay. Valid values are summarized in the following table:

| **Valid ignition types** | |
|---|---|
| ***type* value** | **Description** |
| max | The ignition delay is the time at which the maximum of the target physical property was measured. |
| d/dt max | The ignition delay is the time at which the maximum slope of the target physical property was measured. |
| baseline max intercept from d/dt | Extrapolation to the initial baseline concentration from the maximum slope.<br>Use max if the higher concentration intercept is needed (e.g. the target species concentration is depleted and you want to get the timepoint when the concentration decrease starts).<br>Use min if the lower concentration intercept is needed (e.g. the target species concentration is produced and you want to get the timepoint when the concentration increase ends). |
| baseline min intercept from d/dt | |
| concentration | The ignition delay is the time at which the concentration of the target species reaches a specified concentration value. |
| relative concentration | The ignition delay is the time at which the concentration of the target species reaches a specified concentration value relative to its maximum concentration. |
| relative increase | The ignition delay is the time at which the target physical property increases by the specified value relative to its initial value. (For example, the ignition delay time is the time when the temperature increases by 10%.) |

The attribute *amount* defines the absolute or relative concentration value the target species needs to reach for ignition to occur. This attribute can only be used when the value of *type* is "concentration", "relative concentration" or "relative increase".

The attribute *units* defines the unit of the concentration value defined in the attribute *amount*. This attribute can only be used when the value of *type* is "concentration" or "relative concentration". The same units can be used here as for "concentration" or "composition" type properties (e.g. "mole fractions" or "molecule cm-3").

Attribute value *"unitless"* should be assigned to relative properties ("relative concentration" or "relative increase").

| **timeshift** | | experiment – O/N; see below | kdetermination – N |
|---|---|---|---|
| **Child of** | **- experiment** | **Children** | None |
| **Attributes** | - *target* – M<br>- *type* – M<br>- *amount* – O | **Text content** | None |

**Description**

A **timeshift** element describes how the simulated species profile should be shifted in a species profile measurement file. It is mandatory in such a file and non-handled otherwise.

The time shifting of species profiles is widely used to interpret species profile measurements in flow reactors. To account for an unknown mixing and heating time, the simulated profiles are shifted in time to match a feature (e.g., the time of the half depletion of the fuel) of the experimental profiles. Even if multiple species were measured in a single experiment, each profile uses the same time shift.

The attribute *target* defines the physical property on which the time shift is based. This must be the name of a single measured species.

The attribute *type* defines which part of the specified species profile matches the experiments. The valid types are summarized in the following table.

**Valid timeshift types**

| ***type* value** | **Description** |
|---|---|
| half | The half concentration relative to the maximum concentration of the specified species is matched between the experiment and simulation. |
| inflexion | The inflection point of the specified profile is matched between the experiment and the simulation. |
| relative | A concentration relative to the maximum concentration of the specified species is matched between the experiment and simulation. |

| | |
|---|---|
| | In this case, an amount attribute is mandatory and contains the value of the matched relative concentration. |

**Note**
The *type* value must also be followed by "increase" or "decrease." This defines if the target species is being produced or depleted, respectively.
Therefore, a valid *type* value would be "half decrease" if the half depletion of the species is used for the time shifting.

The attribute *amount* defines the relative concentration value of the target species that is used to match the experiment and the simulation. This attribute can only be used when the value of *type* is "relative increase" or "relative decrease".
In the current version of the ReSpecTh Kinetics Data Format Specification, defining a fixed (i.e., absolute) time shift is impossible.

| **reaction** | | experiment – N | kdetermination – M |
|---|---|---|---|
| **Child of** | - **kdetermination** | **Children** | - **reactant1** – O<br>- **reactant2** – O<br>- **reactant3** – O<br>- **product1** – O<br>- **product2** – O<br>- **product3** – O |
| **Attributes** | - *preferredKey* – M<br>- *order* – M<br>- *bulkgas*– M | **Text content** | None |

**Description**

The **reaction** element defines the reaction for which the rate coefficients recorded in a file were measured.

The *preferredKey* attribute contains the reaction string which defines the reaction. The reaction string must contain "LP" or "HP" before the first species is separated by a space if the rate coefficients measured are at the low-pressure or high-pressure limit, respectively, for pressure-dependent reaction rate coefficients. (e.g. "LP H+O2+M=HO2+M")

The reaction string can contain the word "PRODUCTS" instead of the actual products. In this case, the rate coefficient can be interpreted as the sum of all reaction channels with the same reactants. (e.g., "C2H5OH+M=PRODUCTS" means all ethanol decomposition channels)

The *order* attribute contains the order of the reaction.

The *bulkgas* attribute defines the bath gas (as the name of the species) in which rate coefficient was measured. It is possible to provide a detailed experimental gas composition using

appropriate **property** elements in the **commonProperties** or **dataGroup** elements. If this is provided, the exact composition must be considered, and the *bulkgas* attribute must be ignored.

However, this information is not available in many cases, yet it is important to know the bath gas to account for third-body collision effects. Also, for pressure-independent rate coefficients, the detailed gas composition does not influence the rate coefficients.

Multiple **reaction** elements can be present in a single file. In this case, the sum of the reaction rate coefficients of all **reactions** defined in all **reaction** elements is recorded in the file.

**reactant1, 2, 3** and **product1, 2, 3** child elements are allowed to provide information for search engines for the reactants and products of the reaction.

| **property** | | | |
|---|---|---|---|
| **Child of** | - **commonProperties**<br>- **dataGroup** | **Children** | - **value** – M/N; see below<br>- **component** – M/N; see below<br>- **speciesLink** – M/N; see below |
| **Attributes** | - *id* – M/N; see below<br>- *label* – O<br>- *name* – M<br>- *sourcetype* – M<br>- *units* – M/N; see below<br>- *reference* – M/N; see below<br>- *kind* – M/A/N; see below<br>- *bound* – M/N; see below<br>- *method* – M/N; see below<br>- *sigmarange* – O/N; see below | **Text content** | None |

**Description**

A **property** element describes a physical property measured during the experiment or was one of the initial conditions set for the experiment. A **property** element can occur in a **commonProperties** element, where it describes an initial condition of the experiment, and its numerical value must be given as the value of the element.

Suppose a property element occurs as the child of the **commonProperties** element, and its type (name value) is not „initial composition". In that case, it must have a **value** child element containing its numeric value. If it is an „initial composition" property, it must have **component** child element(s) that define the component species of the initial composition.

A property element can also occur in a **dataGroup** element, which defines a physical property that was varied between experiments or measured as a function of another **property** within a single experiment. The numerical values will be given in the **dataPoint** child elements of the current **dataGroup**, in child elements with names corresponding to the *id* values of the **property** elements of the **dataGroup**.

If a property element occurs as the child of the **dataGroup** element, and it describes data corresponding to a species (a "concentration" or "composition" type property), then a **speciesLink** child element is mandatory, which defines the species to which the **property** corresponds.

The *id* attribute is mandatory only if the property element is the child of a **dataGroup** element. Otherwise, it is non-handled. It contains the name of the child element of the **dataPoint** elements in which the corresponding numerical values will appear. The *id* attributes within a **dataGroup** usually follow the progression "**x1**", "**x2**", "**x3**", but can have any other name.

The *label* attribute contains a string that is the short notation of the physical property, e.g. for a temperature property, the *label* is usually "T".

The *kind* attribute is a string that can define the nature of a physical property (e.g., if a pressure rise is "relative"). It is mandatory for the property *name* "uncertainty" and an optional or non-handled attribute for all other properties.

If the *name* attribute is "pressure" or "volume" and the property describes a pressure–time or volume–time history in a rapid compression machine, the *kind* attribute must be used to describe if the profile corresponds to a reactive or a nonreactive mixture. In this case, it can have "reactive" or "nonreactive" values.

The *name* attribute is a string that defines the type of the physical property. The accepted values are summarized in the following table:

| **Valid property *name* types**<br>(M/N depending on the **experimentType**; "uncertainty", "evaluated standard deviation" and "equivalence ratio" are always A) | |
|---|---|
| temperature | length |
| pressure | density |
| volume | flow rate |
| time | volumetric flow rate |
| residence time | laminar burning velocity |
| distance | initial composition |
| ignition delay | composition |
| rate coefficient | concentration |
| equivalence ratio | uncertainty |
| temperature in reference state | pressure in reference state |
| volumetric flow rate in reference state | reactor length |
| reactor diameter | evaluated standard deviation |
| global heat exchange coefficient | environment temperature |
| exchange area | inlet velocity |
| compressed temperature | compressed pressure |
| branching ratio | maximum wall temperature |
| Nusselt number | stagnation plate temperature |
| plate distance | pressure rise |

If the property *name* type is "uncertainty", three more attributes are mandatory:

- The attribute *reference* contains the *property name* to which the specified uncertainty refers.
- The attribute *kind* describes the kind of uncertainty. It can have the values "absolute" and "relative"
- The attribute *bound* specifies the type of uncertainty bound(s): "plus", "minus" or "plusminus"

The property *name* type "evaluated standard deviation" can be provided to encode the estimated standard deviation for a dataset or a datapoint. These standard deviations are used by the computer program Optima++ to calculate error function values.

If the property *name* type is "evaluated standard deviation", three more attributes are mandatory:

- The attribute *reference* contains the *name* of the property to which the specified standard deviation refers.

- The attribute *kind* describes the scale of the standard deviations. It can have values "absolute" for absolute scale errors or "relative" for relative errors. A relative error can be considered as an absolute error on a natural logarithmic scale. If absolute errors are used, the unit of the standard deviations must also be defined using the *units* attribute.

- The attribute *method* specifies the method and how the standard deviations were evaluated. The accepted values are summarized in the following table:

| **Valid *method* attribute values** | |
|---|---|
| ***method* value** | **Description** |
| generic uncertainty | Sigma reflects a generic uncertainty assumed for this category of measurements. |
| statistical scatter | Sigma is identical to the statistical scatter of the data points. |
| from uncertainty of experimental conditions | Sigma is identical to the experimental uncertainty calculated from the uncertainty of the experimental conditions. |
| reported uncertainty | Sigma is identical to the experimental uncertainty reported in the original paper. |
| combined from scatter and reported uncertainty | Sigma was determined from both the statistical scatter and experimental uncertainty reported in the original paper. |
| combined from scatter and the uncertainty of conditions | Sigma was determined from the statistical scatter, and the experimental uncertainty was calculated from the uncertainty of the experimental conditions. |

If the reference property is *composition* or *concentration,* a **speciesLink** child element is mandatory, which defines the species to which the referenced property corresponds.

If the property *name* type is "uncertainty" or "evaluated standard deviation", the *sigmarange* attribute can be used to define the uncertainty limits. For example, *sigmarange*="2" means the error is reported corresponds to 2σ uncertainty. If the property *name* type is "evaluated standard deviation," the default value of the sigmarange attribute is 1 (e.g., if the *sigmarange* attribute is not specified, the "evaluated standard deviation" corresponds to 1$\sigma$).

If the *name* attribute is "initial composition" the *streamName* attribute can be used to specify if the initial components listed inside the "initial composition" property belong to a specific stream (*e.g.* fuel or oxidizer stream). Multiple "initial composition" properties with different *streamName* attributes are allowed.

The property *name* type "equivalence ratio" is often reported in the literature. An exact knowledge of the composition of the oxidizer, as well as information regarding the dilution of the mixture with additional gases, is required. Although there is a potential for redundancy, the parallel definition of *equivalence ratio* and *composition* (or *concentration*) is legal, as long as the *type* attributes differ (see next paragraph).

The *sourcetype* attribute can be either "reported" (if the **property** was found in the corresponding literature reference), "digitized" (if the **property** was reported, but had to be digitized from a plot by the creator of the XML file), "calculated" (if the **property** was calculated during data processing, e.g., as a result of the unit conversion) or "estimated" (if the **property** was estimated during data processing using some assumption, e.g., a composition calculated using the not explicitly reported composition of air).

The *units* attribute contains the physical unit of the numeric values corresponding to the **property**. It is mandatory in all cases, except if its type (*name* value) is „initial composition", where it is non-handled.

In this case, the units are defined within each **component** child element.

| **component** | | | |
|---|---|---|---|
| **Child of** | - **property** | **Children** | - **amount** – M<br>- **speciesLink** – M |
| **Attributes** | None | **Text content** | None |
| **Description**<br>The **component** element can only occur as a child element of an "initial composition" **property** element as a host for a **speciesLink** element and a corresponding **amount** element. The **speciesLink** is used to identify the species, and the amount element defines the number of species in the initial composition. | | | |
| **speciesLink** | | | |
| **Child of** | - **property**<br>- **component** | **Children** | None |
| **Attributes** | - *preferredKey* – M<br>- *CAS* – O<br>- *InChI* – O<br>- *SMILES* – O<br>- *chemName* – O | **Text content** | None |

**Description**

The **speciesLink** element is used to identify the species to which a "composition" or "concentration" type **property** element or a **component** element refers. It is also necessary when a **property** "uncertainty" or "evaluated standard deviation" has the *reference* "composition" or "concentration".

If a **property** shall be defined as the sum of several species, multiple **speciesLink** blocks occurring after one another should be specified.

The name of the species is stored within the *preferredKey* attribute as a string. The *CAS* attribute serves as an unambiguous form of identification of chemical species. The CAS Registry Number of the species is stored within the *CAS* attribute as a string. Such identification numbers can be found in various online databases, e.g., http://www.commonchemistry.org/index.aspx.

As alternatives to *CAS*, the *InChI* and *SMILES* identifiers can also be used to identify species. Note that the standard InChI string should be used, not the InChIKey, which is a hashed version of the standard InChI string. A canonical identifier should be used if the user prefers using SMILES identifiers. Note that a number of equally valid SMILES strings can typically be written for a single molecule, which may cause ambiguity.

In addition to the mandatory *preferredKey* and the optional attributes *CAS*, *InChI* and *chemName* may be used to denote the chemical name of a certain species.

*Example:*

```
<speciesLink preferredKey="C2H5OH" chemName="ethanol" CAS="64-17-5"
InChI=”1S/C2H6O/c1-2-3/h3H,2H2,1H3 ” SMILES=”CCO”/>
```

| **dataPoint** | | | |
|---|---|---|---|
| **Child of** | **- dataGroup** | **Children** | see below |
| **Attributes** | None | **Text content** | None |

**Description**

Contains as many child elements as many properties were defined in the **dataGroup** of which the **dataPoint** is a child of. These children have names corresponding to the *id* attributes of the **property** elements contained in the **dataGroup**. In each **dataPoint,** the numeric values of the corresponding properties are stored in the corresponding child element.

Each **dataPoint** corresponds to a measured data point, representing an experiment by itself, or a single point measured during an experiment. It contains the values of both the independent and dependent variables of the experiment, and the content of the corresponding **property** elements have the relevant information. If the corresponding property *name* type is "evaluated standard deviation", the attribute *kind* is allowed in the child element of the **dataPoint**. It can have values "absolute" for absolute scale errors or "relative" for relative errors.

## *Specific data elements of root element* **xmlinfo**

| **referenceFileDOI** | | experiment – O | | kdetermination – O |
|---|---|---|---|---|
| **Child of** | **- xmlinfo** | **Children** | None | |
| **Attributes** | None | **Text content** | DOI of the related main XML file as a string – O | |
| **Description** | | | | |
| The **referenceFileDOI** element is the counterpart of **fileDOI** that should have the same content as a text content. A distinction is made to avoid the false assumption that a separate DOI should be requested/assigned for an additional XML file. | | | | |

| **referenceXMLFile** | | experiment – M | | kdetermination – M |
|---|---|---|---|---|
| **Child of** | **- xmlinfo** | **Children** | None | |
| **Attributes** | None | **Text content** | Name of the related XML file as a string – M | |
| **Description** | | | | |
| The **referenceXMLFile** element is mandatory if an additional XML file exists. The naming scheme "*[xmlname]*_info.xml" is recommended. The element should contain the string "*[xmlname]*.xml" as its text content. | | | | |

| **keywords** | | experiment – O | | kdetermination – O |
|---|---|---|---|---|
| **Child of** | **- xmlinfo** | **Children** | - **item** (multiple instances possible) | |
| **Attributes** | None | **Text content** | Keyword(s) as a string in the child element – O | |
| **Description** | | | | |
| The **keywords** element may contain keywords associated with the experiment or the publication. | | | | |

| **modelingInfo** | | experiment – O | | kdetermination – O |
|---|---|---|---|---|
| **Child of** | **- xmlinfo** | **Children** | - **item** (multiple instances possible) | |
| **Attributes** | None | **Text content** | Comment as a string in the child element – O | |
| **Description** | | | | |
| The **modelingInfo** element may be used to provide solver-specific information. | | | | |

<table>
<tr><td colspan="2">plottingInfo</td><td colspan="2">experiment – O</td><td>kdetermination – O</td></tr>
<tr><td>Child of</td><td>- xmlinfo</td><td>Children</td><td colspan="2">- Xaxis – M/N; see below<br>- Yaxis – M/N; see below<br>- speciesLink – M/N; see below</td></tr>
<tr><td>Attributes</td><td>No attributes of the main element. Attributes of the child elements are:<br>- name – M<br>- units – M<br>- scale – M<br>- label – O<br>- reference – M/N; see below<br>- kind – M/N; see below<br>- bound – M/N; see below</td><td>Text content</td><td colspan="2">None</td></tr>
<tr><td colspan="5">Description<br>The element plottingInfo and its children can be used to specify which property names appearing in the main XML file should be plotted. If the element is specified, name, units, and scale are mandatory.<br>While the name must match the name of a property in the main XML file, units can have a different value depending on the type of property (see Section “Summary of valid units”). The attribute scale can take the values “lin” (linear axis), “inv” (inverse axis), “log10” (decadic logarithmic axis), and “ln” (natural logarithmic axis).<br>The label attribute contains a string that is the short notation of the physical property and may be used as the label in plotting, e.g. for a temperature property, the label is usually “T”.<br>If the specified name is “uncertainty”, additional attributes of the child element are mandatory:<br>- reference containing the name of the property to which the specified uncertainty refers.<br>- kind describing the kind of uncertainty. It can have the values “absolute” and “relative”<br>- bound specifying the type of uncertainty bound(s): “plus”, “minus” or “plusminus”<br>Note that several Yaxis child elements may be specified, e.g., for different species to be plotted or when uncertainty information corresponding to a certain property shall be added to the plot.<br>Suppose a property element to be plotted describes data corresponding to a species (a “concentration” or “composition” type property). In that case, a speciesLink child element is mandatory, which defines the species to which the property corresponds. If a property shall be defined as the sum of several species, multiple speciesLink blocks occurring after one another must be specified.<br>Several Xaxis elements may only be used for a selected property and its related uncertainty. If you wish to create plots with different Xaxis properties, please use separate plottingInfo blocks.</td></tr>
</table>

<table>
<tr><td colspan="2">dataGroup</td><td>experiment – O</td><td>kdetermination – O</td></tr>
<tr><td>Child of</td><td>- xmlinfo</td><td>Children</td><td>- property – M<br>- dataPoint – M</td></tr>
<tr><td>Attributes</td><td>- id – M<br>- label – O<br>- dataPointLink – M/N, see below</td><td>Text content</td><td>None</td></tr>
<tr><td colspan="4">Description<br>The dataGroup element as a child of xmlinfo should only be used to report information too large to efficiently handle the main XML file, e.g., raw pressure–time histories. Volume–time histories, which were converted from pressure–time histories (and potentially smoothened and/or subsampled) should occur in the main XML file.<br>The dataGroup element contains property elements. It also includes the corresponding data in the dataPoint elements. For the details of the data storage, see the description of dataPoint.<br>The id attribute is mandatory in xmlinfo files and must match the id attribute of the corresponding dataGroup in the main XML file. These id attributes of data groups also usually follow the progression “dg1”, “dg2”, but can have any other name.<br>The label attribute may contain a string describing the type of data grouped in a dataGroup. This can be useful, e.g., to distinguish a dataGroup containing the properties volume and time from the primary one containing the measured data.<br>A data point link must be provided via the dataPointLink attribute, if the non-primary dataGroup contains a pressure-time history, volume-time history or temperature-time-history. It is by default “all” (which can be specified as such, too). If it shall only be used for selected points of the primary dataGroup, the value of this attribute should be specified e.g. as “1” for the 1st point in order of occurrence. Multiple links may be used. In this case, all linked data points must be separated with a semicolon, e.g. “1;2;5;6;” for the value of the dataPointLink attribute.</td></tr>
</table>

# Description of the XML structure for different experiment types

The ReSpecTh Kinetics Data Format can describe ignition delay, laminar burning velocity measurements, and concentration profiles measured as a function of time, distance, or outlet or stationary concentrations measured as a function of varying experimental conditions (e.g., reactor temperature). These types altogether are called “indirect experiment types”. Reaction rate coefficients can also be stored using the ReSpecTh Kinetics Format, called “direct measurements” or “theoretical rate determinations”.

This section describes which data are mandatory and optional for each experiment type.

## *Common features*

Data files describing indirect experiment types must have a root element named **experiment**, and those describing direct data files must have a root element named **kdetermination**.

The root element must have the following child elements (for details, see section *Elements of the data format*)

- **fileAuthor** – Author of the file (not the data)
- **ReSpecThVersion** – ReSpecTh specification version followed by the file
- **bibliographyLink** – Bibliographic data of the source publication
- **dataGroup** – The measured dataset (experimental conditions, measured values)

A **commonProperties** element is also almost always present in all files. This contains the experimental conditions that are constant over the whole dataset.

The **ReSpecThVersion** element defines which version of the ReSpecTh Kinetics Data Format Specification file was created. This way, even if the RKD format is modified in a non-backward compatible way, the correct interpretation method can be identified for any file.

An **experimentType** and apparatus element is also necessary for indirect experimental files, which are non-handled for direct experiments. These define the type of experiment and experimental apparatus, respectively.

The following subsections list the mandatory and optional types of physical properties and how they are to be interpreted. All physical properties must be defined in **property** elements as children of either the **commonProperties** or **dataGroup** elements. Properties in the **commonProperties** element describe the experimental conditions common for all experiments described in the data files, and those in the **dataGroup** element correspond to those experimental conditions that were varied between the experiments and the measured values.

For each property, it is specified whether it can occur in the **commonProperties** (C for “common”) or in the **dataGroup** (V for “variable”) or in both (C/V). It should be noted that a composition type **property** in the **commonProperties** is defined differently from all other **property** elements. For details, see the detailed description of the **property** element. For each

property, it is specified whether it is mandatory (M, i.e. it is required for the simulations), optional (O, i.e. it can be specified and used, but simulations can generally be set up without it, e.g. used for the more accurate RCM simulations or for plotting), not handled (N, i.e. not needed to simulate the experiment, but provides auxiliary information about it), or forbidden (F, i.e. some properties cannot be used together). The possible units are also given for each type of property in a summarized form in the “Summary of valid units” section.

## experiment: *ignition delay measurement*

Ignition delay measurements can describe data measured in shock tubes or rapid compression machines (RCMs). The initial state of the reactive mixture must be defined by the temperature, pressure, and composition. If it is known that the system cannot be described adiabatically, e.g., due to heat losses in a rapid compression machine or pressure rise in a shock tube, one can also define an equivalent volume–time history or a constant pressure rise factor, respectively, to describe these effects. The measured values are ignition delays, and the definition of the ignition delay time must be defined in the **ignitionType** child element of the root element.

The initial state defined in the file must correspond to the state behind the reflected shock wave (usually denoted by $p_5$ and $T_5$) for shock tube data. It is useful to encapsulate this information in the **apparatus** element.

*Example:* For a reflected shock tube measurement, the child element **kind** must be specified as "shock tube", and the **mode** must be "reflected". Accordingly, the **mode** of an experiment at incident shock wave should be "incident".

For rapid compression machine data, the initial state should correspond to the beginning of the corresponding volume–time history. The volume–time history can begin before the start of the compression phase of the experiment or to the state at the end of the compression phase. In either case, the ignition delay should be interpreted as the delay compared to the end of the compression phase. If the volume–time history includes the compression phase, the "compressed temperature" and "compressed pressure" properties can store the experimentally reported $T_c$ and $p_c$ values.

| **Properties** | | | |
|---|---|---|---|
| **Property** | **C/V** | **M/O/N/F** | **Notes** |
| temperature | C/V | M | The temperature behind the reflected shock wave in a shock tube experiment.<br>For an RCM experiment, this is the temperature either before the start or at the end of compression, depending on the initial state of the corresponding volume–time history. |
| pressure | C/V | M | The pressure behind the reflected shock wave in a shock tube experiment.<br>For an RCM experiment, this is the pressure either before the start or at the end of compression, depending on the accompanying volume–time history. |
| (initial) composition | C/V | M | The composition of the reaction mixture is given in mole fractions.<br>A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |

| | | | |
|---|---|---|---|
| | | | The "composition" and "initial composition" properties are equivalent in ignition delay time measurements. |
| ignition delay | V | M | The measured ignition delay time.<br>For an RCM experiment, the delay should be given compared to the end of compression, even if a volume–time history starts at the beginning of compression or even earlier. |
| volume | V | O | A volume **property** can be given in a **dataGroup** separate from the primary one, to provide a volume–time history for an ignition experiment. It must be accompanied by a time property in the same **dataGroup**, to give the corresponding time values.<br>A data point link must be provided via the *dataPointLink* attribute (use "all" for all data points). If a volume–time history is to be used for only specific points of the primary **dataGroup**, the value of this attribute must be specified e.g. as "1" for the 1st point in order of occurrence. Multiple links may be used. In this case, all linked data points must be separated with a semicolon, e.g. "1;2;5;6;" for the value of the *dataPointLink* attribute.<br>A volume–time history cannot be used with a constant pressure rise value.<br>The *kind* attribute must be used to describe if the profile corresponds to a reactive or a nonreactive mixture. It can have the values "reactive" or "nonreactive". |
| temperature | C/V | O | A temperature **property** can be given in a **dataGroup** separate from the primary one, to provide a temperature–time history for an ignition experiment. It must be accompanied by a time property in the same **dataGroup**, to give the corresponding time values.<br>A *dataPointLink* attribute link must be provided. For details, see the above description of the property "volume". |
| pressure | C/V | O | A pressure **property** can be given in a **dataGroup** separate from the primary one, to provide a pressure–time history for an ignition experiment. It must be accompanied by a time property in the same **dataGroup**, to give the corresponding time values.<br>A pressure–time history cannot be used with a temperature–time history in specific simulation codes (*e.g.*, CHEMKIN-II).<br>A *dataPointLink* attribute link must be provided. For details, see the above description of the property "volume".<br>The *kind* attribute must be used to describe if the profile corresponds to a reactive or a nonreactive mixture. It can have the values "reactive" or "nonreactive". |

| | | | |
|---|---|---|---|
| time | V | O | The time values for a volume–time, temperature–time, or pressure–time history. |
| pressure rise | C | O | For a shock tube experiment, a constant pressure rise can represent the pressure rise behind the reflected shock wave.<br>A constant rise can be defined relative to the initial pressure.<br>*Example:*<br>`<property label="dp/dt" name="pressure rise" sourcetype="reported" units="ms-1" kind="relative"> <value>0.05</value></property>`<br>At an initial pressure of 2 bar, a relative pressure rise value of 0.05 $ms^{-1}$ means that the pressure rises by 0.1 bar every millisecond.<br>Note: if a volume–time history is also defined for the same data point, the pressure rise is ignored. |
| compressed temperature | C/V | O | For an RCM experiment, this is the temperature corresponding to the end of the compression ($T_c$). *Note:* it is unnecessary for the simulations but can be used as an independent variable on plots. |
| compressed pressure | C/V | O | For an RCM experiment, this is the pressure corresponding to the end of the compression ($p_c$). *Note:* it is unnecessary for the simulations but can be used as an independent variable on plots. |

## experiment: *laminar burning velocity measurement*

To describe laminar burning velocity measurements, the composition and state of the initial gas mixture, and the corresponding laminar burning velocity must be defined.

| Properties | | | |
|---|---|---|---|
| **Property** | **C/V** | **M/O/N/F** | **Notes** |
| temperature | C/V | M | Unburned gas temperature. |
| pressure | C/V | M | Inlet gas pressure. |
| (initial) composition | C/V | M | The composition of the reaction mixture is given in mole fractions.<br>A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**.<br>The "composition" and "initial composition" properties are equivalent in laminar burning velocity measurements. |
| laminar burning velocity | V | M | The measured laminar burning velocity. |
| environment temperature | C/V | O | The temperature of the environment. It is used if the simulation is performed with radiative heat transfer. If it is not specified and the simulation is performed with radiative heat transfer, the default environment temperature value of the solver is used (typically 298.15 K) |

## experiment: *concentration time profile measurement*

Concentration time profile measurements describe concentration values measured as a function of the reaction time, typically in a flow reactor or other reactor that can be described by homogeneous kinetics. The state and composition of the inlet or initial gas mixture must be defined, along with the measured time – concentration values.

If the measurements should be compared to the simulated values with a time shifting, then the **timeshift** child element of the root element can be defined.

| Properties | | | |
|---|---|---|---|
| **Property** | **C/V** | **M/O/N/F** | **Notes** |
| temperature | C | M | Inlet gas temperature. |
| pressure | C | M | Inlet gas pressure. |
| initial composition | C/V | M | The composition of the reaction mixture is given in mole fractions.<br>A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |
| time | V | M | The time values at which concentrations were measured. |
| composition or concentration | V | M | The measured mole fractions or concentrations of the species.<br>A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |

## experiment: *outlet concentration measurement*

Outlet concentration measurements describe concentration values that were measured as the outlet of a reactor (e.g. final product distributions measured from tubular flow reactors, shock tubes, or micro flow reactors). Jet-stirred reactor outlet (i.e., end) concentrations are handled as a separate case (see below). The initial state and composition of the gas and the measured outlet concentrations after a given residence time must be defined. The temperature profile can be defined in a dataGroup separate from the primary one (see below). The inlet gas state is often reported in a reference state. This data can be included in the XML file using the property names ending with "in reference state" (see below).

| Properties | | | |
|---|---|---|---|
| **Property** | **C/V** | **M/O/N/F** | **Notes** |
| temperature | C/V | M/O | Inlet gas temperature. It is mandatory if the temperature profile is not included; otherwise, it is optional. |
| pressure | C/V | M | Inlet gas pressure. |
| residence time | C/V | M/O | Residence time of the reactive mixture in the reactor. It is mandatory if the temperature profile is not included; otherwise, it is optional. |
| initial composition | C/V | M | The composition of the reaction mixture is given in mole fractions.<br>A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |
| composition or concentration | V | M | The measured mole fractions or concentrations of the species.<br>A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |
| reactor length | C | M/O | The length of the reactor. It is mandatory if the temperature profile is included; otherwise, it is optional. |
| reactor diameter | C | M/O | The diameter of the reactor. It is mandatory if the temperature profile is included; otherwise, it is optional. |
| volumetric flow rate | C/V | M/O | Inlet gas volumetric flow rate. It is mandatory for tubular flow reactor measurements if the temperature profile is included; otherwise, it is optional. |
| temperature | V | M/O | A temperature **property** can be given in a **dataGroup** separate from the primary one, to provide a temperature profile measured in tubular or micro flow reactors. It must be accompanied by a |

| | | | |
|---|---|---|---|
| | | | distance property in the same **dataGroup** to give the corresponding distance values.<br>A data point link must be provided via the *dataPointLink* attribute, which can be "all". Suppose a temperature profile shall only be used for selected points of the primary dataGroup. In that case, the value of this attribute should be specified, e.g., as "1" for the 1st point in order of occurrence. Multiple links may be used. In this case, all linked data points must be separated with a semicolon, e.g. "1;2;5;6;" for the value of the *dataPointLink* attribute.<br>It is mandatory for micro flow reactor measurements, otherwise optional. |
| Nusselt number | C | M/N | The ratio of convective to conductive heat transfer across the reactor wall. It is mandatory for micro flow reactor measurements, otherwise not handled. |
| inlet velocity | C | M/N | The velocity of the inlet gas mixture. It is mandatory for micro flow reactor measurements, otherwise not handled. |
| maximum wall temperature | V | O/N | The maximum wall temperature measured in a micro flow reactor. *Note:* it is unnecessary for the simulations but can be used as an independent variable on plots. It is optional for micro flow reactor measurements, otherwise not handled. |
| distance | V | M/O | The distance values for a temperature profile. It is mandatory for micro flow reactor measurements otherwise optional. |
| temperature in reference state | C | O | Gas temperature in the reference state, as reported in the publication. |
| pressure in reference state | C | O | Gas pressure in the reference state, as reported in the publication. |
| volumetric flow rate in reference state | C/V | O | Volumetric flow rate in the reference state, as reported in the publication. |

## experiment: *burner stabilized flame speciation measurement*

Burner stabilized flame speciation measurements describe speciated flame measurements. The inlet gas state, composition, and flow rate (or inlet velocity) must be defined, and the measured concentrations must be defined as a function of the distance from the burner.

| Properties | | | |
|---|---|---|---|
| **Property** | **C/V** | **M/O/N/F** | **Notes** |
| temperature | C | M/O | Inlet gas temperature. |
| pressure | C | M | Inlet gas pressure. |
| flow rate | C | M/O | The mass flow rate of the inlet gases. Mandatory if an *inlet velocity* property is not specified, otherwise optional. |
| inlet velocity | C | M/O | The velocity of the inlet gas mixture at the burner surface. Mandatory if a *flow rate* property is not specified, otherwise optional. |
| initial composition | C/V | M | The composition of the reaction mixture is given in mole fractions.<br>A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |
| distance | V | M | The distance values from the burner at which the species concentrations were measured. |
| composition or concentration | V | M | The measured mole fractions or concentrations of the species.<br>A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |
| temperature | V | O | Flame temperature is given as a function of the distance from the burner (temperature profile). |
| distance | V | O | The distance values for a temperature profile. |
| environment temperature | C | O | The temperature of the environment. It is utilized if the simulations are performed with radiative heat transfer. If it is not specified and the simulation is performed with radiative heat transfer, the default environment temperature value of the solver is utilized (typically 298.15 K). |

## experiment: *micro flow reactor concentration profile measurement*

Micro flow reactor concentration profile measurements describe species concentration profile measurements in micro flow reactors. The inlet gas state, composition, and inlet velocity must be defined, and the measured concentrations must be defined as a function of the distance from the inlet of the reactor.

| Mandatory properties | | | |
|---|---|---|---|
| **Property** | **C/V** | **M/O/N/F** | **Notes** |
| temperature | C | M | Inlet gas temperature. |
| pressure | C | M | Inlet gas pressure. |
| inlet velocity | C | M | The velocity of the inlet gas mixture. |
| reactor length | C | M | The length of the reactor. |
| reactor diameter | C | M | The diameter of the reactor. |
| Nusselt number | C | M | The ratio of convective to conductive heat transfer across the reactor wall. Note, this is not an experimental parameter, but must be defined for the simulations to describe heat transfer between the gas and the wall. |
| initial composition | C/V | M | The composition of the reaction mixture is given in mole fractions.<br>A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |
| distance | V | M | The distance values from the inlet of the reactor where the species concentrations were measured. |
| composition or concentration | V | M | The measured mole fractions or concentrations of the species.<br>A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |
| temperature | V | M | Wall temperature is given as a function of the distance from the inlet of the reactor (temperature profile). |
| distance | V | M | The distance values for the temperature profile. |

## experiment: *burner-stabilized stagnation flame concentration measurement*

Burner-stabilized stagnation flame concentration measurements describe speciated flame measurements in a stagnation-flow burner. This flame configuration is visually a flat, strained flame and involves a premixed laminar nozzle burner impinging on a wall. The inlet gas state, composition, and flow rate (or inlet velocity) must be defined, and the measured concentrations must be defined at specific distances from the burner.

| Properties | | | |
|---|---|---|---|
| **Property** | **C/V** | **M/O/N/F** | **Notes** |
| temperature | C/V | M | Inlet gas temperature. |
| pressure | C/V | M | Inlet gas pressure. |
| plate distance | C | M | Distance between the inlet (burner) and the stagnation plate. |
| stagnation plate temperature | V | M | Temperature of the stagnation plate. |
| flow rate | C/V | M/O | The mass flow rate of the inlet gases. Mandatory if an *inlet velocity* property is not specified otherwise optional. |
| inlet velocity | C/V | M/O | Velocity of the inlet gas mixture at the burner surface. Mandatory if a *flow rate* property is not specified otherwise optional. |
| initial composition | C/V | M | Composition of the reaction mixture, given in mole fractions. A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |
| distance | C/V | M | Distance from the burner at which the concentrations of the species were measured. |
| composition or concentration | V | M | The measured mole fractions or concentrations of the species. A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |

## experiment: *jet-stirred reactor measurement*

Jet-stirred reactor measurements describe concentration values measured at the outlet of a jet-stirred reactor (or perfectly stirred reactor), i.e., representing outlet concentrations. The initial state and composition of the gas must be defined, along with the reactor volume and the measured outlet concentrations after a given residence time.

| **Mandatory properties** | | | |
|---|---|---|---|
| **Property** | **C/V** | **M/O/N/F** | **Notes** |
| temperature | C/V | M | Inlet gas temperature. |
| pressure | C/V | M | Inlet gas pressure. |
| residence time | C/V | M | Residence time of the reactive mixture in the reactor. |
| volume | C/V | M | The volume of the reactor. |
| initial composition | C/V | M | The initial composition of the reaction mixture, given in mole fractions.<br>A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |
| composition or concentration | V | M | The measured mole fractions or concentrations of the species.<br>A separate **property** element must be defined for each species, and the species is identified with a **speciesLink** child element of the **property**. |
| global heat exchange coefficient | C | O | Global heat exchange coefficient ($U$): $\dot{Q} = UA(T - T_{\text{env}})$. This property is optional. |
| environment temperature | C/V | M/N | The environment temperature ($T_{\text{env}}$) for calculating heat exchange ($\dot{Q} = UA(T - T_{\text{env}})$). It is mandatory if the *global heat exchange coefficient* is specified; otherwise, it is not handled. |
| exchange area | C | M/N | The exchange area ($A$) for calculating heat exchange ($\dot{Q} = UA(T - T_{\text{env}})$). It is mandatory if the *global heat exchange coefficient* is specified; otherwise, it is not handled. |

## kdetermination: *Rate coefficient determinations*

Reaction rate coefficient measurement files contain the rate coefficients measured at various temperatures, pressures, and gas compositions for a given reaction. Defining the pressure and gas composition in a data file is unnecessary, as these are only relevant for pressure-dependent reactions.

The reaction for which the data are contained in the file is stored in a **reaction** element. If the sum of the rate coefficient of two or more reactions is to be stored in a file, these reactions should be stored in separate **reaction** elements. Alternatively, a single **reaction** element can define the sum of all (or selected) branches for a given set of reactants. For details on specifying the reaction, see the description of the **reaction** element.

Branching ratios of reactions having the same reactants but different products can also be stored in kdetermination type XML files. In this case, two or more **reaction** elements must be provided in the file, and the branching ratio ($\alpha$) as a function of temperature can be defined using the *branching ratio* property type. The branching ratio is defined as follows:

$$\alpha = \frac{k_1}{\sum_{i=1}^{N} k_i}$$

where $k_1$ is the rate coefficient of the reaction defined first in the file and the $k_i$-s are the rate coefficients of the $N$ reactions defined in the file.

| Properties | | | |
|---|---|---|---|
| **Property** | **C/V** | **M/O/N/F** | **Notes** |
| temperature | C/V | M | The temperature at which the rate coefficient or the branching ratio was measured. |
| rate coefficient | V | M/F | Value of the rate coefficient. It is mandatory if a *branching ratio* property is not specified in the file; otherwise, it is forbidden. |
| branching ratio | V | M/F | Value of the branching ratio. It is mandatory if a *rate coefficient* property is not specified in the file; otherwise, it is forbidden. |
| pressure | C/V | O | 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 | O | The gas composition in which the rate coefficient was measured. This is only relevant for pressure-dependent reactions but can be defined in any case. |

## *Summary of valid units*

The following table gives a summary of the unit strings currently handled within the ReSpecTh Kinetics Data Format Specification. Here, all strings are given exactly as they should appear in the file. This means that exponents are not typed as superscripts, and the micro (μ) prefix should be typed as "u" to guarantee that these can be typed in plain text files.

| Property type | Valid units |
|---|---|
| temperature | K |
| environment temperature | K |
| pressure | Pa, kPa, MPa, Torr, torr, bar, mbar, atm |
| volume | m3, dm3, cm3, mm3, L |
| time | s, ms, us, ns, min |
| residence time | s, ms, us, ns, min |
| time | s, ms, us, ns, min |
| distance | m, dm, cm, mm |
| ignition delay | s, ms, us, ns, min |
| length | m, dm, cm, mm |
| density | g m-3, g dm-3, g cm-3, g mm-3,<br>kg m-3, kg dm-3, kg cm-3, kg mm-3 |
| flow rate | g m-2 s-1, g dm-2 s-1, g cm-2 s-1, g mm-2 s-1,<br>kg m-2 s-1, kg dm-2 s-1, kg cm-2 s-1, kg mm-2 s-1 |
| volumetric flow rate | m3 s-1, dm3 s-1, L s-1, cm3 s-1, mL s-1, m3/s, dm3/s, L/s, cm3/s, mL/s, m3 min-1, dm3 min-1, L min-1, cm3 min-1, mL min-1, m3/min, dm3/min, L/min, cm3/min, mL/min |
| inlet velocity | m/s, dm/s, cm/s, mm/s, m s-1, dm s-1, cm s-1, mm s-1 |
| laminar burning velocity | m/s, dm/s, cm/s, mm/s, m s-1, dm s-1, cm s-1, mm s-1 |
| composition | mole fraction, percent, ppm, ppb |
| concentration | mol/m3, mol/dm3, mol/cm3, mol m-3, mol dm-3, mol cm-3,<br>molecule/m3, molecule/dm3, molecule/cm3, molecule m-3,<br>molecule dm-3, molecule cm-3 |
| rate coefficient | s-1,<br>m3 mol-1 s-1, dm3 mol-1 s-1, cm3 mol-1 s-1,<br>m3 molecule-1 s-1, dm3 molecule-1 s-1, cm3 molecule-1 s-1,<br>m6 mol-3 s-1, dm6 mol-2 s-1, cm6 mol-2 s-1,<br>m6 molecule-2 s-1, dm6 molecule-2 s-1, cm6 molecule-2 s-1 |
| pressure rise | ms-1, s-1 |

| | |
|---|---|
| exchange area | m2, dm2, cm2, mm2 |
| global heat exchange coefficient | W m-2 K-1, W/m2/K, J m-2 s-1 K-1, J/s/m2/K, cal m-2 s-1 K-1, kcal m-2 s-1 K-1, cal/s/m2/K, kcal/s/m2/K |
| *all relative properties* | unitless, percent |

# Change log

## *v2.4 to v2.5* (09 April, 2024)

- New name types were added to the element property for RCM
    - “compressed temperature”
    - “compressed pressure”
- A new attribute was added to the property element to specify different streams of the initial species
- A new experiment type, “Burner-stabilized stagnation flame concentration measurement” was added
- A new experiment type, “Micro flow reactor concentration profile measurement” and related new property types were added
- The outlet concentration measurement type was extended to handle outlet concentrations measured in micro flow reactors
- Added optional “environment temperature” property to laminar burning velocity measurement and burner stabilized flame speciation measurement types
- Branching ratio data can be stored in kdetermination type XML files, the related property type was added.

## *v2.3 to v2.4* (08 February, 2022)

- New name types were added to the element property
    - “global heat exchange coefficient”
    - “environment temperature”
    - “exchange area”
    - “inlet velocity”
- A new child node was added to the element apparatus
- New ignition definition type “relative increase” was added

## *v2.2 to v2.3* (19 October, 2020)

- The temperature profile can be included in the flow reactor XML file.
- The *kind* attribute (with values “reactive” or ”nonreactive”) is mandatory in pressure property if it corresponds to a pressure-time profile for rapid compression machine data.
- New name types were added to the element property
    - “reactor length”
    - “reactor diameter”
    - “volumetric flow rate”
    - “temperature in reference state”
    - “pressure in reference state”

    - "volumetric flow rate in reference state"
    - "evaluated standard deviation"
- The encoding of special characters in **referenceDOI** was specified.
- The following optional elements were added:
    - **firstPublicationDate**
    - **lastModificationDate**

## *v2.1 to v2.2* (February 13, 2019)

- Child elements (**reactant1, 2, 3 and product1, 2, 3**) of the **reaction** were introduced to provide information for search engines for the reactants and products of the reaction.

## *v2.0 to v2.1* (August 24, 2018)

- Literature details using standard BibTeX fields can be given in child element **details** of **bibliographyLink**.
- Minor correction: child **method** is denoted as optional for **kdetermination** in the appropriate table
- "all" value for the *dataPointLink* attribute should be specified, there is no default value for it

## *v1.0 to v2.0* (August 14, 2017)

- The root element **kmeasurement** was renamed to **kdetermination**, which allows to encode of the results of theoretical reaction rate determinations in a similar manner
- The optional child element **method** was introduced for **kdetermination**
- Instead of the labels "indirect" and "direct", now the labels "experiment" and "kdetermination" are used throughout the manual
- The root element **xmlinfo** was introduced, which should appear in a separate file named "*[xmlname]*_info.xml". Other than the common data elements, it has the following unique children: **referenceFileDOI, referenceXMLFile, keywords, plottingInfo, modelingInfo**
- The structure of the mandatory element **bibliographyLink** was changed, which necessitated a major version update:
    - The attribute *preferredKey* was replaced by the mandatory child **description**
    - Optional children were added: **referenceDOI**, **location**, **table**, **figure**
- The following optional elements were added:
    - **fileDOI**
    - **comment**
- New *name* types were added to the mandatory element **property**:
    - "uncertainty"
    - "equivalence ratio"
- The *name* type "flame speed" was renamed to "laminar burning velocity"
- New attributes were added to the mandatory element **property**:

    - *sourcetype* (mandatory)
    - *reference, kind, bound* (mandatory if the **property** *name* is “uncertainty”)
- The optional Text contents of **experimentType** were revised:
    - All Text contents now start with lowercase letters (e.g., “ignition delay measurement” instead of “Ignition delay measurement”) in accordance with other specifications
    - “Laminar flame speed measurement” was renamed to “laminar burning velocity measurement”, as this term describes the measured quantity more accurately
- The attribute *description* of the property “pressure rise” was renamed to *kind*
- The optional attributes *CAS, InChI, SMILES,* and *chemName* were added to the **speciesLink** element specification
- The initial composition of a concentration measurement must be defined as “initial composition” – in the old format specification, this was not stated explicitly
- The role of *dataPointLink* in **dataGroup** elements is now detailed in a more consistent manner
- Some missing explanations of existing features were added, and others were corrected. If you notice others missing in this manual, please get in touch with the authors! ☺
- The policy of documentation versioning was changed to avoid confusion

# Appendix: Example files

Example files for each type of **experiment** and **kdetermination** can be found in the ZIP archive "example_files.zip", alongside some additional XML files containing **xmlinfo** blocks.

These contain published data and can be found on http://respecth.hu.

Note that the values of the elements **fileDOI**, **modelingInfo,** and **keywords** contain dummy values.

| Type of data | Example file (with info file) |
|---|---|
| **experiment** | |
| *ignition delay measurement* (shock tube) | x10003006.xml (x10003006_info.xml) |
| *ignition delay measurement* (RCM) | x40003002.xml (x40003002_info.xml) |
| *laminar burning velocity measurement* | x23003038.xml (x23003038_info.xml) |
| *outlet concentration measurement* | x30003004.xml (x30003004_info.xml) |
| *concentration time profile measurement* (flow reactor) | x30003001.xml |
| *concentration time profile measurement* (shock tube) | x50003002.xml |
| *jet stirred reactor measurement* | x00003001.xml |
| *burner stabilized flame speciation measurement* | x60003002.xml |
| **kdetermination** | |
| Experimental/direct rate determination | k10003002.xml (k10003002_info.xml) |
| Theoretical rate determination | t10003001.xml (t10003001_info.xml) |
| Branching ratio determination | k00299010.xml |