

SHORT TERM SCIENTIFIC MISSION (STSM) – SCIENTIFIC REPORT

The STSM applicant submits this report for approval to the STSM coordinator

Action number: CM1404

STSM title: SMARTCATS

STSM start and end date: 29/10/2018 to 02/11/2018

Grantee name: Dr. Kieran P. Somers

PURPOSE OF THE STSM

This STSM is a follow-up to a previous STSM attended by Dr. Ultan Burke and Dr. Matteo Pelucchi, also hosted in RWTH Aachen by Prof. Pitsch. This is the first STSM for this particular researcher (Dr. Kieran Somers)

Following the successful STSM in Aachen in July, focusing on the collation, critical evaluation and design of a working process for efficient review, the current STSM expands upon the number of reactions under consideration and on the methods themselves, in order to garner relevant insight into the statistical evaluation of large sets of data. Ultimately, the goal of this collaboration between COST partners and external partners (National University of Ireland Galway (NUIG), Politecnico di Milano (PoliMi), RWTH Aachen, Argonne National Laboratory (ANL), Denmark Technical University (DTU) and ELTE Budapest) to collect, collate, evaluate and reconcile conflicting results for the existing data within the literature for hydrogen/syngas oxidation, is producing an outcome of outstanding relevance for the entire kinetic modelling community, by compiling the results of the review, into recommendations for each of the elementary reactions. The final outcome will be a kinetic model which is an accurate reflection of our most up to date understanding of the chemical kinetics for such system. This will also ensure that the obtained model can predict the indirect data of interest for more practical application such as, ignition delay times and laminar burning velocities.

The detail of the objectives of this STSM are listed below:

- 1) Consistently format the data collected over the previous 21 months to facilitate dissemination and interpretation. Statistics on the number of data/paper collected are provided in this report.
- 2) Discuss the most suitable methods to perform mathematical fitting of rate constants based on theoretical and experimental determinations. Details of the approach for pressure-dependent reactions are given in this report, and details of the approach used for pressure-independent reactions are provided in the reports of Dr. Ultan Burke, and Dr. Matteo Pelucchi.
- 3) Discuss and provide meaningful methods to define uncertainties.
- 4) Provide an outline for the treatment of every elementary reaction that is suitable for publication and easy use by kinetic modelers and users of kinetic models
- 5) Discuss and provide appropriate treatments of pressure dependent reactions
- 6) Provide a recommendation for additional reactions within the hydrogen/syngas model ($\text{OH} + \text{OH} \rightleftharpoons \text{O} + \text{H}_2\text{O}$ was specific to this researcher, as well as the collection and organization of the

large amount of information on $\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$ and $\text{HCO} + \text{M}$ that was useful to guide a proper treatment of pressure dependent reactions)

Together with these objectives, useful discussions allowed to further improve and extend the methods and approaches defined in the previous meeting. As part of this STSM, this author has contributed to the management of the project, to the collation of data for key reactions, and to the development of a method to fit pressure-dependent rate measurements based on theoretical modelling results.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

Project Management and Project Overview

Project management is a critical component of any project in order to meet targets, and assess progress on an ongoing basis. As the current project is unfunded (with the exception of COST support), involves colocated teams of people with varying expertise, some aspects of project management are necessary to delegate workload amongst contributors, and to assess on-going progress. As part of the current STSM, the current author spent ~20% of their time (1 out of 5 days) familiarising with the procedures and workflows established by the working group as part of their previous COST STMS which was held in Aachen in July 2018. All of the papers and data which were collated as part of the previous STSM were organised into a structured database by this author. Project Gantt Charts and workflows were then constructed to allow the team members to co-ordinate and collaborate effectively and to allow for the project to be managed on a longer term basis when collaborators returned to their home institution. A set of computational tools which manage and analyse the database of papers, and corresponding experimental data were also constructed during this time. The results section of this report provides an overview of the project, the results of which are directly relevant to COST SMARTCATS WG1 – “Smart energy carriers gas phase chemistry: from experiments to kinetic models”, and also WG4 – “Standard definition for data collection and mining toward a virtual chemistry of smart carriers”.

Data Collection and Tabulation for $\text{H}_2 \rightleftharpoons \text{H} + \text{H}$

Approximately 20% (1/5 days) of the current authors STSM was designated to collating data for reaction R2 ($\text{H} + \text{H} + \text{M} \rightleftharpoons \text{H}_2 + \text{M}$). This recombination reaction is an important initiation and termination reaction in combustion systems, and is also the simplest combustion reaction possible. In total, there are 36 experimental rate constant recommendations, 4 theoretical rate constant recommendations, and 1 rate constant recommendation based on detailed chemical kinetic modelling studies, Figure 1. The data must be digitized in order to arrive at a rate constant recommendation, and this will take place as part of future work.

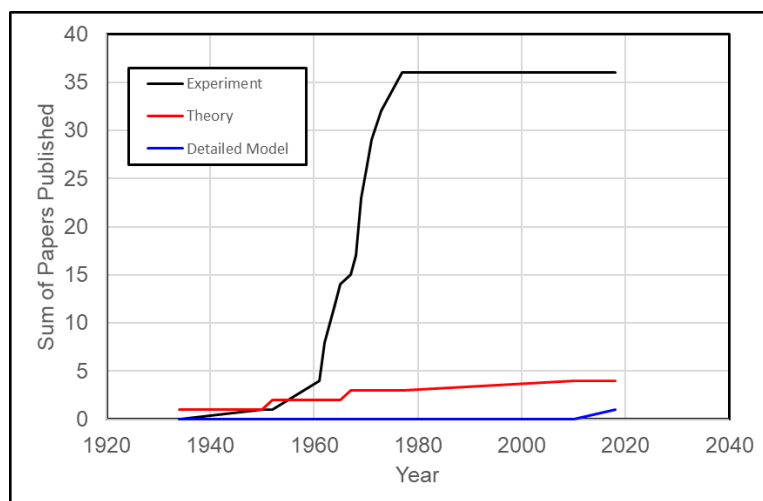


Figure 1: Cumulative number of papers published on the reaction $\text{H} + \text{H} + \text{M} \rightleftharpoons \text{H}_2 + \text{M}$

Data Fitting for Pressure-Dependent Reactions

Of the 50 reactions being considered as part of *this work*, 33 reactions (66%) involve bimolecular reactions proceeding through a single transition state forming bimolecular products, and 17 reactions (33%) involve an energised adduct, which can undergo non-reactive bimolecular collision which transfers ro-vibrational energy between the adduct and collider. Whilst the former 33 reactions tend to be only temperature dependent, those 17 reactions which involve collisional energy transfer (CET) are both temperature- and pressure-dependent, and some form of complex model (e.g. Lindemann Model, Troe Model/Fit, RRKM/Master Equation) is required to interpolate and extrapolate data so that rate constants can be cast in a form that is useful for chemical kinetic modelling studies, but also, a form which is based on a physically meaningful model.

An approach to fitting the majority (66%) of reactions which are only temperature-dependent was developed during this STSM, the details of which are outlined in the report of Dr. Burke who validated a method based available data for the $\text{H} + \text{O}_2 = \text{O} + \text{OH}$ system, which is the most important reaction in combustion. In the case of reactions which are both temperature- and pressure-dependent, data tends to be sparse over all regimes of temperature/pressure/diluent space which is relevant for combustion. A suitable method to fit experimental data is a much more complex task than for reactions which are only temperature-dependent, as the fitting method must retain a fundamentally physical basis such that extrapolation beyond experimental measurement is accurate.

Therefore ~60% (3/5 days) of the current STSM was designated to discuss and design a suitable data-fitting approach for the 17 reactions which are both temperature and pressure-dependent, which ultimately requires a tabulation of all available experimental data and conditions (temperature, pressure, rate constant, collider) coupled with *ab initio* quantum chemistry/statistical rate theories (RRKM/ME). Dr. Somers and Dr. Pelucchi, in collaboration with Dr. Klippenstein, have tabulated experimental data for two key combustion reactions which have been well-studied experimentally: $\text{H} + \text{CO} + \text{M} = \text{HCO}$ and $\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$. A detailed potential energy surface (PES) must first be constructed based on accurate *ab initio* methods. An important contribution of Dr. Klippenstein to this project is the provision of the PES for each reaction classified in the following section of this report. Once the PES has been characterised the experimental data must be provided to a RRKM/ME solver in order for some form of error-minimised fitting to be carried out. As part of this STSM, the current author built a computational tool in order to automatically carry out large-scale RRKM/ME calculations in order to fit available data. The approach is still under development as the error-minimisation approaches are more complex than a simple least-squares regression as the reaction barrier, the bath gas/collider properties, the energy transfer parameters, are all optimisable parameters. Preliminary results are presented in subsequent sections for conditions where the energy transfer parameters were used to fit the experimental data.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

Project Management and Project Overview

Tables 2 and 3 below provide high-level synopses of the current status of the project with Table 1 providing a legend to interpret Gantt Charts and Task Completion Rates shown in Tables 2 and 3. Table 3 gives a reaction-specific breakdown of the current status. Each reaction is classified based on the number of electrons in the system, which is appropriate when considering reactions that take place on a multi-channel or multiple-well potential energy surface, where absolute rate constants may be sensitive to both pressure and temperature, and where relative rate constants (branching ratios) may also be of interest to kinetic modellers. For each reaction, lead investigator(s) are assigned, and a series of tasks must be completed before a reaction data-sheet is written (RDS) and the data sheet is peer-reviewed (DSPR) by all collaborators before final recommendations are made. These tasks are non-trivial and labour-intensive (sourcing and mining data), and includes exhaustive literature review to collate papers (PC), tabulation of experimental data (EDT), tabulation of theoretical data (TDT) before the rate constant can be fitted (RCF) and a rate constant with appropriate uncertainties recommended for use in combustion modelling.

Table 2 below show that approximately 37.5% of all tasks have been carried out when one analyses the set of 50 reactions of interest. The key tasks of PC, EDT, TBT, PES construction are ~50% complete.

Table 1: Legend for Table 2 and Table 3			
Key/Legend		Authors Abbreviations	
PC	Papers Collated into Database	MP	Dr. Matteo Pelucchi
EDT	Experiment Data Tabulated	UB	Dr. Ultan Burke
TDT	Theoretical Data Tabulated	LC	Dr. Liming Cai
PES	Potential Energy Surface Constructed	SJK	Dr. Stephen J. Klippenstein
SRT	Statistical Rate Theory Computed	PG	Prof. Peter Glarborg
RCF	Rate Constant Fitted	KPS	Dr. Kieran P. Somers
RDS	Reaction Data Sheet Written		
DSPR	Reaction Data Sheet Peer-Reviewed		
C	Completed		
IP	In Progress		
X	To be Completed		

Table 2: Task Completion Summary Statistics									
Status	PC	ET	TT	PES	RRKM/ME	RCF	RDS	PR	Total %
Completed	52%	48%	42%	54%	0%	4%	14%	0%	26.75%
In Progress	0%	0	0%	0%	36%	34%	0%	16%	10.75%
To be Completed	48%	52%	58%	46%	64%	62%	86%	84%	62.5%
Completed/In Progress	52%	48%	42%	54%	36%	38%	14%	16%	37.5

Table 3: Reaction Gantt Chart

# Electrons	Reaction	Lead	PC	EDT	TDT	PES	RRKM/ME	RCF	RDS	DSRP
R2	$\text{H}+\text{H}+\text{M} \rightleftharpoons \text{H}_2+\text{M}$	KPS/MP	C	X	X	C	X	X	X	X
R9	$\text{H}+\text{O}+\text{M} \rightleftharpoons \text{OH}+\text{M}$	KPS/MP	X	X	X	C	X	X	X	X
R10a	$\text{H}+\text{OH}+\text{M} \rightleftharpoons \text{H}_2\text{O}$	UB	X	X	X	C	X	X	X	X
R10b	$\text{H}_2+\text{O} \rightleftharpoons \text{OH}+\text{H}$	LC	C	C	X	C	X	IP	X	X
R11	$\text{H}_2+\text{OH} \rightleftharpoons \text{H}+\text{H}_2\text{O}$	MP	C	C	C	X	IP	IP	X	X
R15	$\text{HCO}+\text{M} \rightleftharpoons \text{H}+\text{CO}+\text{M}$	KPS/SJK	C	C	C	X	IP	IP	X	X
R16a	$\text{HCO}+\text{H} \rightleftharpoons \text{CH}_2\text{O}$	KPS	X	X	X	X	X	X	X	X
R16b	$\text{HCO}+\text{H} \rightleftharpoons \text{CO}+\text{H}_2$	MP	X	X	X	X	X	X	X	X
R16p	$\text{O}+\text{O}+\text{M} \rightleftharpoons \text{O}_2+\text{M}$	KPS/MP	X	X	X	X	X	X	X	X
R17a	$\text{H}+\text{O}_2+\text{M} \rightleftharpoons \text{HO}_2+\text{M}$	SJK	C	C	C	X	IP	X	X	X
R17b	$\text{H}+\text{O}_2 \rightleftharpoons \text{O}+\text{OH}$	UB	C	C	C	X	X	C	X	X
R18a	$\text{OH}+\text{OH}+\text{M} \rightleftharpoons \text{H}_2\text{O}_2+\text{M}$	UB	C	C	C	C	X	IP	X	X
R18b	$\text{OH}+\text{OH} \rightleftharpoons \text{O}+\text{H}_2\text{O}$	LC	C	C	C	C	X	C	X	IP
R18c	$\text{H}+\text{HO}_2 \rightleftharpoons \text{H}_2+\text{O}_2$	PG	C	C	C	C	IP	X	X	X
R18d	$\text{H}+\text{HO}_2 \rightleftharpoons \text{OH}+\text{OH}$	PG	C	C	C	C	IP	X	X	X
R18e	$\text{H}+\text{H}+\text{O}_2 \rightleftharpoons \text{H}_2+\text{O}_2$	KPS/MP	X	X	X	C	IP	X	X	X
R18f	$\text{H}+\text{H}+\text{O}_2 \rightleftharpoons \text{OH}+\text{OH}$	KPS/MP	X	X	X	C	X	X	X	X
R19a	$\text{H}_2\text{O}_2+\text{H} \rightleftharpoons \text{H}_2\text{O}+\text{OH}$	SJK	C	C	C	C	IP	IP	X	X
R19b	$\text{H}_2\text{O}_2+\text{H} \rightleftharpoons \text{HO}_2+\text{H}_2$	SJK	C	C	C	C	IP	IP	X	X
R22	$\text{CO}+\text{O}+\text{M} \rightleftharpoons \text{CO}_2+\text{M}$	PG	X	X	X	X	X	X	X	X
R23a	$\text{H}+\text{CO}_2+\text{M} \rightleftharpoons \text{HOCO}+\text{M}$	PG/SJK	C	C	C	C	X	IP	X	X
R23b	$\text{CO}+\text{OH}+\text{M} \rightleftharpoons \text{HOCO}+\text{M}$	PG/SJK	C	C	C	C	X	IP	X	X
R23c	$\text{CO}+\text{OH} \rightleftharpoons \text{CO}_2+\text{H}$	PG/SJK	C	C	C	C	X	X	X	X
R23d	$\text{HCO}+\text{O} \rightleftharpoons \text{CO}_2+\text{H}$	UB	X	X	X	C	X	X	X	X
R23e	$\text{HCO}+\text{O} \rightleftharpoons \text{CO}+\text{OH}$	UB	X	X	X	C	X	X	X	X
R24a	$\text{HCO}+\text{OH} \rightleftharpoons \text{CO}_2+\text{H}_2$	UB	X	X	X	X	X	X	X	X
R24b	$\text{HCO}+\text{OH} \rightleftharpoons \text{CO}+\text{H}_2\text{O}$	UB	X	X	X	X	X	X	X	X
R24p	$\text{O}_2+\text{O}+\text{M} \rightleftharpoons \text{O}_3+\text{M}$	MP	X	X	X	X	X	X	X	X
R25a	$\text{O}+\text{HO}_2 \rightleftharpoons \text{O}_2+\text{OH}$	LC	X	X	X	X	X	X	X	X
R25b	$\text{H}+\text{O}+\text{O}_2 \rightleftharpoons \text{OH}+\text{O}_2$	KPS/MP	X	X	X	X	IP	X	X	X
R26a	$\text{HO}_2+\text{OH} \rightleftharpoons \text{H}_2\text{O}+\text{O}_2$	KPS	C	C	X	X	X	X	X	X
R26b	$\text{H}_2\text{O}_2+\text{O} \rightleftharpoons \text{OH}+\text{HO}_2$	UB	X	X	X	X	X	X	X	X
R26c	$\text{H}+\text{OH}+\text{O}_2 \rightleftharpoons \text{H}_2\text{O}+\text{O}_2$	KPS/MP	X	X	X	X	IP	X	X	X
R27	$\text{H}_2\text{O}_2+\text{OH} \rightleftharpoons \text{HO}_2+\text{H}_2\text{O}$	UB	C	C	X	X	IP	IP	X	X
R30a	$\text{HCO}+\text{HCO} \rightleftharpoons \text{OCHCHO}$	UB	X	X	X	X	X	X	X	X
R30b	$\text{HCO}+\text{HCO} \rightleftharpoons \text{CO}+\text{CH}_2\text{O}$	UB	X	X	X	X	X	X	X	X
R30c	$\text{HCO}+\text{HCO} \rightleftharpoons \text{CO}+\text{CO}+\text{H}_2$	UB	X	X	X	X	X	X	X	X
R30p	$\text{CO}+\text{O}_2 \rightleftharpoons \text{CO}_2+\text{O}$	LC	C	X	X	X	X	X	X	X
R31a	$\text{OHC}(\text{O})\text{O}+\text{M} \rightleftharpoons \text{OHOCO}+\text{M}$	LC	X	X	X	C	X	X	X	X
R31b	$\text{CO}_2+\text{OH}+\text{M} \rightleftharpoons \text{OHC}(\text{O})\text{O}+\text{M}$	LC	X	X	X	C	X	X	X	X
R31c	$\text{CO}_2+\text{OH}+\text{M} \rightleftharpoons \text{OHOCO}$	LC	X	X	X	C	X	X	X	X
R31d	$\text{CO}+\text{HO}_2 \rightleftharpoons \text{OHC}(\text{O})\text{O}$	LC	C	C	C	C	IP	IP	C	IP
R31e	$\text{CO}+\text{HO}_2+\text{M} \rightleftharpoons \text{OHOCO}+\text{M}$	LC	C	C	C	C	IP	IP	C	IP

R31f	$\text{CO} + \text{HO}_2 \rightleftharpoons \text{CO}_2 + \text{OH}$	LC	C	C	C	C	IP	IP	C	IP
R31g	$\text{HCO} + \text{O}_2 + \text{M} \rightleftharpoons \text{OHC(O)O} + \text{M}$	UB	C	C	C	C	IP	IP	C	IP
R31h	$\text{HCO} + \text{O}_2 + \text{M} \rightleftharpoons \text{OHOCO} + \text{M}$	UB	C	C	C	C	IP	IP	C	IP
R31i	$\text{HCO} + \text{O}_2 \rightleftharpoons \text{CO}_2 + \text{OH}$	UB	C	C	C	C	IP	IP	C	IP
R31j	$\text{HCO} + \text{O}_2 \rightleftharpoons \text{CO} + \text{HO}_2$	UB	C	C	C	C	IP	IP	C	IP
R32	$\text{HCO} + \text{HO}_2 \rightleftharpoons \text{CO} + \text{H}_2 + \text{O}_2$	UB	X	X	X	X	X	X	X	X
R34	$\text{HO}_2 + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	MP	C	C	C	X	X	IP	X	X

Table 4: Overview of the papers collected for each potential energy surface/reaction and the method use to derive rate constants therein.

# Electrons	Reaction	Experimental	Theoretical	Detailed Chemical Kinetic Modelling	Total
R2	$\text{H} + \text{H} + \text{M} = \text{H}_2 + \text{M}$	36	4	1	41
R9	$\text{H} + \text{O} + \text{M} = \text{OH} + \text{M}$	0	0	0	0
R10	H_2O	35	46	0	81
R11	$\text{H}_2 + \text{OH} = \text{H}_2\text{O} + \text{H}$	14	29	0	43
R15	$\text{HCO} + \text{M} = \text{CO} + \text{H} + \text{M}$	18	12	0	30
R16	H_2CO	0	0	0	0
R16p	$\text{O} + \text{O} + \text{M} = \text{O}_2 + \text{M}$	1	0	0	1
R17	HO_2	82	22	3	107
R18	H_2O_2	0	0	0	0
R19	H_3O_2	8	6	0	14
R22	$\text{CO} + \text{O} + \text{M} = \text{CO}_2 + \text{M}$	0	2	0	2
R23	HCO_2	24	29	0	53
R24	$\text{O}_2 + \text{O} + \text{M} = \text{O}_3 + \text{M}$	0	3	0	3
R24p	H_2CO_2	0	0	0	0
R25	HO_3	10	6	0	16
R26	H_2O_3	0	0	0	0
R27	$\text{H}_2\text{O}_2 + \text{OH} = \text{H}_2\text{O} + \text{HO}_2$	5	0	0	5
R30	$\text{H}_2\text{C}_2\text{O}_2$	3	1	0	4
R30p	$\text{CO} + \text{O}_2 = \text{O} + \text{CO}_2$	1	2	0	3
R31	HCO_3	16	4	0	20
R32	$\text{HCO} + \text{HO}_2 = \text{CO} + \text{H}_2 + \text{O}_2$	0	0	0	0
R34	$\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$	40	4	0	44
	Sum	293	170	4	467

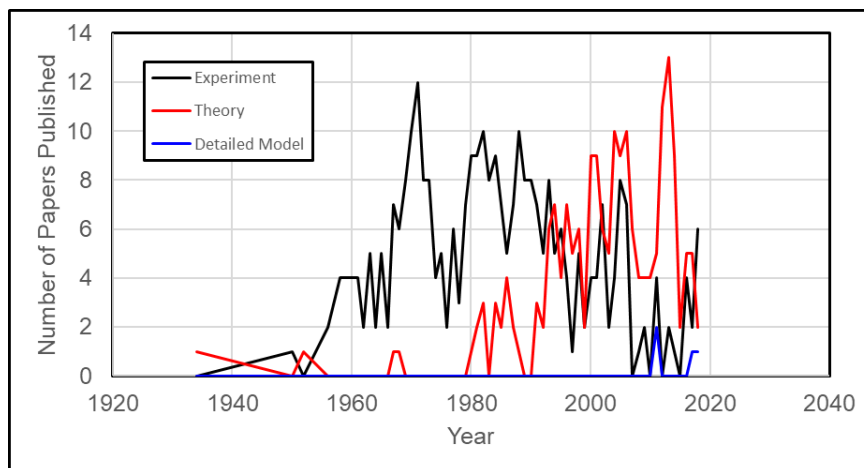


Figure 2: Number of papers published each year with recommended rate constants for reactions in Table 4

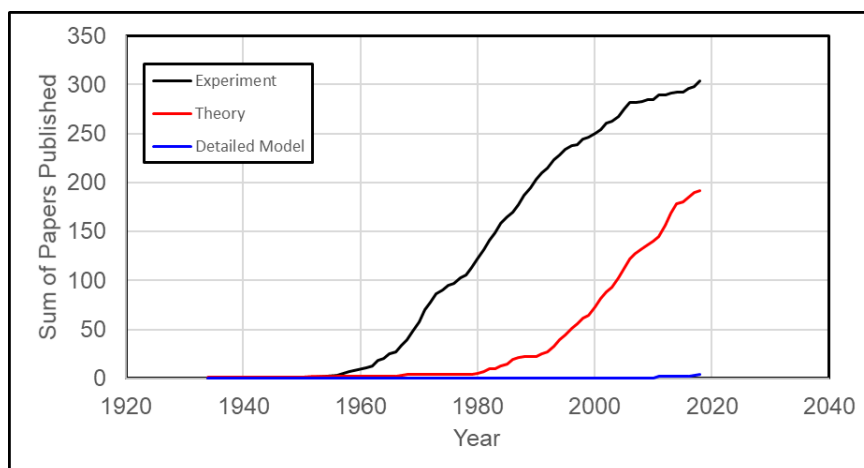


Figure 3: Cumulative number of papers published by a given year which recommend rate constants for reactions in Table 4.

Data Fitting for Pressure-Dependent Reactions

For the reaction $\text{HCO} + \text{M} = \text{H} + \text{CO} + \text{M}$, approximately 400 unique rate constant measurements have been tabulated based on results from ~17 independent studies, where gas density/pressure, temperature, and bath gas are all variables which influence the reported rate constant, Figure 4. As part of this STSM we have commenced development of a useful procedure to model these data and provide rate constants fits that are both physically meaningful, and useful for combustion modelling.

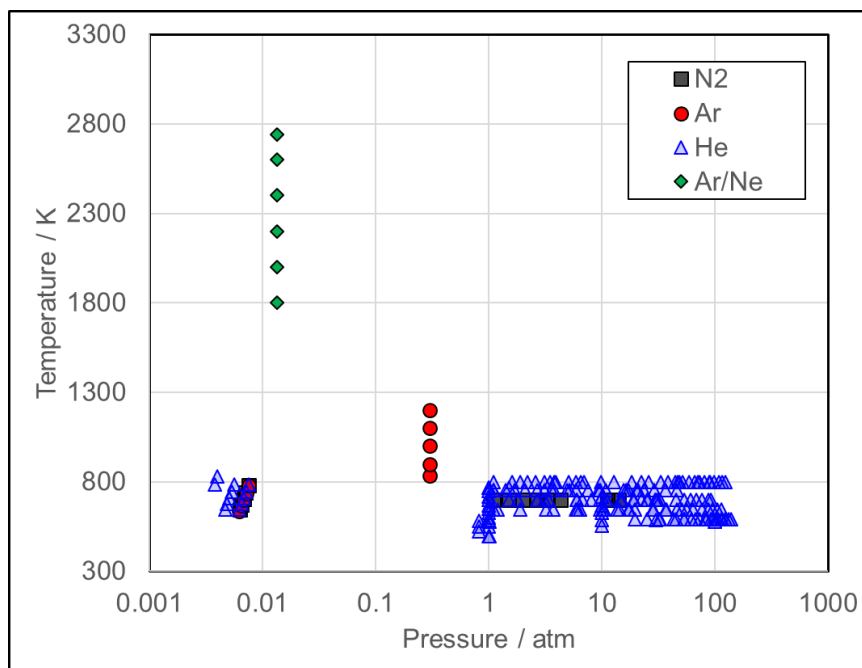


Figure 4: Temperatures and pressures at which the rate constant for $\text{HCO} + \text{M} = \text{H} + \text{CO} + \text{M}$ has been experimentally measured in various bath gases

For each individual experimental measurement, an RRKM/ME input file for use with the MESS solver is constructed based on *ab initio* quantum chemistry results using highly accurate ANLO calculations. The specific temperature, pressure, and bath gas of the experiment is accounted for and each experiment receives an individual treatment. The RRKM/ME master equation results are then compared directly with experimental results.

In order to arrive at optimum fits, some form, the average energy transferred in a collision $\Delta E_d(T)$ must be described as a function of temperature. A common functional form is $\Delta E_d(T) = \Delta E_{300}(T/300)^n$ where ΔE_{300} is the energy transferred in a collision at 300 K, T , is the temperature, and n is an exponent that describes the temperature dependence of the energy transfer parameter. As part of this STSM, this author develop a computational tool to run large scale RRKM/ME calculations, where ΔE_{300} and n are used as variable parameters in the rate constant fitting process. Figure 5-7 below show the result of running approximately 60,000 RRKM/ME calculation in order to find the bath-gas specific values of ΔE_{300} and n which give optimal agreement with the available experimental data, as measured by the maximum absolute deviation of the theoretical results from the experimental predictions.

Figure X below shows the results of this work, where heatmaps of the maximum average deviation in the RRKM/ME results are presented as a function of ΔE_{300} and the fitting exponent n . What is clear is that there are potentially multiple minima as part of this fitting procedure, and there may not be unique values of ΔE_{300} and the fitting exponent n which give best agreement with the data.

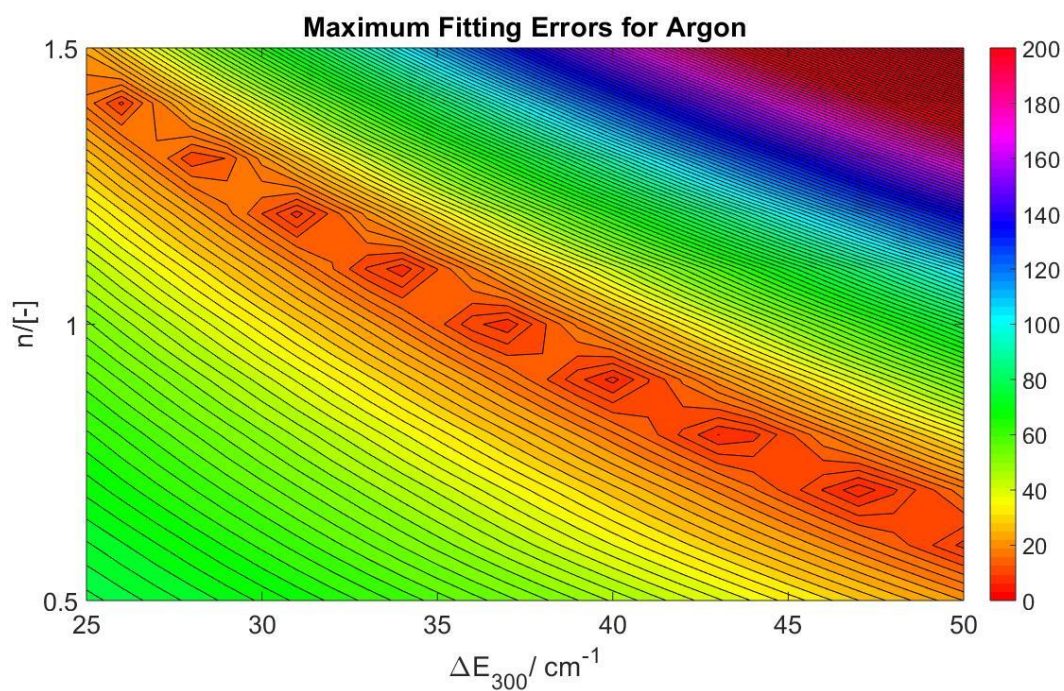


Figure 5: Fitting errors (Maximum Absolute Deviation) of the RRKM/ME calculations, from the experimental data for Ar bath gas.

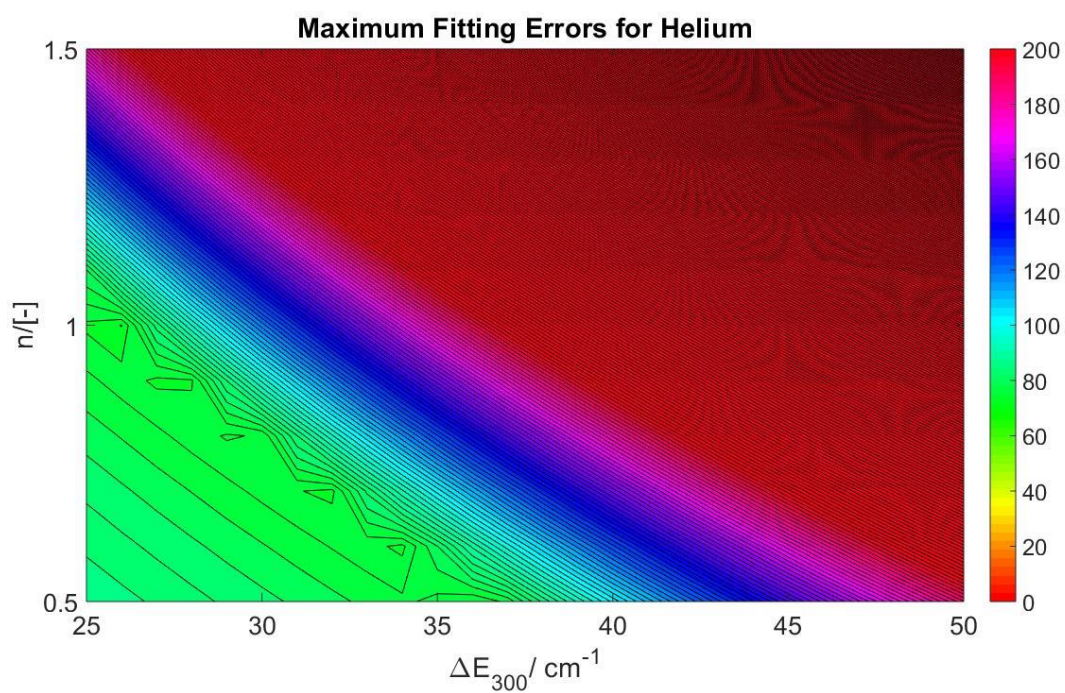


Figure 6: Fitting errors (Maximum Absolute Deviation) of the RRKM/ME calculations, from the experimental data for He bath gas.

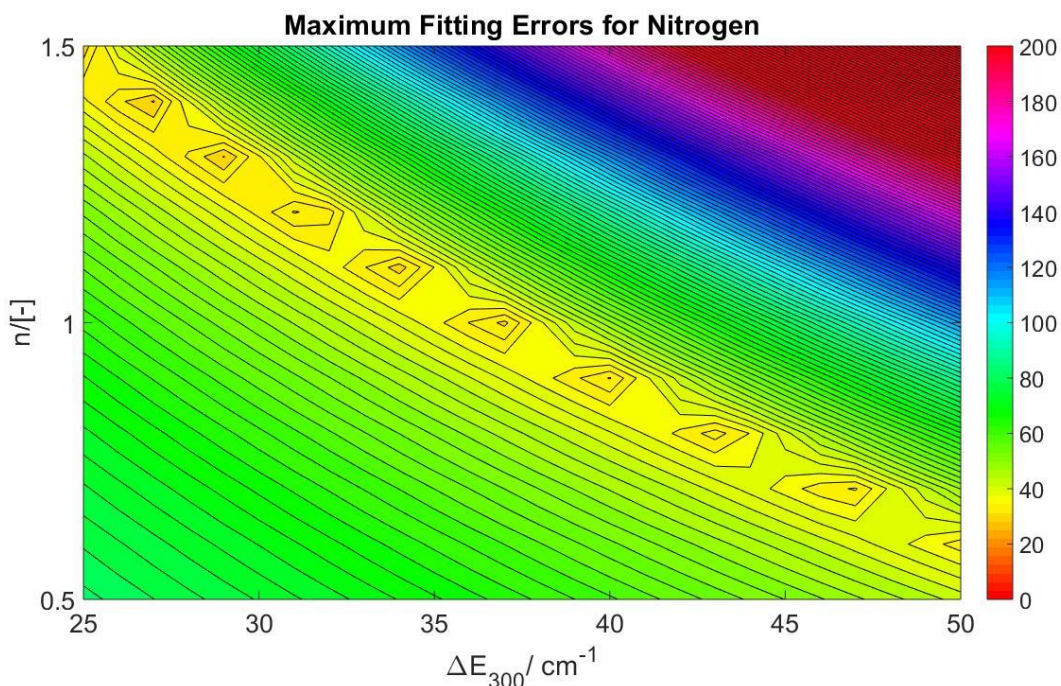
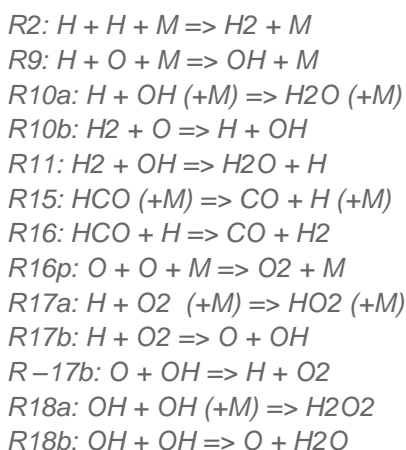


Figure 7: Fitting errors (Maximum Absolute Deviation) of the RRKM/ME calculations, from the experimental data for N₂ bath gas.

The results presented above are also bath-gas specific, with different values of ΔE_{300} and the fitting exponent n found to best reproduce the data in different bath gases. For a given bath gas, the lack of a unique values of ΔE_{300} and the fitting exponent n complicate the procedure of producing rate constants for use in kinetic models, as these parameters will become increasingly sensitive under high temperature and low-pressure conditions which are beyond the temperature pressure range of the current kinetic data, but which are typical of combustion conditions (e.g. shock tubes, flames, engines). Future work will aim to refine this fitting procedure to incorporate other aspects of the potential energy surface, including the reaction barrier, and the imaginary frequency of the reaction path.

FUTURE COLLABORATIONS (if applicable)

The same approach will be applied to all of the remaining reactions listed below:



R18c: $H + HO_2 \Rightarrow H_2 + O_2$
R18d: $H + HO_2 \Rightarrow OH + OH$
R18e: $H + H + O_2 \Rightarrow H_2 + O_2$
R18f: $H + H + O_2 \Rightarrow OH + OH$
R22: $CO + O (+M) \Rightarrow CO_2 (+M)$
R23a: $CO_2 + H \Rightarrow HOCO$
R23b: $CO + OH \Rightarrow HOCO$
R23c: $CO + OH \Rightarrow CO_2 + H$
R23d: $HCO + O \Rightarrow CO_2 + H$
R23e: $HCO + O \Rightarrow CO + OH$
R24: $O_2 + O (+M) \Rightarrow O_3 (+M)$
R24pa: $HCO + OH \Rightarrow CO_2 + H_2$
R24pb: $HCO + OH \Rightarrow CO + H_2O$
R25a: $O + HO_2 \Rightarrow O_2 + OH$
R25b: $H + O + O_2 \Rightarrow OH + O_2$
R26a: $OH + HO_2 \Rightarrow H_2O + O_2$
R26b: $H_2O_2 + O \Rightarrow H_2O + O_2$
R26c: $H + OH + O_2 \Rightarrow H_2O + O_2$
R27: $H_2O_2 + OH \Rightarrow H_2O + HO_2$
R30a: $HCO + HCO \Rightarrow OCHCHO$
R30b: $HCO + HCO \Rightarrow CO + H_2CO$
R30c: $HCO + HCO \Rightarrow CO + CO + H_2$
R30p: $CO + O_2 \Rightarrow CO_2 + O$
R31a: $OHC(O)O (+M) \Rightarrow OHOCO (+M)$
R31b: $CO_2 + OH (+M) \Rightarrow OHC(O)O (+M)$
R31c: $CO_2 + OH (+M) \Rightarrow OHOCO (+M)$
R31d: $CO + HO_2 \Rightarrow OHC(O)O (+M)$
R31e: $CO + HO_2 (+M) \Rightarrow OHOCO (+M)$
R31f: $CO + HO_2 \Rightarrow CO_2 + OH$
R31g: $HCO + O_2 (+M) \Rightarrow OHC(O)O (+M)$
R31h: $HCO + O_2 (+M) \Rightarrow OHOCO (+M)$
R31i: $HCO + O_2 \Rightarrow CO_2 + OH$
R32: $HCO + HO_2 \Rightarrow CO + O_2 + H_2$
R34: $HO_2 + HO_2 \Rightarrow H_2O_2 + O_2$

The working group has decided to meet on bi-weekly telecons, in order to continue progress on the review of the above listed reactions.

A publication to be submitted to Progress in Energy and Combustion Science or, alternatively, to the Journal of Physical and Chemical Reference Data is expected by March 2019.

The progresses of this activity will be presented at the final SMARTCATs meeting and 1st International Conference on Smart Energy Carrier to be held in Naples on the 21st-23rd of January 2019.

As part of this author's future work, a scientific exchange to Dr. Stephen Klippenstein at Argonne National Laboratory is planned in order to continue developing the methods described herein. That trip is due to take place in Spring 2019.