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Report on the SmartCats Training School Analysis of Combustion Mechanisms Budapest, 4-7 July, 2016

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2nd SmartCats General Meeting
Lisbon, Portugal, 14-16 November, 2016

Topic of the school



Official title of the school:

COST CM1404 Training School on the
analysis, uncertainty quantification, validation,
optimization and reduction of detailed combustion
mechanisms for practical use of smart energy carriers

Short title of the school:

COST Training School on the
Analysis of Combustion Mechanisms

http://garfield.chem.elte.hu/COST_Training_School_2016/



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Venue



The lectures and practices were in the building of the Institute of Chemistry, Eötvös Loránd University (ELTE)

Dorm accommodation was offered in the **Martos Hostel** of the Budapest University of Technology and Economics

Networking event (school banquet) in the **Trófea Grill Restaurant** with unlimited food and drink consumption („all you can eat”)



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Hosts of the Training School



Most of the costs were covered by the SmartCats COST Action in the form of „Local Organizer Support”.



Hungarian Section of The Combustion Institute paid the bills and also provided in kind contribution (cost of accounting, poster boards).



Eötvös Loránd University (ELTE) provided the free usage of a lecture theatre and a large room. Also, technical equipment was provided free of charge.



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School setup



Lectures in the mornings from 8:30 to 13:10

The .pdf version of the lecture slides were downloadable from the web site of the school before the lecture in most cases.

Hands-on computer practices in the afternoons from 14:00 to 16:30

The computer codes were available well before the school on the web site. Everyone brought her/his own laptop.

Local support was provided for the installation.

The picture on the laptop of the trainer was presented by a beamer.

Posters of the trainees

The posters were on display during the whole week in the same room where the refreshments were served.



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Topics of the lectures



Reaction kinetics basics for combustion simulations

Pathway analysis

Local sensitivity analysis

Uncertainty of data and parameters

Validation and optimization of detailed combustion mechanisms

Chemical kinetics data

Global uncertainty analysis

Timescale analysis

Reduction of reaction mechanisms

Uncertainty of ab initio rate coefficient calculations

Uncertainty of spectroscopic data

Uncertainty of computed thermodynamic data



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Trainers



Lecturers

Tamás Turányi (ELTE, Budapest)
Alison S. Tomlin (Leeds University, Leeds)
Dimitris Goussis (NTUA, Athens)
György Lendvay (HAS RCNS, Budapest)
Tibor Nagy (HAS RCNS, Budapest)
István Gy. Zsély (ELTE, Budapest)
Attila G. Császár (ELTE, Budapest)



Hand-on computer practices were performed by

Tibor Nagy (HAS RCNS, Budapest)
Carsten Olm (ELTE, Budapest)
Éva Valkó (ELTE, Budapest)
Tamás Varga (ELTE, Budapest)



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Trainees



61 trainees from 19 countries

27 received travel grant from the
SmartCats COST Action

The participants were mainly,
but not exclusively,
PhD students and
Early-Career Investigators
involved in the COST Action.

There was at least one participant present
from each research group in Europe
dealing with combustion modelling
using detailed mechanisms.

Distribution of the countries:

Austria	1
Belgium	4
China	4
Cyprus	1
Denmark	1
Germany	9
Greece	2
Hungary	19
Iran	1
Ireland	1
Italy	4
Lithuania	1
Mexico	1
Poland	4
Serbia	2
Spain	1
Sweden	1
Turkey	1
UK	3



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Feedback



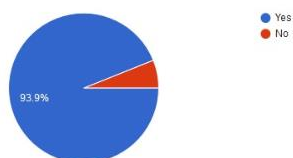
A feedback questionnaire was available for the participants from 10 July to 10 August.

33 participants answered

1. Which was the topic you primarily interested in prior to attending the School?

- mechanism reduction 16
- uncertainty quantification and uncertainty analysis 11
- mechanism development, validation and optimization 8
- general reaction kinetics and applications of combustion mechanisms 6

2. Did you get more knowledge in this topic?

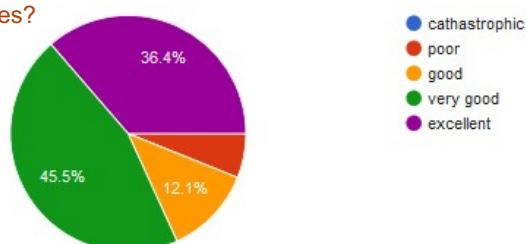


Feedback 2



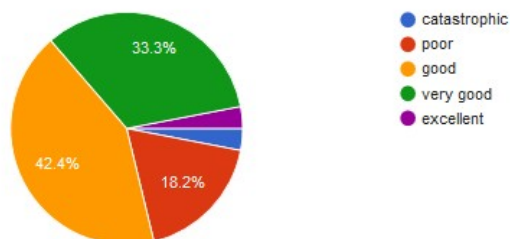
What was the general level of lectures?

36% excellent
46% very good
12% good



What was the general level of hands-on-practices?

5% excellent
33% very good
42% good

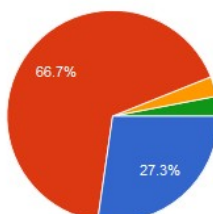


Feedback 3



Was it a good occasion for networking?

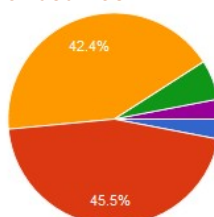
67% new connections
27% good for networking



- It was very good for networking, I established connections with several interesting people.
- It was good for networking, I made connections with some people I did not know previously.
- No new social connections were made.
- I even lost my previous friends.

The length of the 4-day Training School as compared to the amount of information provided was

46% slightly short
42% just appropriate



- much too short
- slightly short
- just appropriate
- slightly long
- much too long



Feedback 4



General comments:

A new school with future developments in combustion should be organized in two years time again

All in all, a very good training school.

Unfortunately the weather was very hot, so it was hard to concentrate on the lectures and practises.

In overall I really enjoyed the Training School and I believe I benefited tremendously from this experience. I am looking forward to start applying the obtained knowledge to my research. Thank you very much for this great experience.

A lecture on adaptive chemistry reduction would have been interesting

I would like to take part to the next Training school again. Budapest was a very good choice.

Maybe it was not for everybody interested in combustion kinetics but more for people working on kinetic mechanisms. There wasn't much for someone performing experiments in combustion.

No comments

Great Training School!

The full evaluation of the feedbacks is available on the web site of the Training School.





Thank you for your attention!

