BUILD-IT2023 Workshop

Talk 38

SOME CHALLENGES AND METHODS FOR DIGITAL DEVELOPMENT OF NEW GENERATION FUELS

FRANCESCO SAVERIO MARRA

CNR-STEMS, NAPOLI, ITALY

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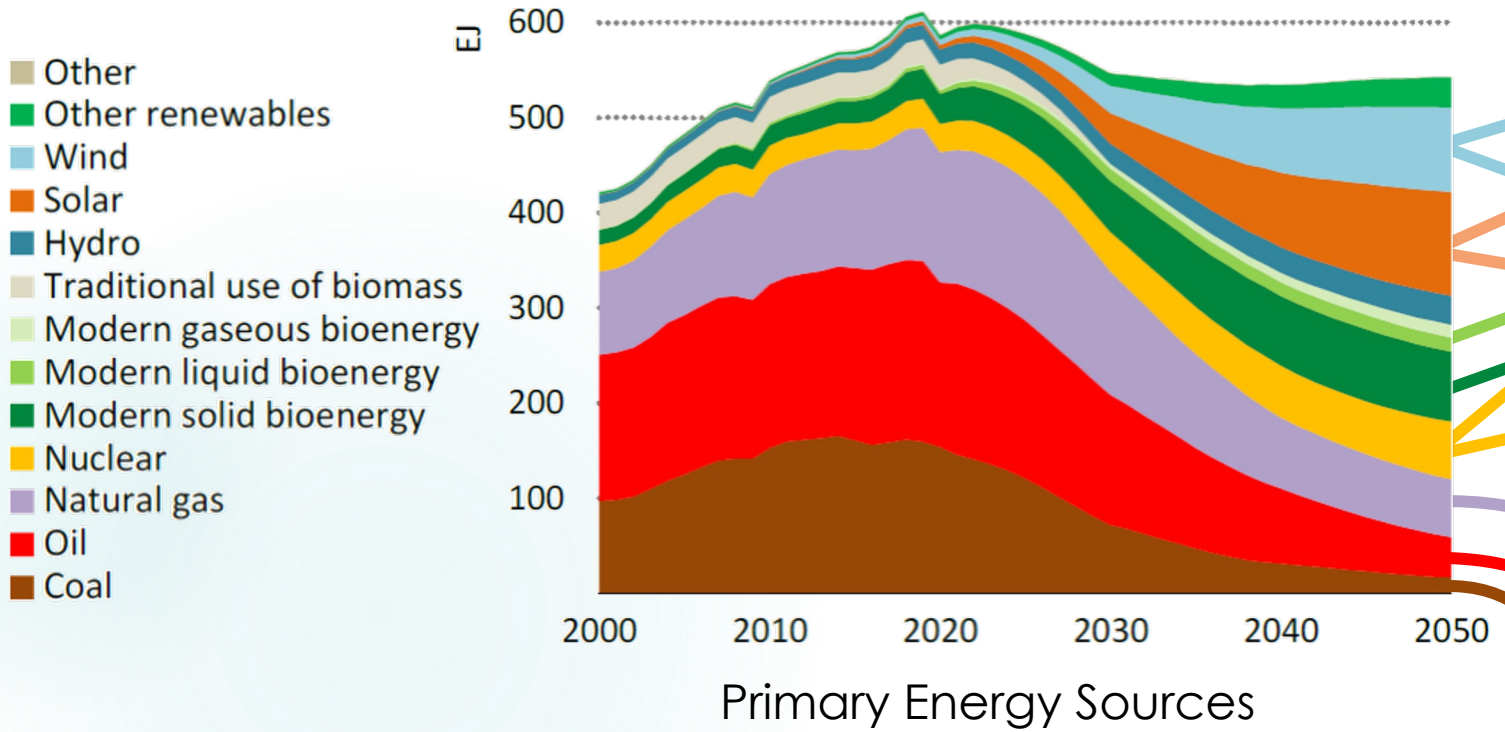
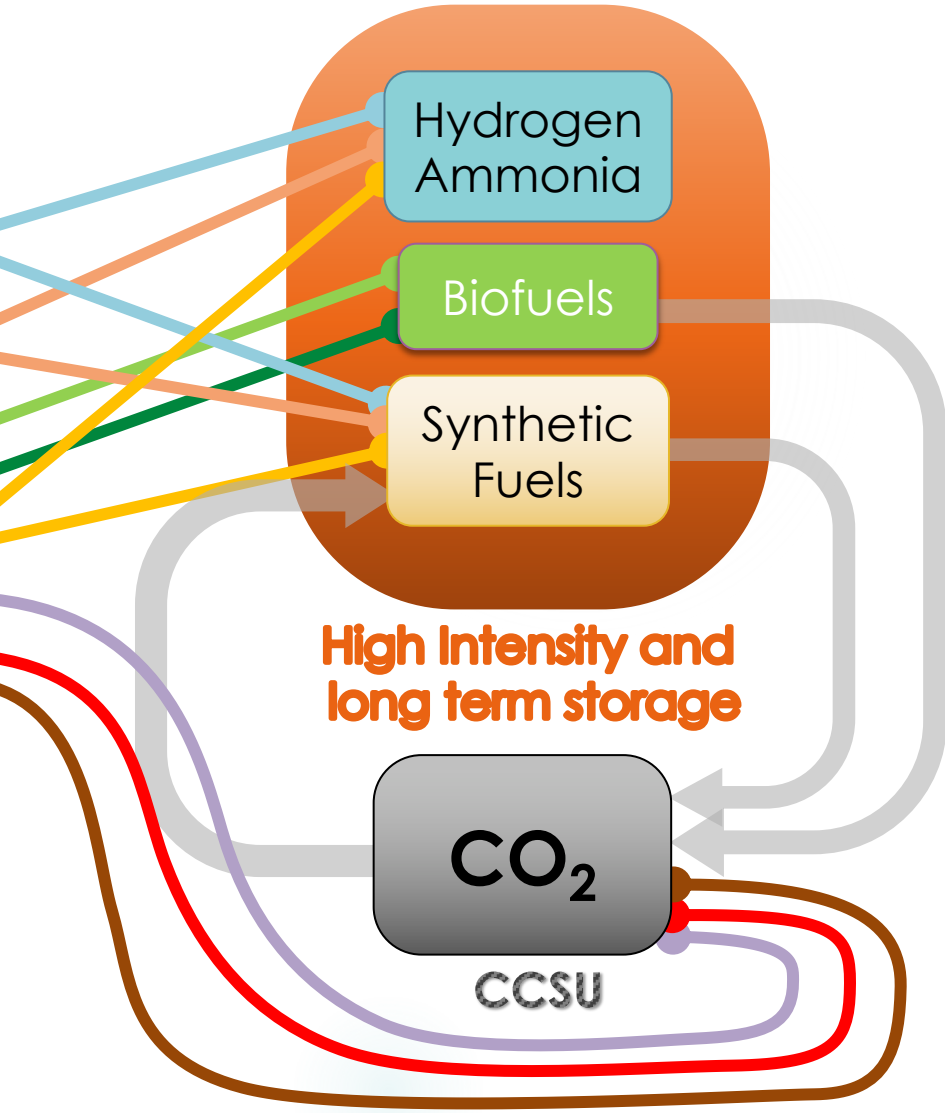
New fuels in the energy transition

Wide variety of new fuels and combustion processes



Primary Energy Sources

Net Zero Emissions by 2050 Scenario (NZE)
IEA 2023



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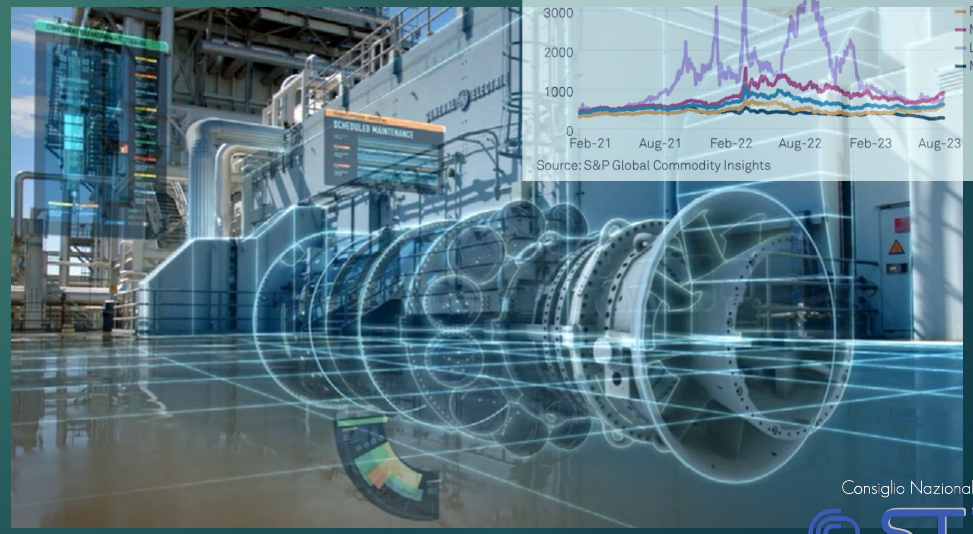
Fuels and Digital Twins

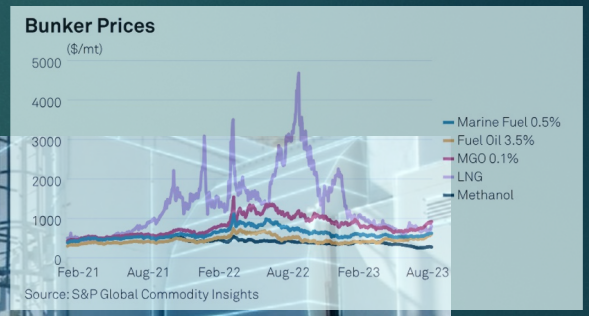
Building digital twins of the entire processes could be of great help to assess new fuels production and their performances and emissions when used in new combustors/conditions and in the training of operators (plants design and management, failures drivers and maintenance schedules, safety issues, economics, etc.).

Current applications are mainly limited to:

- ✓ Plants management
  (improve efficiency, avoid critical conditions, …)
- ✓ Maintenance schedules
  (predict components failure, detect deteriorated functioning, …)
- ✓ Economics
  (Predict supply requirements and market of sources, balance physical emissions with emissions trading system, …)

Mostly based on Data-Driven approaches





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Fuels and Digital Twins

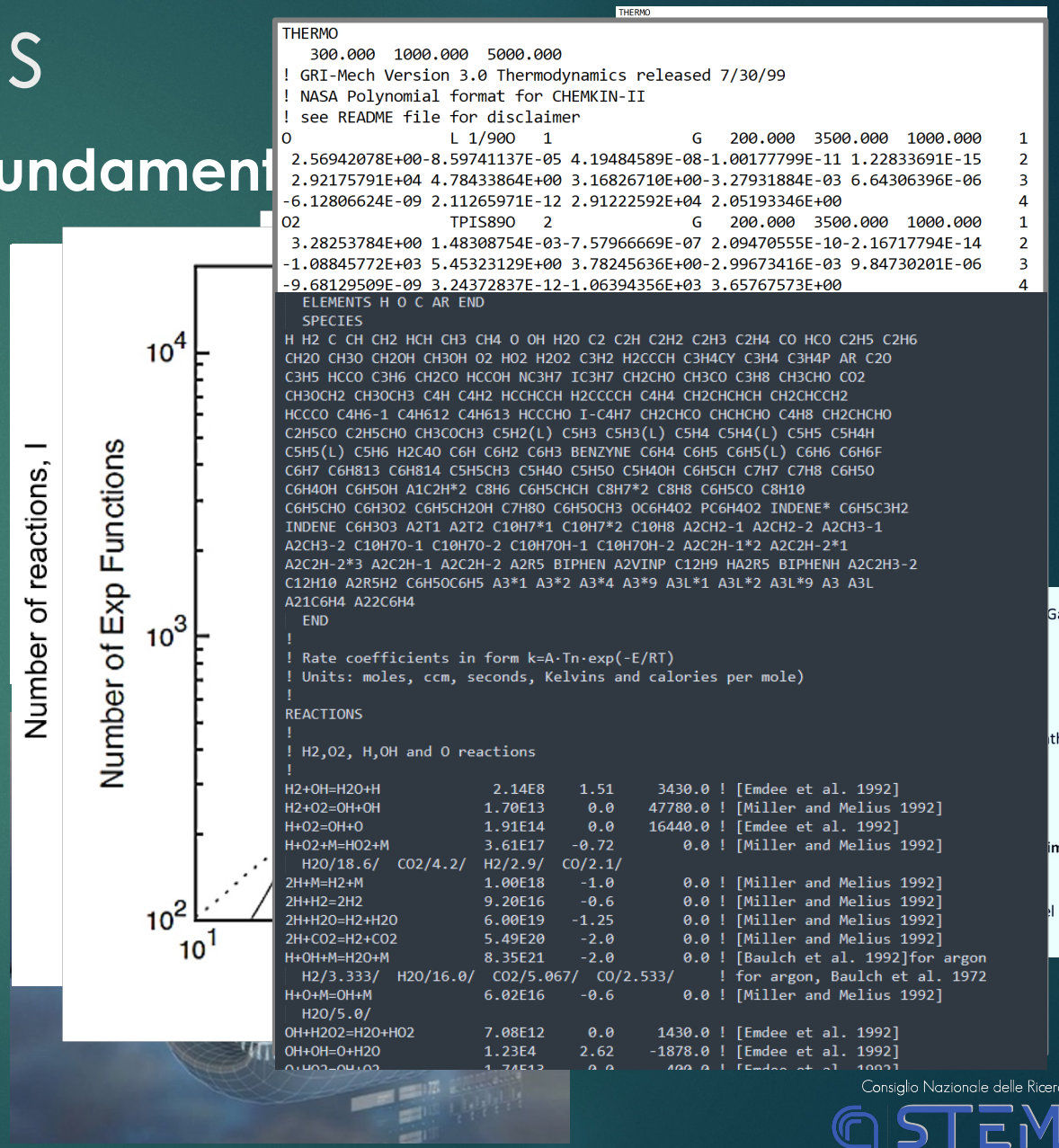
Digital Twins almost missing in more fundament

Intrinsic properties

- Fuel and flammable mixture composition (surrogate fuel composition, physical properties, thermodynamic properties, chemical properties…)

Interaction properties

- Design of fuel manufacturing processes (process design, reactor prototype and scale-up, process efficiency, resilience, use of primary sources, emissions predictions, …)
- Development of proper combustors (geometry, materials resistance, fluidynamic regime, …)

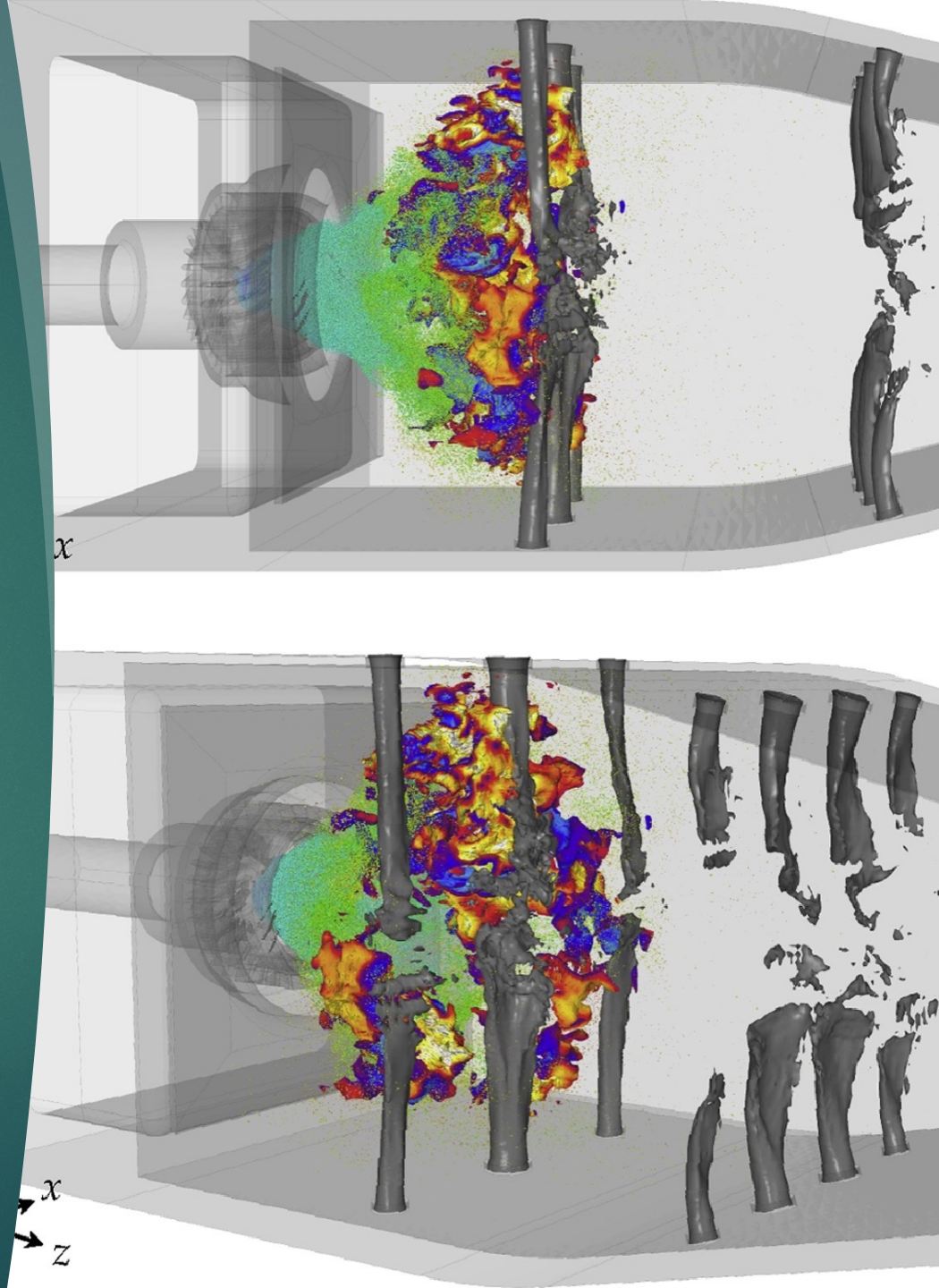


Main challenges

Simulations driven development of Digital Twins

Mathematical modelling of processes involving new generation fuels, **to be predictive**, requires the introduction of a huge number of variables and parameters, posing further issues:

- *Error estimation*
- *Model reduction*
- *Results interpretation*



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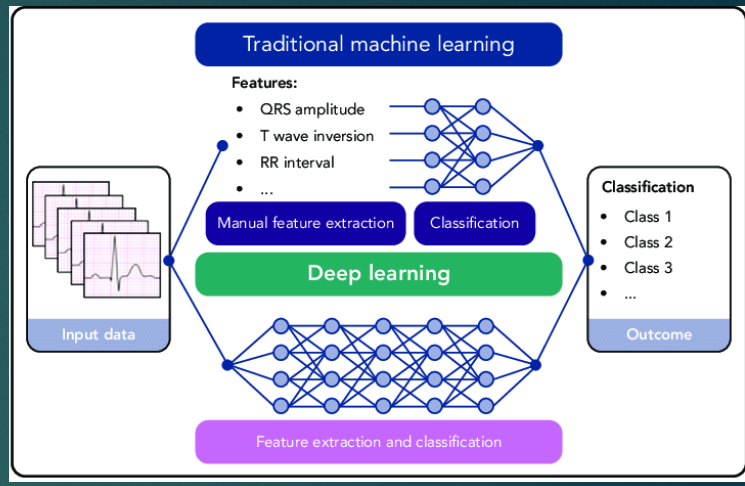
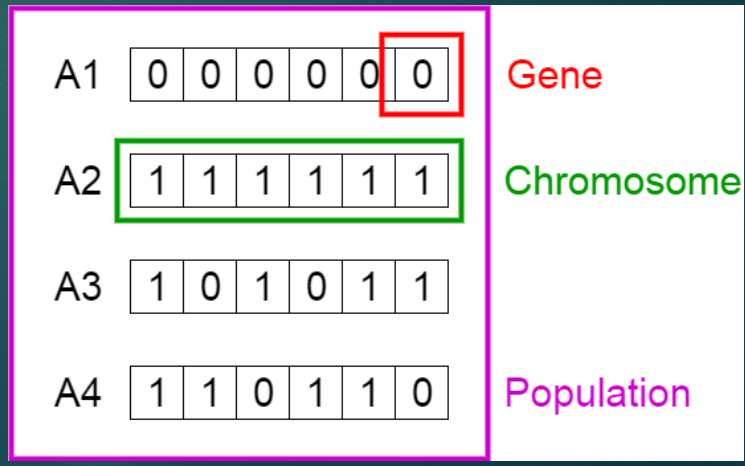
Current Approaches

- Machine Learning to reduce the computational effort:
  - *effective in substituting data retrieval techniques (In Situ Adaptive Tabulation)*
  - *employable to face the high stiffness of the equations deriving from the adoption of detailed chemical mechanisms*
  - *limited capabilities to cope with the large differences in the solutions for small variation of the parameters in specific points*
  - *limited capabilities in the interpretation of the result (identify the driving phenomenon)*



- Genetics algorithms
  - effective in determining the many parameters of an extremely simplified chemical mechanism (Virtual Chemistry)

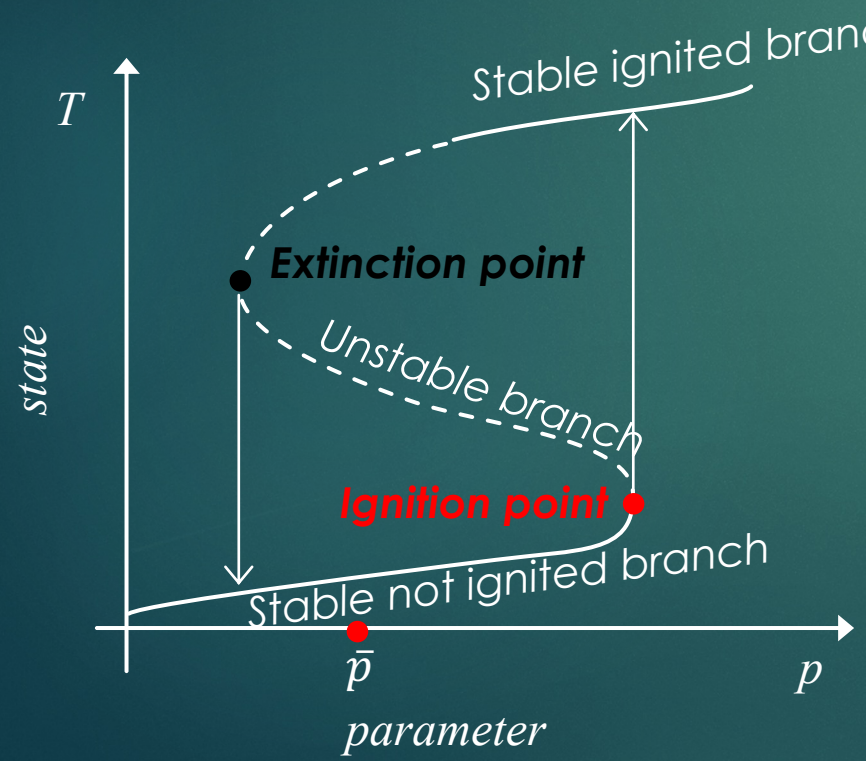


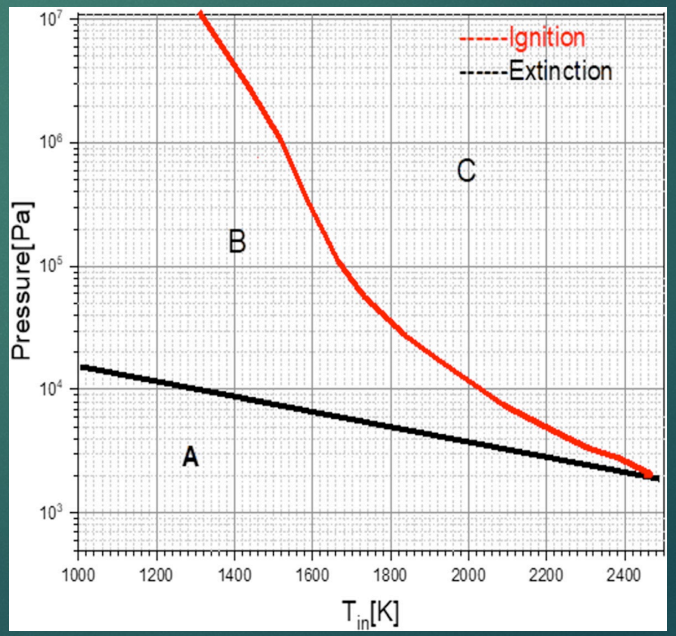
New directions of development

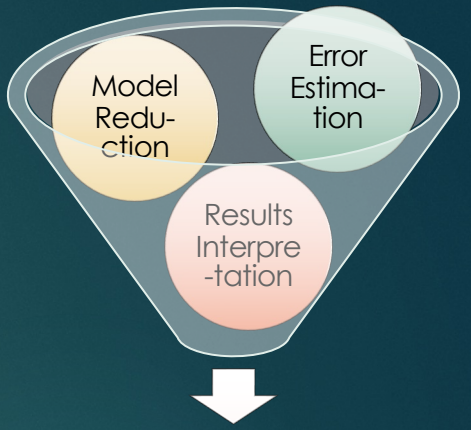
Continuation maps

Obtain knowledge on the system

Community analysis







Acampora, L., Marra, F.S., *Computers and Chemical Engineering*, **82** (2015).

Multi-parameter maps

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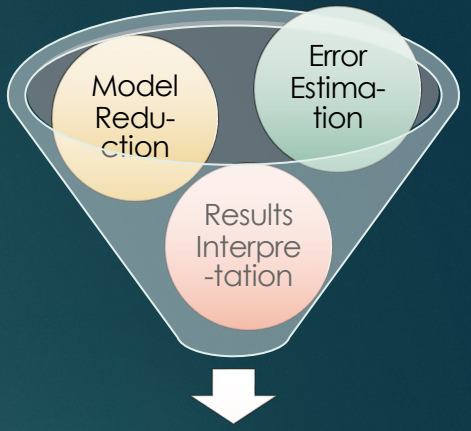
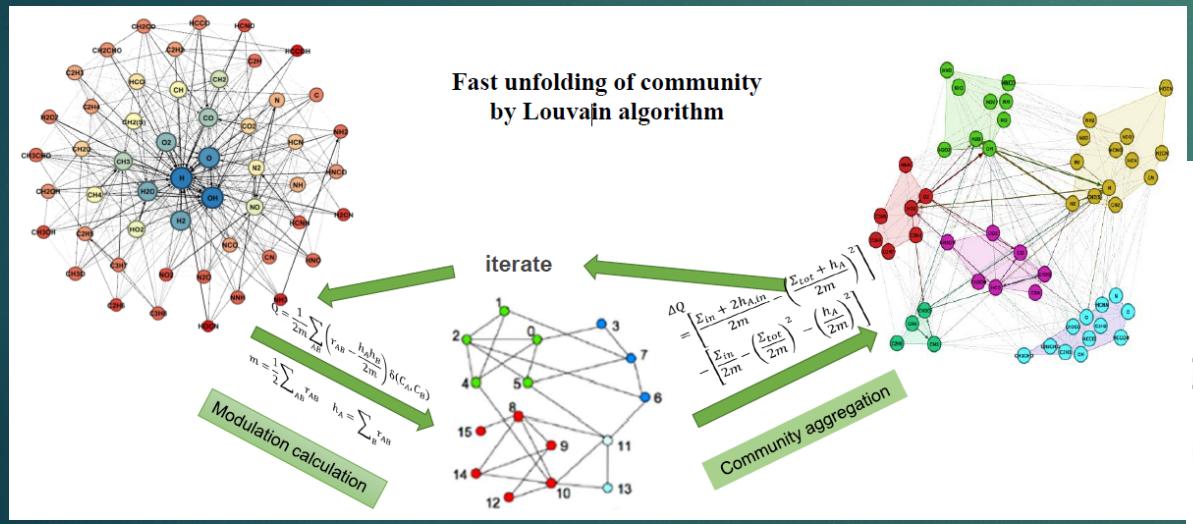
New directions of development



Continuation maps

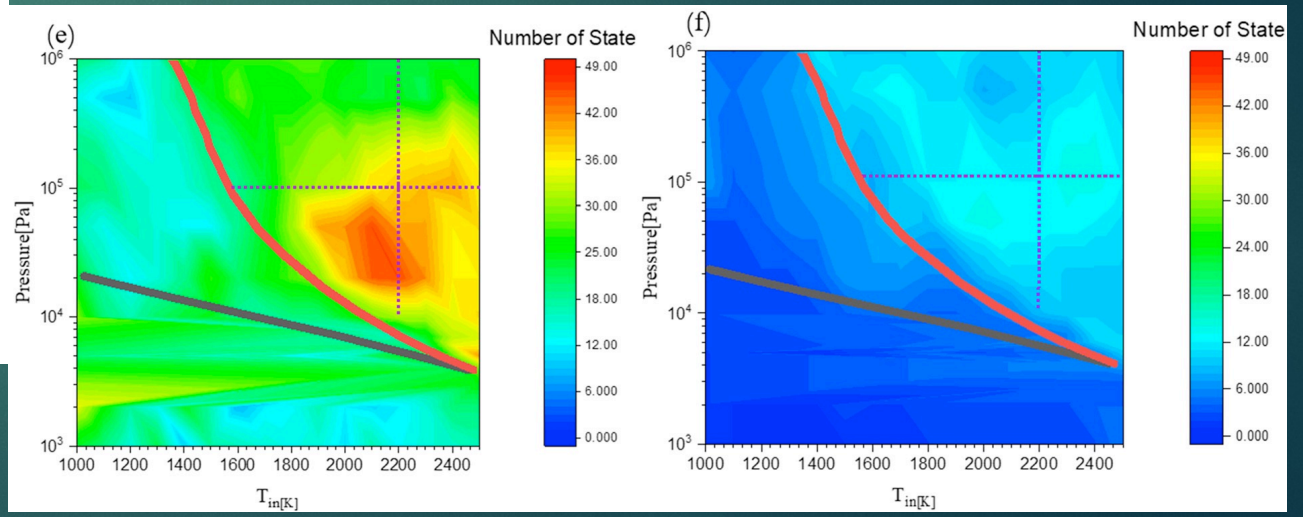
Obtain knowledge on the system

Community analysis



Communities' detection (CH_4 combustion)

Coarse grained states (CH_4 combustion)



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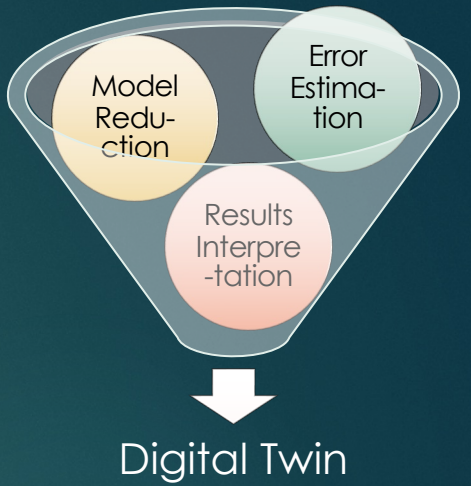
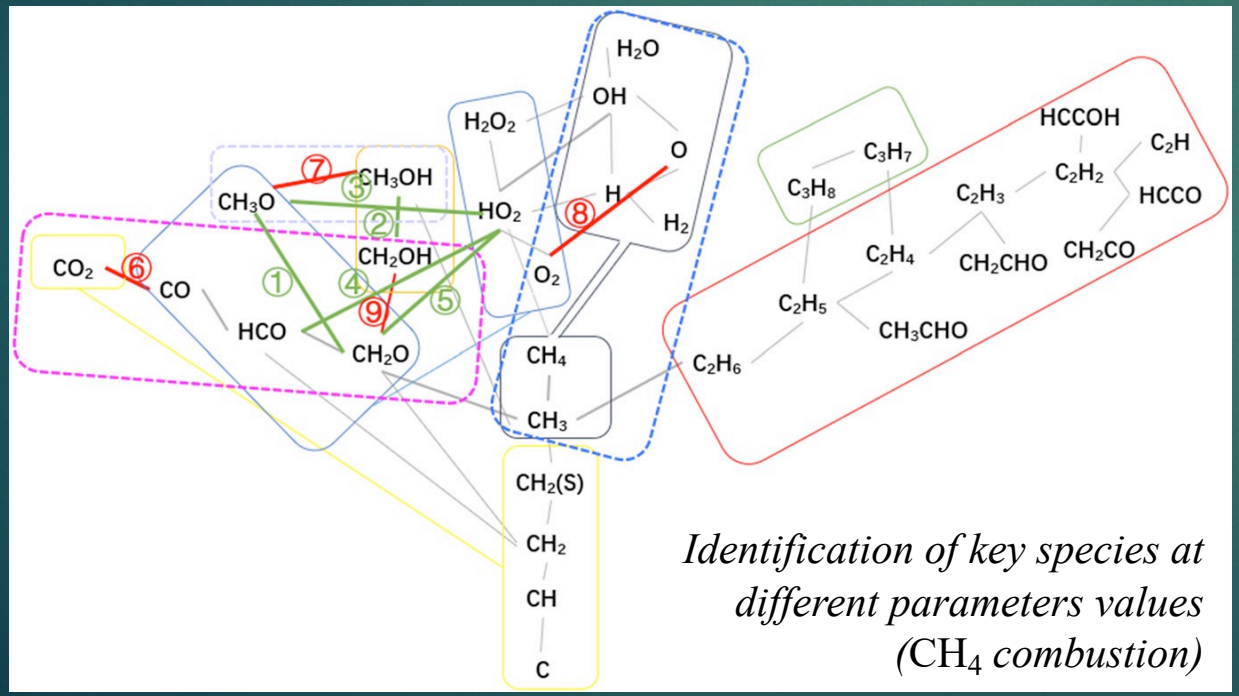


Continuation maps

Obtain knowledge on the system

Community analysis

Du, P., Li, M., Liang, S., Ji, L., Acampora, L., Marra, F.S., *Reaction Chemistry & Engineering*, 10.1039.D2RE00579D, (2023).



Identification of key species at different parameters values (CH_4 combustion)

Note that, due to the strongly non-linear character of chemical kinetics, key species NOT NECESSARILY are the most important from a quantitative point of view.

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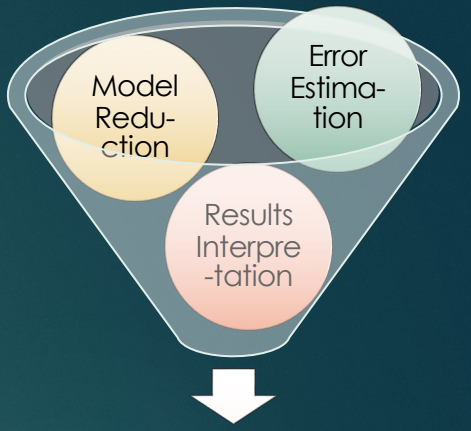
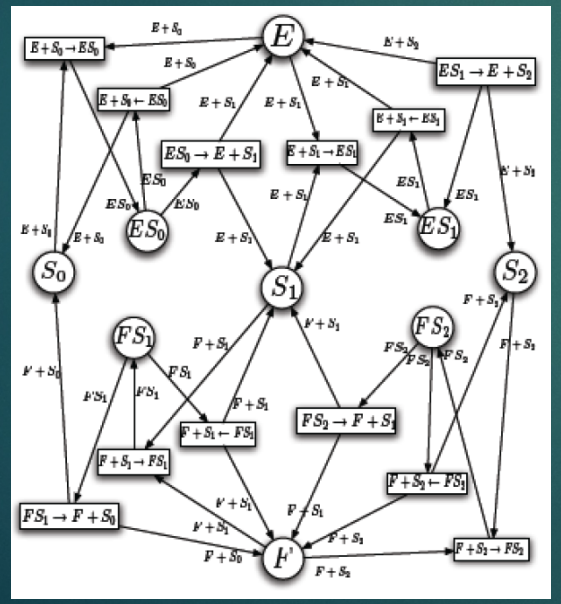
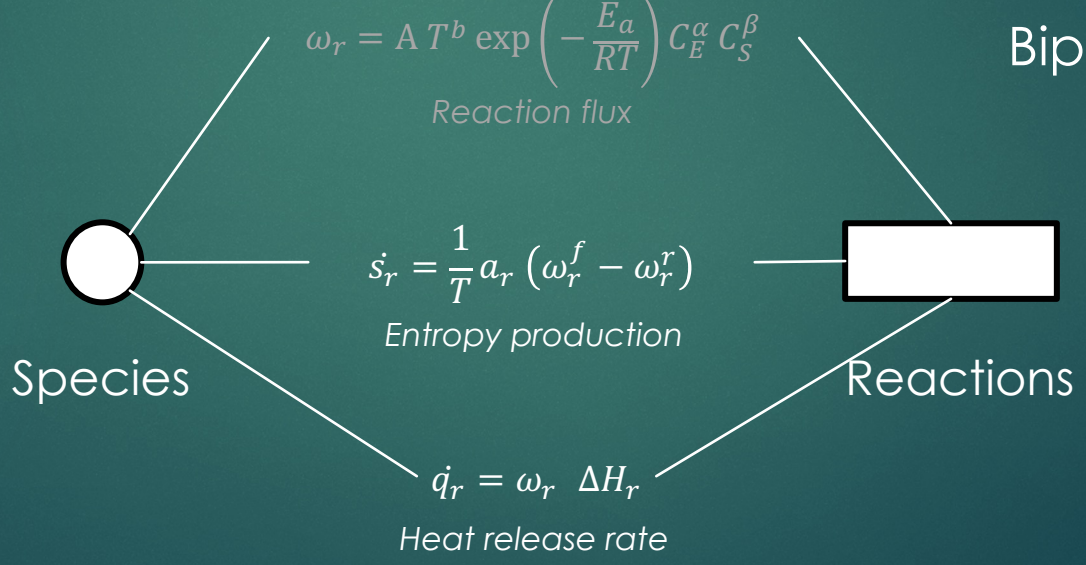


Obtain knowledge on the system

Model reduction

Chemical Mechanisms as networks





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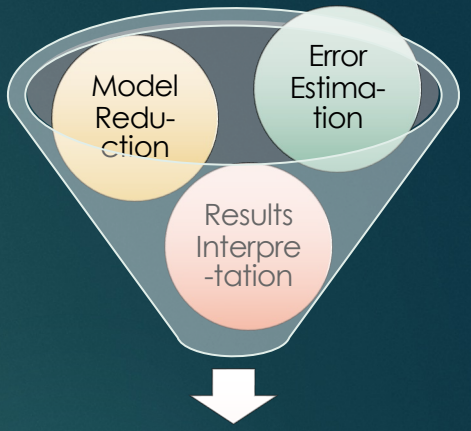
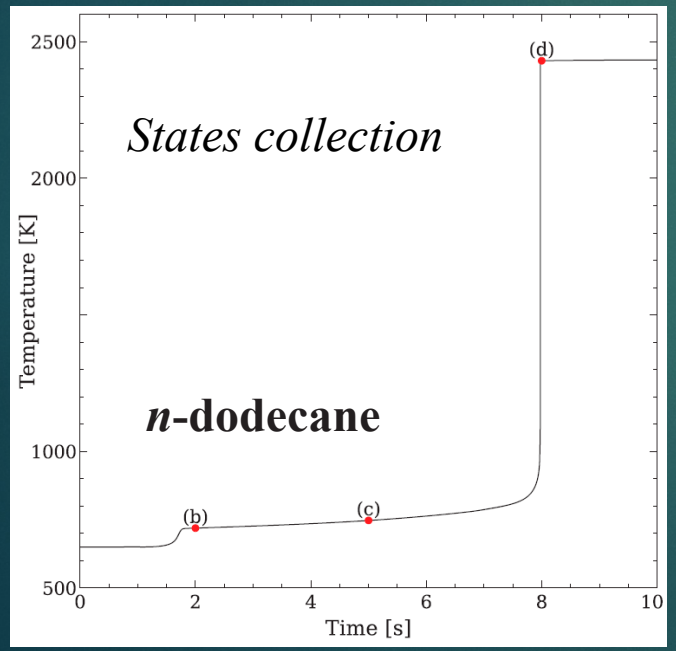


Obtain knowledge on the system

Model reduction

Acampora, L., Kooshkbaghi, M. Frouzakis, C.E., Marra, F.S., *Combustion Theory and Modelling*, **23**, (2019).



$$\omega_r = \mathrm{A}\, T^b \exp\left(-\frac{E_a}{RT}\right) C_E^{\alpha}\, C_S^{\beta}$$

Reaction flux

$$\dot{s_r} = \frac{1}{T} a_r \left(\omega_r^f - \omega_r^r\right)$$

Entropy production

Species

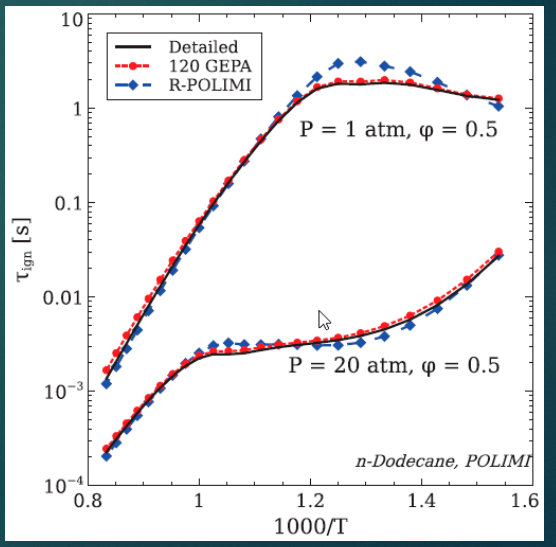
Reactions

$$\dot{q_r} = \omega_r \;\; \Delta H_r$$

Heat release rate

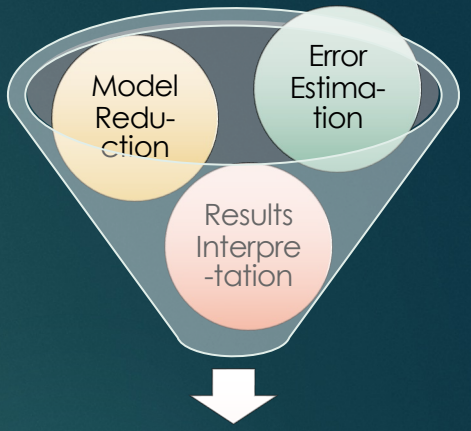
States analysis

Skeletal reduction



From 451 to 120 species

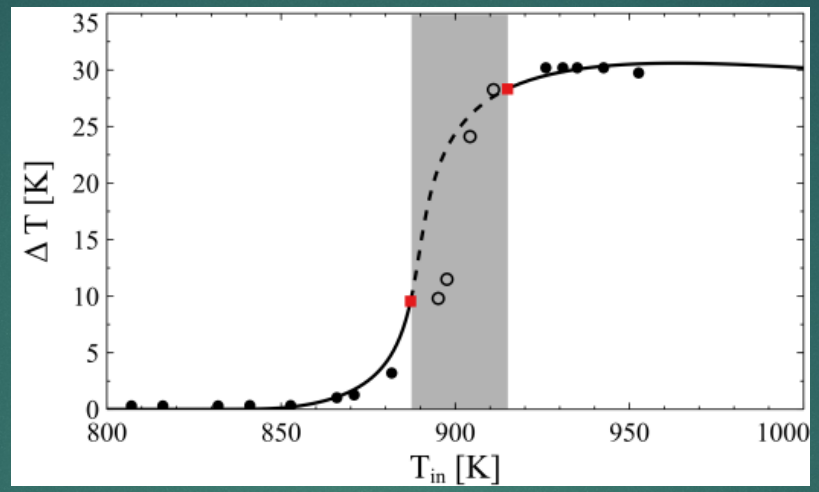
New directions of development



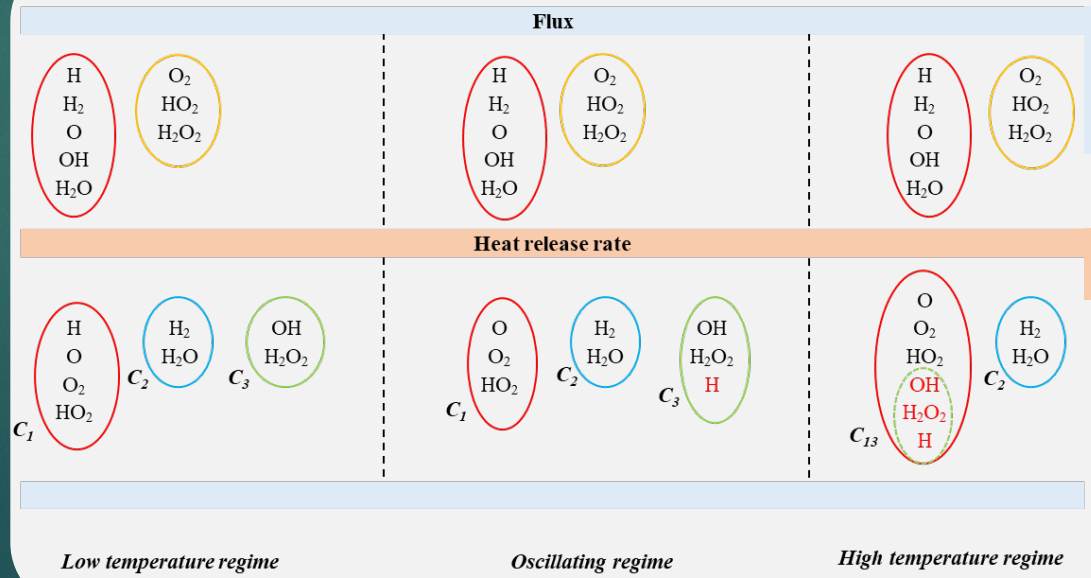
Obtain knowledge on the system

Results Interpretation

Communities' analysis



J. He, Y. Li, L. Acampora, F.S. Marra, L. Ji, *International Journal of Hydrogen Energy*. (2023) S0360319923033700.



$$\omega_r = \mathrm{A}\, T^b \exp\left(-\frac{E_a}{RT}\right) C_E^{\alpha}\, C_S^{\beta}$$

$$\dot{q}_r = \omega_r \;\; \Delta H_r$$

Jumping of species from one community to another at regime transition

Final remarks

- Digital Twins technologies could greatly increase the penetration of sustainable fuels from renewable sources
- Some approaches to overcomes current barriers to their development in the fuel's technologies have been illustrated
- Several issues still need consideration:
  - Further decrease the computational demand for almost real time simulations
  - Include the capability to deal with multi-physics effects
  - Develop the ability to recognize the effective probing function for results interpretation

Thank you for your kind attention!

Acknowledgements
L. Acampora, P. Du, M. Li, S. Liang, L. Ji, M. Kooshkbaghi, C.E. Frouzakis, J. He, Y. Li

Contacts:
francescosaverio.marra@stems.cnr.it

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