Kinetic Analysis and CFD Modelling of Hydrogen-Air Combustion Applied to Scramjet Vehicles

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Virtual, 8th April 2022, 7th International Conference on Combustion Science and Processes

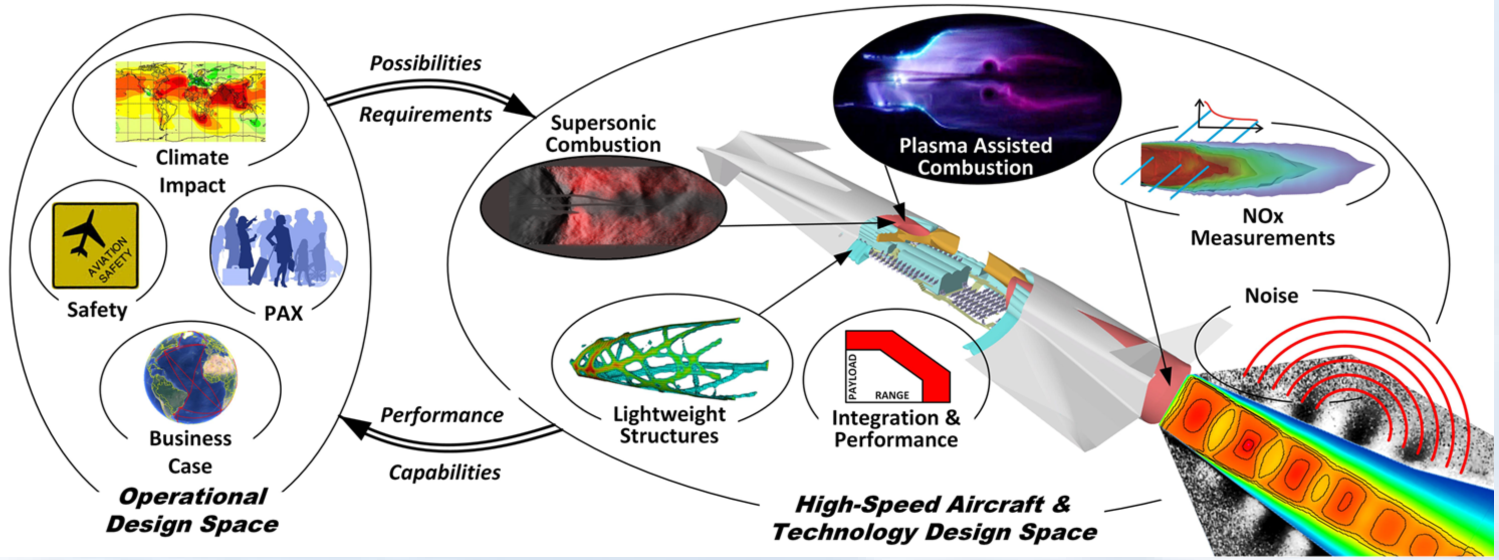
STRATOFLY PROJECT

Stratospheric Flying Opportunities for High-Speed Propulsion (STRATOFLY)

- Project co-funded by **Horizon2020** programme of **European Commission** involving **10 partners** (**POLITO, VKI, CIRA, NLR, DLR, ONERA, CNRS, FOI, LTH, TUHH, FICG**)
- Duration: **30 months** (June 2018-November 2020 + **6 months extension**)
- Stemming from a series of **EC-funded projects**, STRATOFLY is a **highly multidisciplinary** project combining technological and operative issues for **hypersonic civil aircrafts** studying the feasibility of **high-speed passenger stratospheric flight**
- Technological, environmental, operational and economic factors were taken into account, allowing global sustainability of new air space’s exploitation and drastically **reducing transfer time** (antipodal flights in less than 2÷4 hours), **emissions and noise**, and guaranteeing the **required safety**

- Main objectives:
  - ✓ *to refine design and CONOPS of the **LAPCAT-II MR2.4 vehicle***
  - ✓ *to reach **TRL = 6 by 2035** for the concept*

- STRATOFLY crucial technologies may represent a step forward to **future reusable space transportation systems**



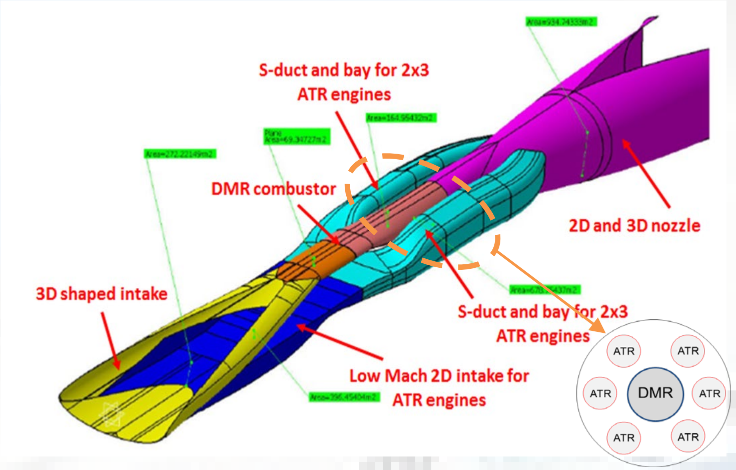
STRATOFLY VEHICLE

STRATOFLY MR3 in numbers

- Length: 94 m
- Wingspan: 41 m
- Maximum Take-Off Mass: 400 t
- Fuel Mass: 200 t
- **Liquid hydrogen as fuel**
- Available Thrust at Take-Off: 4000 kN
- **Mach 8 Cruise at 32÷33.5 km**
- L/D ≈ 7 in hypersonic cruise
- DMR shutdown at 33.5 km, Mach 8

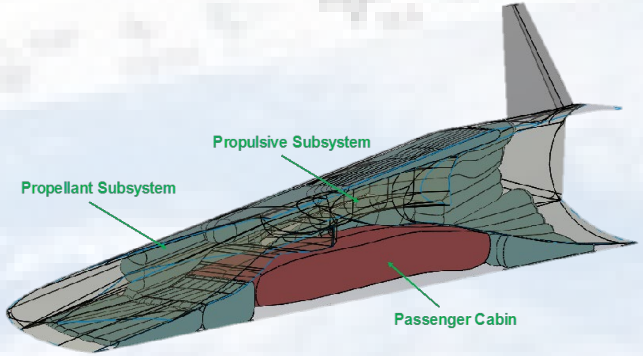
- 300 passengers
- 19,000 km in 3 hours (BRU-SYD)
- Ticket Price 3500 €

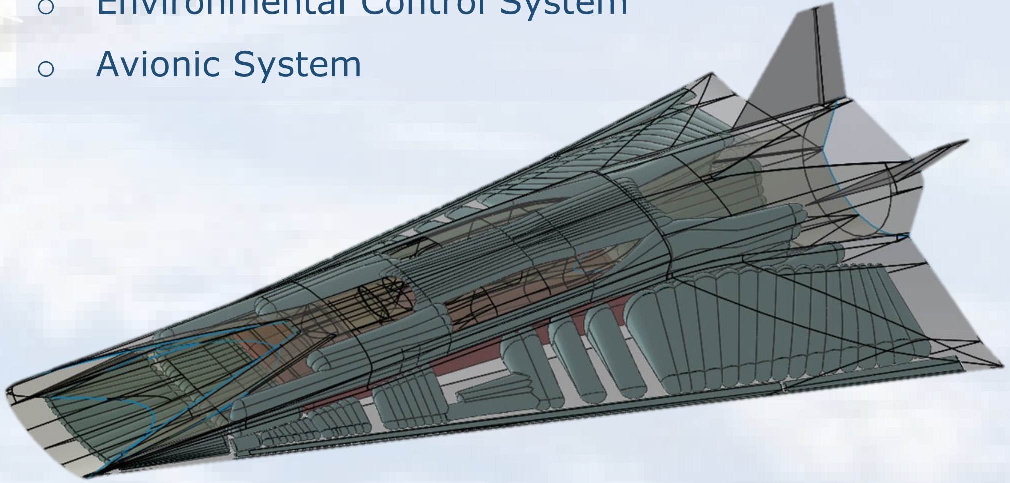
- **Zero CO_2 emissions**
- **Reduced NO_x emissions**



What's inside MR3?

- Bubble structure configuration, to optimize volume effectiveness and structural resistance (Structures)
- **Propulsive ducts for the air intake, combustor, turbomachinery (ATR only) and nozzle (Propulsive System)**
- Cryogenic tanks (Propellant System)
- Landing gear (Landing Gear System)
- Cabin layout (Payload)
- Thermal and Energy Management Subsystem
- Thermal Protection System
- Environmental Control System
- Avionic System





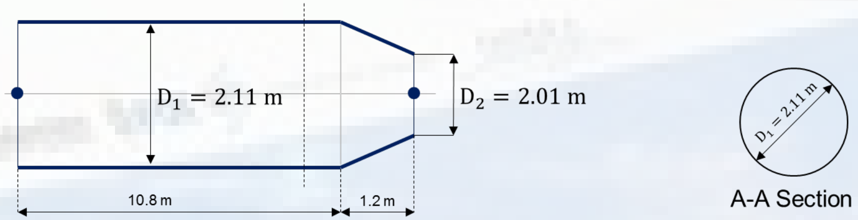
HYDROGEN COMBUSTION PROPERTIES

- ✓ **H_2** gas is strongly diffusive and highly buoyant
- ✓ Overall product of its complete **oxy-combustion** is only **water** → **clean fuel** with **zero carbon emissions**
- ✓ Combustion with **air** produces also **NO_x** due to the achievement of **elevated flame temperatures**

- ✓ **Supersonic hydrogen combustion** is a challenging process for several reasons as:
  - injection
  - compressible mixing
  - **chemical kinetics**
  - **ignition**
  - flame holding
  - vortices generation
  - turbulence combustion modelling
  - interactions among shock waves
  - boundary layer and heat release

- ✓ **Very short residence time τ (~ 10^{-3} s)** of the flow through the combustor chamber that is of the **same order of magnitude of chemical kinetic ignition time**

ATR Combustion chamber:



- ✓ **Experimental measurements** of **multispecies, reacting, high-speed, unsteady, turbulent** flow fields are **very challenging**
- ✓ The most convenient way to preliminary design and develop **scramjet vehicles** often relies on **CFD modelling**
- ✓ Chemical modelling of **hydrogen/air combustion** is of fundamental importance → need of a **suitable kinetic mechanism**

0D KINETIC ANALYSIS

- ✓ Open-source **thermodynamic** and **kinetic Cantera** tool under **Python** interface
- ✓ **Homogeneous, isochoric, batch reactors**
- ✓ **Ignition delay times** calculations at several **initial** operative conditions ***(T, P, φ)***

$$
\begin{cases}
m_{tot} = \sum_{k=1}^{K} m_k = const. \Leftrightarrow \dfrac{dm_{tot}}{dt} = 0 \\
\dfrac{dm_k}{dt} = V r_k M_{w,k} \\
c_p \dfrac{dT}{dt} + v \cdot \sum_{k=1}^{K} h_k \cdot r_k \cdot M_{w,k} = 0
\end{cases}
$$

→ ✓ Total reacting mixture **matter** balance equation

→ ✓ Single k-th chemical component **matter** balance equation

→ ✓ **Energy** balance equation

- ✓ The net reaction rates for every ***k-th*** **chemical component** is determined by **Arrhenius** expressions, according to the **kinetic mechanism** under investigation
- ✓ The gaseous mixture averaged density ***ρ*** was calculated assuming an **ideal gas** behaviour
- ✓ **Mass transport** to the **reactor walls** is infinitely fast

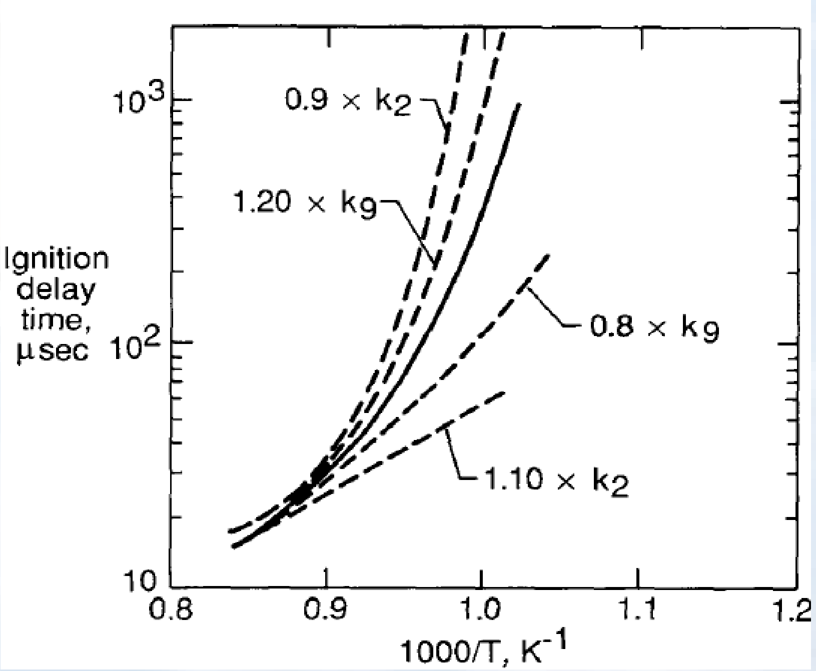
JACHIMOWSKI - 1988

- ✓ Developed in **1988** at **NASA Langley Research Centre** in the framework of the **National Aero-Space Plane (NASP)**
- ✓ **Supersonic scramjet combustion** at flight speed up to **Mach 25**
- ✓ **33 radical, reversible, elementary reactions** involving **13 chemical species** (including the **inert bath gases**)
- ✓ Rate coefficients for certain reactions were adjusted in order to obtain the best agreement with the **experimental measurements of *real* hydrogen-air mixtures** of **ignition delay times** reported by **Slack**
- ✓ At pressures of **0.5, 1** and **2 atm** for **stoichiometric hydrogen/air mixtures**, induction times are very sensitive to the rate coefficients, assigned to the second and ninth reactions of the whole scheme

[R2] $H + O_2 \rightarrow OH + O$

[R9] $H + O_2 + M \rightarrow HO_2 + M$

- ✓ **At high flight Mach numbers (M > 12) conditions**, reactions involving nitric oxides become greatly important
- ✓ **Experimental data** by **Slack** and **Grillo** show that a limited addition of NO_x to stoichiometric hydrogen/air mixtures **decreases** the **ignition delay times**
- ✓ Conversion of the **chain-terminating** species HO_2 to the very reactive **OH radical**



[R30] $HO_2 + NO \rightarrow NO_2 + OH$

[R31] $H + NO_2 \rightarrow NO + OH$

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KEROMNÈS – 2013

- ✓ **Detailed** kinetic mechanism suitably conceived for investigating the oxidation of **syngas mixture consisting in** $\mathbf{H_2/CO/O_2/N_2/Ar}$ at pressures from **1 to 70 bar**, over a temperature range of **900-2550 K** and equivalence ratios from **0.1** to **4**
- ✓ **11 chemical species** comprising also the **excited** radical **OH*** and interacting among them through **30 reversible reactions**
- ✓ **Hydrogen reactivity** is mainly controlled by the **competition** between

✓ **Chain-branching**

[R1] $H + O_2 \rightarrow O + OH$

VS

✓ **Pressure dependent chain-propagating**

[R9] $H + O_2 (+M) \rightarrow HO_2 (+M)$

- ✓ **Hydrogen ignition** under **high pressure** and **intermediate temperature conditions** is governed by the fundamental reactions:

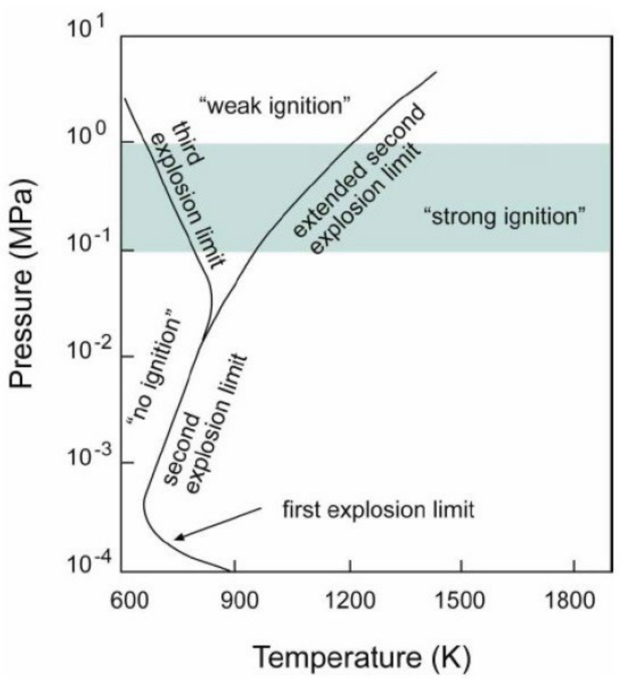
[R17] $H_2 + HO_2 \rightarrow H + H_2O_2$

[R15] $H_2O_2 (+M) \rightarrow OH + OH (+M)$

- ✓ **T < 1000 K (RCM):** hydrogen oxidation is predominantly controlled by reaction **[R9]** → **hydroperoxyl radical i.e.,** $\mathbf{HO_2 \rightarrow H_2O_2}$ according to reaction **[R17]**
- ✓ **Oxygenated water** decomposes to two **OH radicals** as prescribed by reaction **[R15]**
- ✓ **T > 1100 K (Shock Tube Experiments):** Competition between **[R1]** and **[R9]** leads to a **pressure dependence** of τ_{ign} governed by reaction **[R1]**

Z25 – 2018

- **22 irreversible steps** plus the **3 Zel'dovich NO** generation reactions involving **10 chemical species**



✓ **T < 900 K: R4** competes with **R12**

✓ $\mathbf{HO_2}$ concentration increases and **alternative** reactions **R16**, **R20** become more important and produce $\mathbf{H_2O_2}$ in greater amount

[R4] $H + O_2 \rightarrow O + OH$

[R12] $H + O_2 (+M) \rightarrow HO_2 (+M)$

VS

[R16] $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$

[R20]: $H_2O + HO_2 \rightarrow H_2O_2 + OH$

✓ **T > 1100 K: R1**, **R4**, **R5** and **R8** well describe **branched-chain explosion**

[R1] $H_2 + O_2 \rightarrow H + HO_2$ **[R5]** $OH + O \rightarrow H + O_2$ **[R8]** $H_2 + OH \rightarrow H_2O + H$

✓ **R17** is furthermore essential since it consumes $\mathbf{H_2O_2}$ and creates **OH** radicals **decreasing** τ_{ign}

[R17]: $H_2O_2 (+M) \rightarrow OH + OH (+M)$

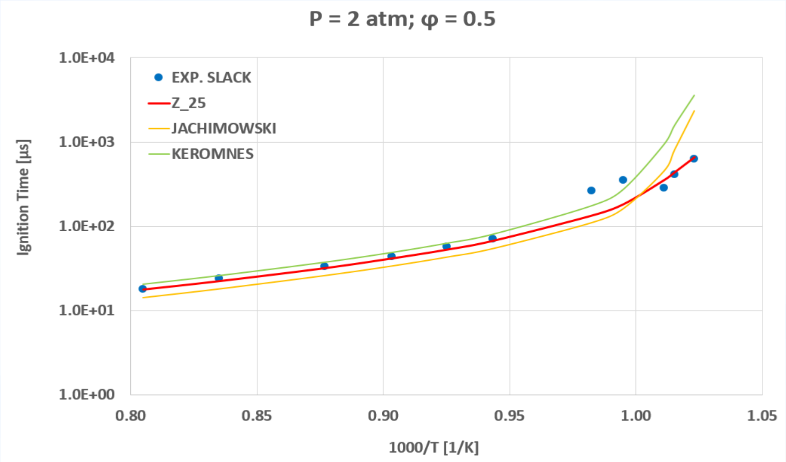
✓ **Crossover region →** corresponding to **900 K < T < 1100 K**

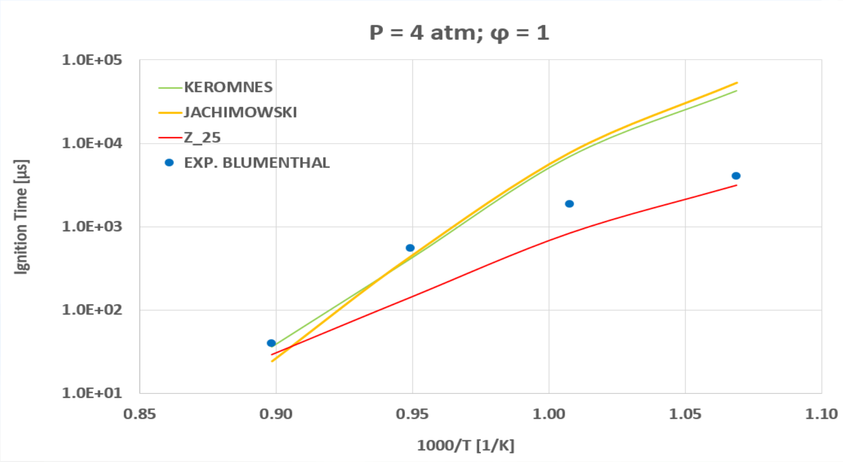
✓ Dominated by extremely **complex chemical processes**

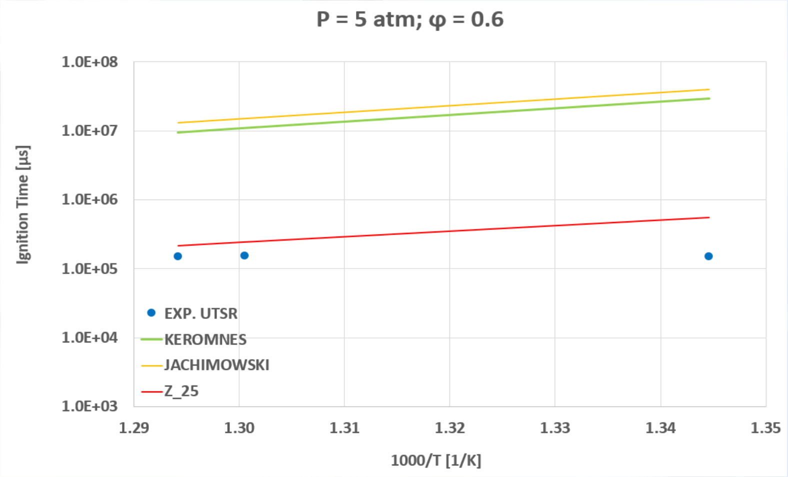
✓ Several **ramjets, scramjets** and **dual mode engines** operate exactly in this **connecting critical zone**

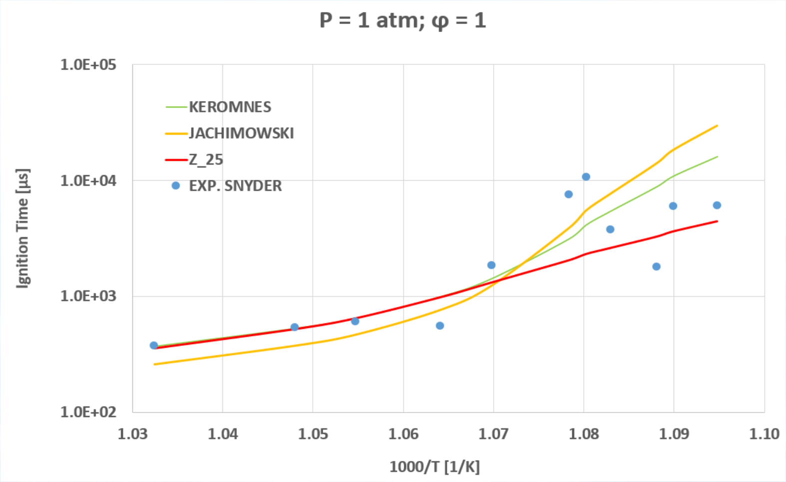
KINETIC RESULTS - I

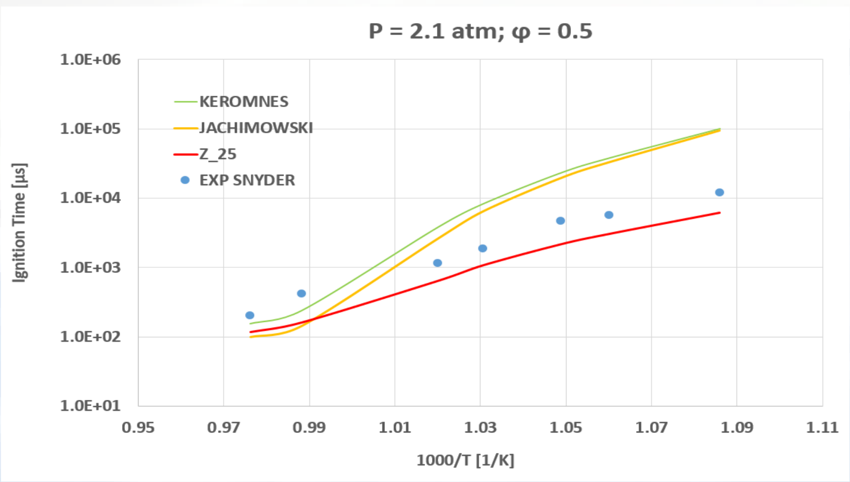
✓ Comparison between the **0D ignition delay times** and the **experimental data** at the same **initial temperature, pressure** and **equivalence ratios,** measured in **shock tube** and/or **RCM tests**

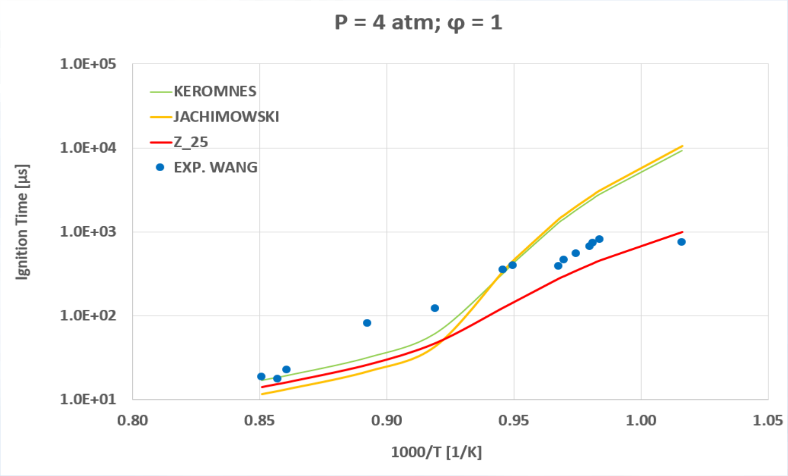




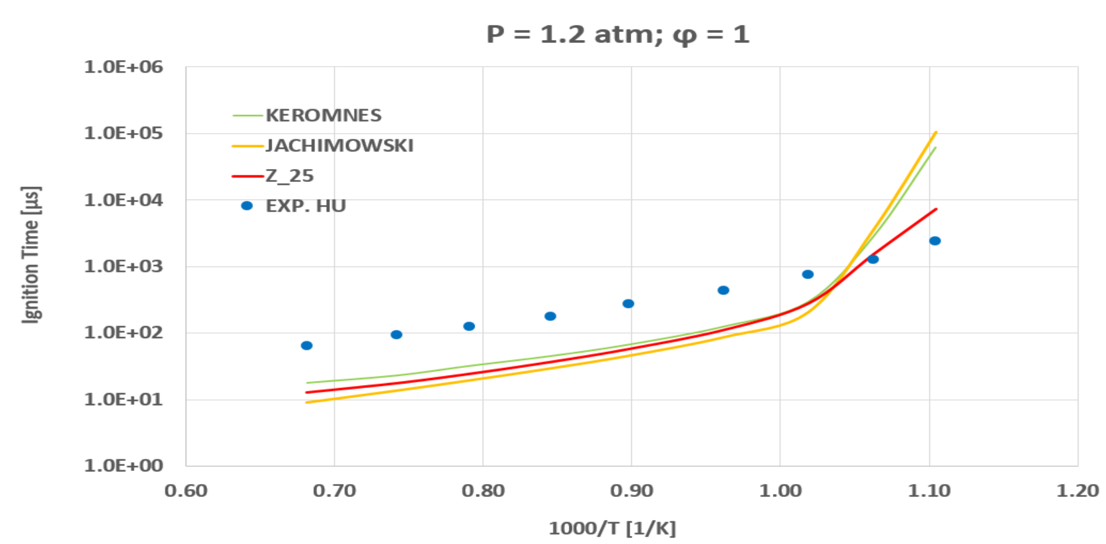


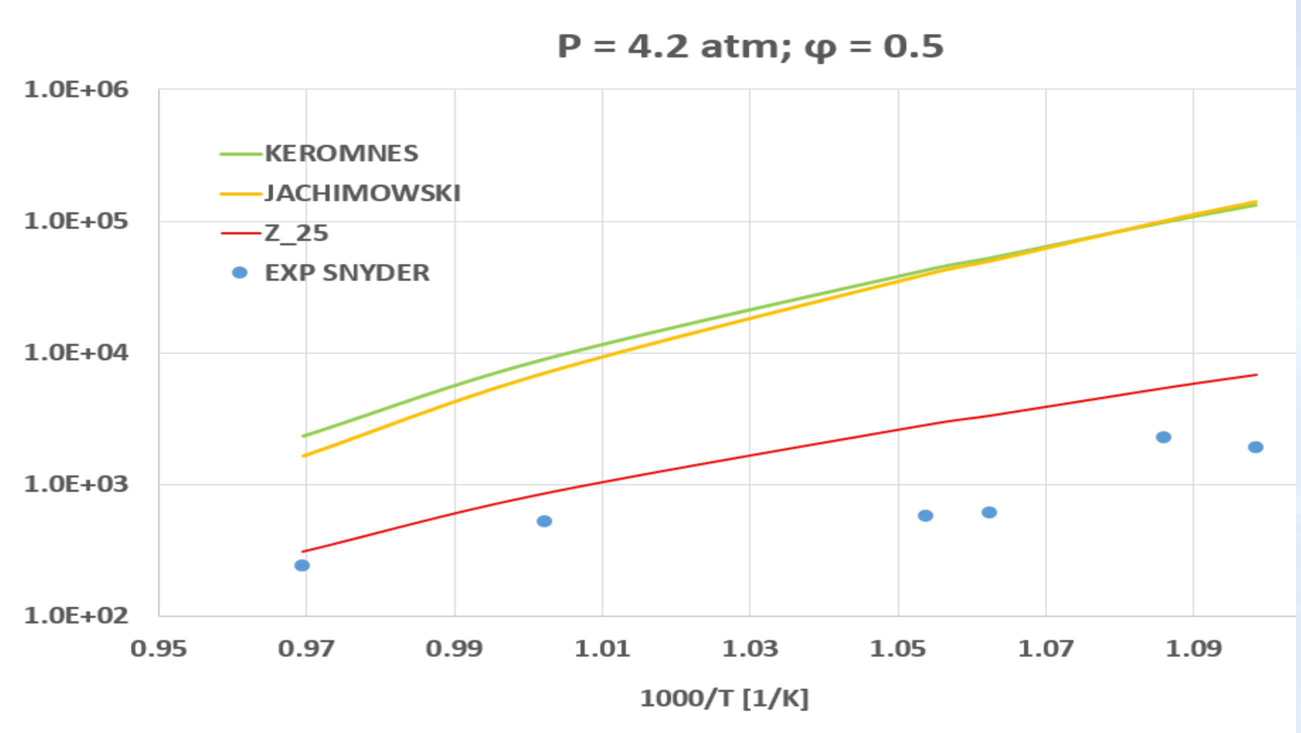


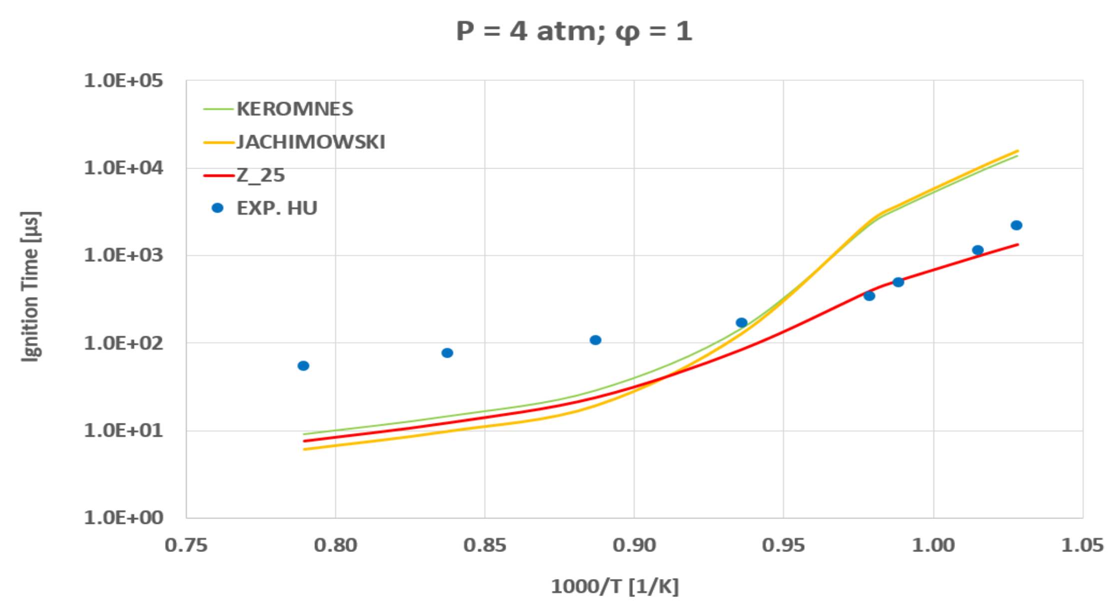




KINETIC RESULST - II



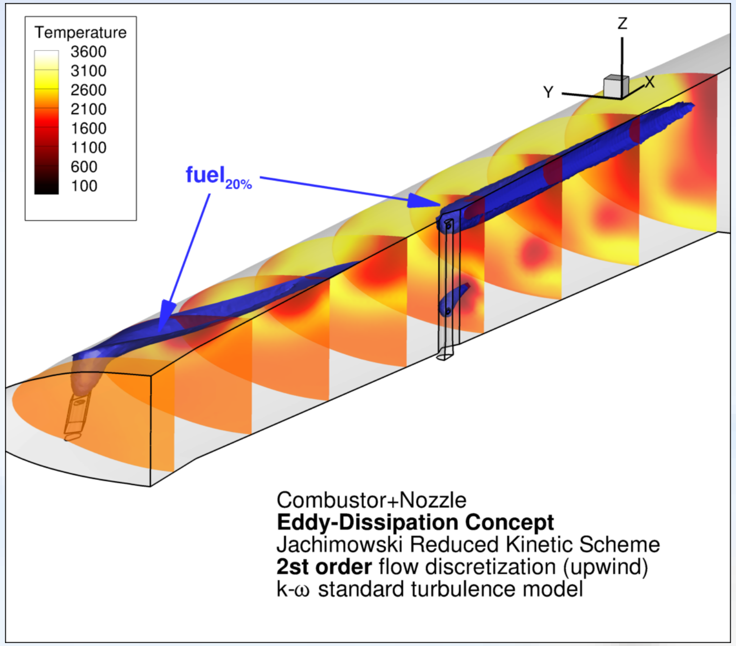




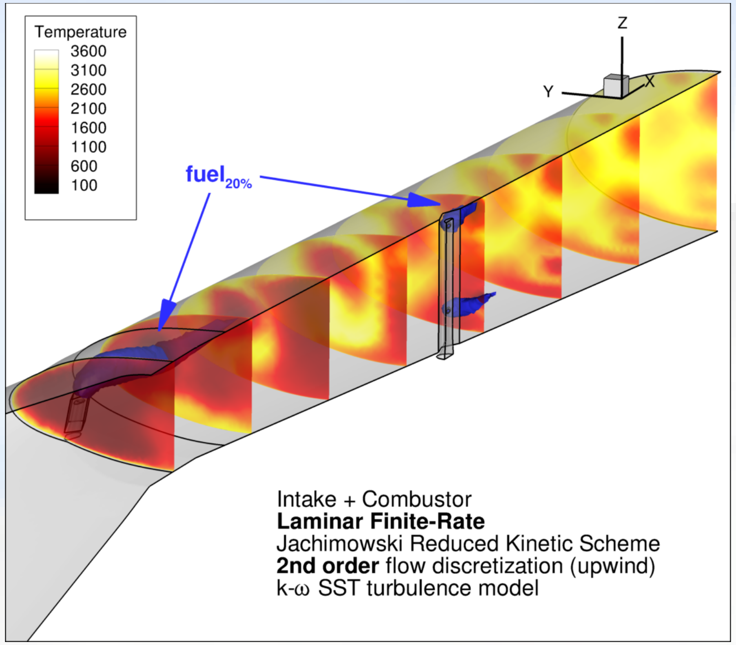
- ✓ The best agreement was achieved by the **Z25** kinetic mechanism
- ✓ The matching of **Jachimowski** and **Kéromnés** kinetic schemes are satisfactory only for **high temperature** and **low pressure conditions**
- ✓ In the **crossover region** and **pressure above 2 bar** only the **Z25** exhibits a quite good behaviour

FULLY-3D CFD MODELLING

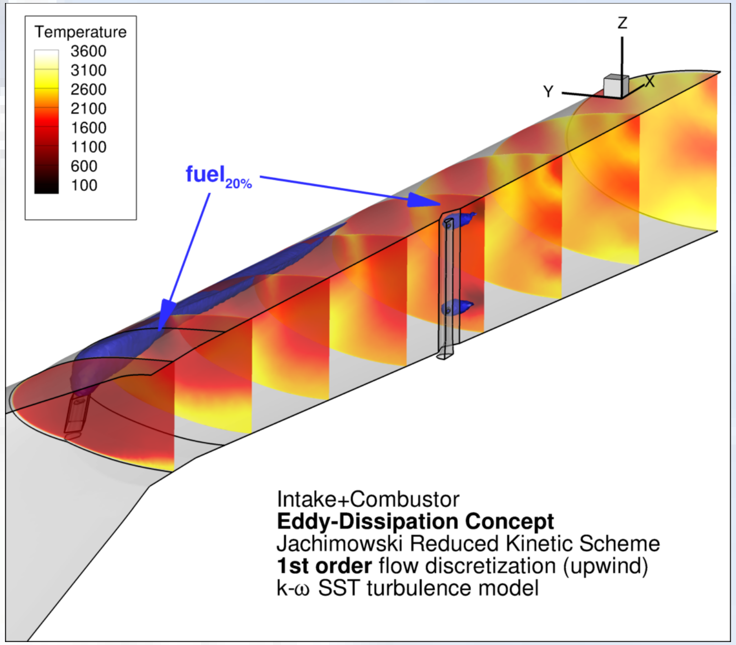
Combustor + Nozzle result



R3 result (LFR 2^{nd} order)



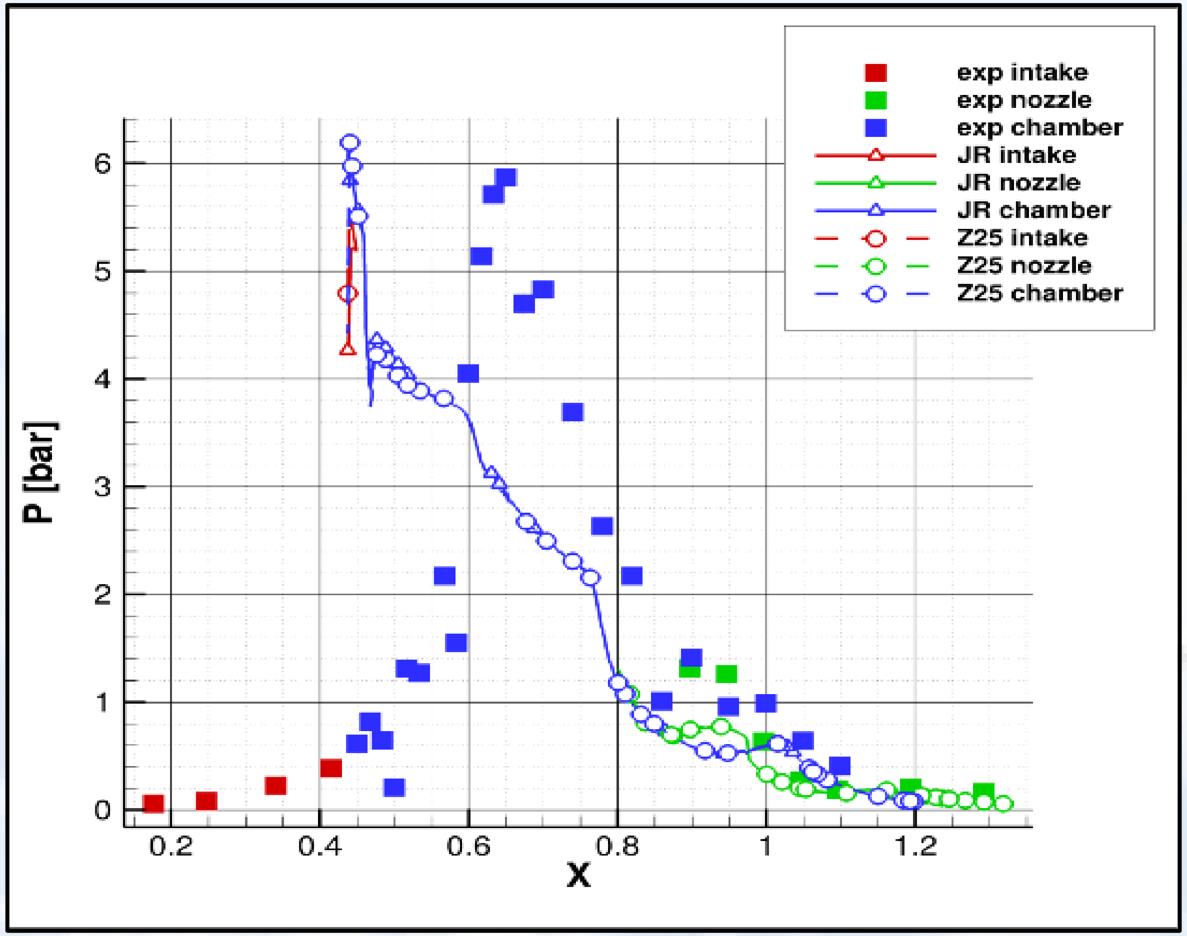
R4 result (EDM 1^{st} order)



- ✓ **Ansys Fluent®** software
- ✓ **Temperature contour plots** over some slices of the **combustion chamber**
- ✓ Solution with **JR mechanism**
- ✓ In order to better understand **temperature distribution**, iso-surfaces of **20% mass-fraction** of $\mathbf{H_2}$ are also reported
- ✓ The **CFD** run was carried out using both **Laminar Finite Rate (LFR)** and **Eddy Dissipation Model (EDM)** combustion models, along with a **standard k-ε turbulence** model and **2^{nd} order up-wind** discretization scheme

CFD VALIDATION

- ✓ The **ground-based testing** of M8 flight experiment configuration, conducted in **HEG** wind tunnel at the **German Aerospace Center - DLR** , was used as experimental **test reference**



- ✓ Vehicle geometry was simplified removing the **intake**
- ✓ Only combustion process along with **nozzle expansion** was simulated
- ✓ Inlet temperature > **1100 K**
- ✓ Unexpected **compression** that is a consequence of the **abrupt temperature increasing** caused by the combustion process
- ✓ **Predicted pressure peak value** is consistent with the **experimental measurement**
- ✓ **Both kinetic schemes** (**JR** as well as **Z25**) are reliable for **3D CFD** simulations of the **H_2-O_2 combustion**

CONCLUSIONS

- **Hydrogen/air supersonic combustion** process was analysed both on **chemical kinetic** and **CFD** points of view
- **0D kinetic assessment** in the operative conditions experienced in **scramjet engines** was carried out on literature available combustion mechanisms
- The **best agreement** with experimental **shock ignition delay times measurements** was achieved with **Z25** scheme
- **Fully-3D CFD simulations** confirmed that **kinetic schemes** due to **Zettervall** and also **Jachimowski** are quite good for **pressure predictions** when the engine inlet temperature is above **1100 K**

✓ **THANK YOU FOR YOUR ATTENTION**

✓ **QUESTIONS?**

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