

# PARUPM: A SIMULATION CODE FOR PASSIVE AUTOCATALYTIC RECOMBINERS





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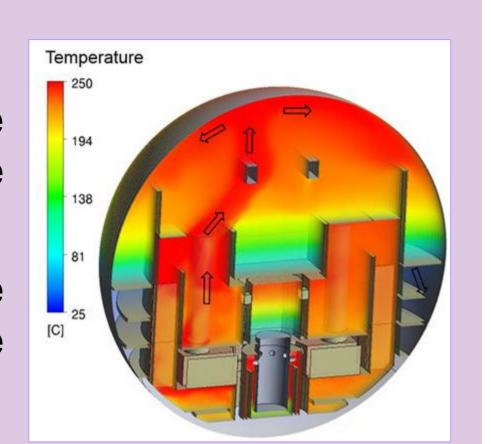
#### **BACKGROUND**

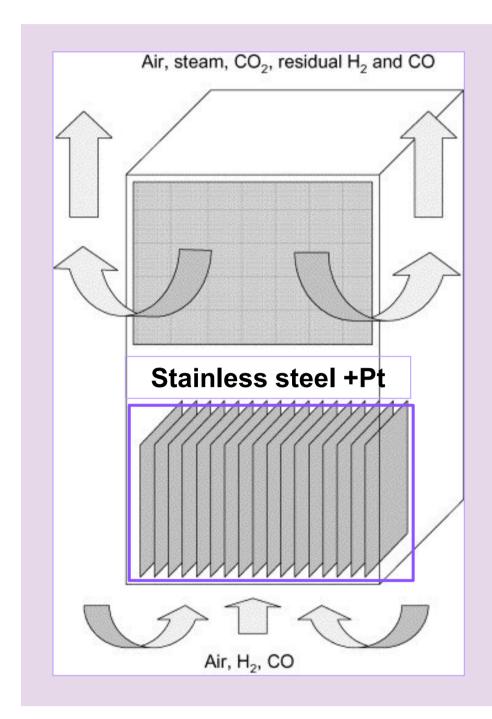
- In severe accidents (SAs) large amounts of combustible gases may get released into the containment atmosphere, generating a risk of combustion.
- To mitigate this hazard, PARs have been installed inside containment buildings.
- These devices can convert H<sub>2</sub> and CO into H<sub>2</sub>O and CO<sub>2</sub>, reducing the risk of combustion.



#### **AMHYCO PROJECT**

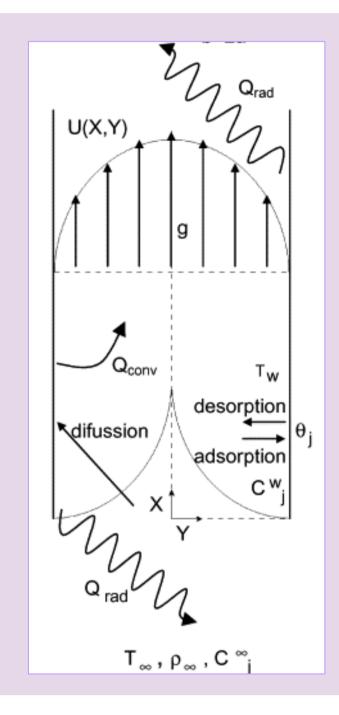
- The AMHYCO project aims to improve the knowledge and simulation capabilities for the H<sub>2</sub>/CO combustion risk management in SAs.
- The enhancement of the available knowledge related to PAR operational performance is one key point of the project.





#### PARUPM MODEL

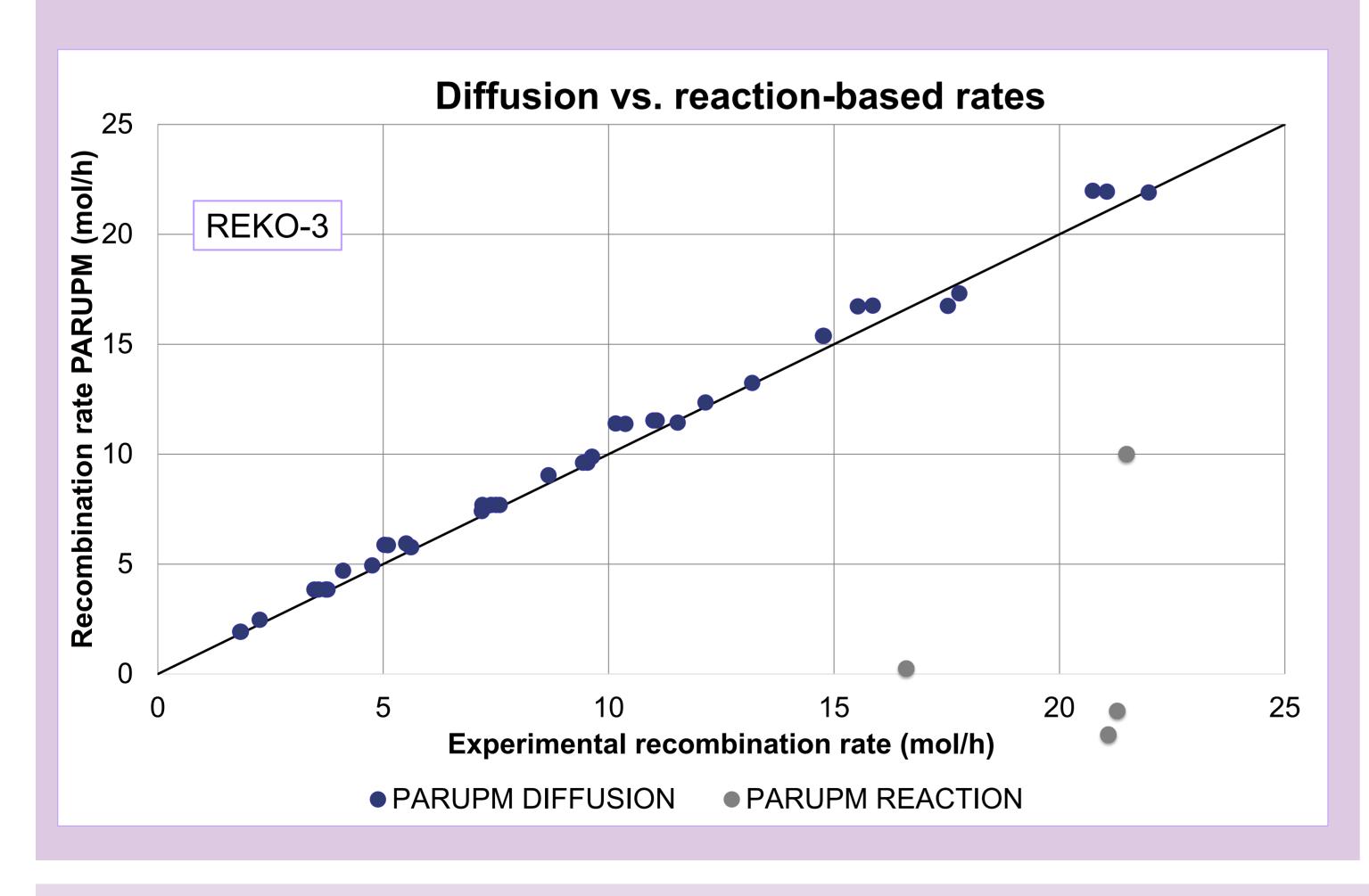
- Numerical code capable of simulating the behaviour of a PAR device through a physical-chemical approach.
- This code will be implemented into containment analysis codes to study the effect of recombiners in SAs scenarios.
- Relevant phenomena considered in the recombination model:
- Mass transfer
- Adsorption/desorption of species
- Surface chemical reactions and heat release
- Convective and radiative heat exchange.



#### MODEL ENHANCEMENT: DIFFUSION RATE

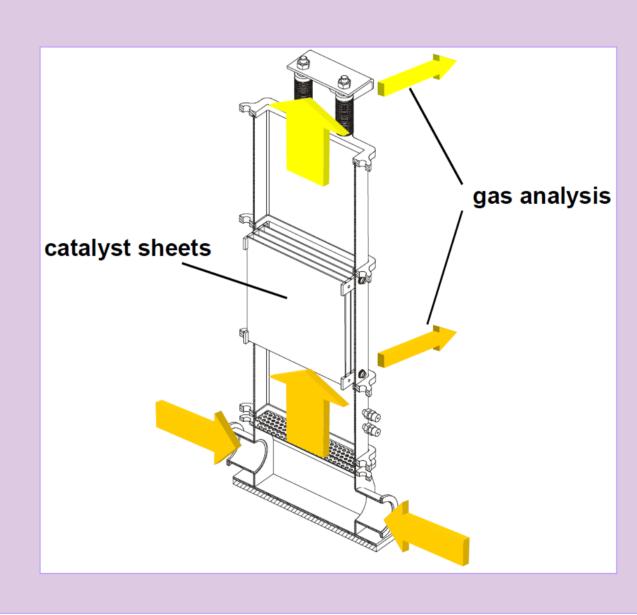
- Heterogenous catalytic reactions involve both surface and transport phenomena. Initially, the recombination rate inside PARUPM was determined by the surface reactions of the species over the catalytic plates.
- A mass transfer model has been added to the code to consider the diffusion through the boundary layer and to study the effect of this phenomenon on the recombination rate.

$$Rate_{H_2,dif} = \frac{Sh_{H_2} D_{dif}}{D_h} \left(\frac{p_{H_2}}{RT}\right)$$



### **CODE VALIDATION AGAINST REKO-3 DATA**

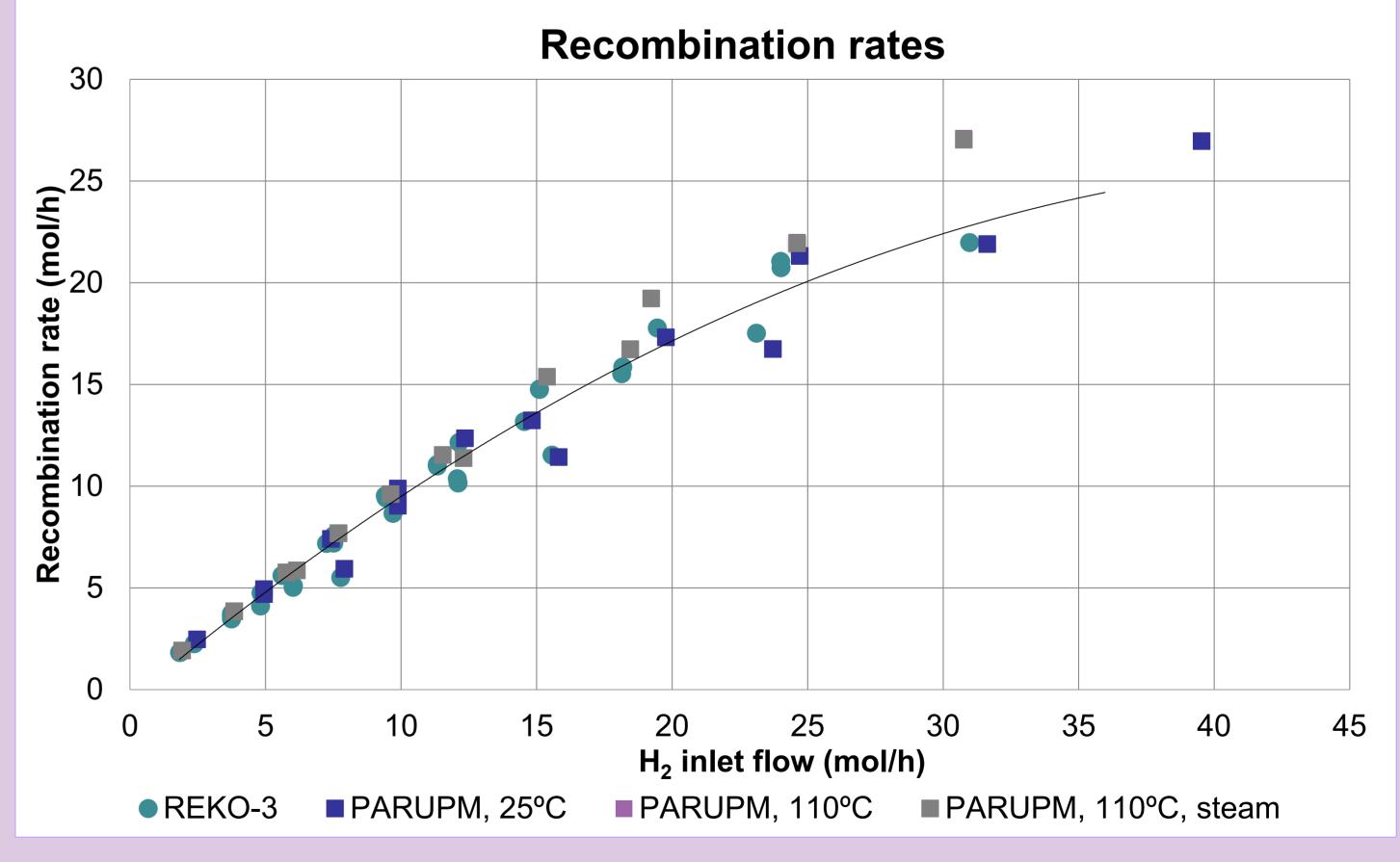
 Analysis of the code capabilities comparing the numerical results with experimental data obtained from the REKO-3 experimental facility.



#### 3 main cases

- Gas temperature 25°C and steam 0%
- Gas temperature 110°C and steam 0%
- Gas temperature 110°C and steam 20%

3 inlet velocities: 0.25 m/s , 0.5 m/s, 0.8 m/s



#### **CONCLUSIONS**

- The introduction of the diffusion model significantly improves the results, independently of the velocity of the inlet gas. With the reaction-based rates, the recombination rate was overpredicted at lower velocities by an average ≈40% and was underpredicted for higher velocities by an average ≈40% as well.
- Good predictions of the recombination rate are achieved with the diffusion model. The biggest deviation appears for low H<sub>2</sub> inlet concentrations, higher inlet temperatures, and higher velocities, though the average deviation is ≈5%.
- After the completion of the model development process, PARUPM will be coupled to thermohydraulic codes for SA analysis with PARs presence.

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