Validation of the PAR code REKO-DIREKT against large scale experiments performed in the frame of the OECD/NEA-THAI project

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- REKO-DIREKT code
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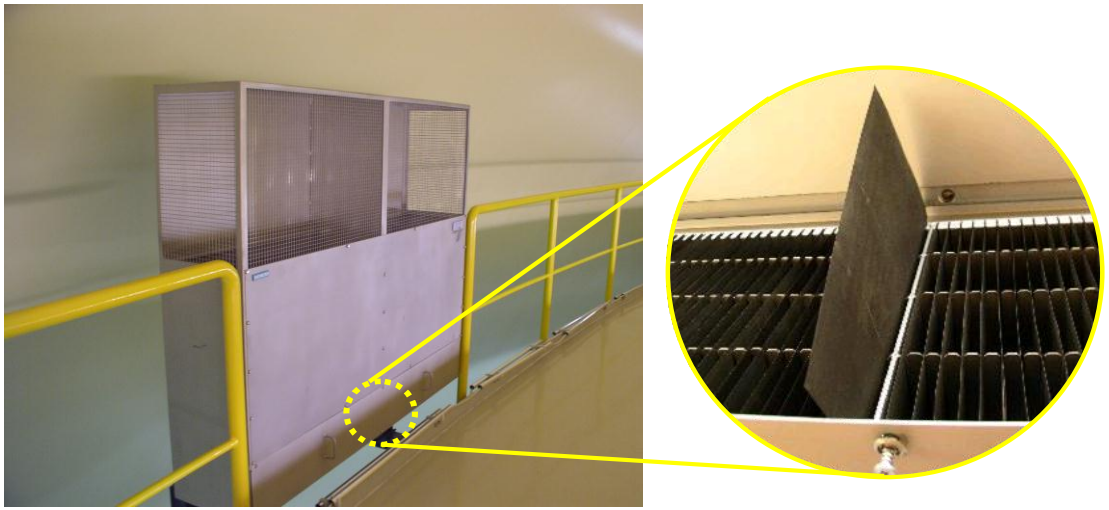
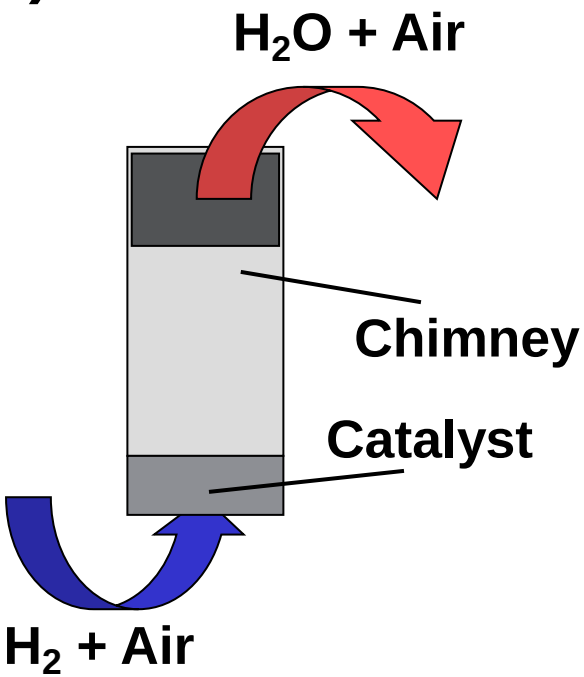
- Outlook

Passive auto-catalytic Recombiners (PAR)

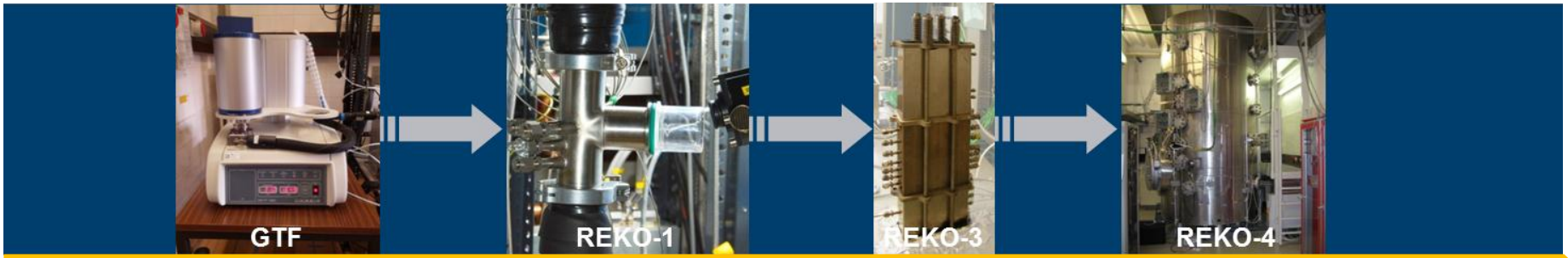




Key element in hydrogen mitigation strategy

- Passive operation
- Hydrogen removal already at low hydrogen concentrations (below ignition limits)
- Comprehensive qualification programme
  (conversion rates, earth quake resistance, catalyst poisoning)

PAR research at JÜLICH and RWTH

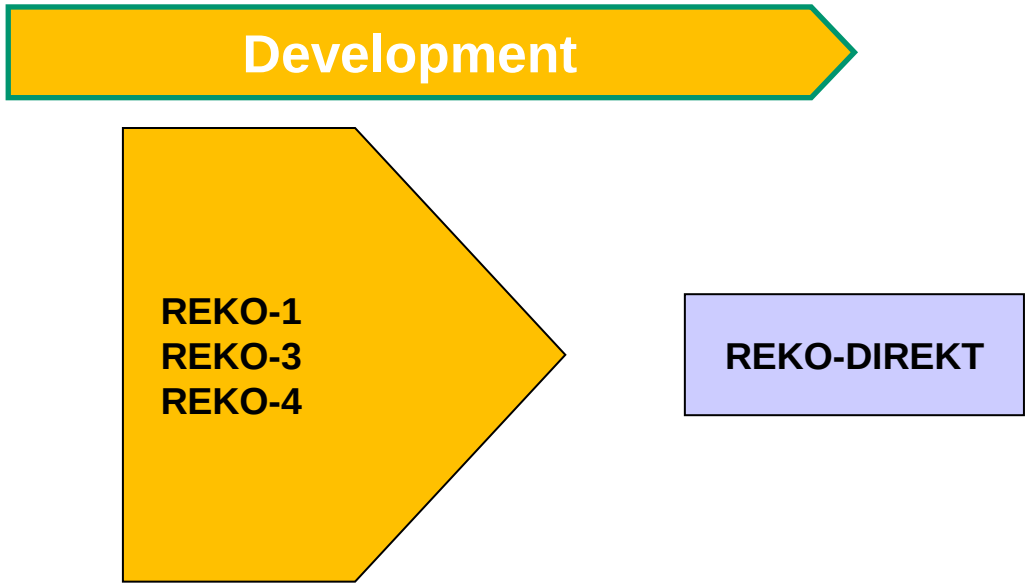


Model development (REKO-DIREKT/JÜLICH, SPARK/IRSN)

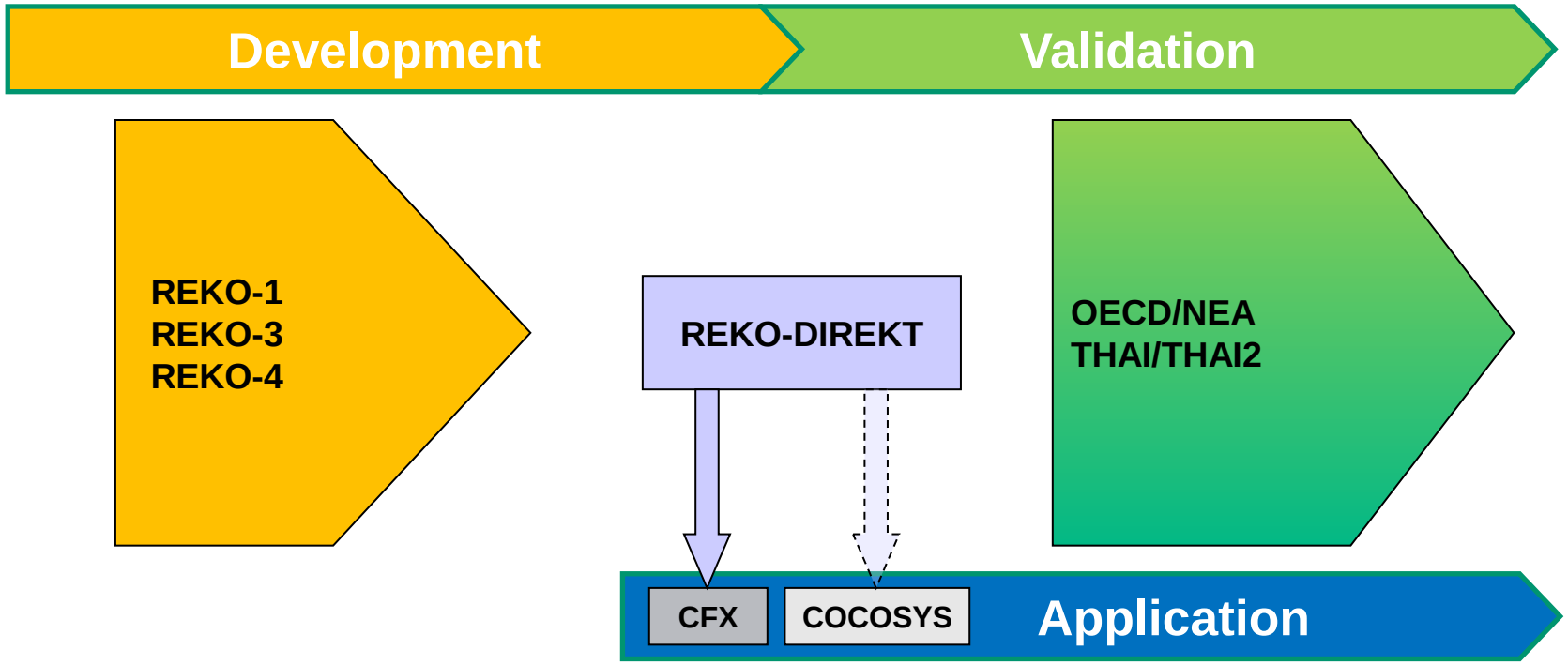
Open modelling issues

- Start-up behaviour (delay under certain conditions)
- Interaction with CO (Poisoning ←→ Recombination)
- Ignition (hot catalyst elements)
- Adverse flow conditions (PAR-atmosphere interaction)

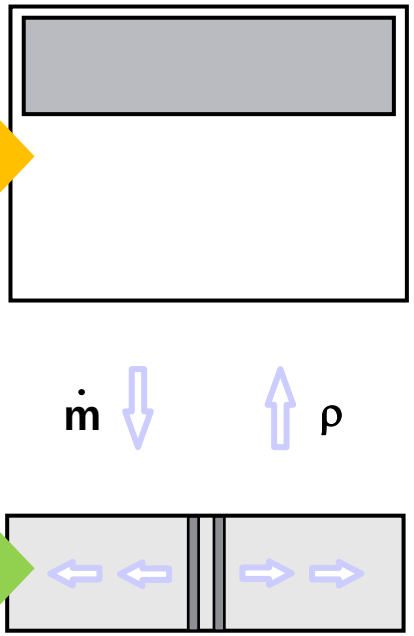
PAR code REKO-DIREKT: Development



PAR code REKO-DIREKT: Validation & Application



PAR code REKO-DIREKT: Modelling strategy



Mechanistic chimney model

$$\dot{m} = A \cdot \sqrt{\frac{g \cdot H \cdot (\rho_0 - \rho)}{\left(\frac{1}{\rho} - \frac{1}{2 \cdot \rho_0} + \underbrace{\frac{\xi \cdot H}{2 \cdot d_h \cdot \rho}}_{\omega_r}\right)}}$$

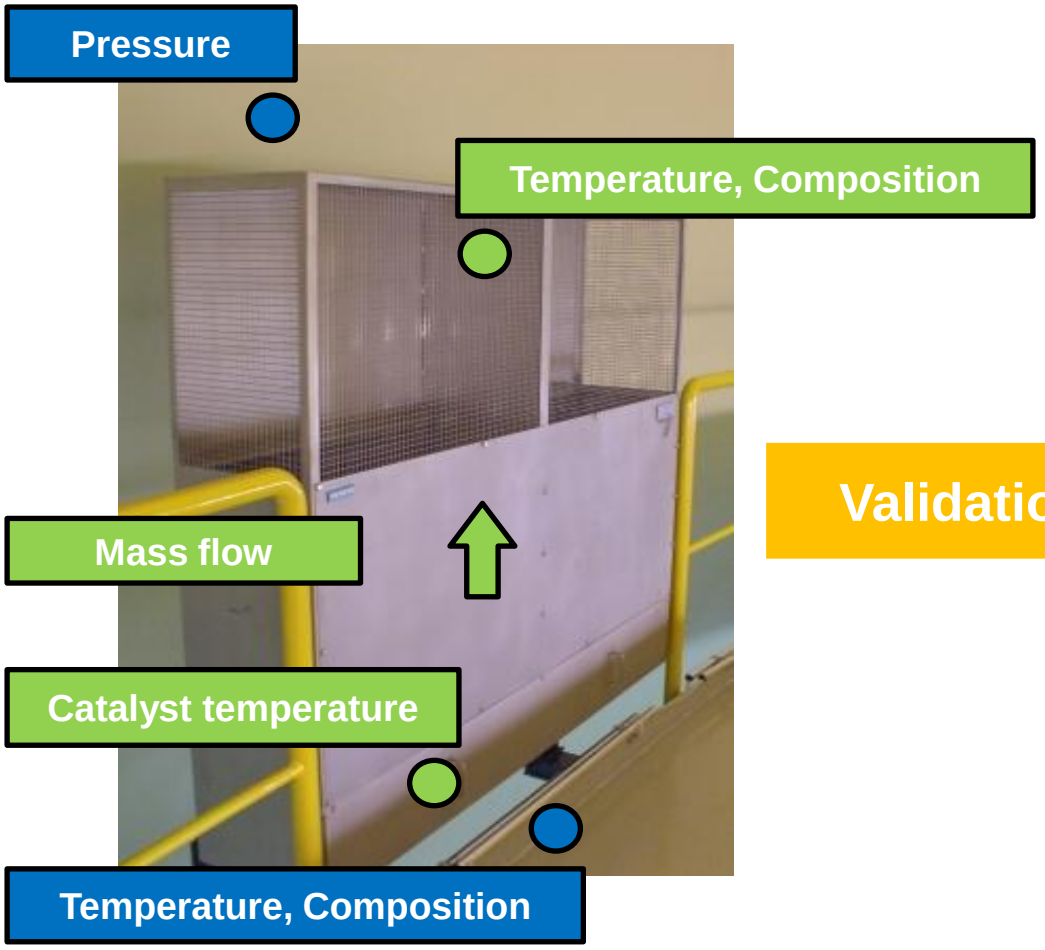
Diffusion controlled reaction kinetics:

$$\dot{r} = \beta \cdot \Delta C_i$$

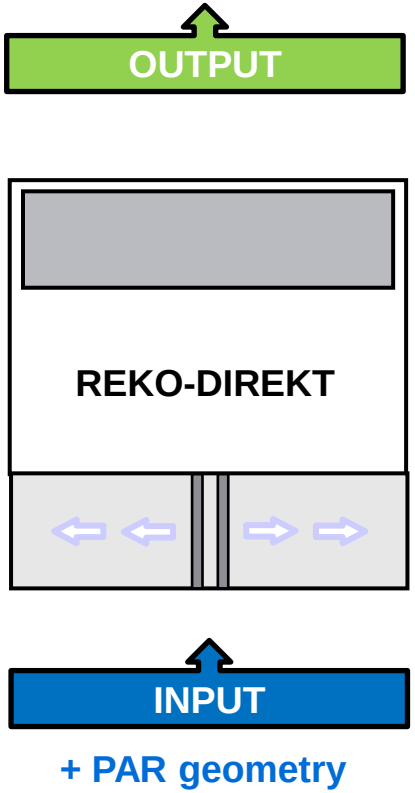
$$\beta = Sh \cdot \frac{D_{i,m}}{d_h}$$

$$Sh = f\left(Re, Sc_i\right)$$

Code validation: Needs



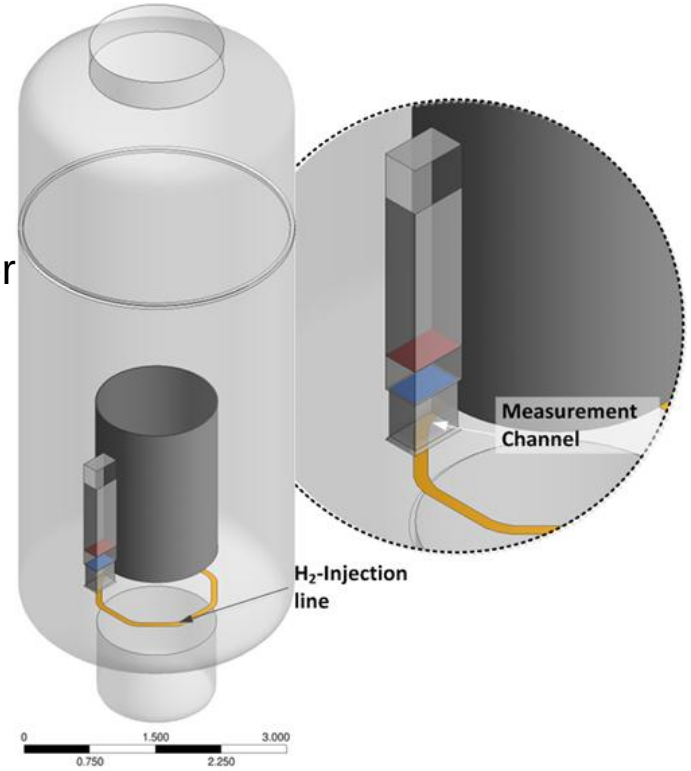
Validation



OECD/NEA-THAI: Test facility

THAI

- 60 m³
- H_2 injection line
- PARs attached to inner cylinder



PARs	AREVA	AECL
Chimney geometry		
Height	0.880 m	0.299 m
Width	0.205 m	0.340 m
Depth	0.320 m	0.320 m
Width outlet	0.202 m*	0.335 m
Height outlet	0.300 m	0.300 m
	*0.187 + 0.285/19	
Catalyst sheet geometry		
Number	19	16
Height	140 mm	180 mm
Depth	280 mm	296 mm
Thickness	0.2 mm	2.0 mm
Distance	9.8 mm	18 mm

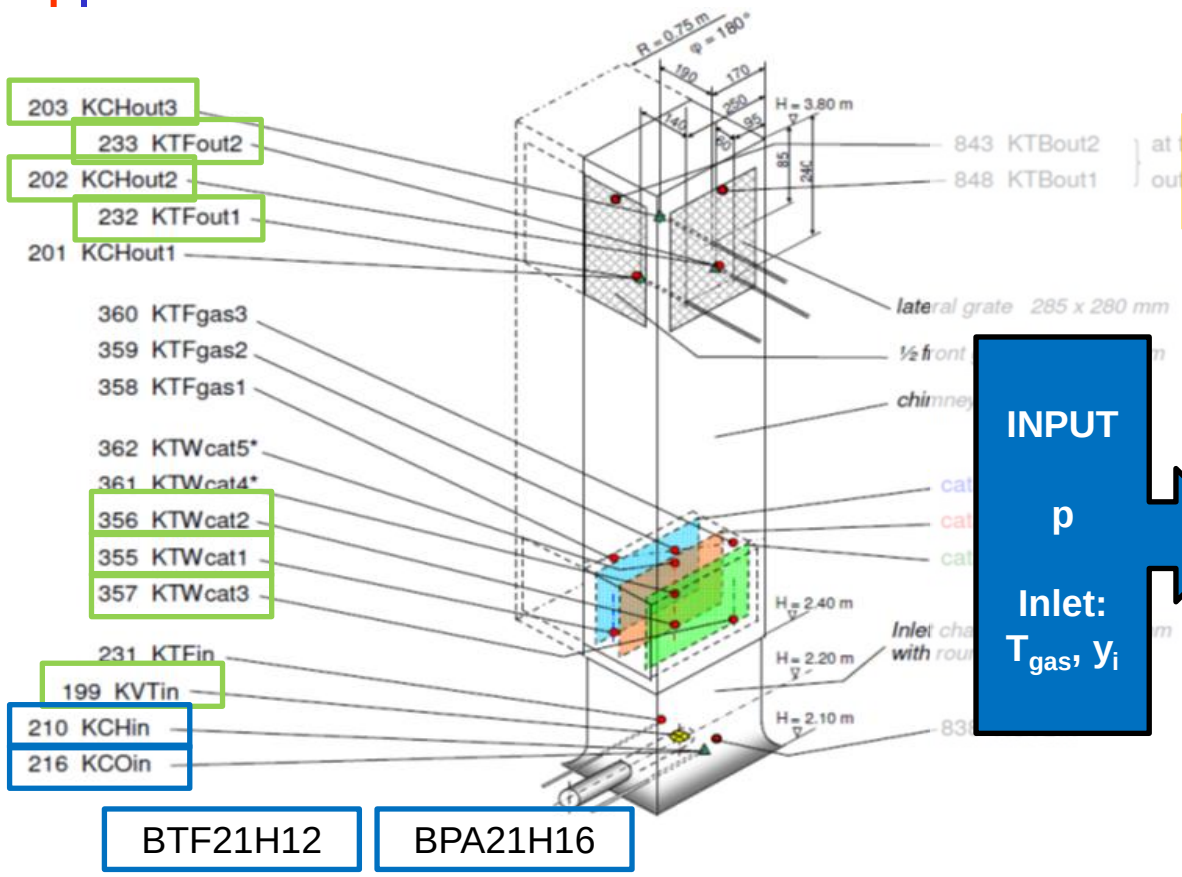
OECD/NEA-THAI: HR test programme

- 37 experiments
  - 22 with AREVA PAR
  - 10 with AECL PAR

  } Selected for validation

- Test parameters
  - Initial vessel pressure (1.0 bar – 3.0 bar)
  - Steam amount (0 – 60 vol.% corresponding to elevated temperatures)
  - Oxygen concentration partially or permanently below the required minimum for optimum hydrogen conversion (‚oxygen starvation‘)
  - Intentionally provoked ignitions

Code validation: Input & Output data (AREVA)



Validation

INPUT

p

Inlet: T_{gas}, y_i

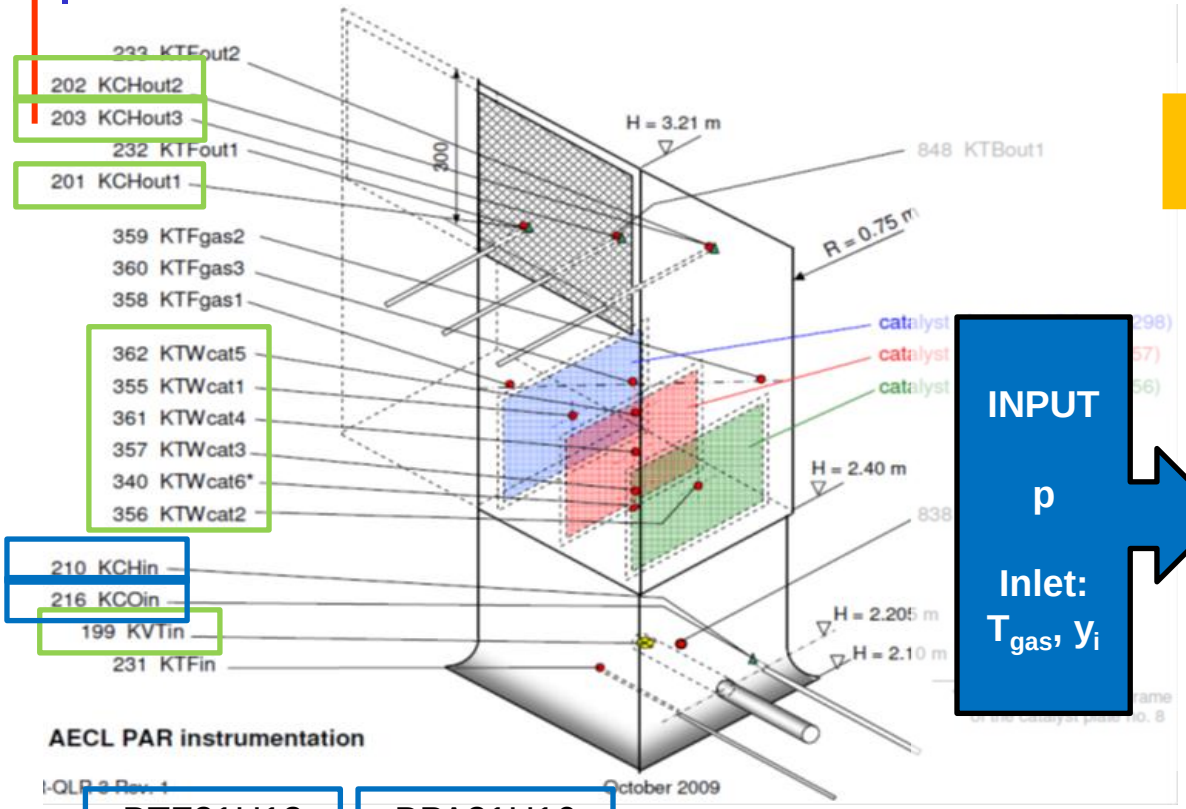
REKO-DIREKT

OUTPUT

v, T_{cat}

Outlet: T_{gas}, y_i

Code validation: Input & Output data (AECL)



BTF21H12 BPA21H16

Validation

INPUT

p

Inlet: T_{gas}, y_i

REKO-DIREKT

OUTPUT

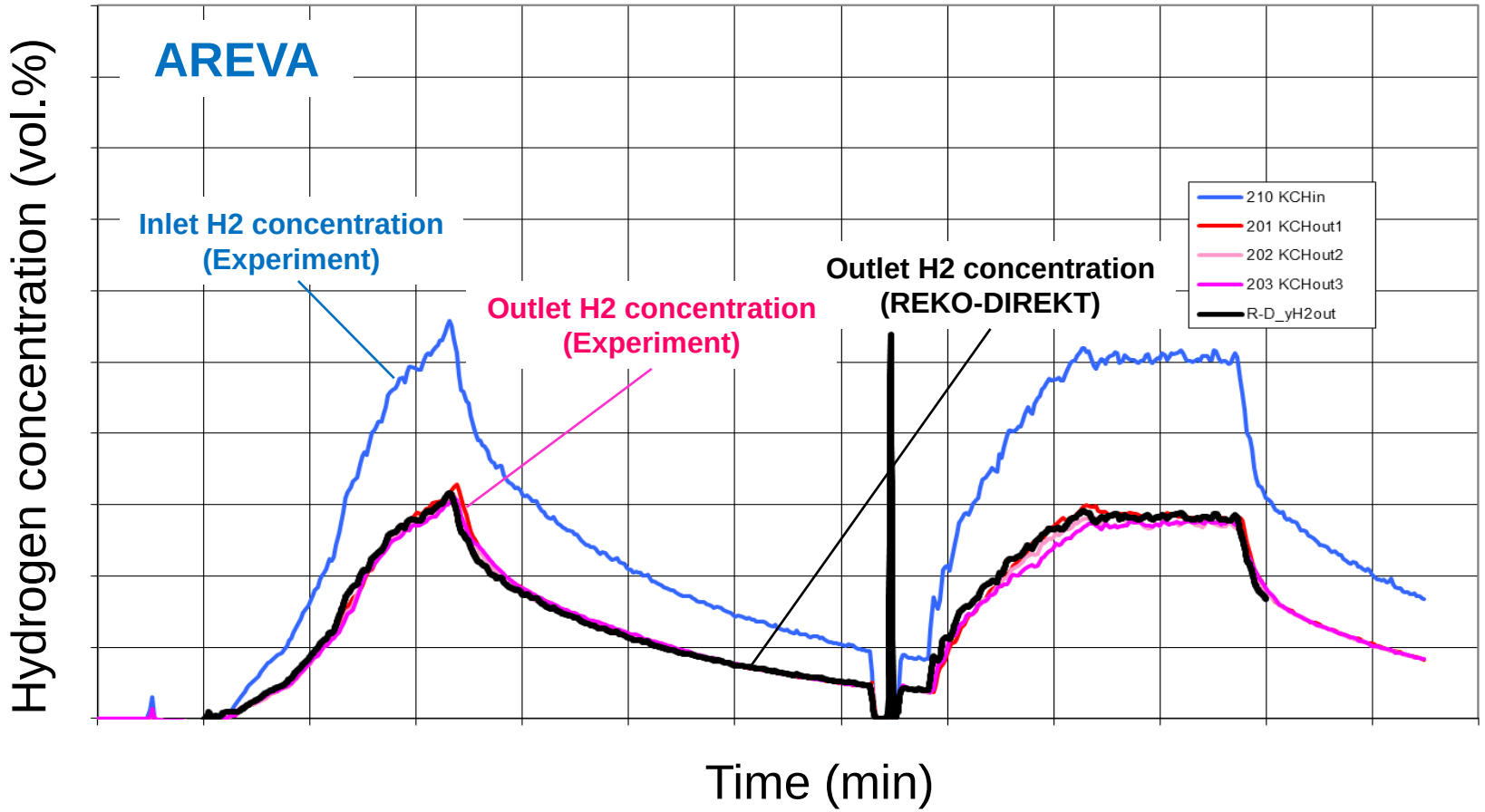
v, T_{cat}

Outlet: T_{gas}, y_i

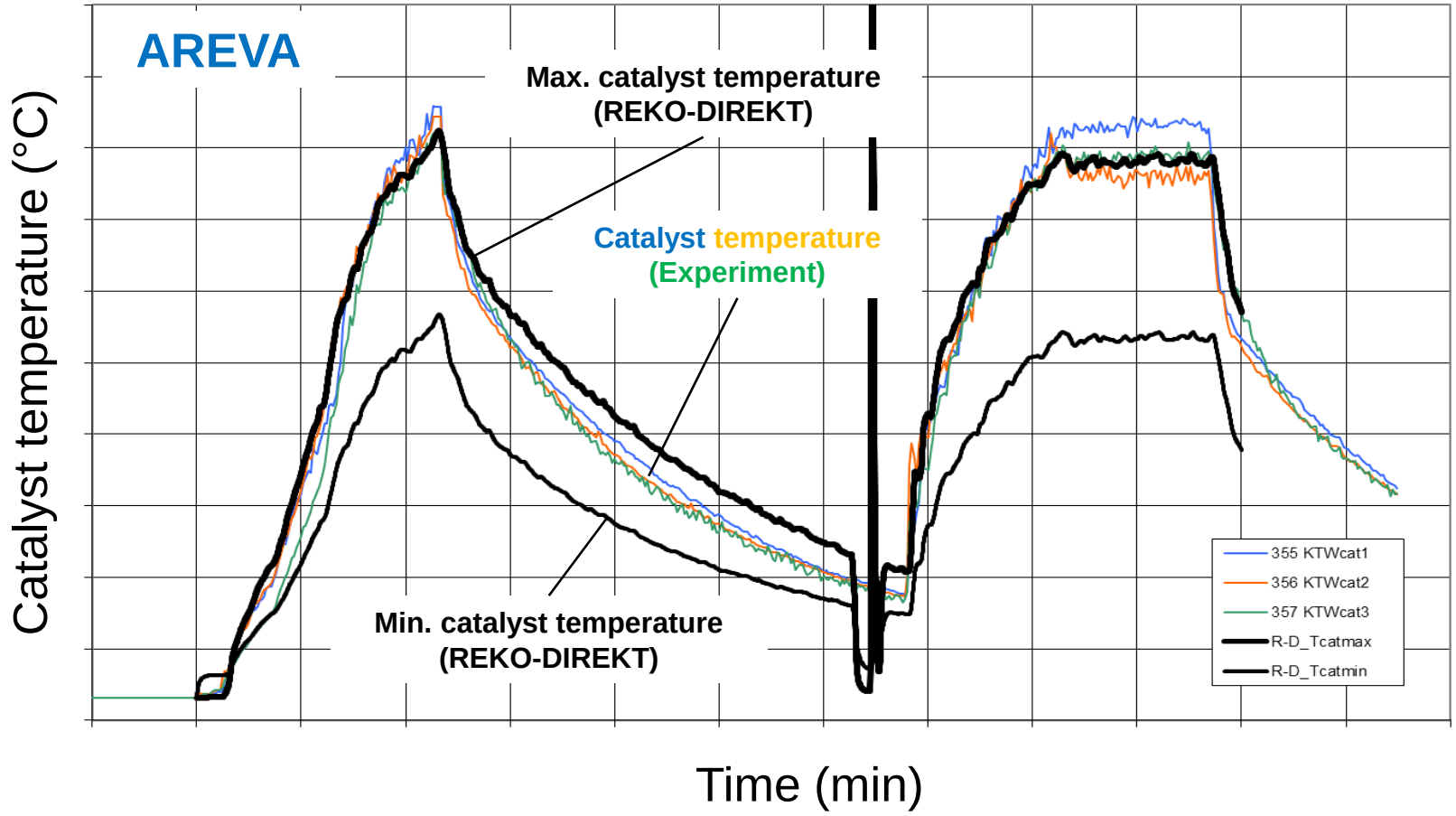
OECD/NEA-THAI HR test series (AREVA)

Test	PAR	Pressure	Temperature	Steam	Oxygen	Ignition
HR-1, HR-2	AREVA	1.0 bar	25°C			Ignition
HR-3, HR-27, HR-28	AREVA	1.5 bar	25°C			Ignition
HR-4	AREVA	2.2 bar	25°C			Multi ignition
HR-5	AREVA	3.0 bar	25°C			
HR-6, HR-7, HR-8	AREVA	1.5 bar	74°C	25%		Ignition
HR-9, HR-10	AREVA	1.5 bar	90°C	47%	O_2 starvation (9)	Ignition (10)
HR-11, HR-29	AREVA	1.5 bar	97°C	60%	O_2 starvation	Ignition (29)
HR-12, HR-30	AREVA	3.0 bar	117 °C	60%	O_2 starvation	Ignition (30)
HR-13	AREVA	1.0 bar	86°C	60%	O_2 starvation	
HR-33	AREVA	1.5 bar	105°C		O_2 starvation (start)	
HR-34	AREVA	1.5 bar	105°C	40%	O_2 starvation (start)	
HR-35	AREVA	3.0 bar	117°C	60%	O_2 starvation (start)	
HR-36	AREVA	1.5 bar	70°C	20%	O_2 starvation	Ignition
HR-37	AREVA	1.5 bar	90°C	30%	O_2 starvation	

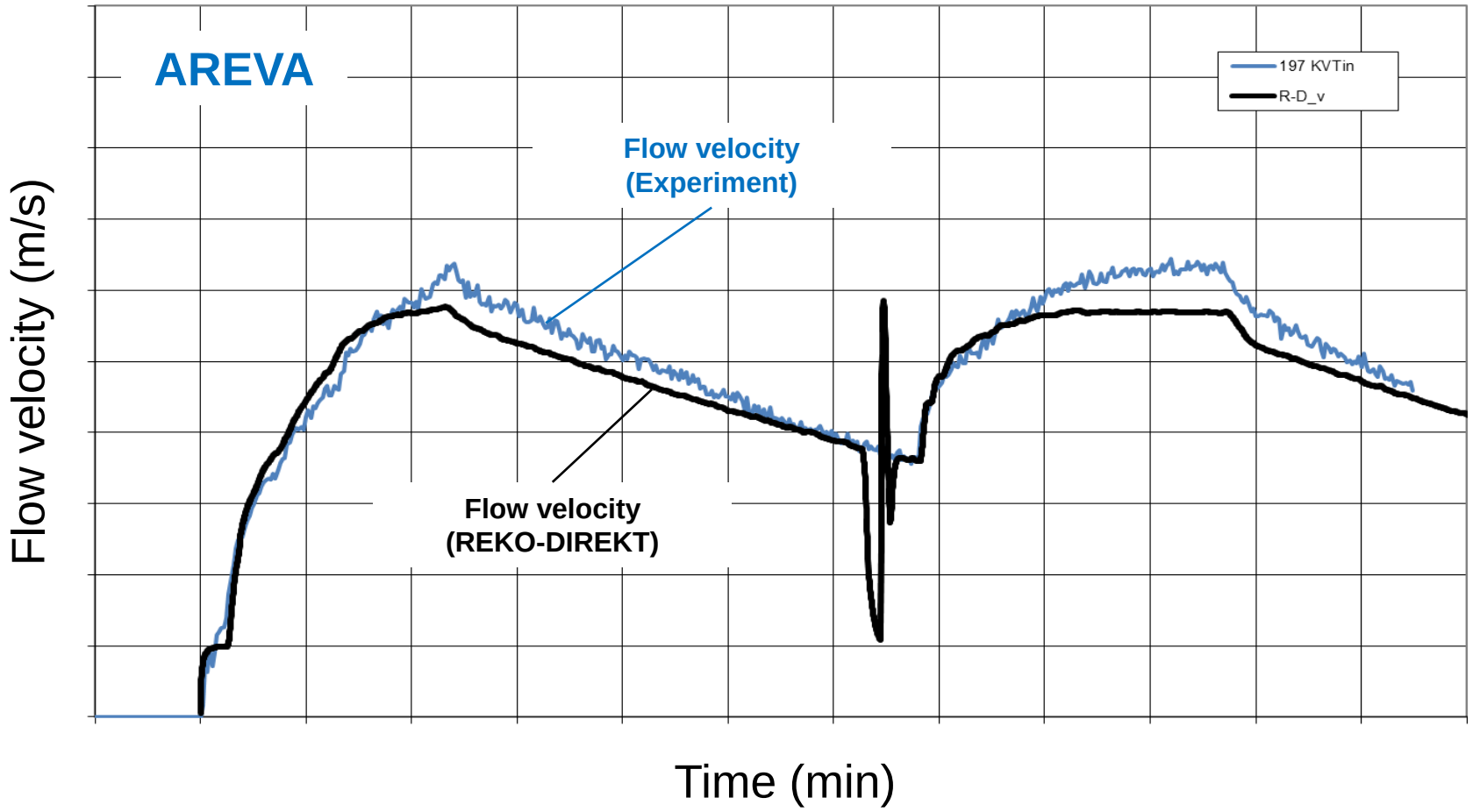
Results: HR-5 – outlet concentration



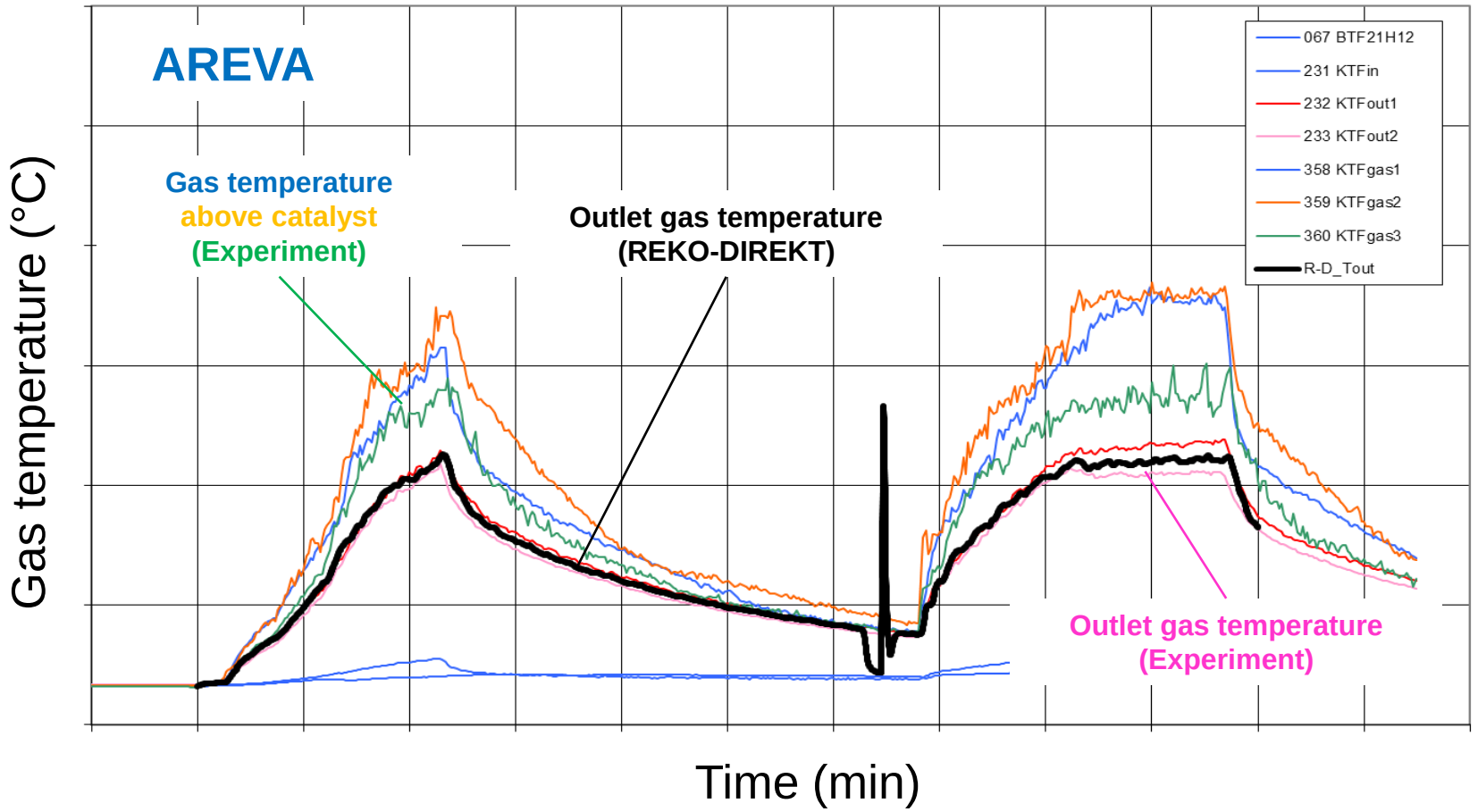
Results: HR-5 – catalyst temperature



Results: HR-5 – flow velocity



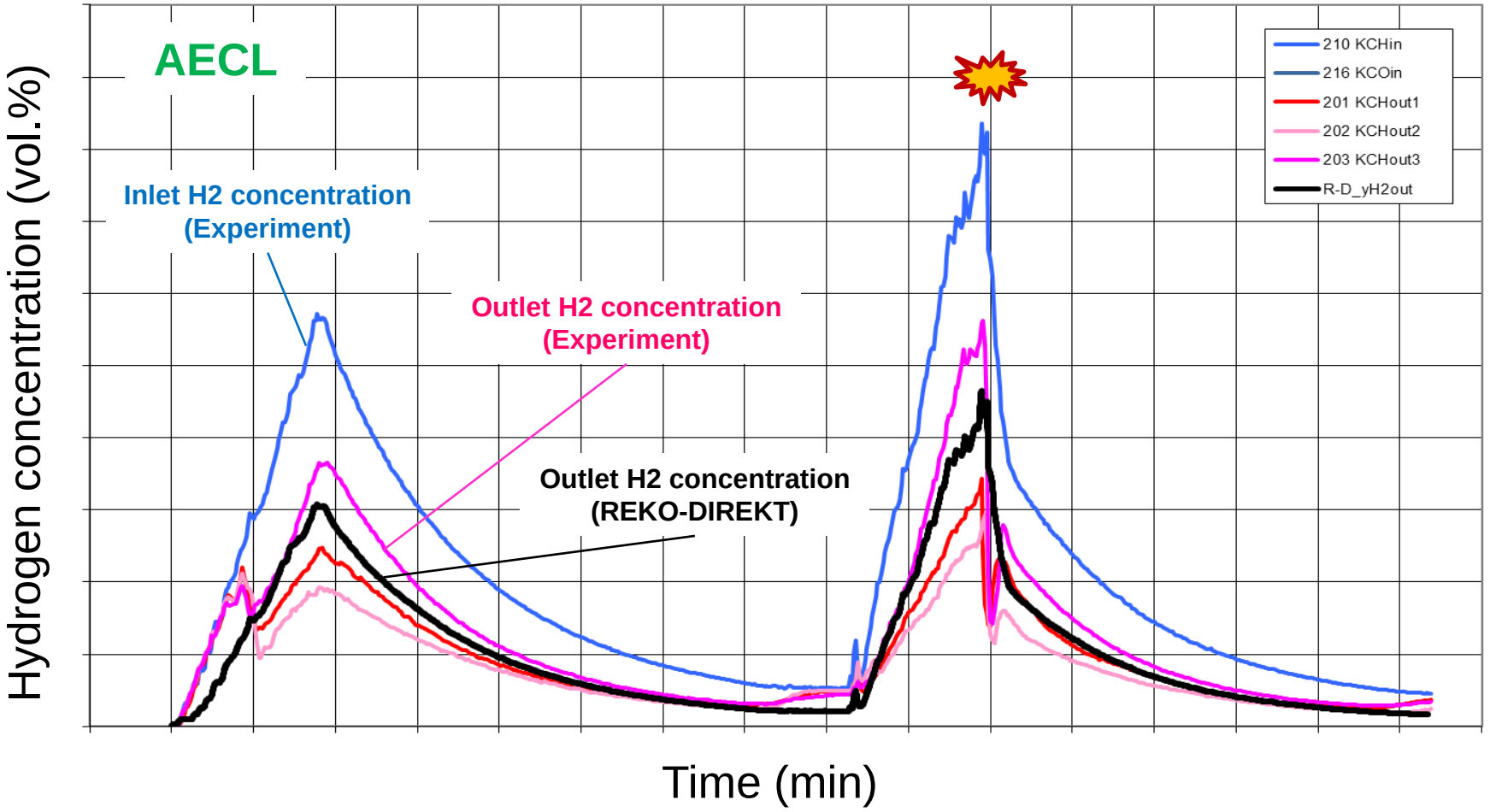
Results: HR-5 – outlet gas temperature



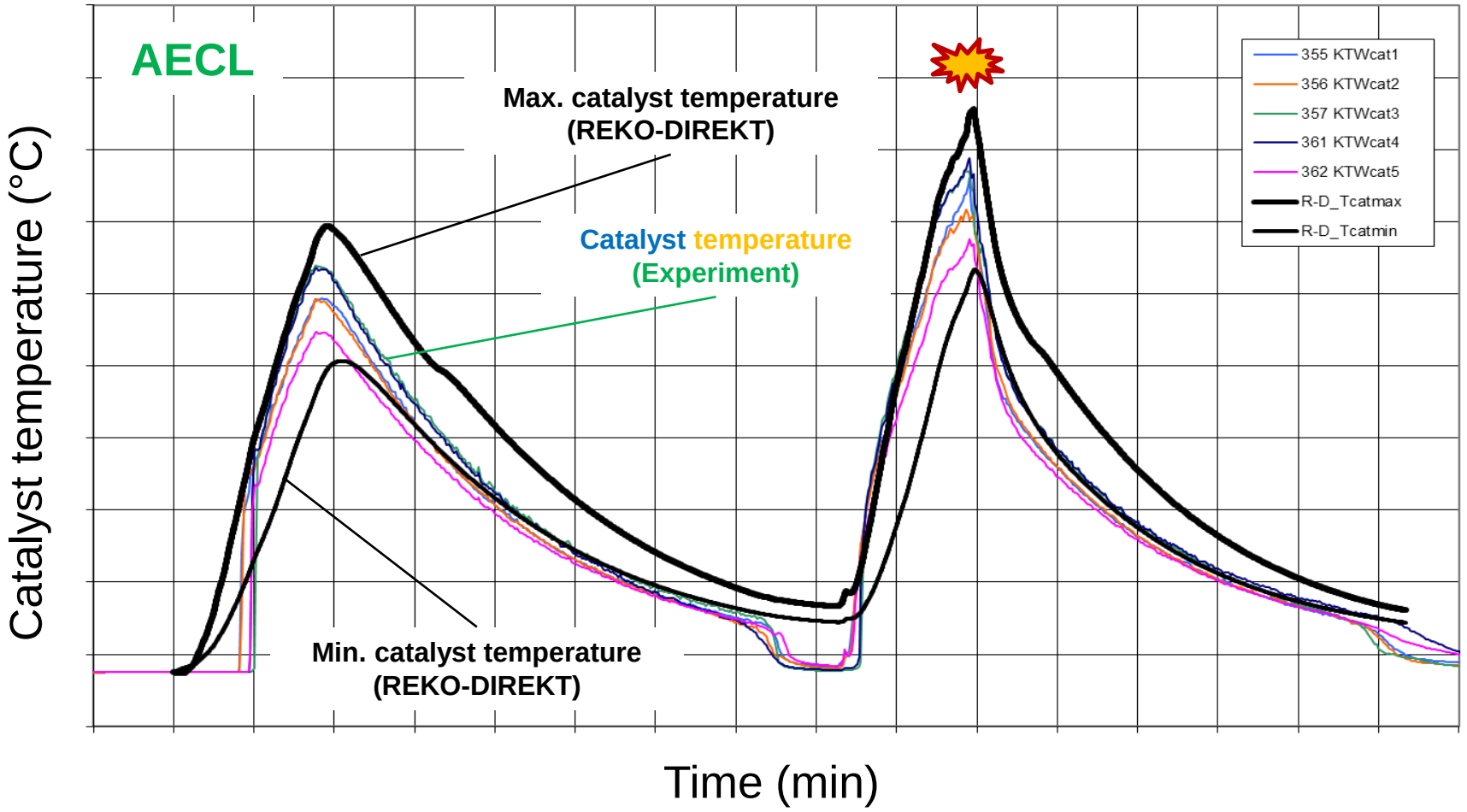
OECD/NEA-THAI HR test series (AECL)

Test	PAR	Pressure	Temperature	Steam	Oxygen	Ignition
HR-17, HR-18	AECL	1.5 bar	25°C			Ignition
HR-19	AECL	1.5 bar	74°C	25%		Ignition
HR-20	AECL	1.5 bar	90°C	47%		Ignition
HR-21	AECL	2.2 bar	108°C	34%	O_2 starvation	
HR-22	AECL	1.5 bar	97 °C	60%	O_2 starvation	
HR-23	AECL	1.0 bar	25°C			Ignition
HR-24, HR-25, HR-26	AECL	2.2 bar	25°C			Ignition

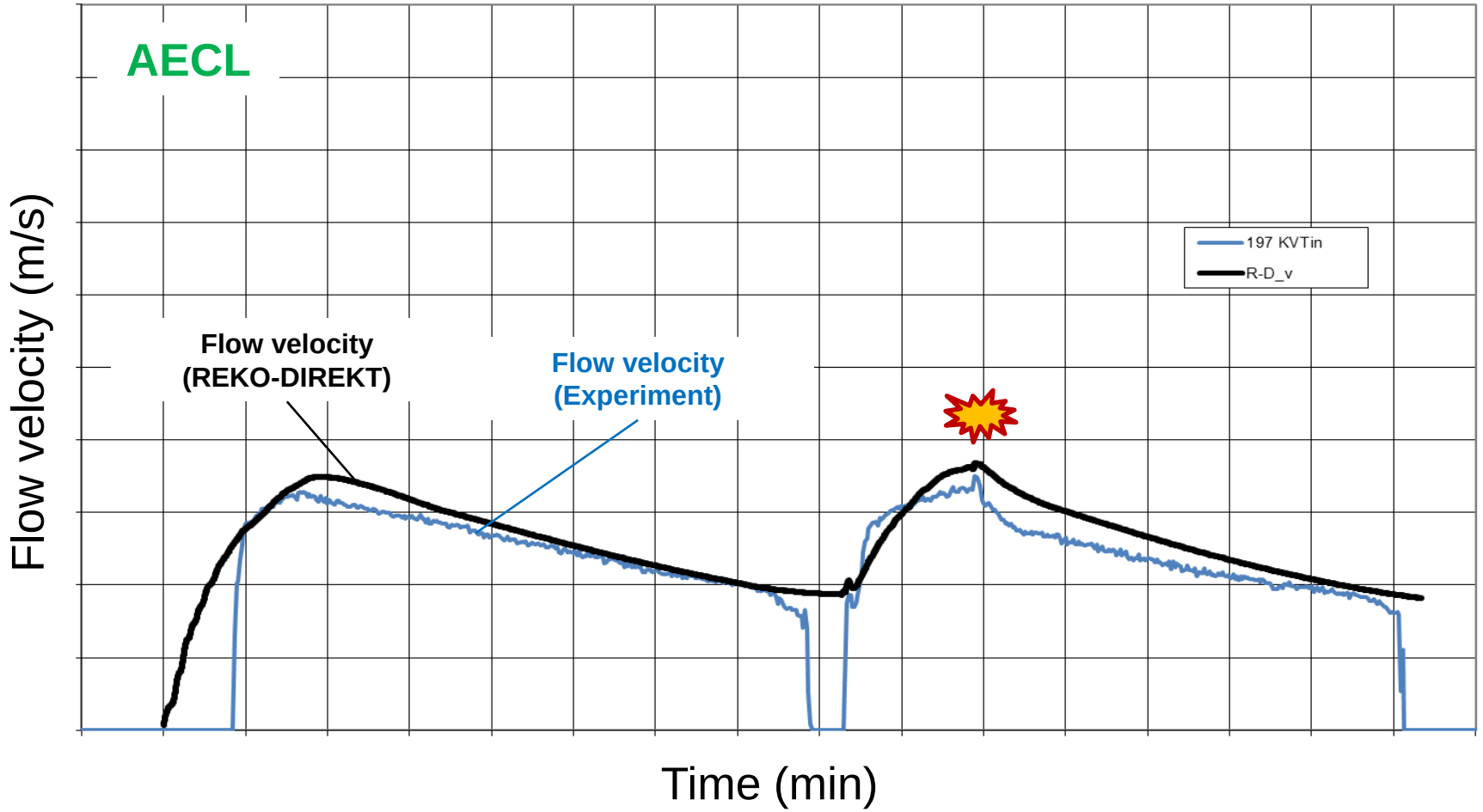
Results: HR-19 – outlet concentration



Results: HR-19 – catalyst temperature



Results: HR-19 – flow velocity



Overall results

Test	PAR	Pressure	Temperature	Steam	Oxygen	Ignition
HR-1, HR-2	AREVA	1.0 bar	25°C			Ignition
HR-3, HR-27, HR-28	AREVA	1.5 bar	25°C			Ignition
HR-4	AREVA	2.2 bar	25°C			Multi ignition
HR-5	AREVA	3.0 bar	25°C			
HR-6, HR-7, HR-8	AREVA	1.5 bar	74°C	25%		Ignition
HR-9, HR-10	AREVA	1.5 bar	90°C	47%	O_2 starvation (9)	Ignition (10)
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HR-37	AREVA	1.5 bar	90°C	30%	O_2 starvation	

AREVA

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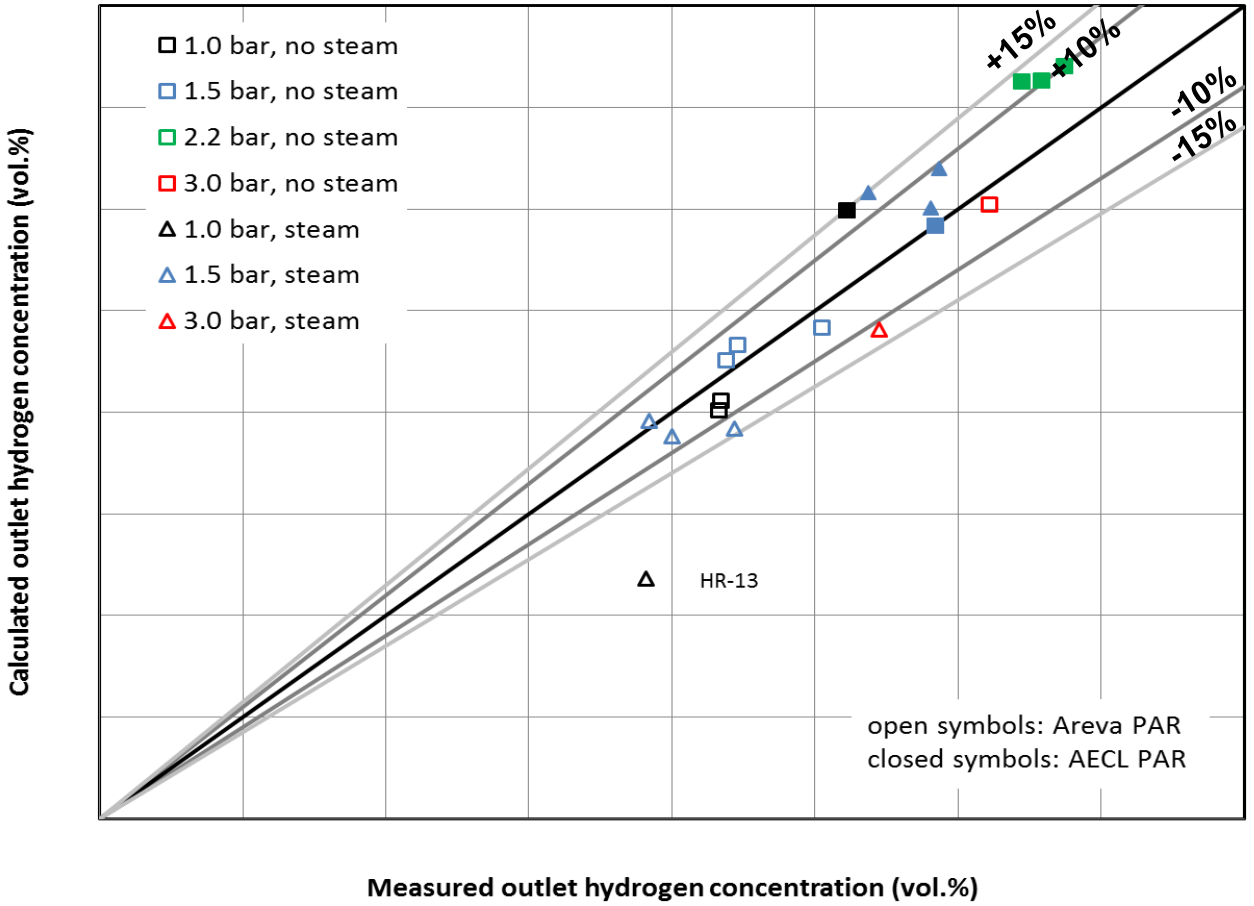
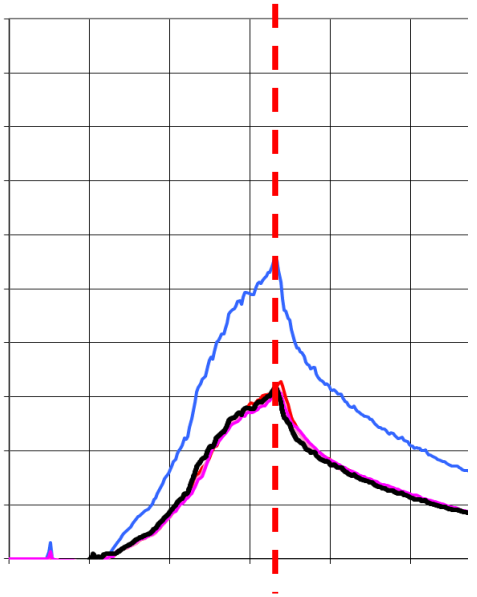
HR-23	AECL	1.0 bar	25°C			Ignition
HR-24, HR-25, HR-26	AECL	2.2 bar	25°C			Ignition

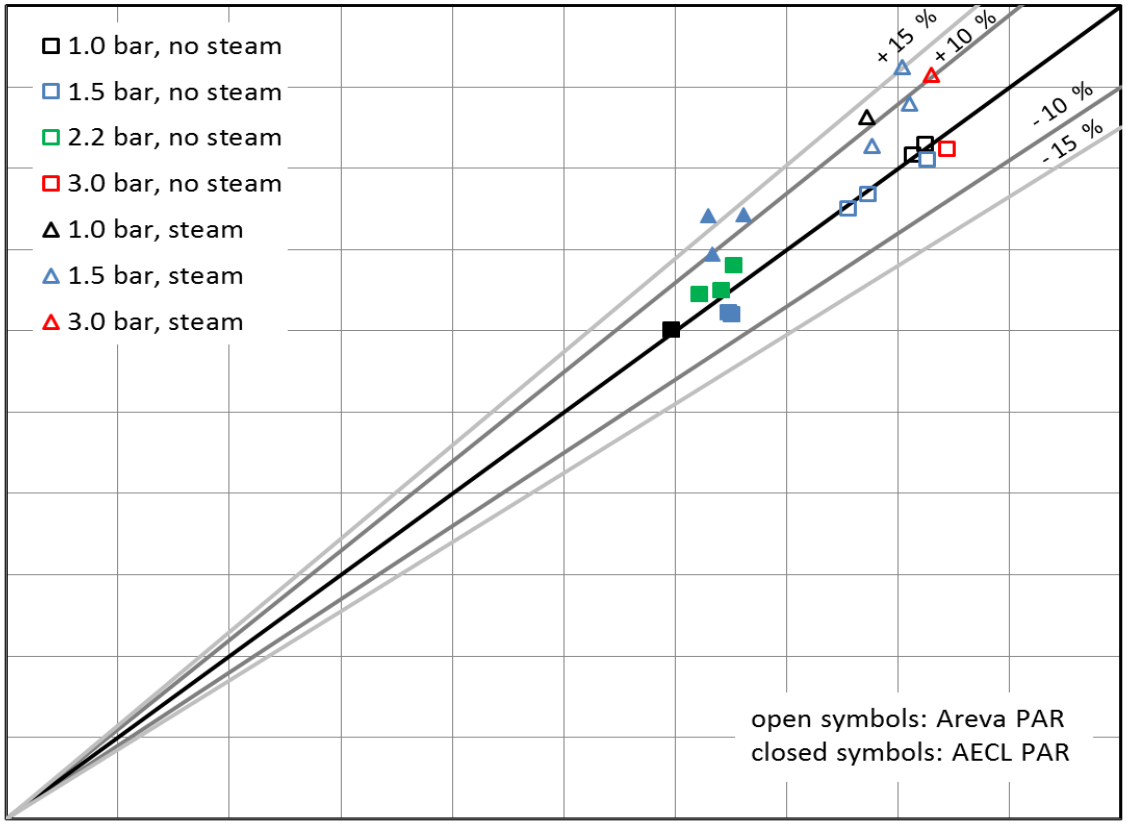
AECL

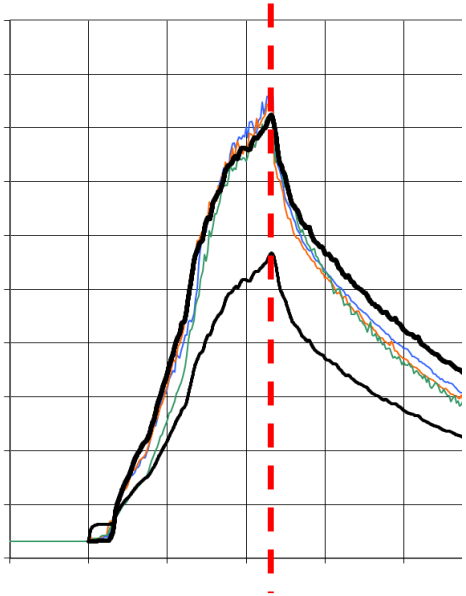
Overall results: outlet concentration



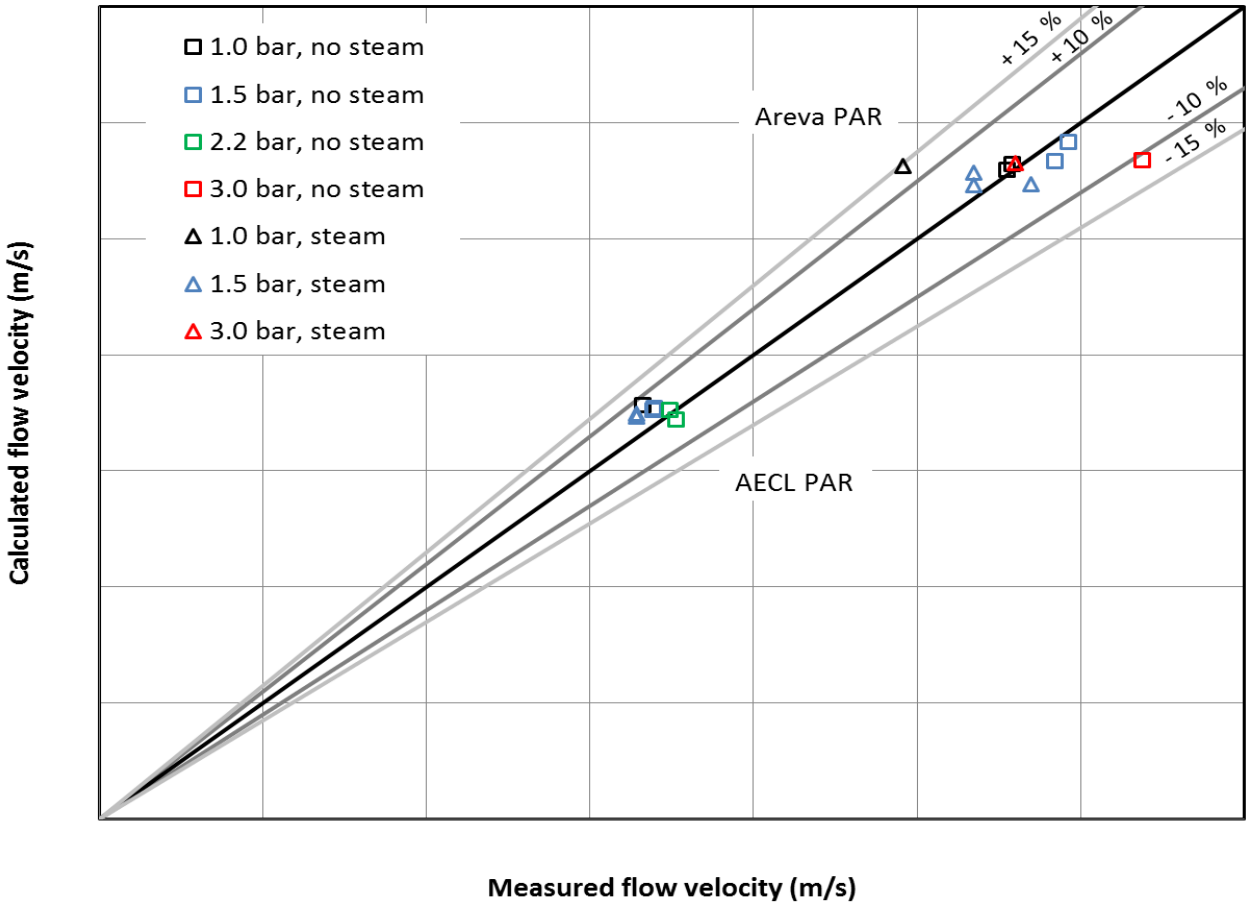


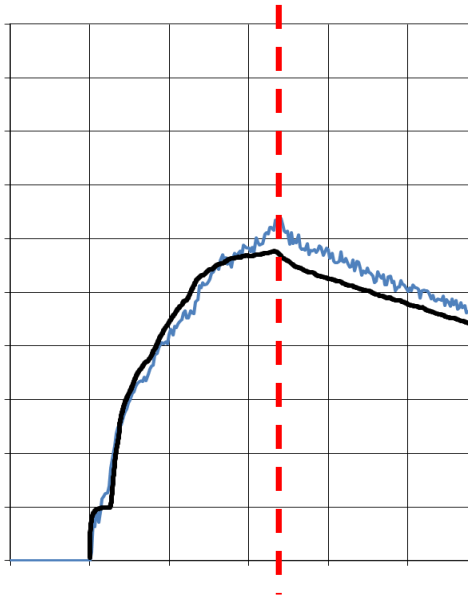
Overall results: catalyst temperature





Overall results: flow velocity





Conclusions

- OECD/NEA-THAI-HR: Comprehensive data base for the validation of stand-alone PAR models and coupled PAR-TH codes
- Broad range of boundary conditions (pressure, gas composition) and PAR geometry
- 32 HR experiments including AREVA and AECL PARs have been simulated with REKO-DIREKT
- Convincing validation results support the modelling approach used in REKO-DIREKT

Outlook

- Room for improvement (REKO-DIREKT)
  - Transient catalyst temperature and flow velocity
  - Catalyst temperature in presence of steam
  - Ignition modelling
- Open issues in understanding PAR behaviour in OECD/NEA-THAI
  - Start-up behaviour
  - Ignition mechanism

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