

Modeling of hydrogen sulfide removal from hot coal syngas in a coal-to-hydrogen pilot plant

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CO.HY.GEN project research: Partners



Ansaldo Ricerche S.r.l.



Università di Cagliari



ENEA

(Ente Nazionale Energie Alternative)

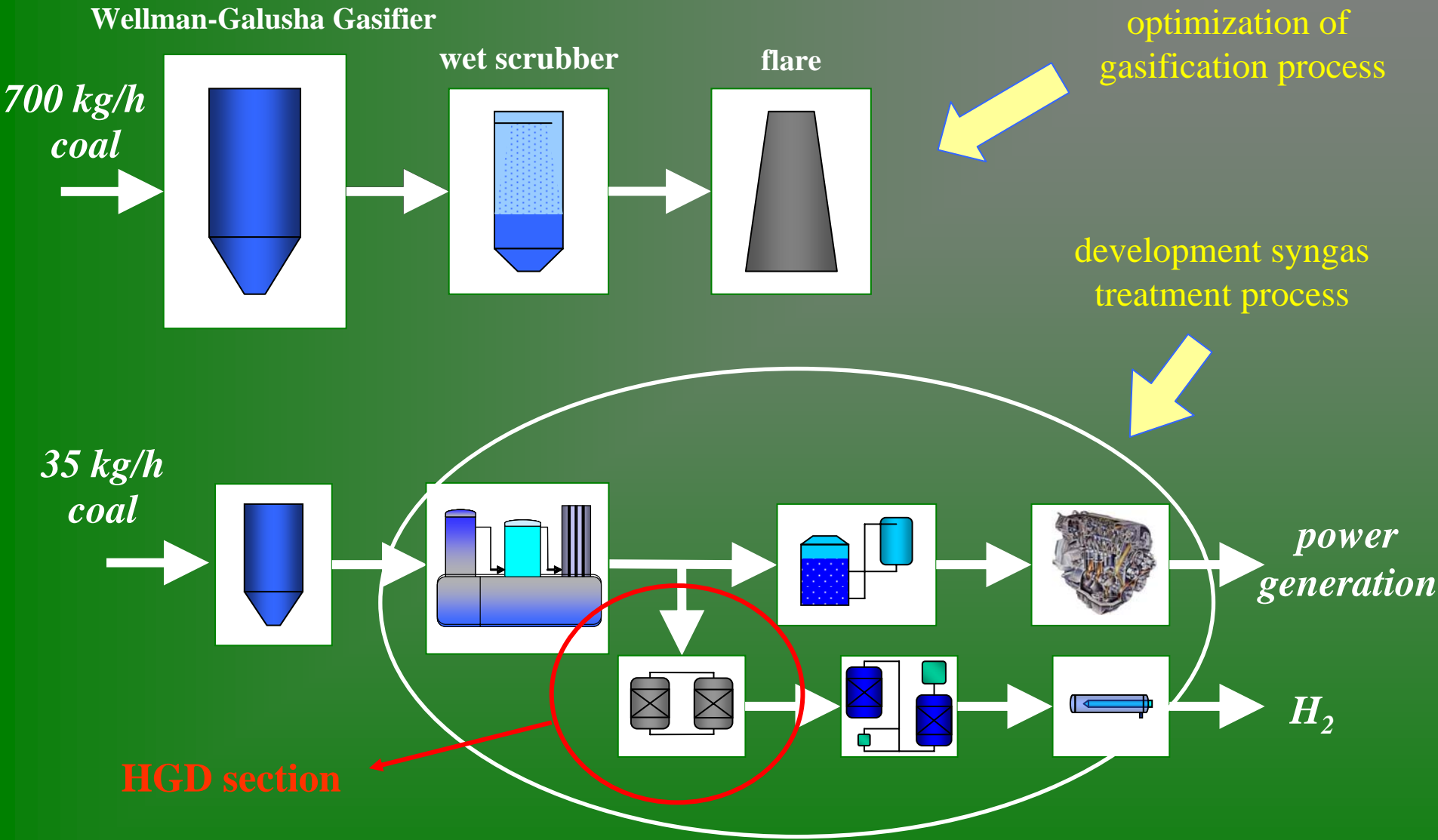
CO_{mbustion} to HY_{drogen} GEN_{eration}

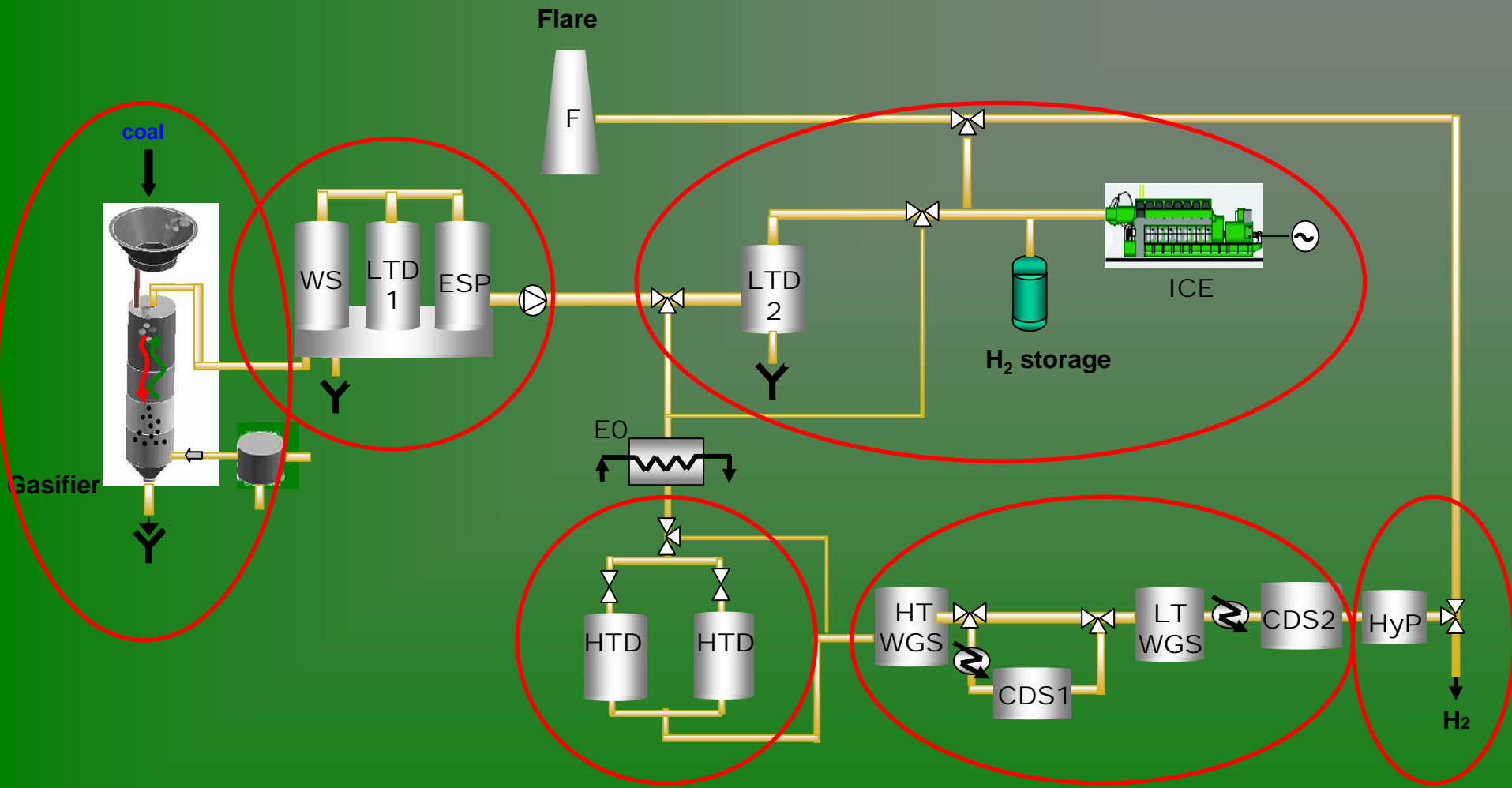


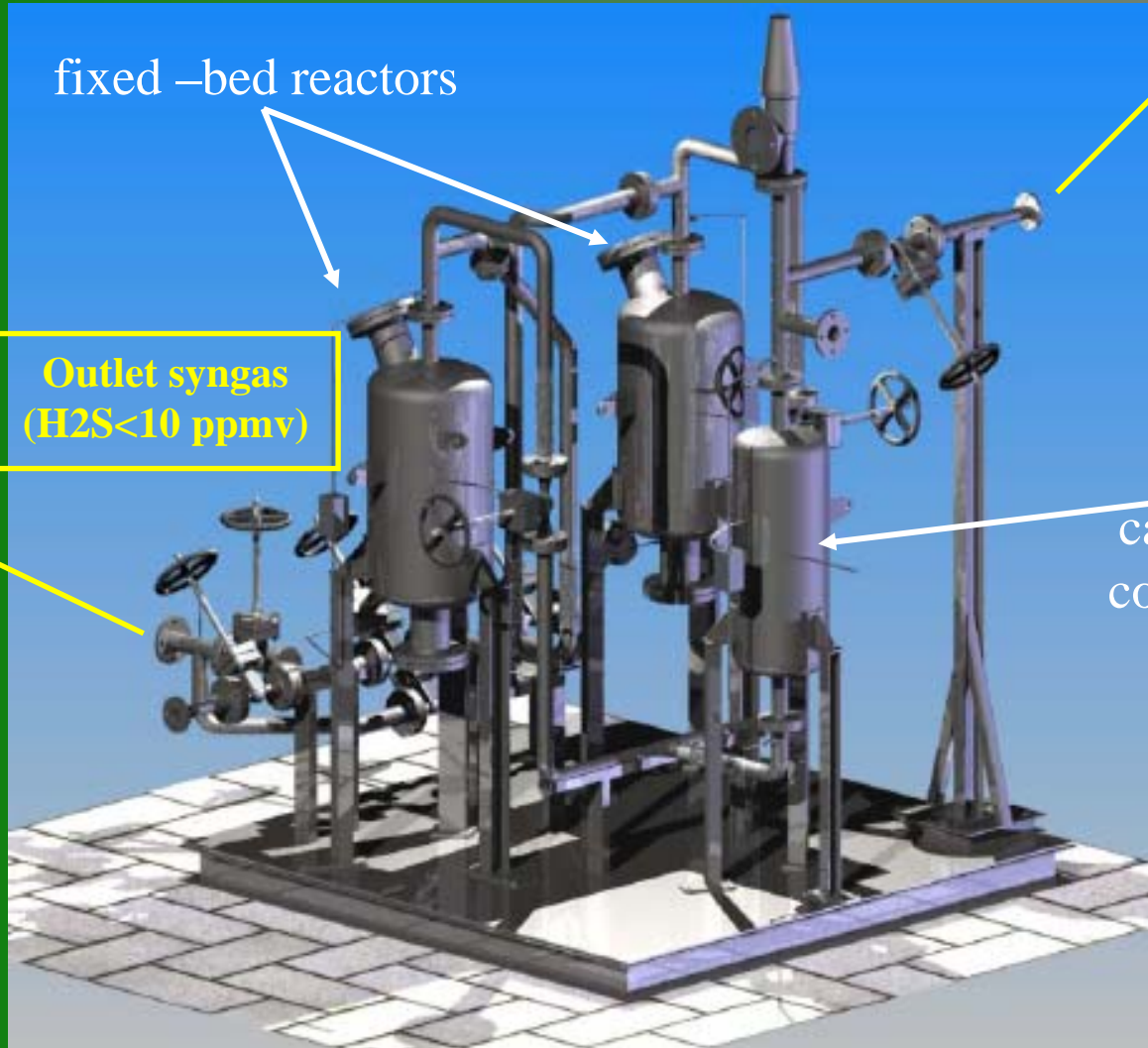
*MIUR – Ministero dell'educazione,
dell'università e della ricerca scientifica*



European structural funds







fixed-bed reactors

Outlet syngas
(H₂S < 10 ppmv)

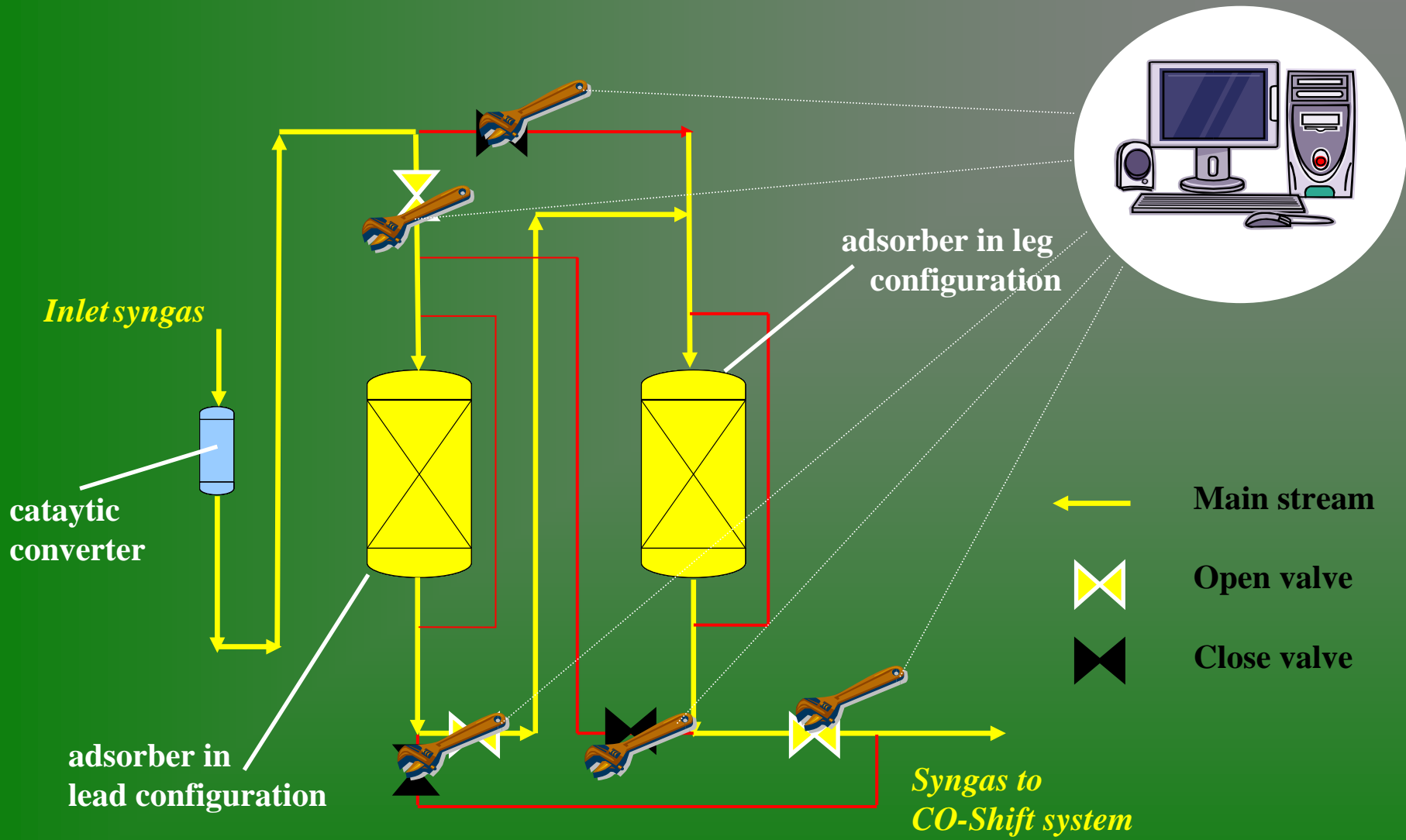
Inlet syngas
(H₂S 10⁴-10³ ppmv)

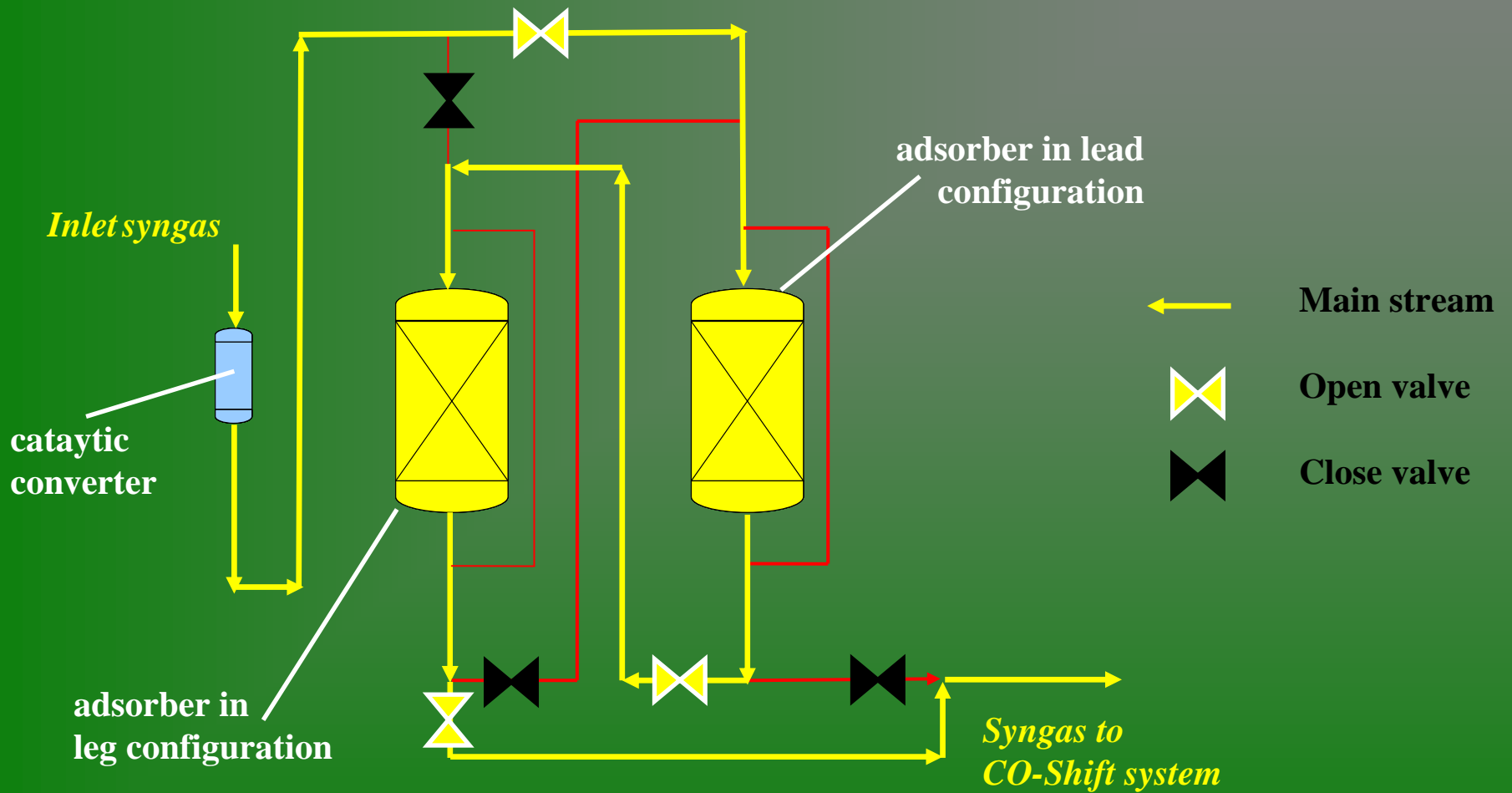
catalytic converter

Operating conditions:

T=300-425 °C

P=1.4 bars

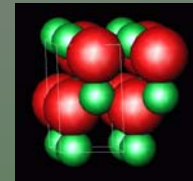




Metal oxides

Fe_2O_3
 $\text{Fe}_2\text{O}_3 * \text{ZnO}$
 ZnO
 $\text{ZnO} * \text{TiO}_2$

ZnO

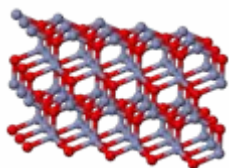


KATALCO 32-5 Hydrogen Sulphide Absorbent



Product Benefits

- Low and stable pressure drop due to high particle strength
- Very high H₂S capacity due to high density coupled with high porosity giving a high accessible zinc oxide content per volume of absorbent
- Optimized for systems with “lead/lag” operation
- Reliable performance and long predictable lives
- Excellent performance over a wide range of operating conditions
- Sulphur removal to very low levels
- Easier disposal because sulphur is chemically absorbed to give stable zinc sulphide



General Description

- **KATALCO 32-5** is a high porosity, spherical zinc oxide absorbent

	Physical Properties (Typical)		Chemical Composition (Typical)	
	Form	Spherical granules		ZnO
Size	2.8 – 4.75 mm diameter		Binder	Balance
Bulk Density	1400 kg/m ³		(CaO/Al ₂ O ₃)	
Surface Area	35 m ² /g			
Pore Volume	0.26 ml/g			

Assumptions:

→ gas- solid reaction: $\text{H}_2\text{S} + \text{ZnO} = \text{H}_2\text{O} + \text{ZnS}$

→ DP negligible → Momentum equation is neglected

→ No radial mixing ($DR/dp > 10$)
Axial back-mixing negligible → Ideal plug-flow reactor

Mass-balance equations

- Gas-phase reactans
- Inert-phase

Energy-balance equation

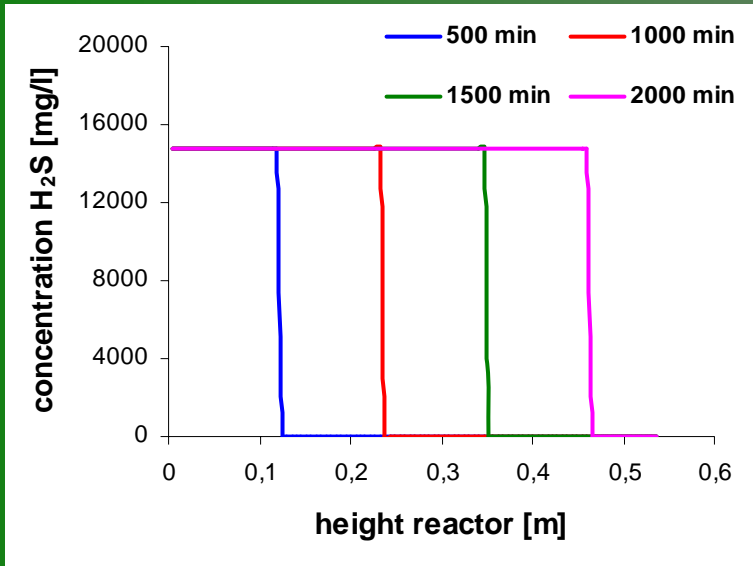
$$\left\{ \begin{array}{l} \frac{dN_{H_2S}}{dz} = -S\rho_s(1-\mathcal{G})R_{H_2S} \\ \frac{dH}{dz} = R_{H_2S}S\rho_s(1-\mathcal{G})(-\Delta H_r) - \pi D_r U(T - T_e) - S\rho_s(1-\mathcal{G})C_{psol} \frac{dT}{dt} \end{array} \right.$$

Shrinking core model

Limiting steps:

mass transfert and internal pores diffusion

Implementation using **FORTRAN** code with contribution of **DICM**



Breakthrough curves
(T= 375°C, Sulcis coal feed)

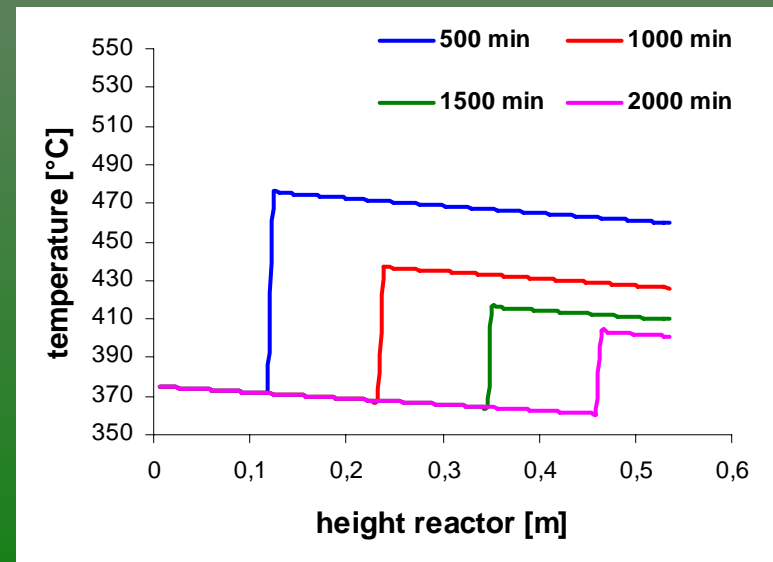


Breakthrough time in about 3,5 h

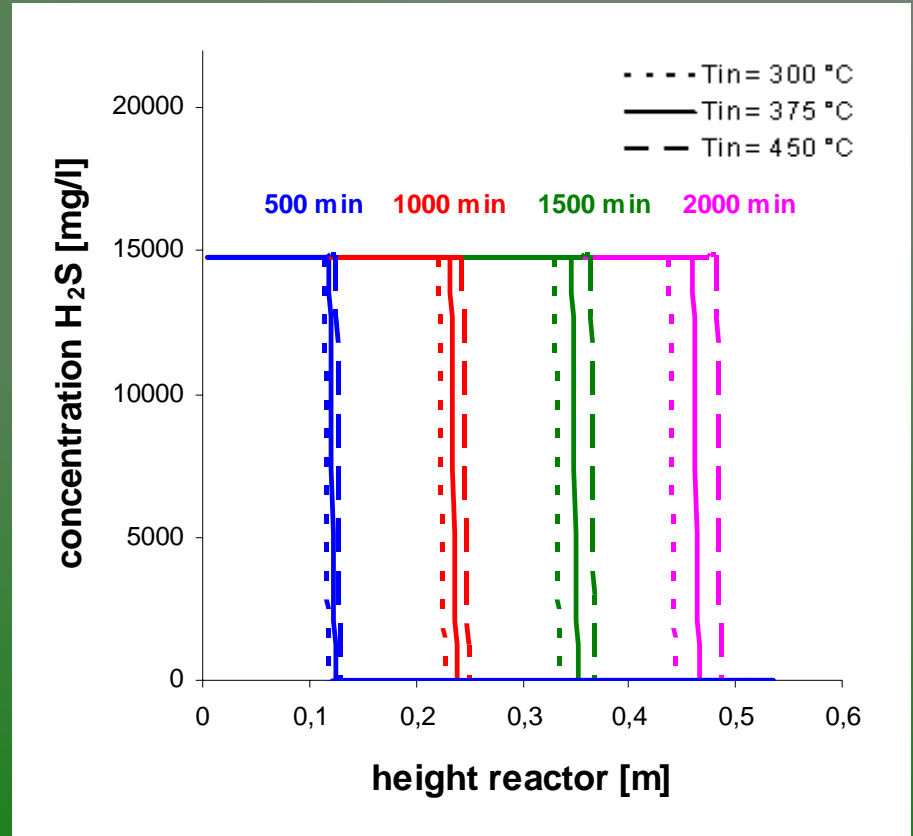
Thermal profile
(T= 375°C, Sulcis coal feed)



Hot spot due to reaction front



**Comparison of
different operating temperature
(Sulcis coal syngas derived)**

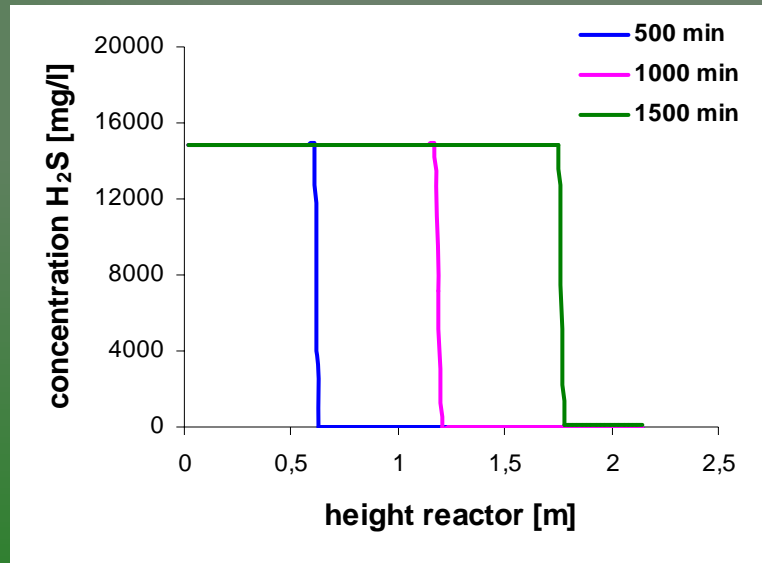


Model limits

Ideal PFR assumption



**Step-shape of
breakthrough
curves**

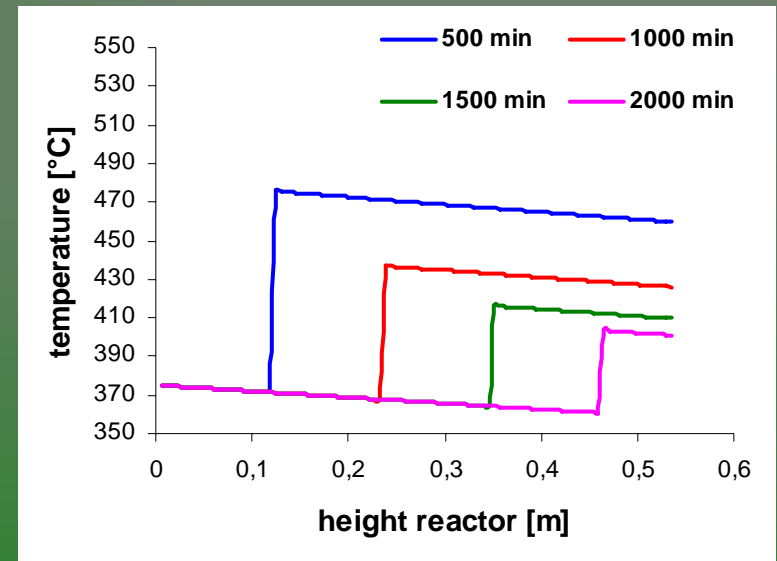


Model limits

Effect of scale-up
on heat exchange

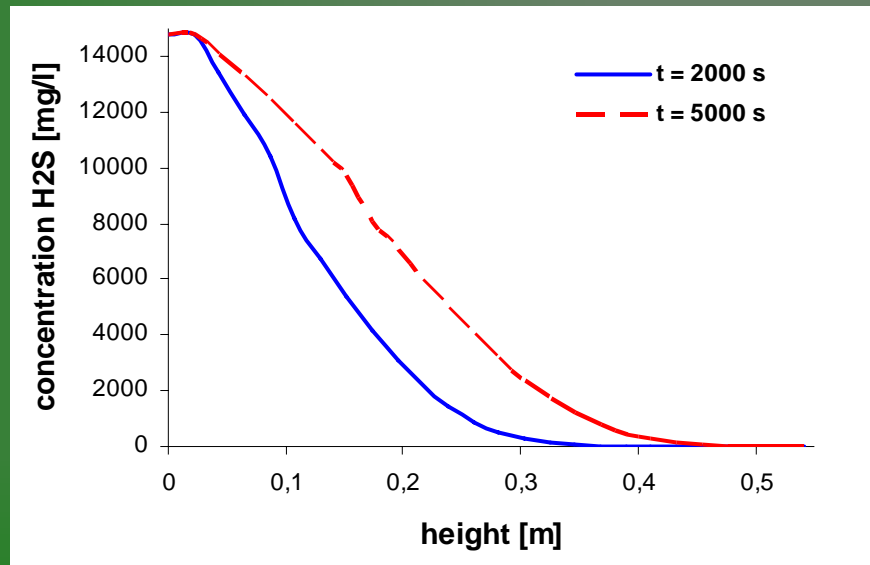


**Decreasing of
reaction
temperature**



Model improvements

Effect of axial back-mixing (*preliminary results*)



Activities in modeling of hydrogen sulfide removal from hot coal syngas in a coal-to-hydrogen pilot plant

- Process analysis of hot gas removal system adopted model improvements
- Development of a ideal assumptions-based mathematical model
- Analysis of model results and limits
- Bases for model improvements

Studies for model improvements are still in progress

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