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Validation strategy for CFD models describing safety-relevant scenarios including LH2/GH2 release and the use of passive autocatalytic recombiners

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Motivation

Safety during storage and transportation of liquid hydrogen (LH2) is essential.

Prediction of the distribution of accidently released gaseous and liquid hydrogen and mitigate the consequences is needed.

Usage of a commercial CFD code:

the model can be easily combined, exchange of experience and models easily possible.

Storage and Transportation

1)

3)

4)

2)

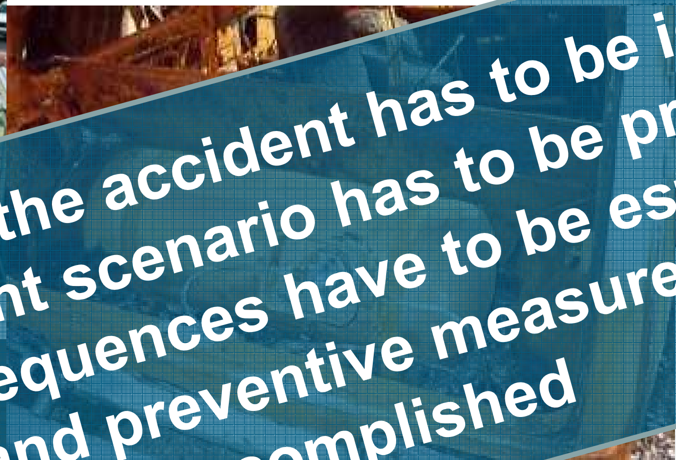
5)

1) http://www.lngworldnews.com/french-fos-tonkin-terminal-receives-5500th-lng-tanker/
2) http://www.jari.or.jp/jhfc/e/station/kanto/ariake.html
3) http://www.blewbury.co.uk/energy/hydrogen.htm
4) http://www.energy-without-carbon.org/HydrogenDistribution

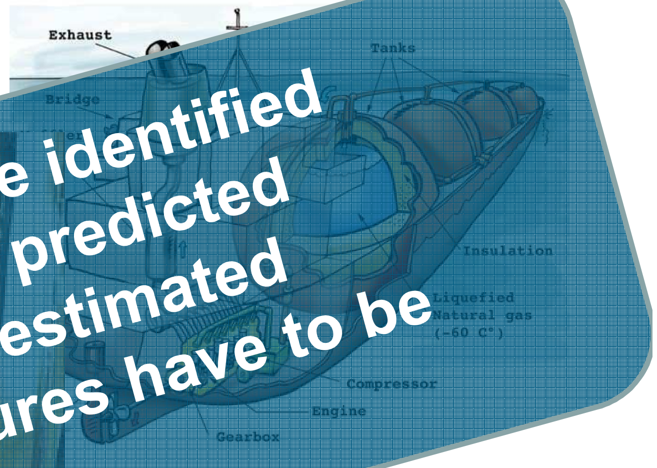
Accident scenarios

1)

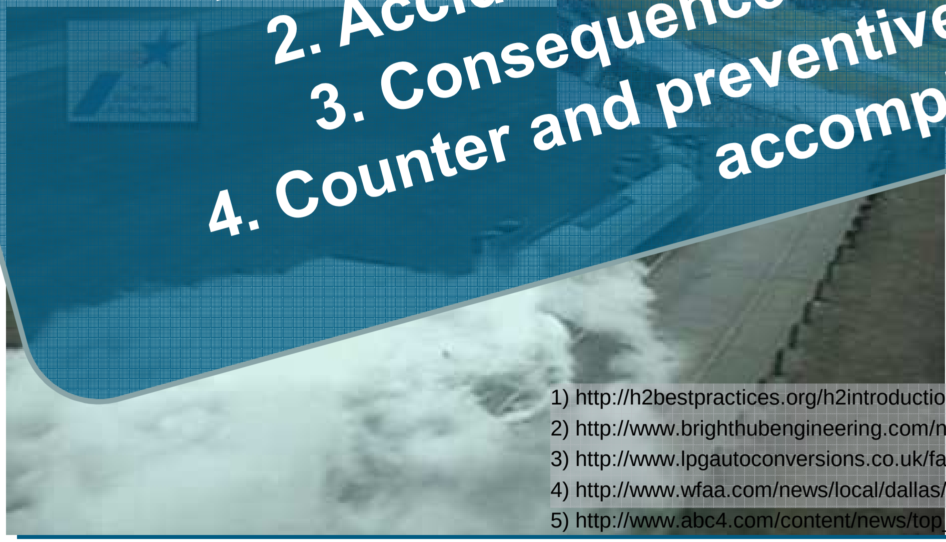
3)



4)



2)

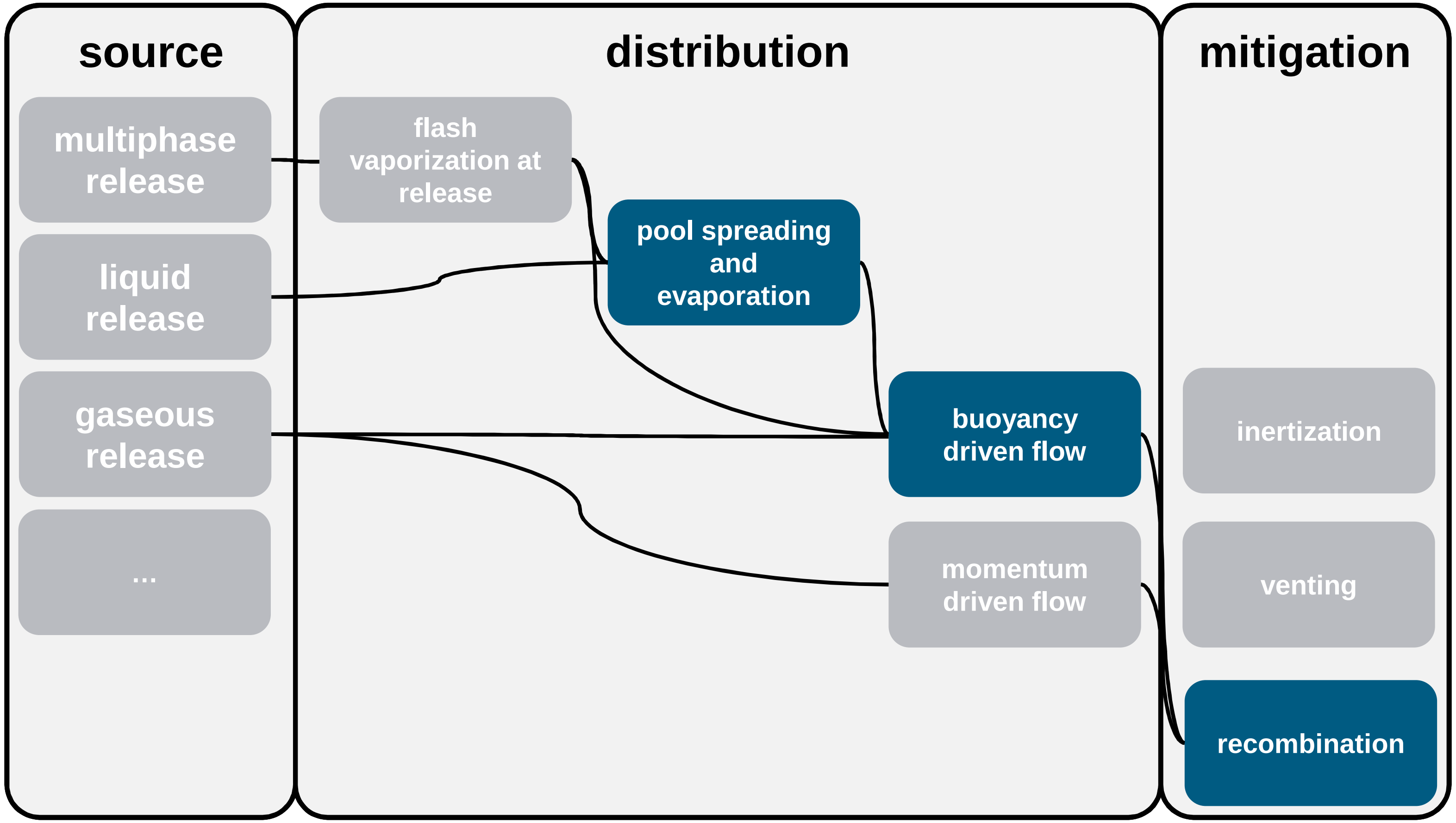


5)

1. Cause of the accident has to be identified
2. Accident scenario has to be predicted
3. Consequences have to be estimated
4. Counter and preventive measures have to be accomplished

1) http://h2bestpractices.org/h2introduction/basics/liquid_behaviors.asp
2) http://www.brighthubengineering.com/naval-architecture/111619-propulsion-methods-for-modern-lng-tankers/
3) http://www.lpgautoconversions.co.uk/faq/index.php
4) http://www.wfaa.com/news/local/dallas/Overturned-tanker-truck-leaking-liquid-nitrogen-near-I-20-in-S-Dallas-215564771.html
5) http://www.abc4.com/content/news/top_stories/story/Liquid-nitrogen-leak-in-Salt-Lake-City/cfiKMUdQhEyLXSYRmie8yQ.cspx

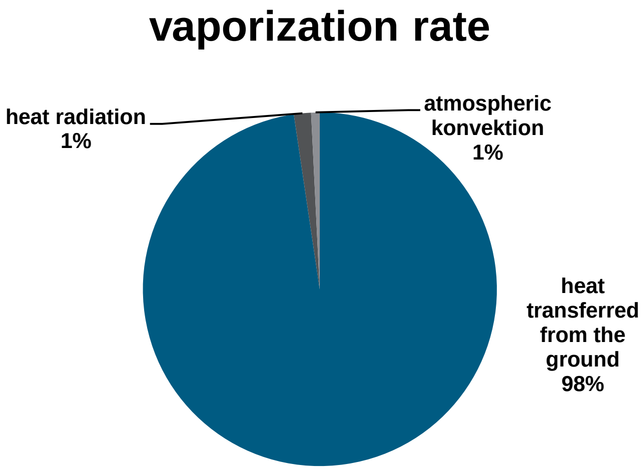
Generic accident sequence

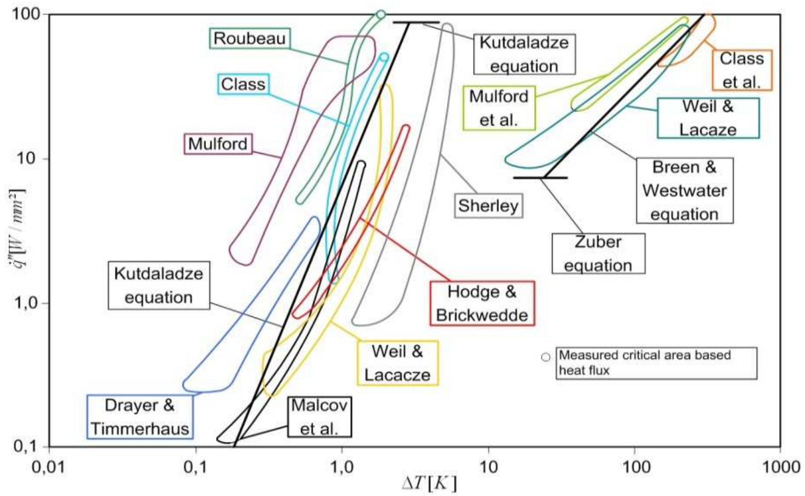


Validation Matrix

	Test / Phenomenon	NASA	HSL	BAM	Garage (CEA)	THAI (Becker Technologies)	REKO-3/4 (JÜLICH)	MISTAR (CEA)	PANDA (PSI)
pool spreading and evaporation	LH2 release	X	X						
	LH2 flash vaporization	(X)	(X)						
	LH2 pool spreading	(X)	X	X					
buoyancy driven flow	GH2 cloud distribution	X	X						
	GH2 transport and mixing				X	X	X	X	X
recombination	PAR thermal effects							X	X
	PAR atmosphere interaction					X	X		

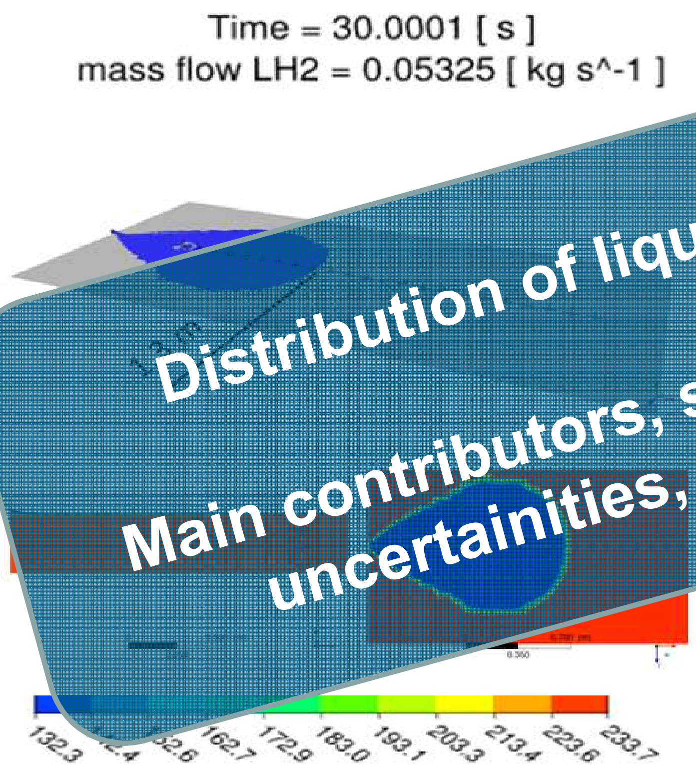
Pool distribution and wall vaporization rate - model



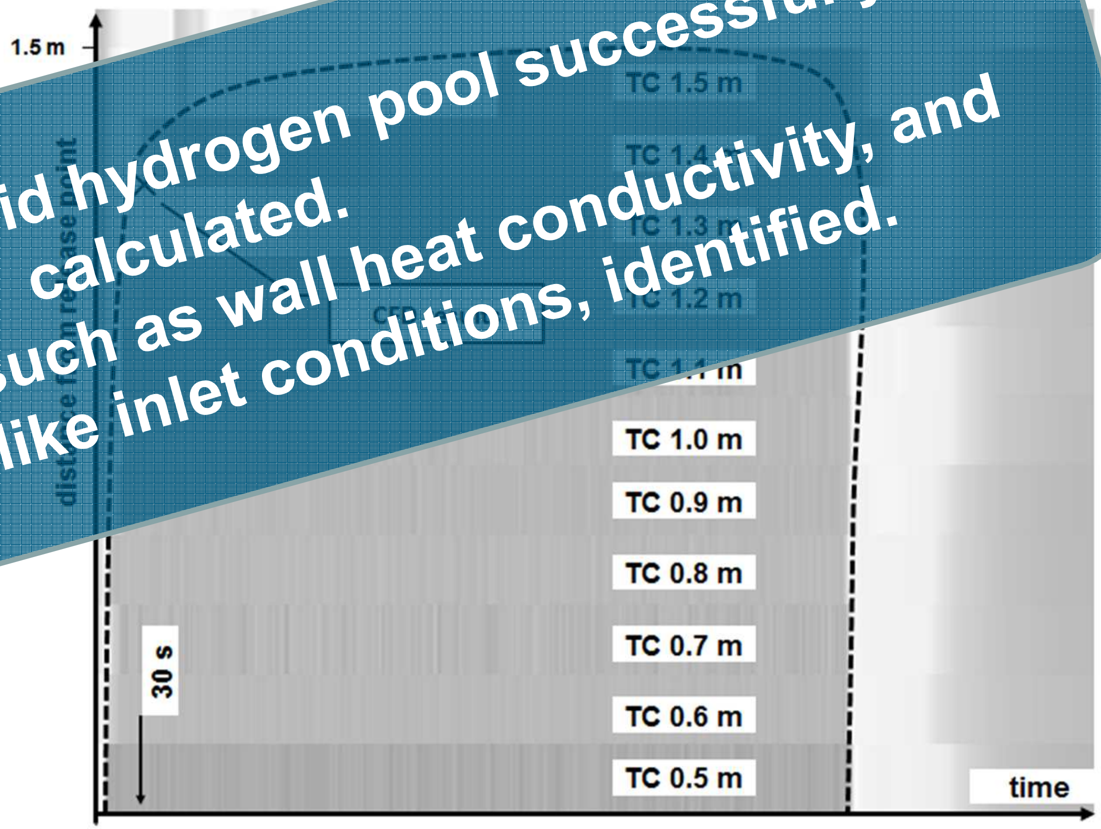


- Heat transfered from the wall/ground is a main contributing factor for pool distribution
- Heat transfered using hydrogen Nukiyama diagramm for hydrogen in dependence of the wall temperature
- Implemented into CFX using CEL user routines

Pool distribution and wall vaporization rate - validation



HSL experiment



Distribution of liquid hydrogen pool successfully calculated.

Main contributors, such as wall heat conductivity, and uncertainities, like inlet conditions, identified.

1. Jaekel C., Verfondern K., Kelm S., Jahn W., Allelein H.-J., 3D Modeling of the Different Boiling Regimes During Spill and Spreading of Liquid Hydrogen, Energy Procedia, Volume 29, 2012, Pages 244-253, ISSN 1876-6102, 10.1016/j.egypro.2012.09.030.

Gas dispersion of hydrogen

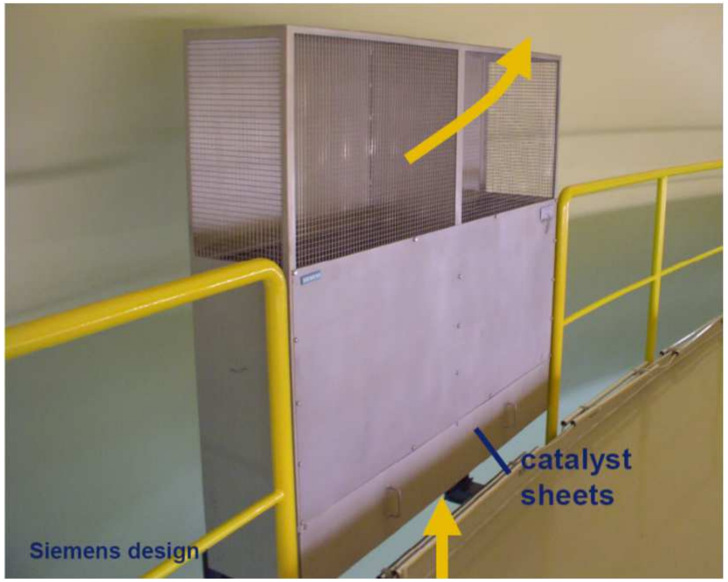
- Gas dispersion mainly driven by buoyancy
- Buoyancy and mixing gas is predicted by using models implemented in ANSYS CFX
- Production and dissipation of turbulence due to buoyancy considered by means of additional terms in the k and ω equation
- Modeling and validation is performed under consideration of well-known best-practice guideline, such as ERCOFTAC and ECORA

1. Menter F. et al. “CFD Best Practice Guidelines for CFD Codel Validation for Reactor Safety Applications, EU-ECORA Project, EC Contract No FIKS-CT-2001-00154, 2001
2. Casey M., T. Wintergerste, “ERCOFTAC Special Interest group on Quality and Trust in Industrial CFD – Best Practice Guidelines”, ERCOFTAC (2000)

Gas dispersion and mitigation

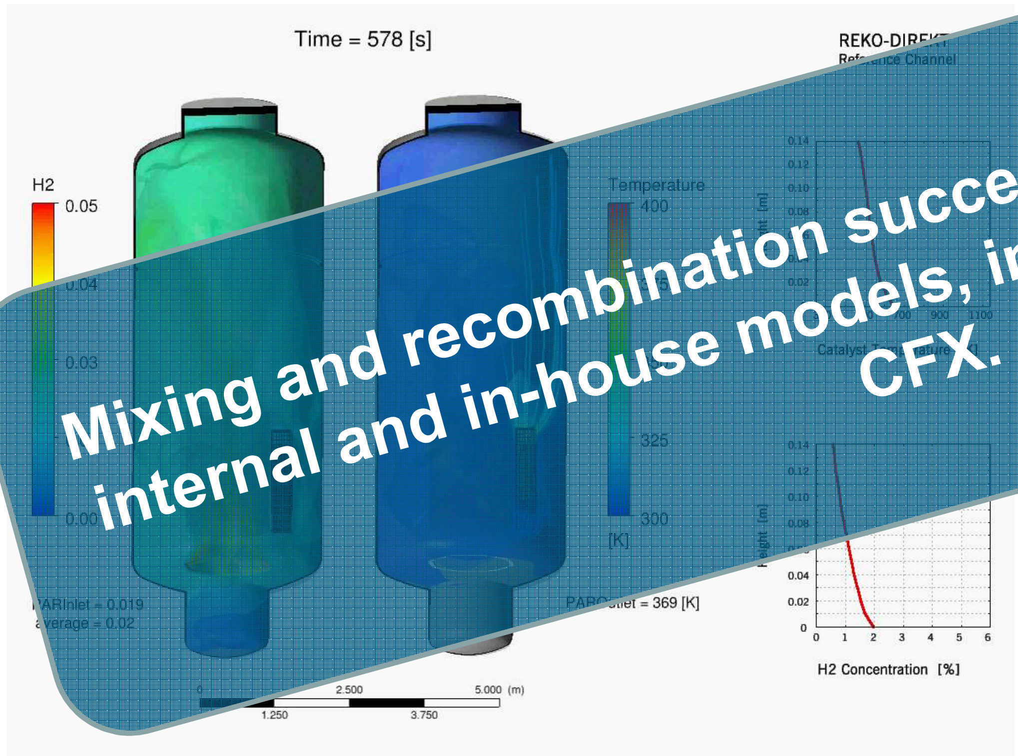
Auto-catalytic recombiners (PAR) provide a hydrogen sink even in situations where dilution and venting is limited or impossible.

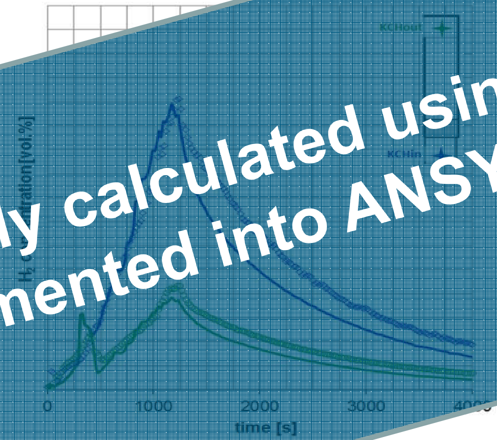
- In-house code REKO-DIREKT describes all relevant aspects of the operational behavior of PARs
- Calculates the conditions at the PAR outlet (i.e. gas temperature and concentrations, mass flow) as well as the local catalyst temperature and local gas concentrations along the catalyst sheets
- Reaction model of the heterogeneous catalytic reaction is based among others on mass transfer correlations

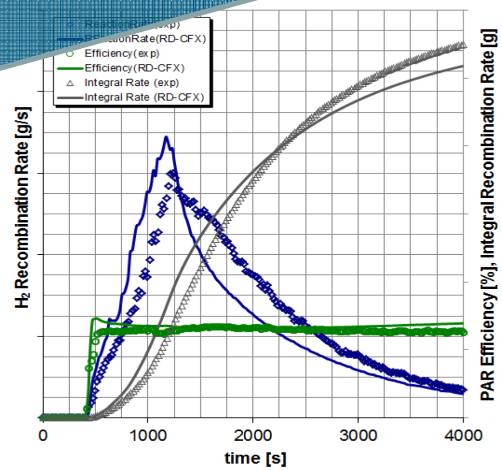


Recombiner modeling - validation

Mixing and recombination successfully calculated using internal and in-house models, implemented into ANSYS CFX.







1. Reinecke E.A., Kelm S., Jahn W., Jäkel C., . Allelein H.-J., Simulation of the efficiency of hydrogen recombiners as safety devices, International Journal of Hydrogen Energy, Available online 11 October 2012, ISSN 0360-3199, 10.1016/j.ijhydene.2012.09.093.
2. Kelm, S., Jahn, W., Reinecke, E.-A., Schulze, A. "Passive auto-catalytic recombiner operation - validation of a CFD approach against OECD-THAI HR2-test", Proc. OECD/NEA & IAEA Workshop on Experiments and CFD Codes Application to Nuclear Reactor Safety (XCFD4NRS), Deajon, South Korea, September 9-13, 2012

Volume phase change of hydrogen – modeling approach

- Link is needed combining liquid and gaseous phase
- Thermodynamic equilibrium model approach seems accurate enough
- Thermodynamic equilibrium model contained in ANSYS CFX seems not to be sufficient for this application
- Any thermodynamic equilibrium model can be expanded to other contributing fluids such as oxygen, nitrogen and water
- Correct modeling of fluid properties is essential → Models based on the Helmholtz energy approach considered most accurate

→ A volume based enthalpy model is going to be developed at Forschungszentrum Jülich

Conclusion and future work

AIM and STRATEGY	• Possible accident phenomena identified • Implement and validate different models into a commercial CFD code in combination with the release of hydrogen
RESULTS	• First models implemented and first successful validation of pool distribution, mixing and recombination • Uncertainties identified and addressed for further analysis
FUTURE STEPS	• Enthalpy based equilibrium model has to implemented and validated • Link models in a generic or even better realistic accident scenario

Questions?

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