## Enabling technologies for precombustion

### TCCS-6

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# Outline

Numerical methods for hydrogen combustion modeling



- Development of a lean premixed hydrogen gas turbine re-heat combustor

Optimization of hydrogen rich fuel supply system







# **The Pencil-Code**

- High order Direct Numerical Simulation (DNS) code
- Open source
  - http://www.nordita.org/software/pencil-code/
- Detailed chemistry combustion implemented
- No libraries required
  - Unix/linux
  - Fortran compiler
- Journal of Computational Physics 230, 1-12 (2011)
  - http://arxiv.org/abs/1005.5301





### Chemical kinetics combustion model validated at LPM and SEV conditions

Background: "Operation of SEV burners involves accurate knowledge and monitoring of both flame speed and ignition delay time."

Results:

- H2 chemical kinetic models have been compared and partly validated at the high temperature and pressure conditions (up to 30 bar) relevant to LPM and SEV conditions.
- At these conditions the mechanisms that are thoroughly validated for hydrogen at lower pressures, predict a factor 3 different ignition delay times.
- To reduce the uncertainties in predictions with hydrogen mechanisms at the high temperature and pressure condition more experiments are needed.

#### Accepted publ: Int. J. Hydrogen Energy. http://arxiv.org/abs/1104.4925



Ignition delay results with 2% H2, 1% O2, 97% Ar at 33atm. Comparison of predictions with various chemical mechanisms and shock tube data of Petersen et al.





## Provide fundamental combustion data for H2-rich fuels at high temperature and high pressure

Background:"Direct
Numerical Simulations
(DNS) may be seen as a
numerical experiment as
nothing except the chemical
kinetics is modeled"

### Results:

- DNS of flames propagating in isotropic decaying turbulence have been performed to find the dependence of the turbulence on the turbulent flame velocity
- DNS of flame propagating in a turbulent channel flow shows the mode of propagation.







#### Submitted for publication in J. Fluid Mech.

Improved combustion model: Linear Eddy Model (LEM3D) integrated with RANS

Background: "LEM3D provides high fidelity resolution at a significantly lower cost than Direct Numerical Simulation (DNS)"

#### Results:

- The LEM3D mixing-reaction model has been coupled to the in-house CFD-code SPIDER and with FLUENT through User Defined Functions (UDFs)
- The coupled model LEM3D-RANS has been verified against experimental data for the turbulent non-premixed jet flame denoted DLR A.



**Snapshot of LEM3D-RANS simulation:** Mixture fraction contours in a non-premixed turbulent jet flame (DLR-A)

















## Selection of piping and sealing materials

- Material Selection for Section 1 and Section 2: carbon steel 1.5415 / 1.0425 / 1.0345. CO has no effect on carbon steel due to low T, no H2O.
- Section 3: Austenitic stainless steel necessary: 1.4571 / 1.4404 since condensed water can not be avoided (dissolution of CO2 in H2O)
- Section 4: Austenitic stainless steel favorable: 1.4571 / 1.4404.
   H2O condensation and formation of H2CO3 can occur at start up or shut down

		-1-2-cc-ccs 3-4-			
		Clean syngas at entry Syngas Fuel System	after Waste-N2 admixing	after saturation by water	Diluted and saturated Syngas after overheating
Composition [vol %]	H <sub>2</sub>	85,32	46,34	42,54	42,54
	N <sub>2</sub>	8,37	49,45	45,40	45,40
	Ar	1,04	0,69	0,64	0,64
	H₂O	-	-	8,20	8,20
	со	4,76	2,59	2,37	2,37
	CO2	0,50	0,27	0,25	0,25
	CH4	0,01	0,01	0,00	0,00
	O <sub>2</sub>	-	0,65	0,60	0,60
	others	-	-	-	-
p [bar(a)]		25,25	25,25	25	24,5
T [°C]		28	86,4	119,1	200
m_punkt [Kg/s]		20,508	100,83	110,895	110,895
LHV [MJ/kg]		36,436	7,411	6,796	6,796





## Selection of piping and sealing materials (2)

- Hydrogen embrittlement is no substantial problem since H2 partial pressures and maximum temperatures are too low
- In the presence of CO, carbon steel (section 1&2) can suffer from Carbonyl formation (Fe(CO)5), S is catalyst, Carbonyls less problematic for IGCC-CCS
- Inconel Alloy 82 (or similar) as joining (carbon austenitic)





## Auto-oxidation effects and self ignition

- Auto-oxidation experiments with plug-flow reactor made of stainless steel 1.4517 (selected material) at atmospheric pressure
  - For residence times in a realistic modular fuel system (ca. 4 s) only 3% of the residual oxygen (3 vol%) will be consumed by auto-oxidation
  - Only traces of ammonia are found due to the presence of about 2 % carbon monoxide that acts as a catalyst poison for this reaction. Equilibrium composition of a typical syngas contains more than 9 % ammonia; cannot be neglected for pre-combustion concepts with very high rates of carbon capture.
- Experimental self ignition tests up to 50 bar for 3 vol%, 4 vol% and 5 vol% oxygen in the syngas
  - No risk of self-ignition if oxygen<3 vol% and T<400°C (for typical pressure and syngas composition)





## Optimised design of the fuel system

- Redundant pumps at saturator recommended ("saturator failure")
- High packing size in saturator recommended ("saturator failure")
- Moving steam admixing upstream of heat exchanger recommended ("saturator failure")
- Moving NG admixing closer to gas turbine ("gasifier failure")
- Ensure fast-switch-back function of gas turbine ("waste N2 failure")





## Conclusion

- Two high fidelity simulation methods previously only used for academic applications; Direct Numerical Simulations (DNS) and the three dimensional Linear Eddy Model (3D-LEM), have proven useful for guidance in development of industrial applications
- SIEMENS has studied safety, availability and material issues for the Hydrogen fuel supply system and have used the results to design an optimized fuel supply system.







Thank you for your attention!



