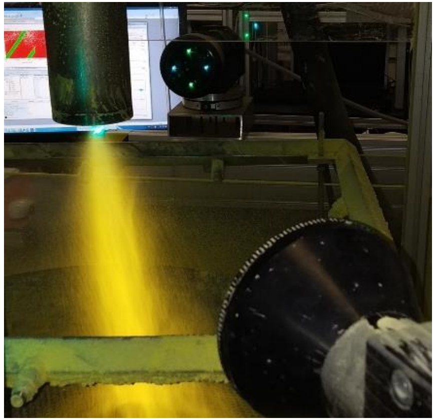
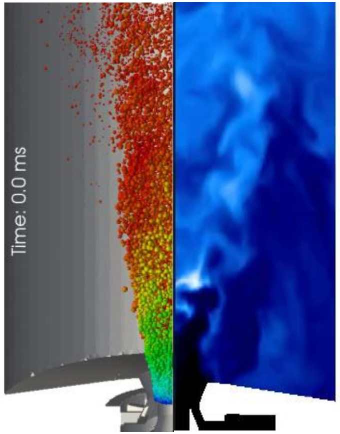
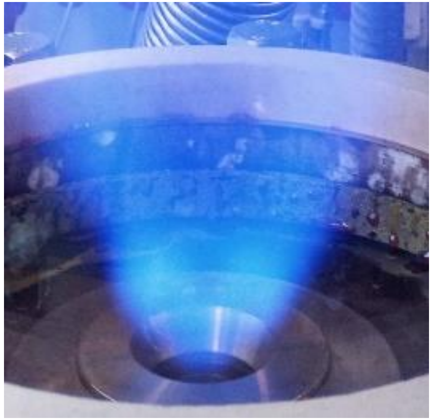
Sulphur combustion at high power density

PEGASUS workshop 09/09/2021

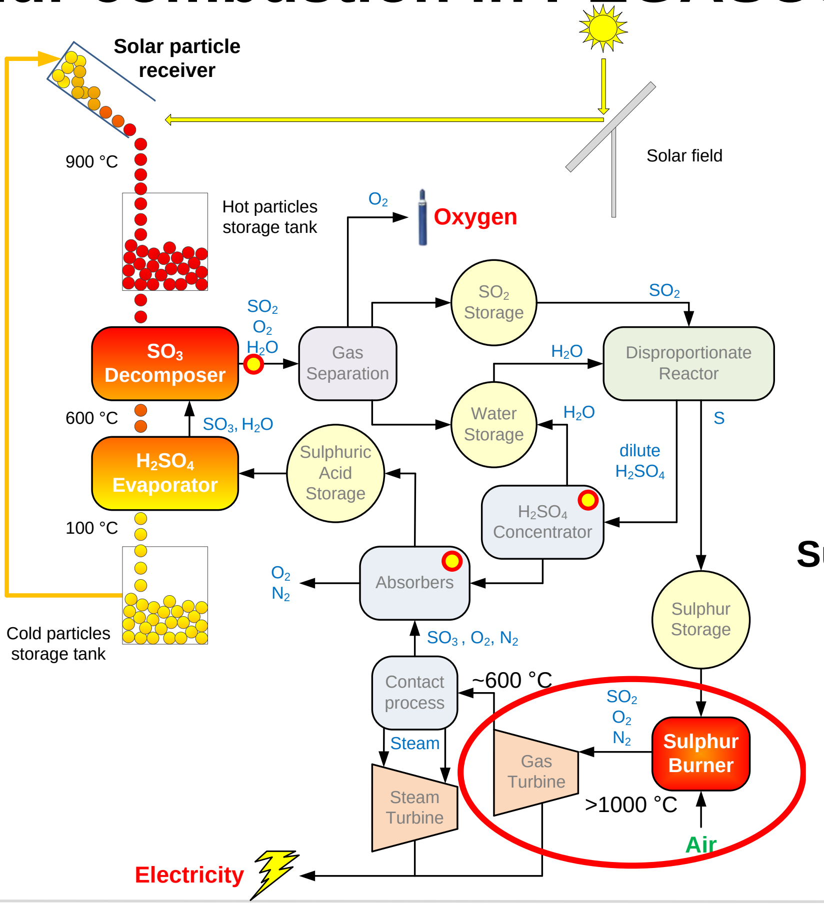
M. Fedoryk, N. Sebbar, S. Harth, D. Trimis







Sulphur combustion in PEGASUS cycle

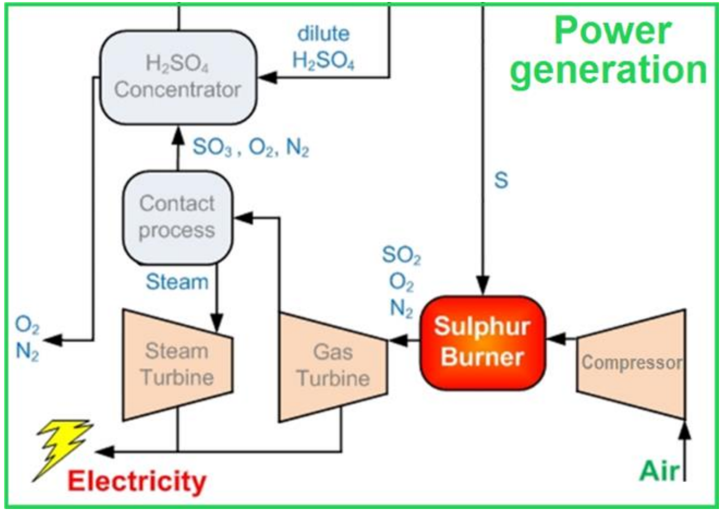


Sulphur burner

High power density sulphur burner and laboratory scale facility at KIT

Development of sulphur burner with high power density suitable for integration in gas turbine

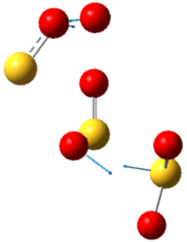
- Definition of operating conditions for sulphur burner
  - Oxidator: air
  - Air compression ratio of gas turbine: 15 bar
  - Combustor air inlet temperature: 720 K
  - Thermal power:
    - 20 kW – laboratory scale (1 burner in tubular combustor, 1 bar)
    - 5 MW - full-scale (multiple burners in annular combustor, 15 bar)
    - Power density target >1.5 MW/m^3 (1 bar)
  - Turbine inlet temperature shall be in the range of 1530 K – 1700 K
    - Combustion in the burner to mainly SO_2
    - Excess oxygen needed for the following contact process ($SO_2 \rightarrow SO_3$)
    - Preferred air/sulphur equivalence ratio $\lambda \approx 2$ (min. 1.5)



Sulphur combustor development methodology

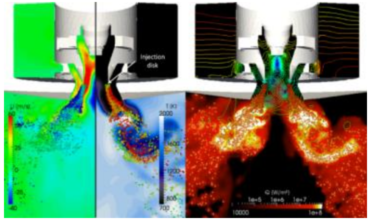
- Development of Sulphur combustor with **high power density**
- Development of **chemical kinetics mechanism** for Sulphur combustion
- **CFD simulations** to support burner development
- Design of laboratory test rigs for
  - **atomization** of Sulphur at isothermal condition
  - **combustion** of Sulphur
- Experimental investigation of elemental **Sulphur atomization**
- Experimental validation of lab-scale **Sulphur combustor**

Sulphur kinetics needed for further development steps



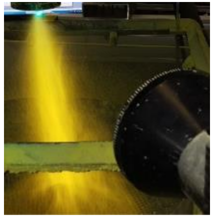
Combustion kinetics development

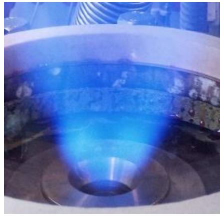
CFD Simulations



Sulphur Atomization (lab scale)

Sulphur Combustion (lab scale)





- **<u>Kinetics – not available / validated for pure Sulphur</u>**
- Flame speed for premixed condition (unknown)
- Auto ignition time (unknown)

Sulphur combustion kinetics: Reactions from literature

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$$k_r = AT^b \exp\left(-\frac{T_a}{T}\right)$$

A b T_a

```
REACTIONS    MOLES   KELVINS
S+O2       = SO+O                  5.200E+06   1.8100     -600.00
S2+M       = 2S+M                  4.800E+13   0.00      38800.00
S2+O       = SO+S                  1.000E+13   0.0000        0.00
SO3+O      = SO2+O2                2.000E+12   0.0000    10000.00
SO3+SO     = 2SO2                  1.000E+12   0.0000     5000.00
SO+O(+M)   = SO2(+M)               3.200E+13   0.0000        0.00
 N2/1.5/  SO2/10/
    LOW /                          1.200E+21  -1.54          0.00 /
    TROE /                         0.5500      1.0e-30      1e+30 /
SO2+O(+M)  = SO3(+M)               9.200E+10   0.0000     1200.00
    LOW /                          2.400E+28  -4.00       2640.00 /
SO+M    =  S+O+M                   4.000E+14   0.0000    54000.00
 N2/1.5/  SO2/10/
SO+O2   =  SO2+O                   7.600E+03   2.3700     1500.00
2SO     =  SO2+S                   2.000E+12   0.0000     2000.00
SO3+S  =   SO+SO2                  5.120E+11   0.00          0.00
```

- Numerical predictions with CHEMKIN
- Target: Burning velocities

Extracted from a hydrocarbon combustion mechanism (ca. 430 react.) which includes treatment/oxidation of sulfur present in the system

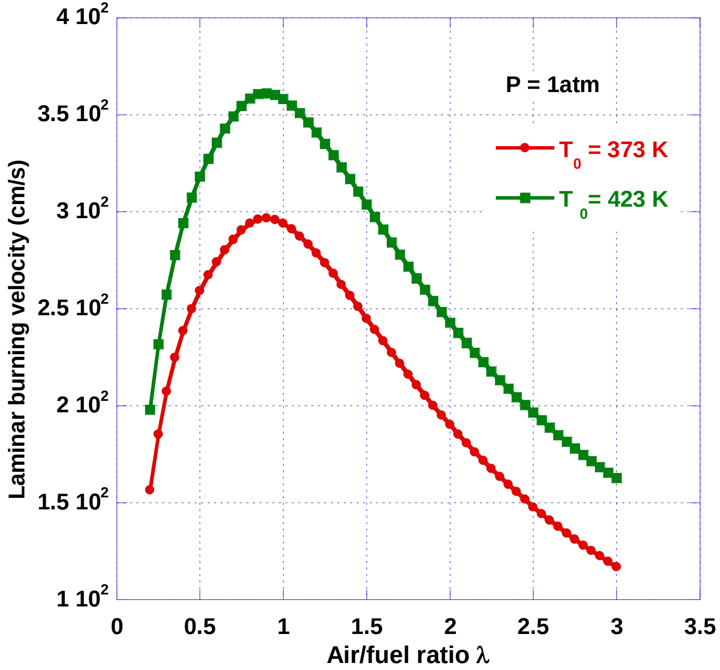
[1] Hughes, K. J.; Blitz, M. A.; Pilling, M. J. Robertson, S. H. *Proc. Comb. Inst.* 29: 2431−2437 (2002).

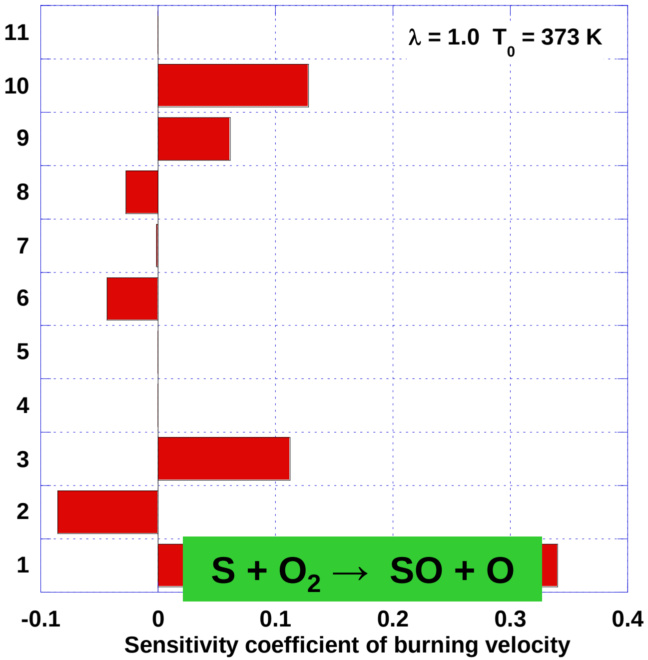
Sulphur combustion kinetics: Laminar burning velocity
Reactions from literature

Laminar burning velocity for $S_2 + O_2$

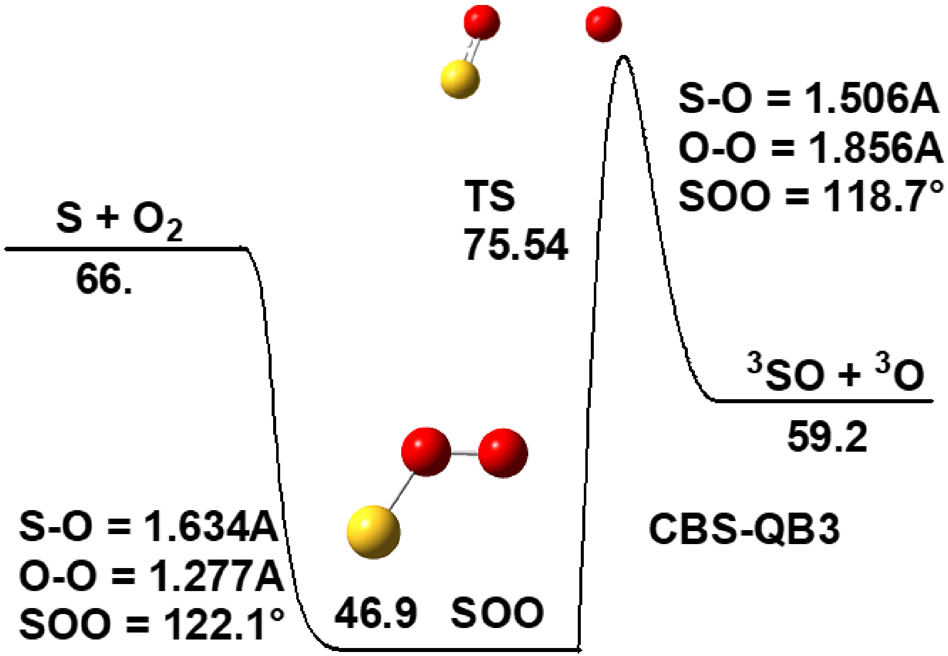
Sensitivity analysis (λ=1)

With Literature mechanism: 11 Reactions





Sulphur combustion kinetics:
Own estimation of $S + O_2 \rightarrow SO + O$



Overall Reaction Rate from Master Equation Analysis	$k = A\,T^b \exp(-Ta/T)$		
	A	b	Ta
$S + O_2 \rightarrow SO + O$ singlet	2.69E+10	0.15	5358.8
k(1600 K) = 2.86E+09			
$S + O_2 \rightarrow SO + O$ triplet	1.09E+11	0.15	2369.4
k(1600 K) = 7.50E+10			

N. Sebbar, T. Zirwes, P. Habisreuther, J.W. Bozzelli, H. Bockhorn, D. Trimis. *Energy & Fuels* **2018** *32* (10), 10184-10193

Sulphur combustion kinetics: Modification of literature mechanism

Karlsruhe Institute of Technology

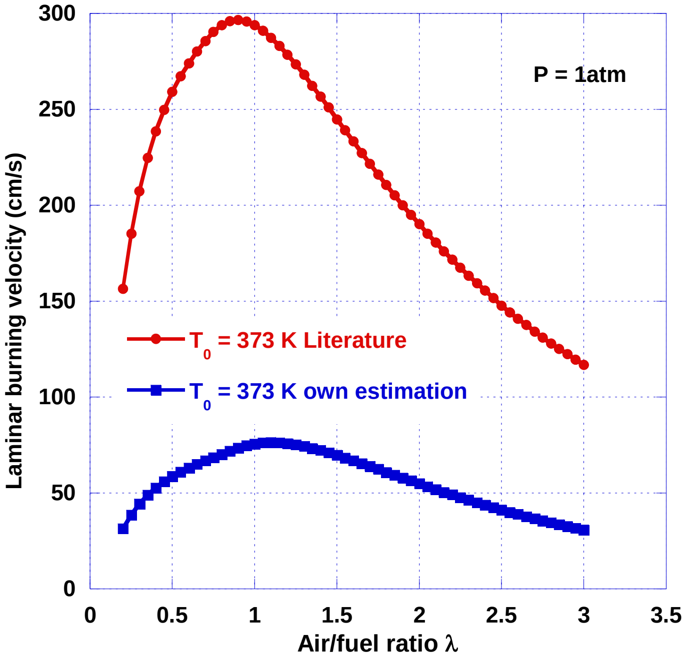
- lit. mechanism [1]
  „base mechanism"

REACTIONS MOLES KELVINS	A	b	T_a
S+O2 = SO+O	**5.200E+06**	**1.8100**	**-600.00**
S2+M = 2S+M	4.800E+13	0.00	38800.00
S2+O = SO+S	1.000E+13	0.0000	0.00
SO3+O = SO2+O2	2.000E+12	0.0000	10000.00
SO3+SO = 2SO2	1.000E+12	0.0000	5000.00
SO+O(+M) = SO2(+M)	3.200E+13	0.0000	0.00
N2/1.5/ SO2/10/			
LOW /	1.200E+21	-1.54	0.00 /
TROE /	0.5500	1.0e-30	1e+30 /
SO2+O(+M) = SO3(+M)	9.200E+10	0.0000	1200.00
LOW /	2.400E+28	-4.00	2640.00 /
SO+M = S+O+M	4.000E+14	0.0000	54000.00
N2/1.5/ SO2/10/			
SO+O2 = SO2+O	7.600E+03	2.3700	1500.00
2SO = SO2+S	2.000E+12	0.0000	2000.00
SO3+S = SO+SO2	5.120E+11	0.00	0.00

- $S + O_2 \rightarrow SO + O$ is replaced by two reactions [2]
  "modified mechanism"

REACTIONS MOLES KELVINS			
S + O2 = SO + O	2.69E+10	0.15	5358.8
DUP			
S + O2 = SO + O	1.09E+11	0.15	2369.4
DUP			

Significant impact of new kinetics on flame speed

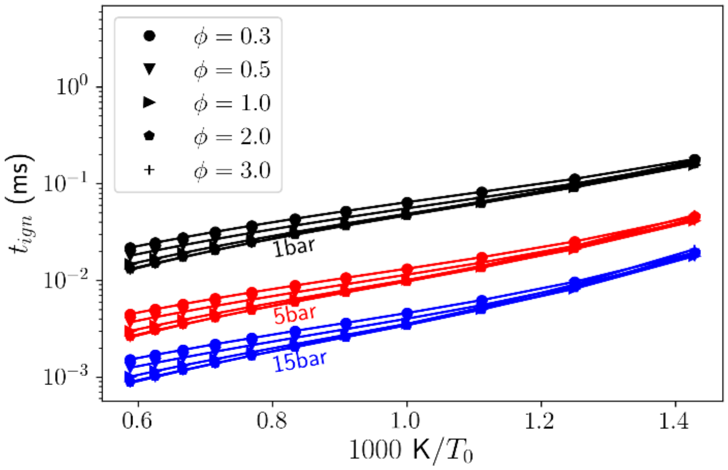


[1] Hughes, K. J.; Blitz, M. A.; Pilling, M. J. Robertson, S. H. *Proc. Comb. Inst.* 29: 2431−2437 (2002).
[2] Sebbar, N.; Zirwes, T.; Habisreuther, P. Bozzelli, J. W.; Bockhorn, H.; Trimis, D. Energy Fuels 2018, 32, 10184−10193

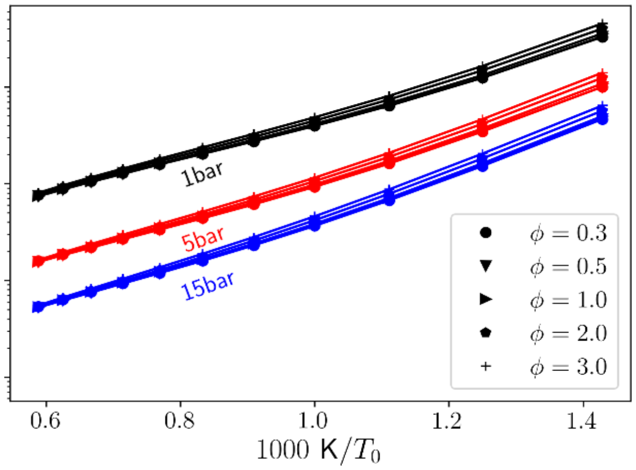
Sulphur combustion kinetics: Ignition delay time

- In the modified mechanism, ignition delay times are about 5 times larger
- The influence of equivalence ratio is negligible
- Ignition delay times decrease with increasing pressure

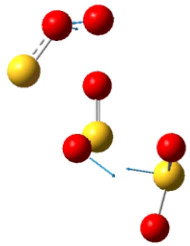
Base mechanism



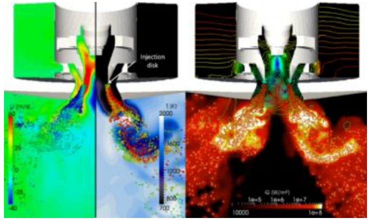
Modified mechanism



Burner design and sulphur atomization



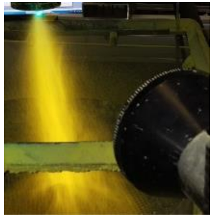
Combustion kinetics development ⇄ CFD Simulations

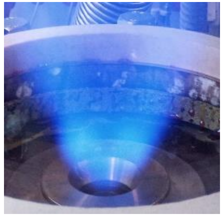


CFD Simulations ⇅ Sulphur Atomization (lab scale)

CFD Simulations ⇅ Sulphur Combustion (lab scale)

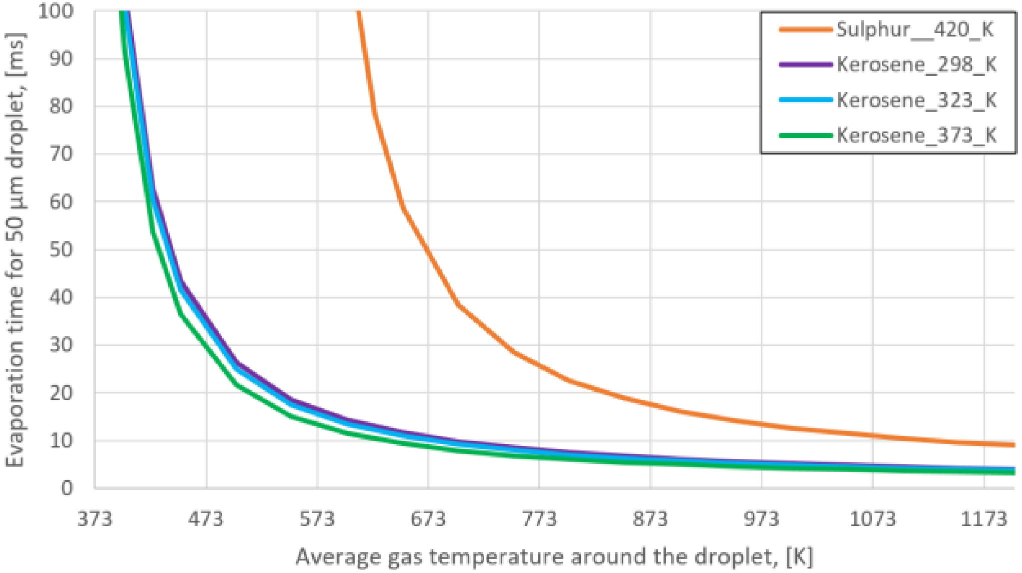
Sulphur Atomization (lab scale) → Sulphur Combustion (lab scale)





Atomization is key factor in burner design

Sulphur droplets require more time for evaporation compared to typical liquid fuels



Atomizer selection

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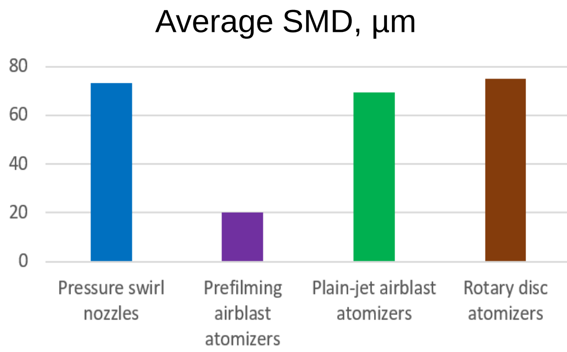
Performance of 4 types of atomizers for sulphur atomization were analyzed by correlations based on key parameters for atomization (We, Oh, Re) → **Sauter Mean Diameter** (SMD)

SMD can be defined as the diameter of a drop having the same **volume/surface** area ratio as the entire spray.

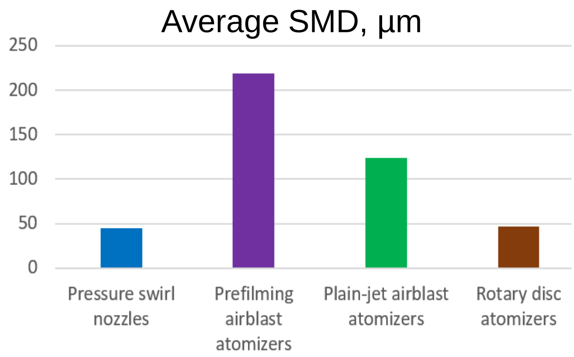
- **Pressure swirl atomizer**
- **Prefilming airblast atomizer**
- **Plain-jet airblast orifice diameter**
- **Rotary atomizer**

Best performance in laboratory scale (right)

Best performance for real scale gas turbine conditions (left)



p_{air} = <u>15 bar</u>
T_{fuel} = 423 K
T_{air} = 720 K
$\Delta p/p$ = 3 %
P_{burner} = 300 kW_{th}

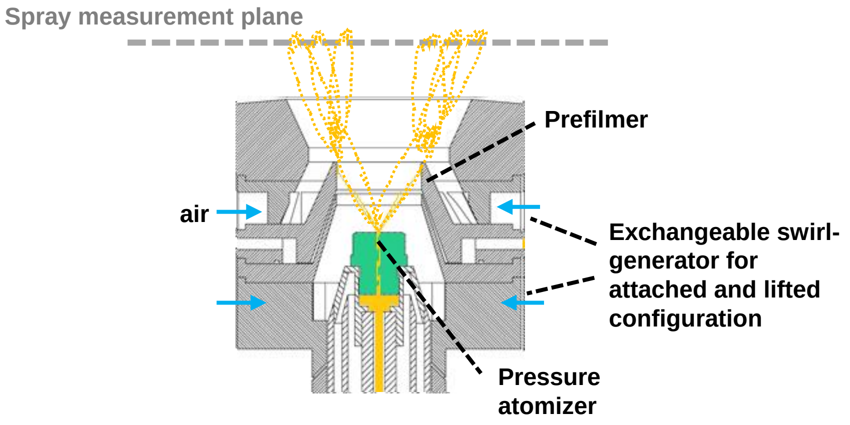


p_{air} = <u>1 bar</u>
T_{fuel} = 423 K
T_{air} = 720 K
$\Delta p/p$ = 3 %
P_{burner} = 20 kW_{th}

Burner design

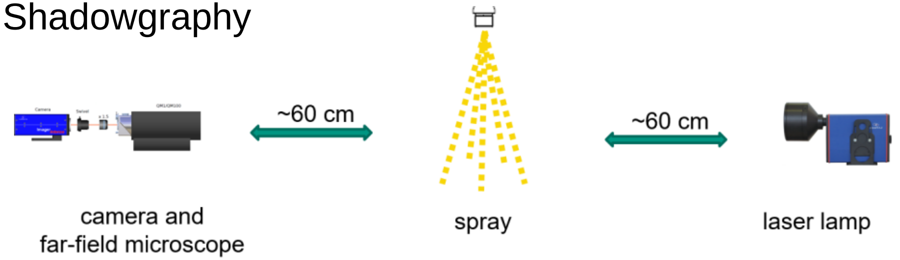
Prototypes for experiments

- Can be operated with pressure atomizer or prefilming airblast atomizer
- Modular burner construction allows to investigate lifted and attached flame configuration by changing swirl generators

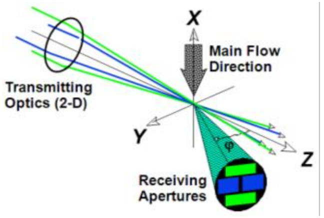


Experimental setup - spray test rig

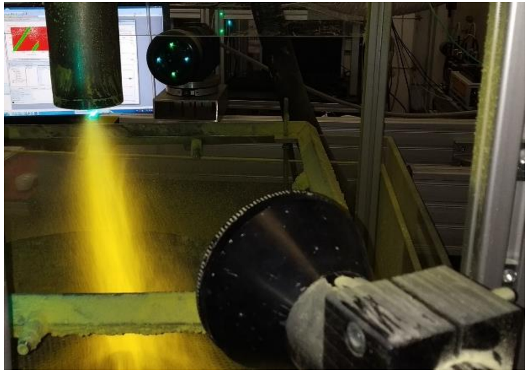
- Liquid sulphur supply at up to 200 bar, 413 K
- Inlet air temperature set to 413 K
- Measurement techniques:
  - Shadowgraphy



  - Phase Doppler Anemometry (PDA)



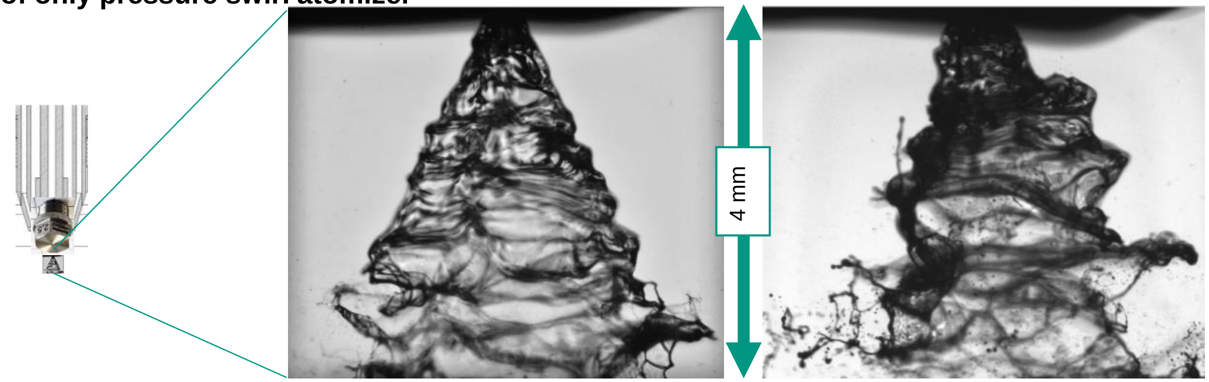
PDA principle, Dantec



Sulphur spray results

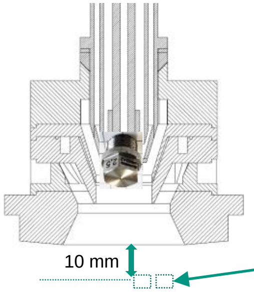
- Shadowgraphy with far field microscope: Qualitative analysis of primary atomization

Operation of only pressure swirl atomizer

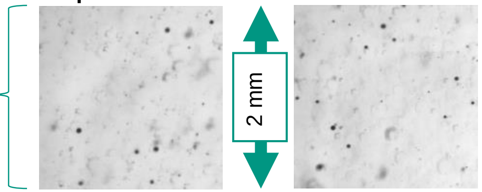


Complete burner nozzle (with swirled air)

Cone angle ~70° (Hollow cone)



Primary atomization is completed at selected measurement plane for PDA measurements



Sulphur spray – Sauter Mean Diameter (SMD)

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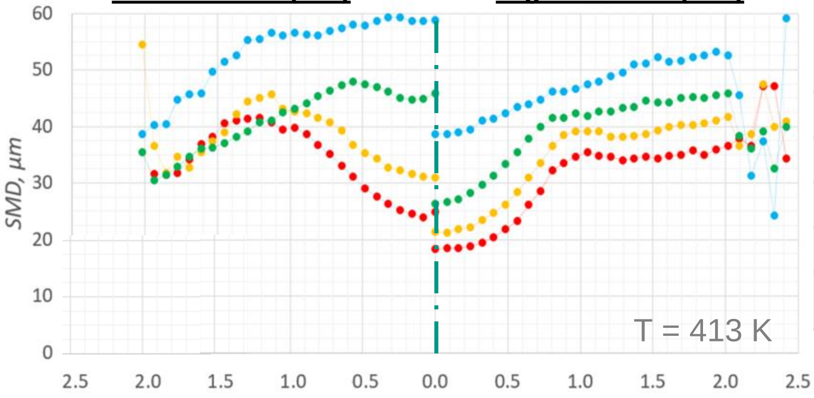
SMD for different type of air flow fields

Low air swirl (LSI) **High air swirl (HSI)**

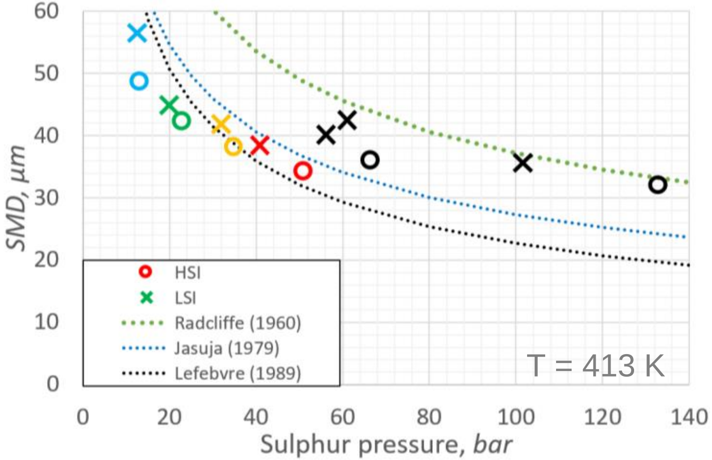


radial position r/r_0

$$SMD = \frac{\sum_i d_i^3}{\sum_i d_i^2}$$

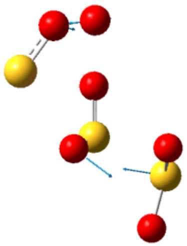
Eq. thermal power [kW]	Sulphur atomization pressure [bar]
22.5	46
20.0	33
17.0	22
13.5	13
>22.5	>46 (richer mixtures)

Global SMD vs atomization pressure



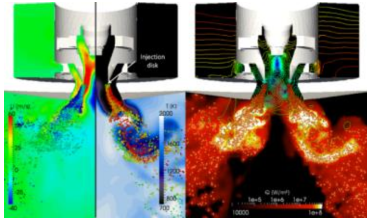
⇨ Measured particle size distribution is used as input to CFD simulations

CFD simulations



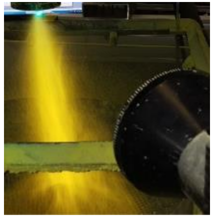
Combustion kinetics development

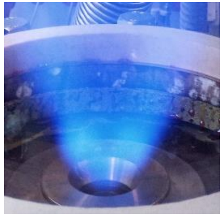
CFD Simulations



Sulphur Atomization (lab scale)

Sulphur Combustion (lab scale)





Low and High Swirl Intensity Burner (LSI vs HSI)

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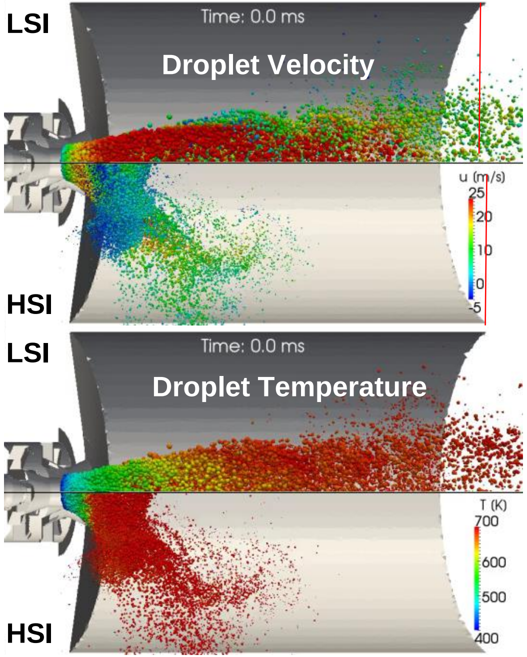
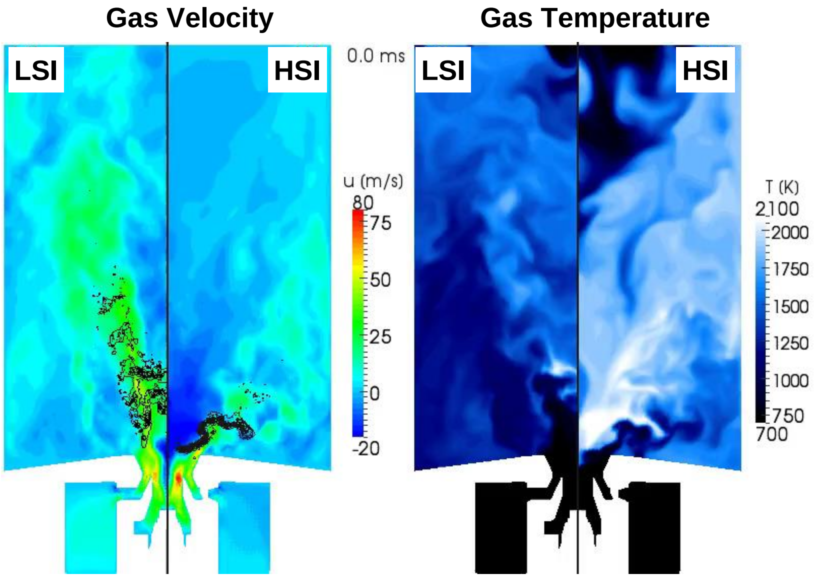
- LES simulation (8 million cells) with OpenFOAM
  - Lagrangian-Eulerian method for multiphase
  - PaSR [– partially stirred Reactor] combustion model based on sulphur kinetics

	Inlet D_{32} $[\mu m]$	L_p $[mm]$ - (95%)	Evap	$\dot{Q}$ $[kW]$
LSI	50	148	99.4%	19.7
HSI	50	90	100%	19.1

(Combustor air inlet temperature 720 K, combustor pressure 1 bar)





Evaluation of two Nozzle Designs

HSI

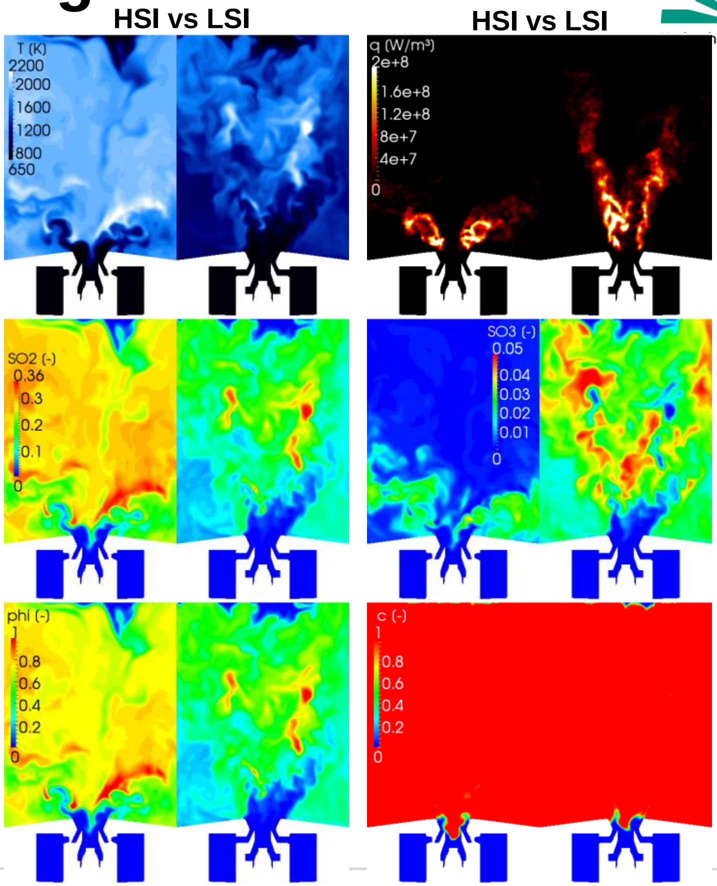
- Compact reaction zone
- High local flame temperature
- High SO_2, low SO_3
- High local Φ

LSI

- Long narrow reaction zone
- Low local flame temperature
- Low SO_2, high SO_3
- Low local Φ

➡ **LSI Burner Preferred**

Next step: high pressure operations



Pilot scale design - elevated pressure

Combustion laboratory scale:

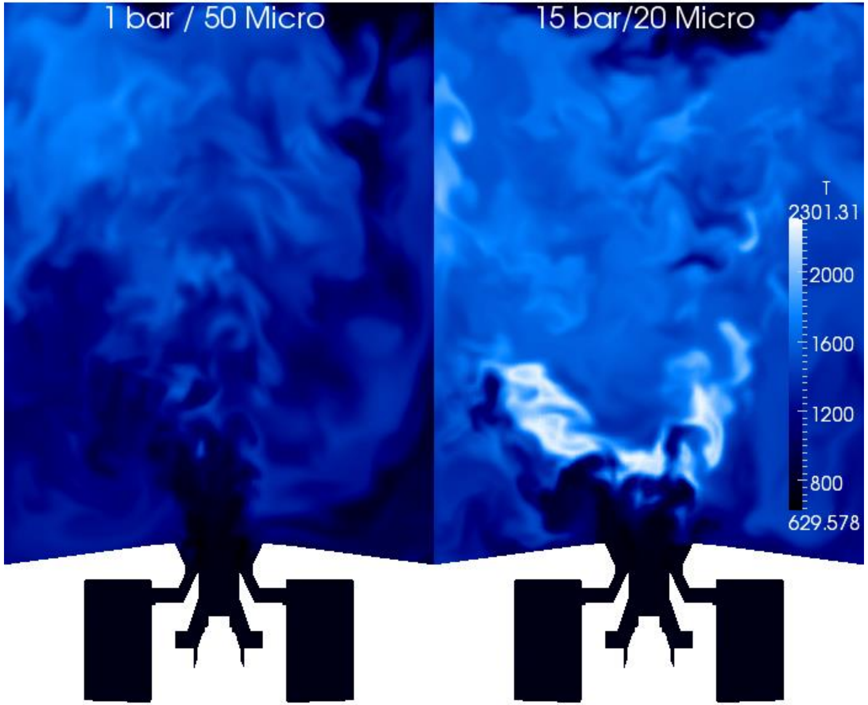
- Pressure: 1 bar
- Thermal load ca. 20 kW
- Power density over combustion chamber volume: 5 MW/m³

  (target: > 1.5 MW/m³)

Combustion at elevated pressure:

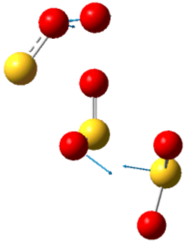
- Pressure: 15 bar
- Thermal load ca. 300 kW
- Power density over combustion chamber volume: 72 MW/m³

Comparison at 1 and 15 bar combustor pressure

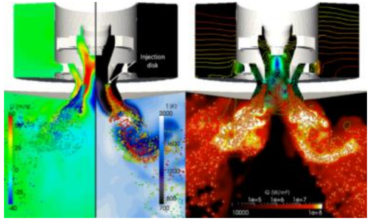


Higher overall combustion temperature at elevated pressure

Sulphur combustion (lab scale)



Combustion kinetics development ⇄ CFD Simulations



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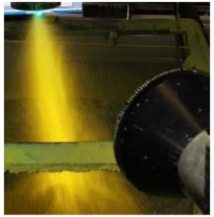
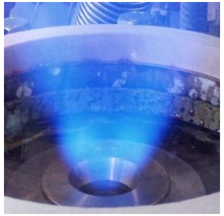
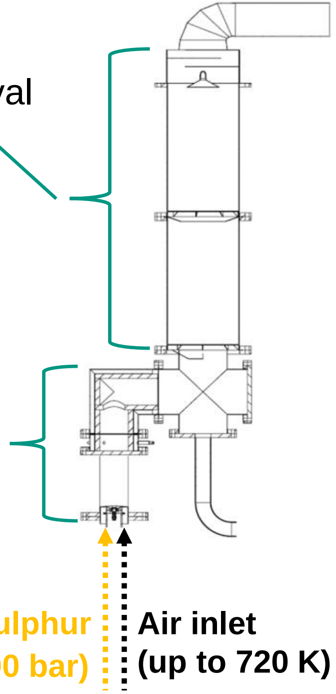
Sulphur Atomization (lab scale) → Sulphur Combustion (lab scale)





Experimental setup - Combustion test rig

- Components
  - Exhaust gas treatment for SO_2 removal
    - Scrubber with NaOH solution
    - Closed circuit for liquids
  - Combustion chamber
    - Optical access
    - Ceramic inlays
  - Sulphur preparation unit
    - Liquid sulphur supply



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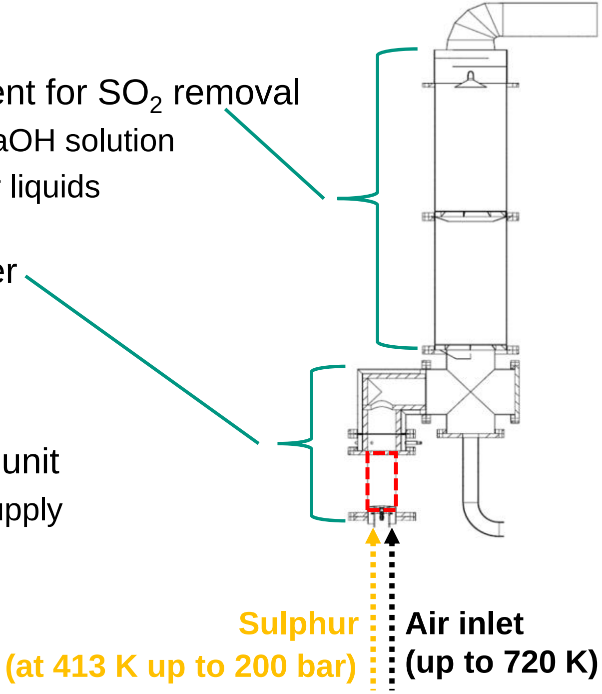
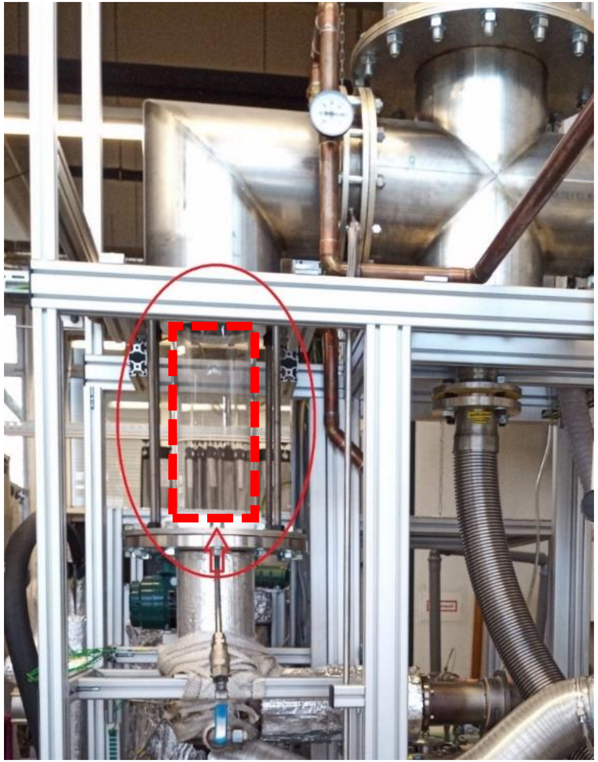
  - Sulphur preparation unit
    - Liquid sulphur supply





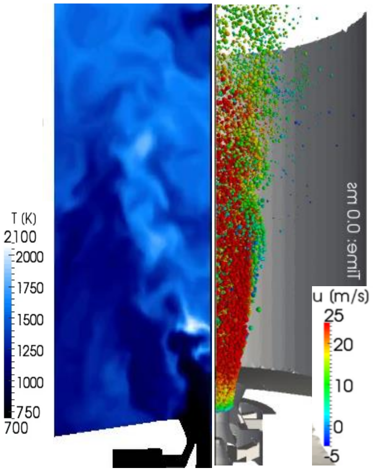
Combustion experiments

Results for LSI configuration

- Ignition by auto ignition (air inlet temperature 720 K)
- Power density > 5 MW/m³ (ambient pressure)
  target: > 1.5 MW/m³
- Very large stability range
  (also for low air inlet temperatures 367 K)

LSI configuration

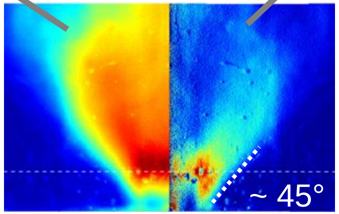
16 kW (air inlet temperature=720 K)



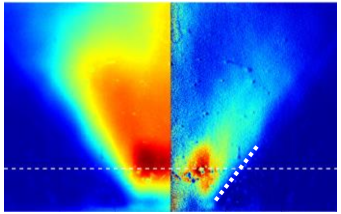
CFD simulation

Flame structure in LSI configuration

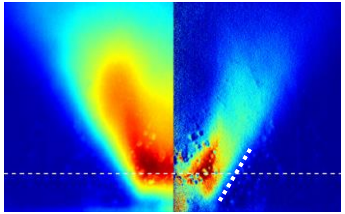
Line-of-sight **Abel-transformed**



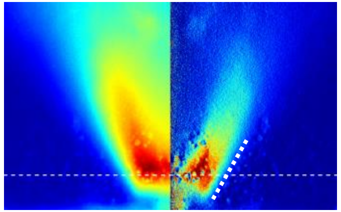
P = 21.4 kW
λ = 1.56
P_S = 110 bar



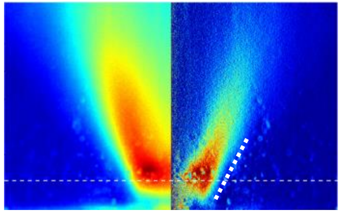
P = 20.7 kW
λ = 1.62
P_S = 101 bar



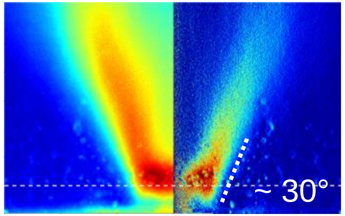
P = 18.1 kW
λ = 1.85
P_S = 87 bar



P = 15.5 kW
λ = 2.16
P_S = 62 bar



P = 12.9 kW
λ = 2.59
P_S = 43 bar



P = 10.3 kW
λ = 3.24
P_S = 27 bar

($\Delta p/p_{air}$= 3 %, T_{inlet} = 450 °C)

Flame structure in LSI configuration

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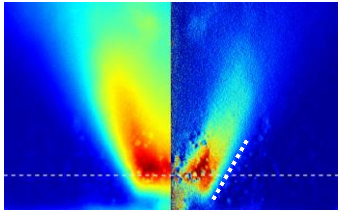
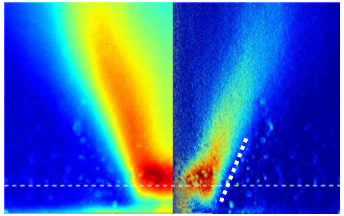
- **Flame shape is dependent on Sulphur atomization pressure**



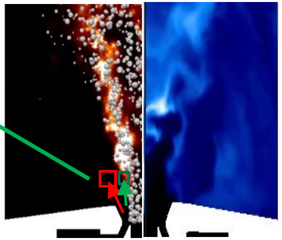
P_S = 62 bar



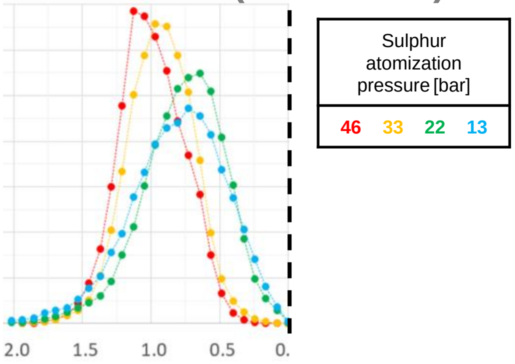
P_S = 27 bar

- **Initial velocity vectors of spray in CFD simulations have be adapted to allow precise simulations for varied operating conditions**

spray is more narrow compared to experiment



Measured mass flow distribution at burner exit (isothermal)



Conclusions

- **Refined CFD simulations for burner development based on**
  - Developed sulphur kinetics
  - Atomization of sulphur at relevant conditions

- **High power density combustion seems feasible**
  - Lab scale experiments and simulations show

    Power density > 5 MW/m^3 at ambient pressure (target > 1.5 MW/m^3)
  - Burner works well for elevated pressure conditions based on simulations

    Power density > 72 MW/m^3 at 15 bar - gas turbine condition

- **More research required:**
  - Measurement of laminar flame speed & auto ignition times
  - Detailed validation of kinetics
  - Burner upscaling and optimization
  - Study on combustor and turbine blade materials for sulphur combustion

Acknowledgements

Karlsruhe Institute of Technology

Thank you

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Sulphur - properties

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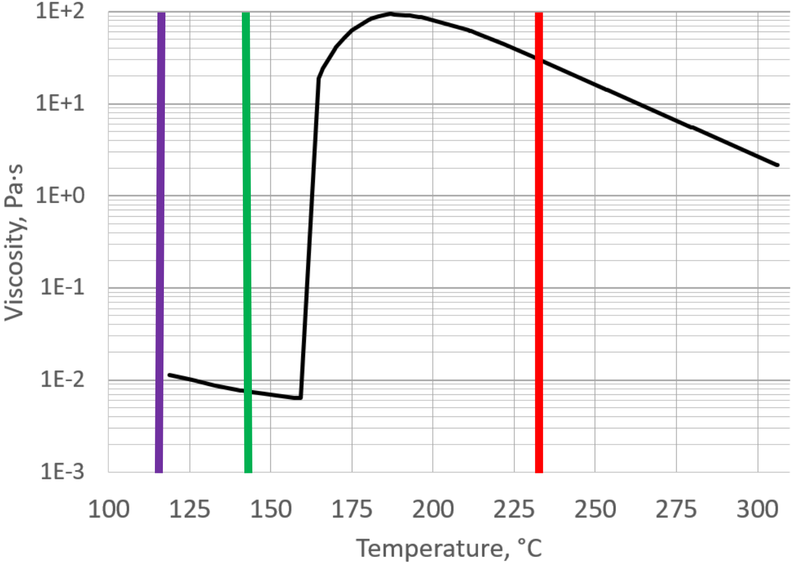
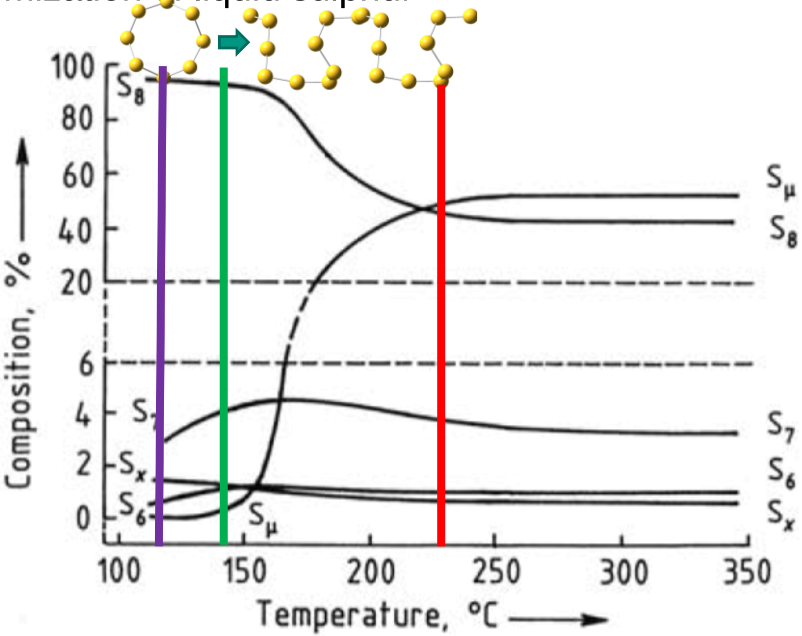
- Viscosity of liquid sulphur strongly dependent on temperature due to polymerization
- Steep viscosity increase shall be avoided before atomization of liquid sulphur



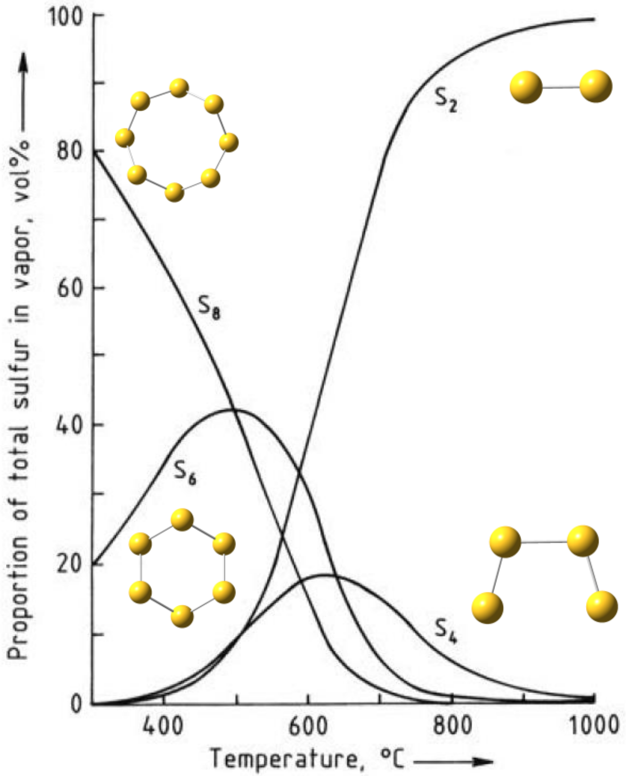


- 115 °C – Melting temperature
- 140 °C – Temperature of liquid sulphur supply
- 230 °C – Autoignition temperature
- 450 °C – Air inlet temperature of gas turbine combustor

Source: W. NEHB, K. VYDRA (ULLMANN'S encyclopedia of industrial chemistry)

Sulphur - properties

- Composition of sulphur vapor



Source: W. NEHB, K. VYDRA (ULLMANN'S encyclopedia of industrial chemistry)

Sulphur - properties

Parameter	Unit	Liquid sulphur @ 423 K	Kerosene, Jet-A1 @ 298 K
Density	kg/m^3	1780	810
Surface tension	mN/m	61	26
Viscosity	mPa·s	7.0	1.5
Specific heat	kJ/(kg·K)	1.1	2.0
Heat of vaporization	kJ/kg	290	363
Heat of combustion (LHV for kerosene)	kJ/kg	-9 300 (for solid)	-43 000
Vapor pressure	Pa	26	185

Particle size distribution

- Measured particle size distribution is used as input to CFD simulations as Rosin-Rammler distribution