

## Integration and Verification of a SO<sub>2</sub>-Chemisorption Model for Computational Spray-Tower Analysis

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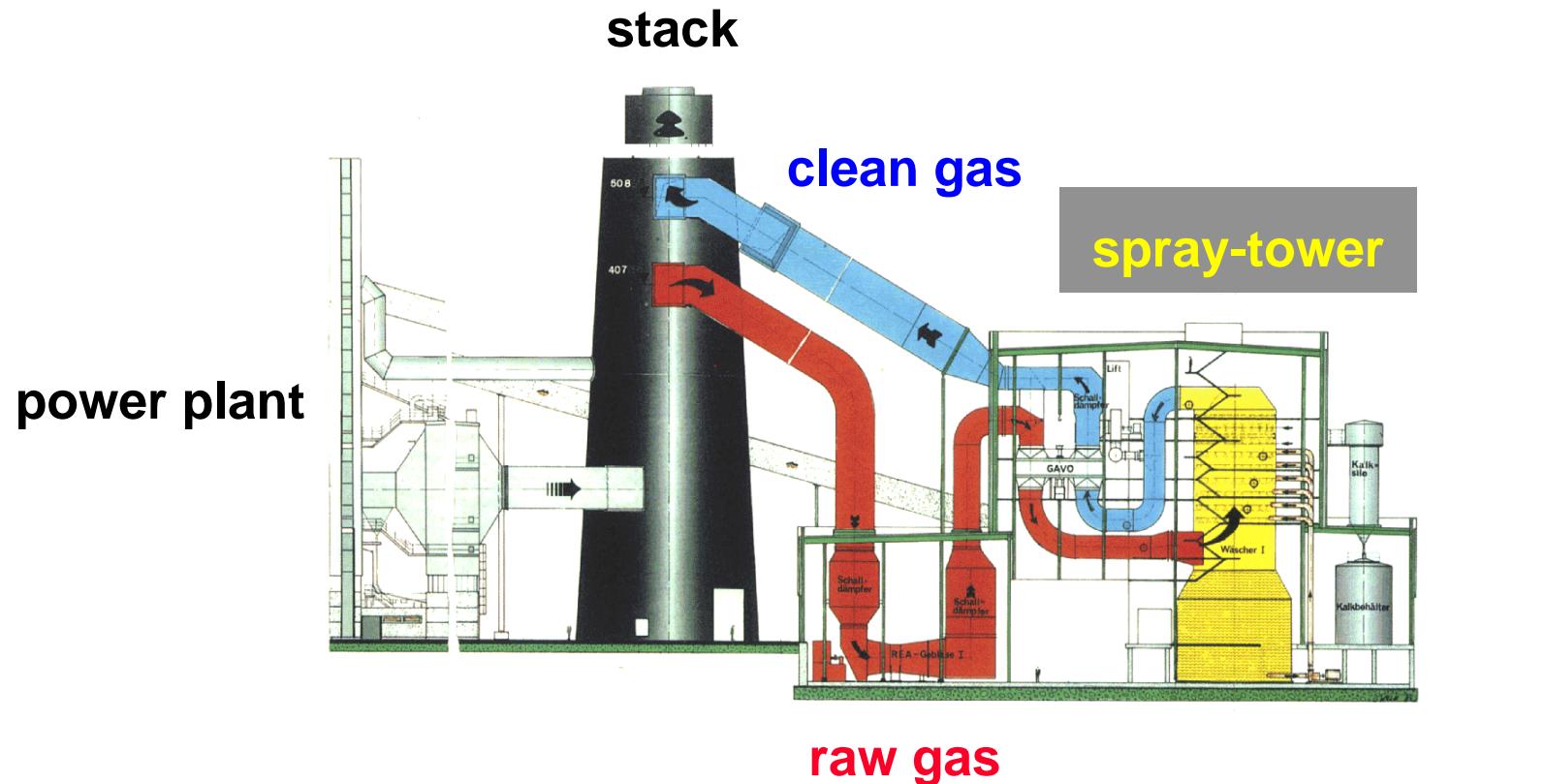
## General

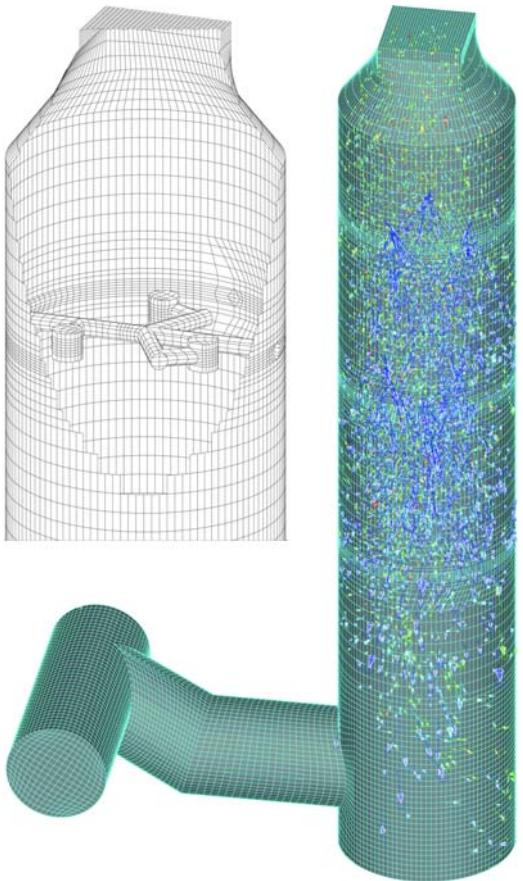
- Introduction spray-tower
  - Overview CFD-setup
  - SO<sub>2</sub>-chemisorption model

## Verification

- Pending droplet experiment (pH-value progression)
  - Pilot-scale scrubber (1.4 m diameter)
- Industrial-scale scrubbers (4.2 m, 15.3 m , 20 m diameter)

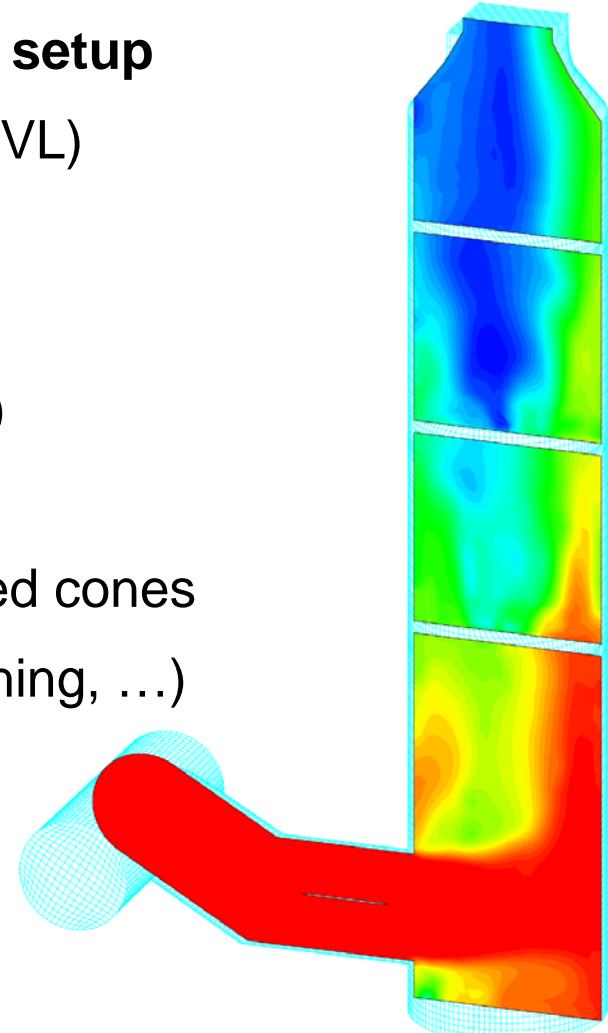
### Injection of limestone slurry into the flue-gas stream for SO<sub>2</sub>-absorption



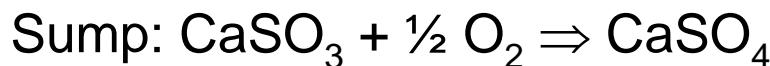


## Computational fluid dynamics - setup

- Commercial code: Fire 7.3 (AVL)
  - Euler-Lagrange
  - Mesh: Hexahedrons only
  - Transient (time-step 5 ms)
    - $k-\varepsilon$ -turbulence-model
- Spray: Two-way-coupling, modelled cones
- Wall-interaction (impinging, splashing, ...)
  - $\text{SO}_2$  - absorption



### Reactions:



- **Components:** CaCO<sub>3</sub>, CaSO<sub>3</sub>, CaSO<sub>4</sub>, H<sub>2</sub>O, SO<sub>2</sub>, CO<sub>2</sub>, air
- **Species:** [SO<sub>2</sub>], [CO<sub>2</sub>]; [H<sup>+</sup>], [OH<sup>-</sup>], [HSO<sub>3</sub><sup>-</sup>], [SO<sub>3</sub><sup>2-</sup>], [HCO<sub>3</sub><sup>-</sup>], [CO<sub>3</sub><sup>2-</sup>]
- **Equations (8):** Ion-product H<sub>2</sub>O, diss.1 H<sub>2</sub>SO<sub>3</sub>, diss.2 H<sub>2</sub>SO<sub>3</sub>, S-total, diss.2 H<sub>2</sub>CO<sub>3</sub>, C-total, electro-negativity, mass-balance

### 2-step-absorption

- SO<sub>2</sub>(gas) → absorption → SO<sub>2</sub>(droplet) [kinetics]
- Droplet chemistry (CaCO<sub>3</sub>/CaSO<sub>3</sub>/CaSO<sub>4</sub>/H<sub>2</sub>O/SO<sub>2</sub>/CO<sub>2</sub>/air) [equilibrium]  
(normally computed iteratively by solving 8 independent algebraic equations)

### „ion-lookup-table“

- All quasi-instantaneous chemical reactions combined and precalculated
  - 5 input, 8 output-parameters
  - 5 steps, linear inter- und extrapolation
  - Reduction of computation-time!

### General

- Introduction spray-tower
- Overview CFD-methods
- SO<sub>2</sub>-chemisorption model

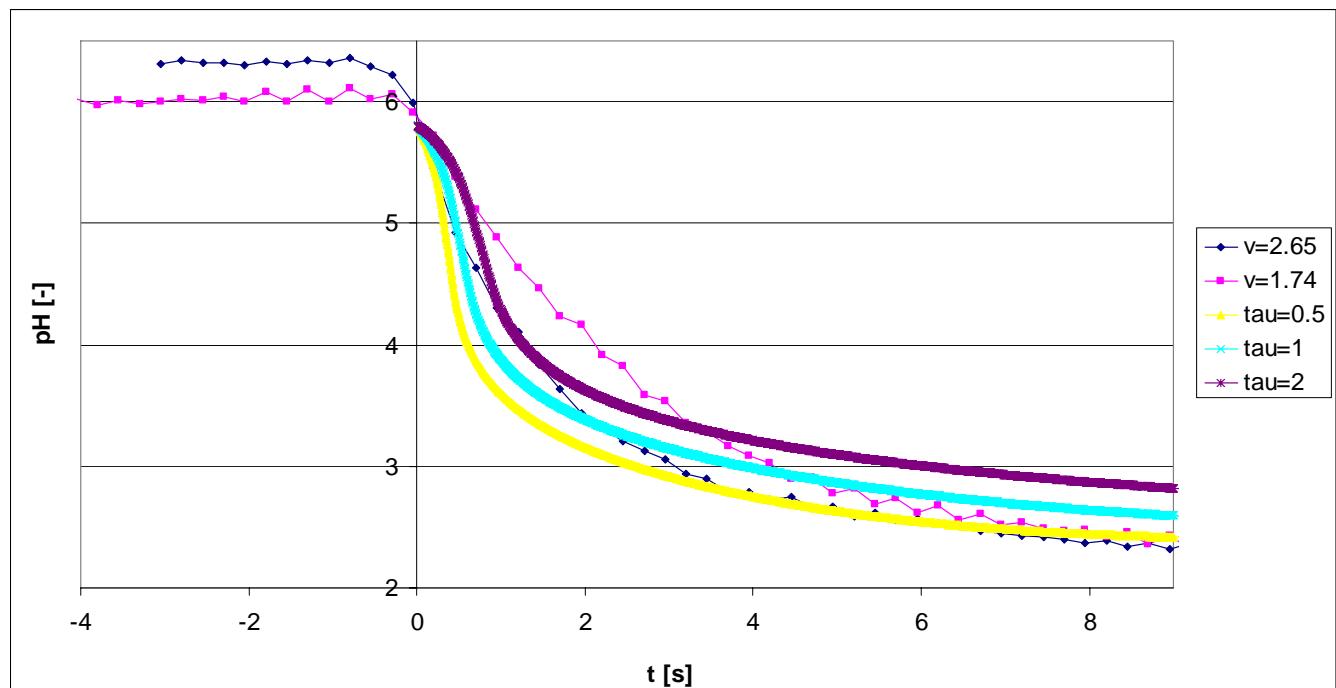
### Verification

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Variation of  $\tau_{\text{exp}}$  until similar ph-value progression is reached  
(some parameters are far out of the scale of those in scrubbers);  
faster decrease because of instantaneous mixing (simulation);  
even though, good resemblance

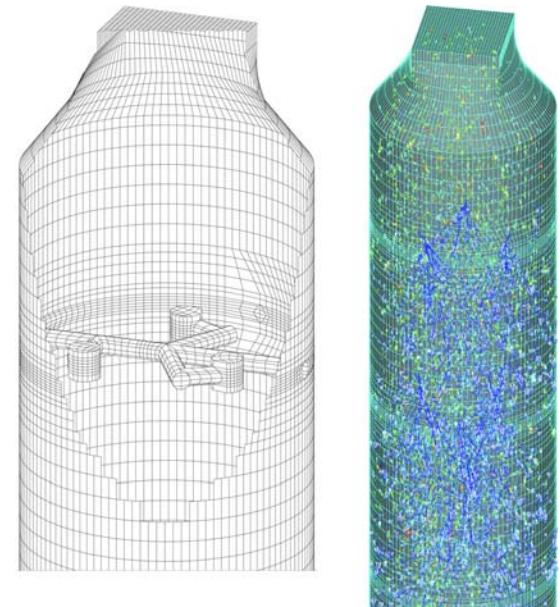
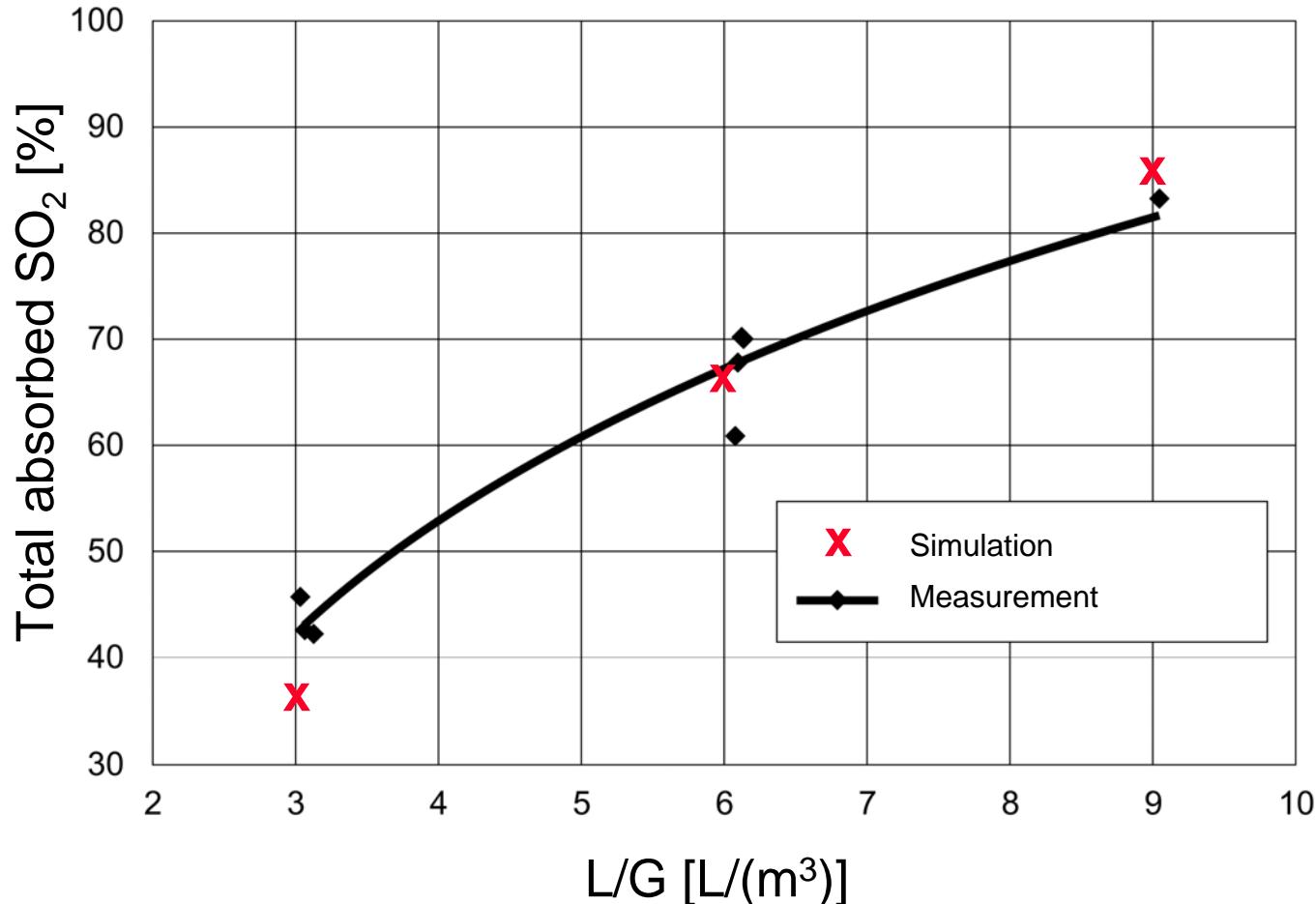
### „pending droplet“

- 2.7 mm droplet
- no alkalinity
- layer model
- $v_{\text{Gas}} = 2 \text{ m/s}$  (about)
- 4000 vol.ppm  $\text{SO}_2$



# Pilot-scale scrubber Sostanj (1.4 m diameter)

Total absorbed SO<sub>2</sub> over L/G



## Simulation

- good trend coverage
- stronger effect of the influence: ratio L/G

# Industrial-scale scrubber (4.2 m diameter)

## Total absorbed SO<sub>2</sub> and measurement (outlet)

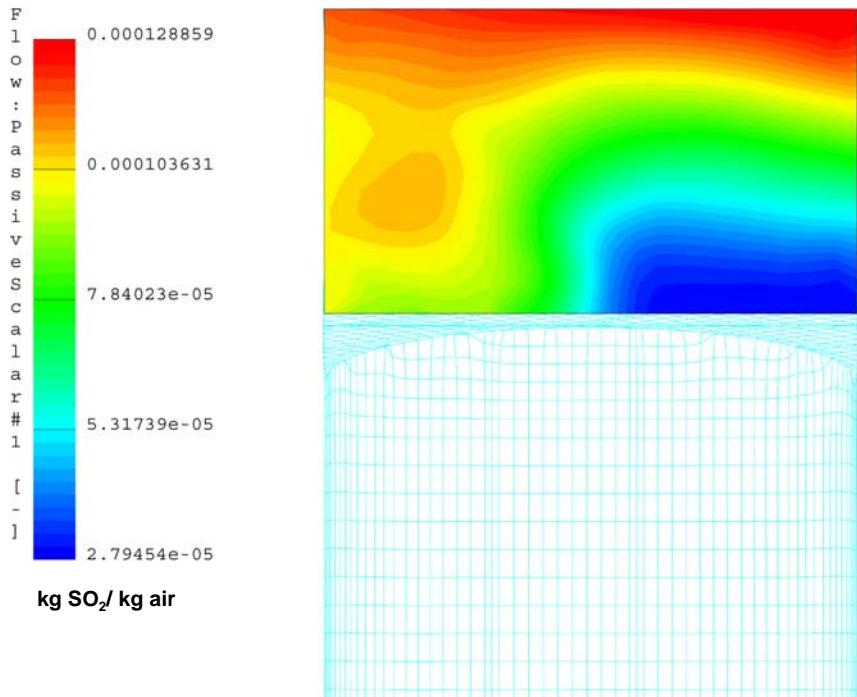


### Total absorbed SO<sub>2</sub>

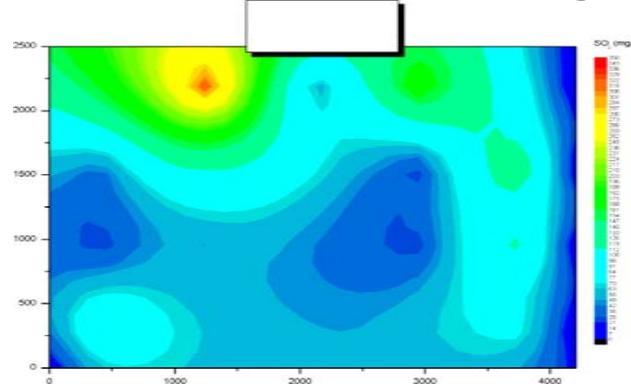
Measurement: 90 %

Simulation: 88 %

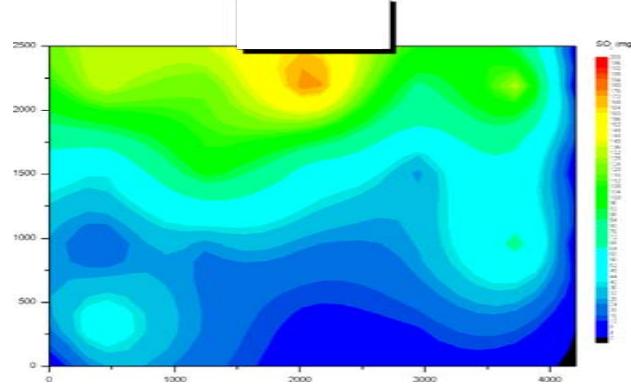
max: 250 mg SO<sub>2</sub> / m<sub>N</sub><sup>3</sup>



max: 350 mg SO<sub>2</sub> / m<sub>N</sub><sup>3</sup>



max: 200 mg SO<sub>2</sub> / m<sub>N</sub><sup>3</sup>



# Industrial-scale scrubber (15.3 m diameter)

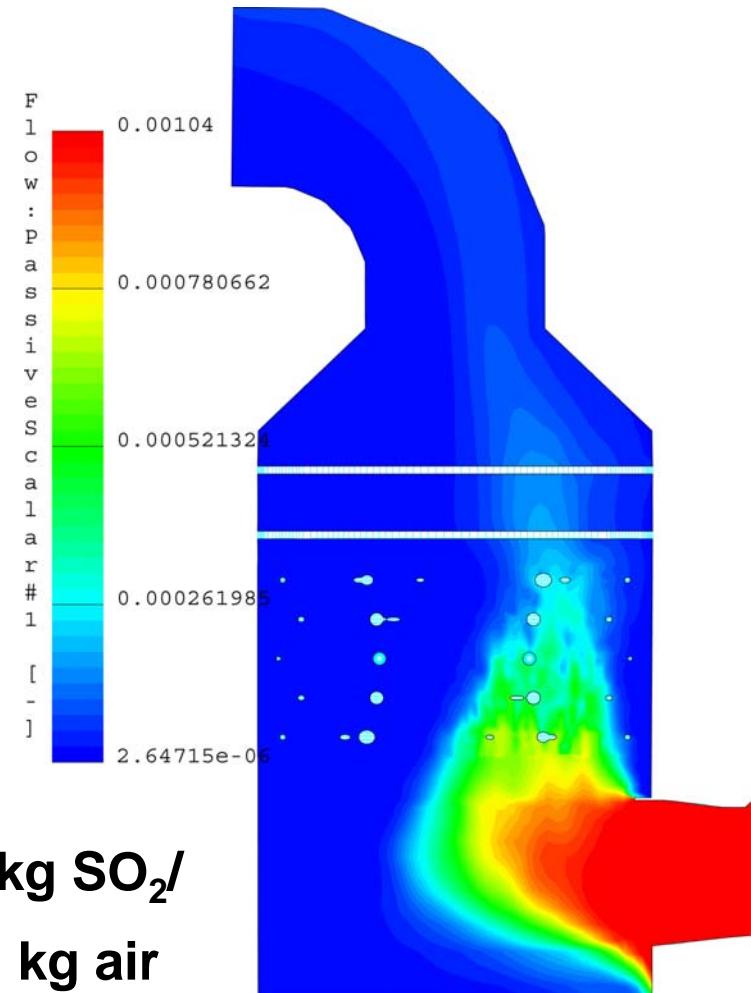
Total absorbed SO<sub>2</sub>



**Total absorbed SO<sub>2</sub>**

**Measurement: 95 %**  
**(spray banks 2-4)**

**Simulation: 96.5 %**  
**(spray banks 1-4)**

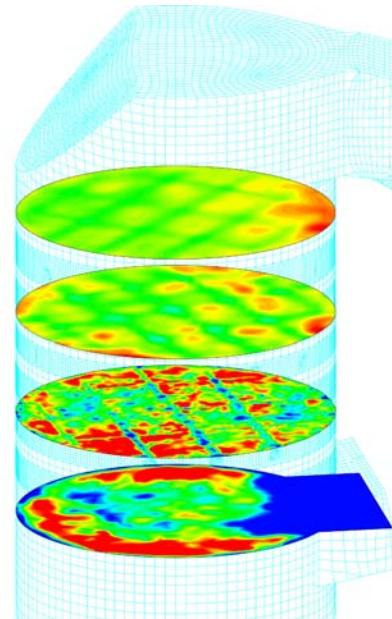
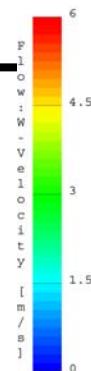
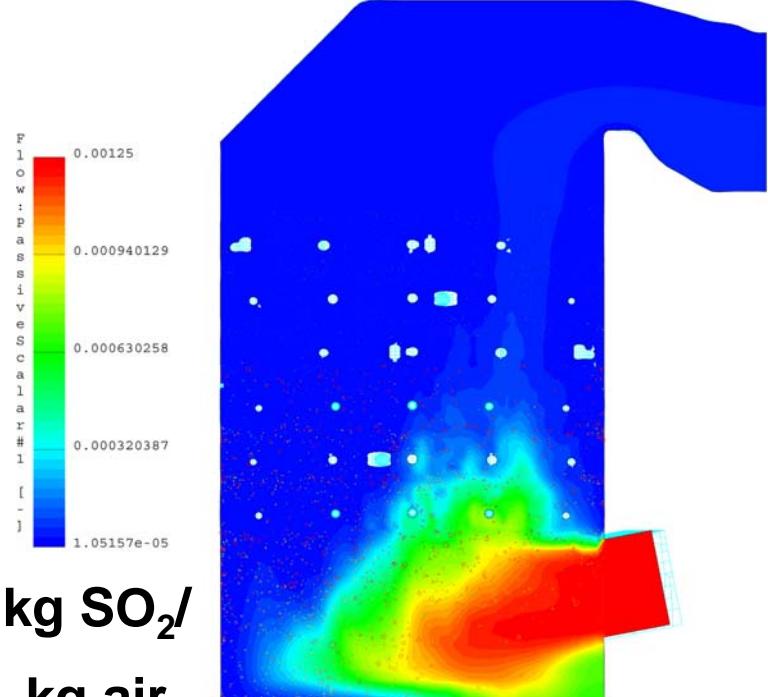


# Industrial-scale scrubber Heyden (20 m diameter)

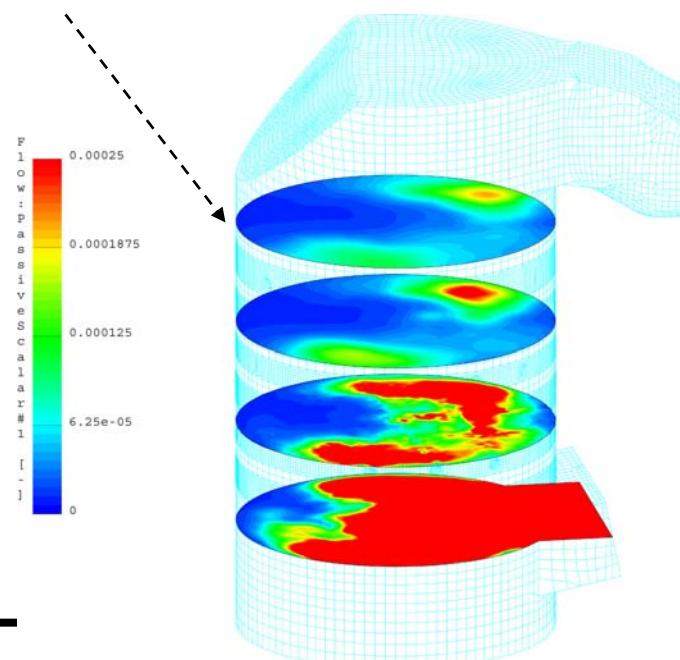
Total absorbed SO<sub>2</sub>

- 1600 mg SO<sub>2</sub> / (m<sub>N</sub><sup>3</sup>) at the entry
- Lower 4 spray-banks activated

**Total absorbed SO<sub>2</sub> 95.5 %**



Measurement (at this level)



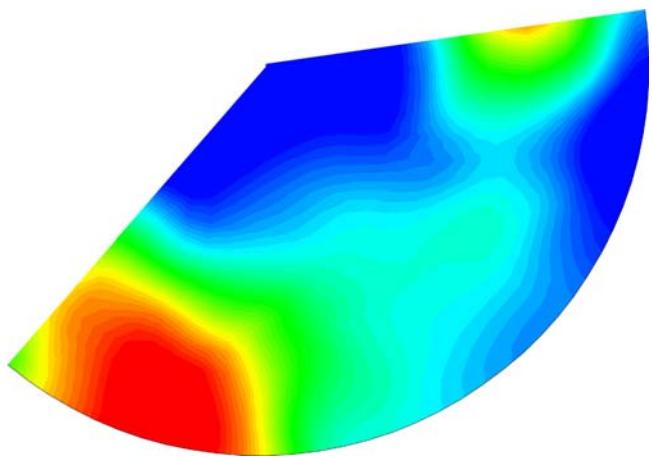
# Industrial-scale scrubber Heyden (20 m diameter)

Comparison: Measurement and simulation



Simulation

Cut z = 39 m (rotated)



Scale: 15 – 50 ppm SO<sub>2</sub>

Measurement

