DAIMLER

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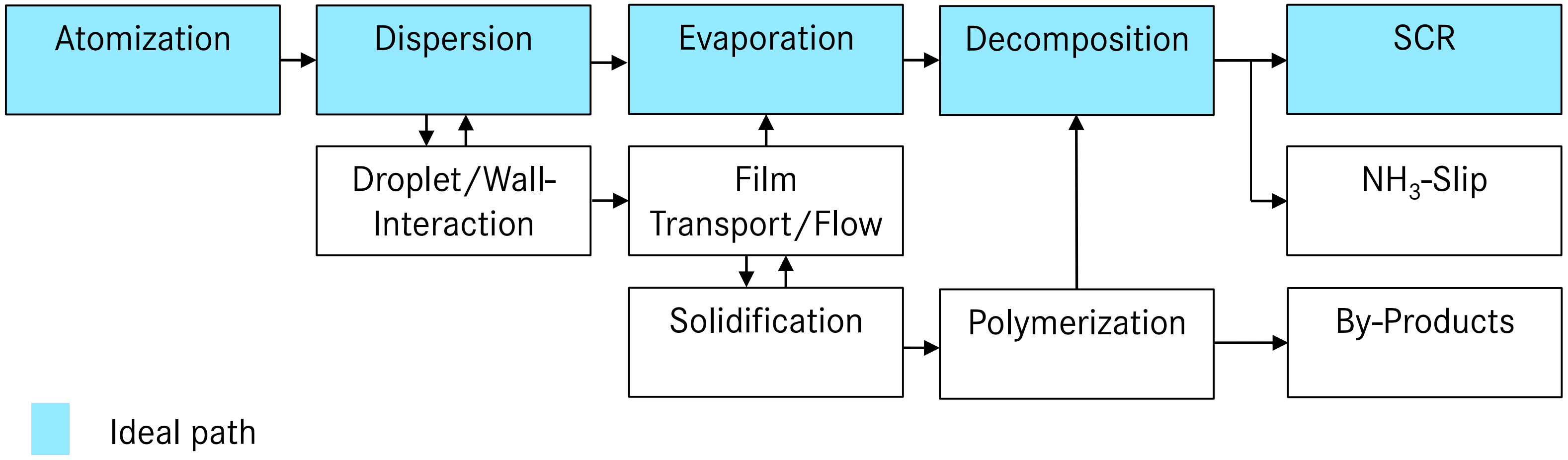
Urea to Ammonia Preparation for SCR-Systems in Commercial Vehicles – Fundamentals and Demands within the Product Development

Ludwigsburg, February 20th, 2018

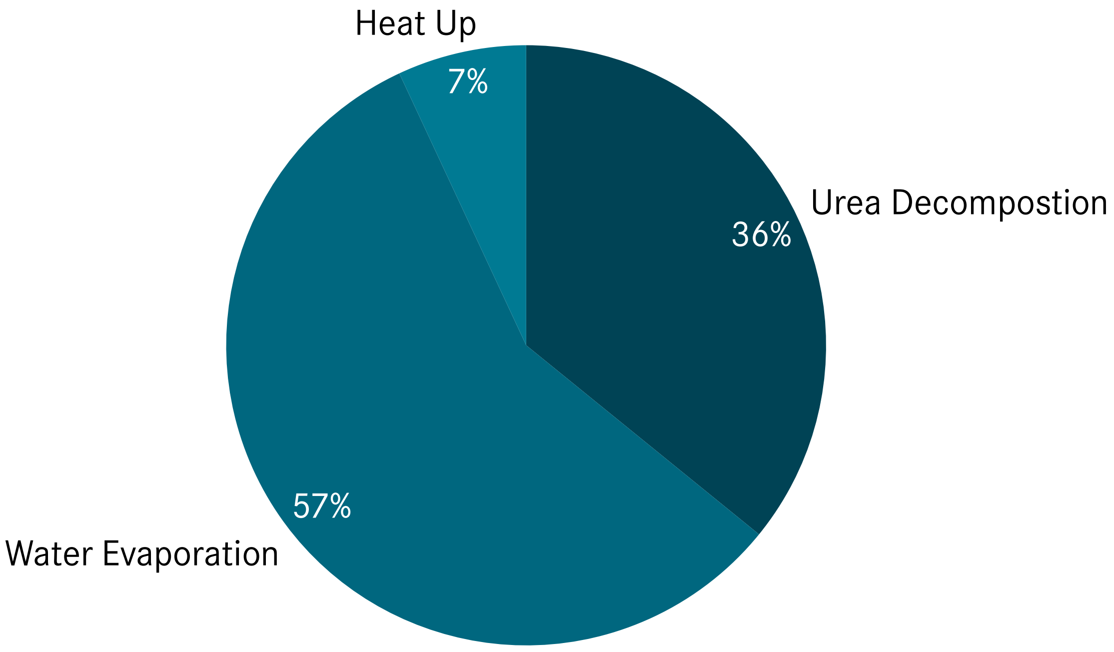
Daimler Trucks

Governing Process Steps
Overview of Phenomena



- Ideally spray preparation w/o
  - wall contact / wall film
  - solid by-products
- In reality restrictions by
  - packaging
  - spray quality
  - low temperatures
- Aggregate trade-offs
  - backpressure
  - costs

Required Energy for Preparation



Stagnant, 573K hot surrounding

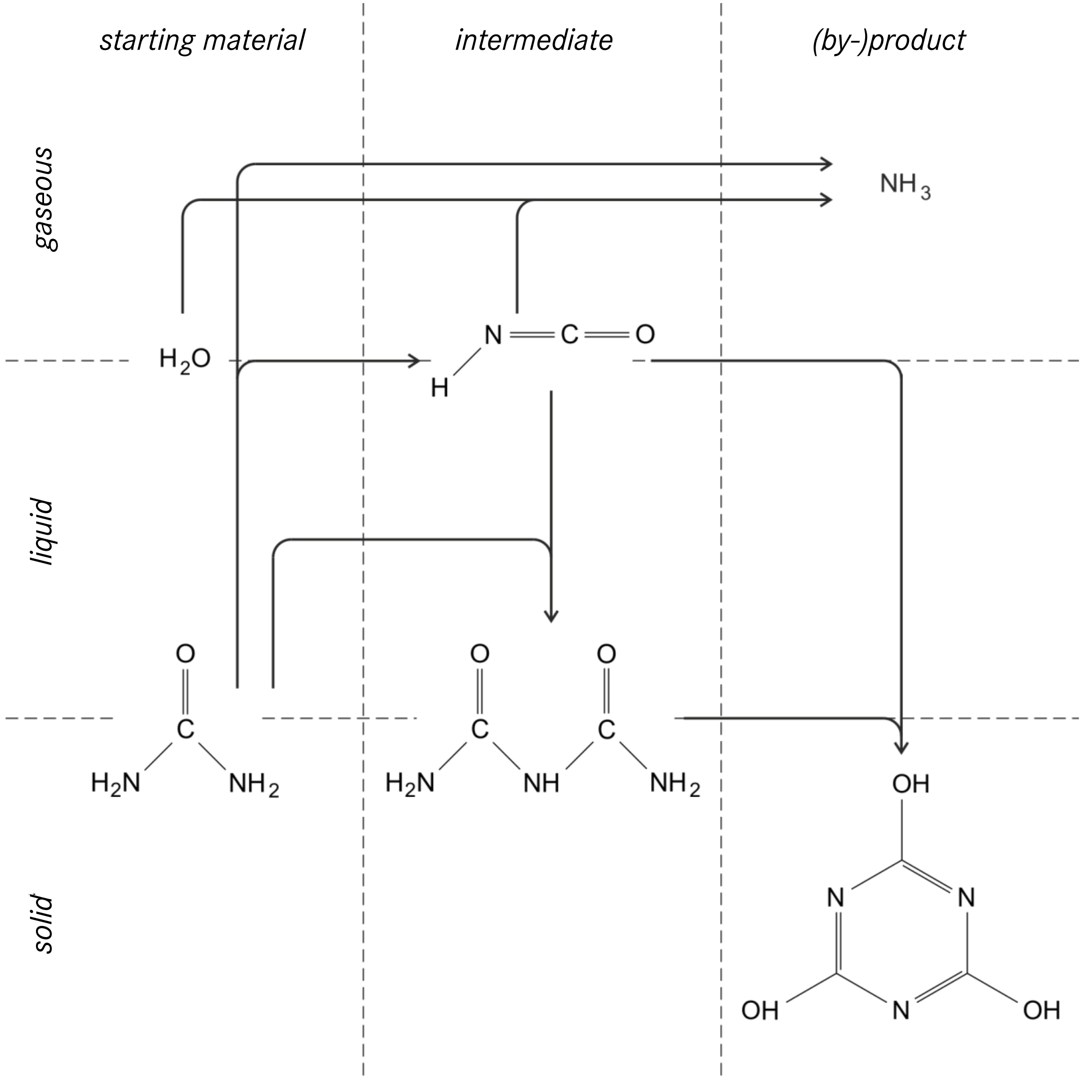
- Calculated for representative single droplet
- Starting conditions
  - 32.5% by weight
  - diameter of 70µm
  - temperature of 293K
- Decomposition consumes 1/3 of overall energy needed

Available Deposit Assessments (Selection)

Authors	Key equation	Comment
Brack et al. (2014)	$\frac{dn_r}{dt} = A_0 \cdot e^{\frac{-E_A}{RT}} \cdot V_R \cdot \prod^{j} c_j^{\gamma_j}, \quad r \in \{II, III, \ldots, XIV\}$	Liquid phase reaction for each potential paths of urea towards by-products
Becker et al. (2014)	-	Empirical regime map of spray impingement surface load vs. wall temperatur
Ebrahimian (2012)	$r_k^{reaction} = \sum_{i=1}^{Nreactions} \nu_{ki} A_i' \exp\left(-\frac{E_{a,i}}{RT}\right) \prod_{j=1}^{Nspecies} Cs_j^{\nu_{ji}} \quad [\mathrm{mol.cm^{-2}.s}]$	Solid phase reaction with active surface for each species; each potential reaction considered
Gan et al. (2016)	$\frac{\partial A_s}{\partial t} + \frac{\partial A_s u}{\partial x} = \frac{S_m Y_u}{W \varepsilon},$	Active reaction surface for each species; each potential reaction considered; see Ebrahimian above
Schiller et al. (2015)	$EER = \frac{\dot{m}_{exhaust} * c_{p_{air}} * T_{exhaust}}{\dot{m}_{DEF} * c_{p_{water}} * (100 - 70) + \dot{m}_{DEF} * h_{fg_{water}}}$	Ratio of exhaust energy available and required energy for water evaporation
Smith et al. (2014)	-	Local deposit risk based on combination of injection rate, HNCO concentration, temperature etc.
Qian et al. (2017)	-	Only urea crystallization by phase diagram of uws considered
Zhang et al. (2017)	$F_D(T) = \sum_i y_i' \cdot F_i(T)$	Empirical correlation for urea decomposition
Zheng (2016)	$\mathrm{DFP} = \alpha \frac{\mathrm{film\_height}}{\max(\mathrm{film\_height})} + (1 - \alpha) \frac{\max(\mathrm{heat\_flux})}{\mathrm{heat\_flux}}$	Appraisal index based on local film thickness, heat flux and weighting factor

- Numerous methods available
- Detail level and effort covered
  - from simple indices
  - to reaction kinetics
- Generally thermal conditions considered by all methods
- Topic is still work in progress indicated by ongoing activities

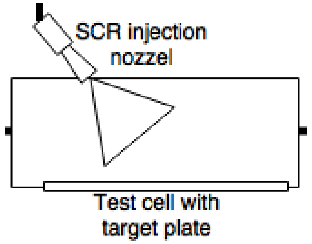
Reaction Scheme w/ Aggregation States



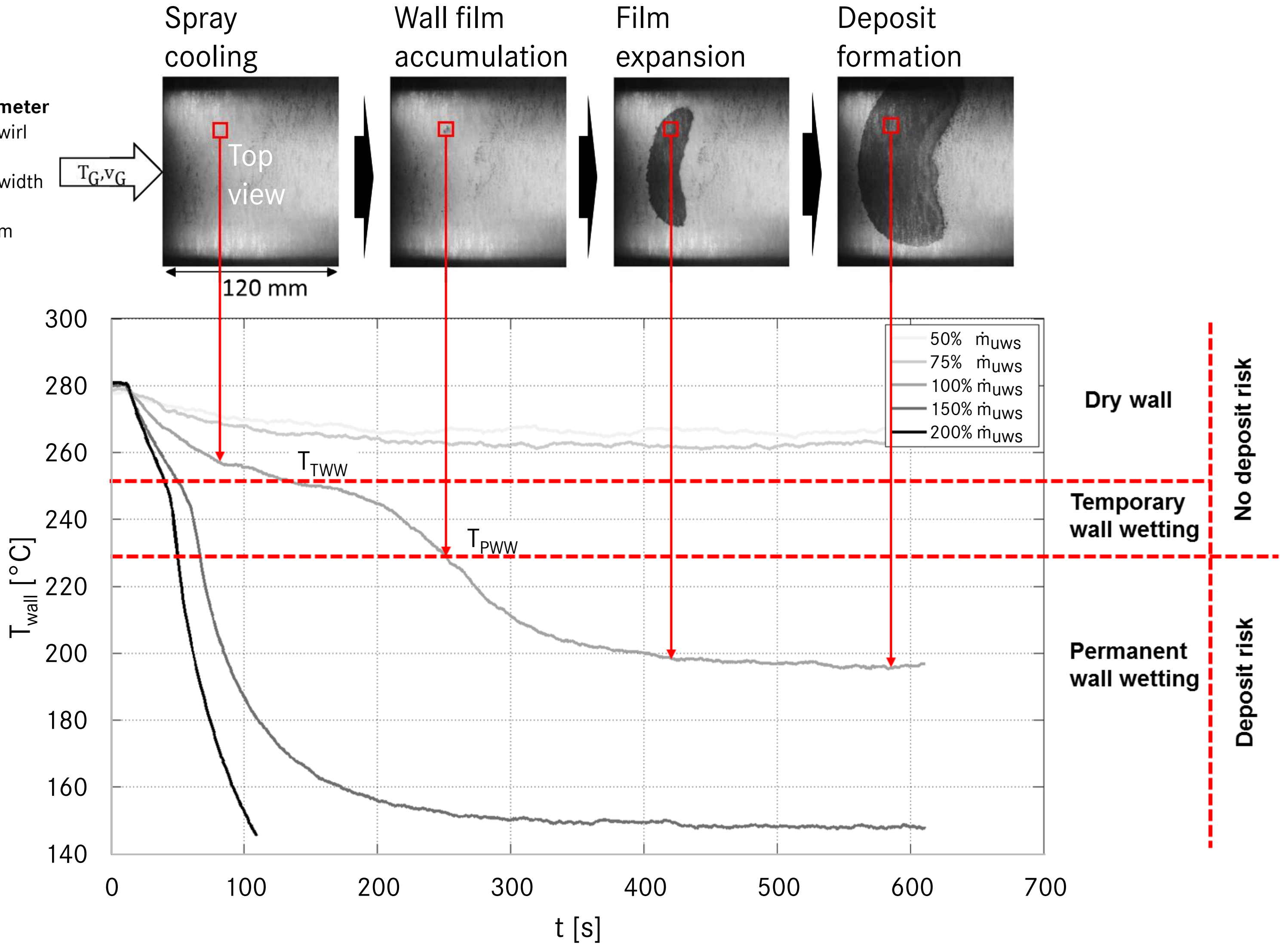
- Urea converted to HNCO and Biuret as intermediates
- Cyanuric acid identified as main component in solid by-products
- Deposit build-up rate more pronounced in temperature span of 200…225 °C

By-product reaction paths located in the vicinity of liquid interfaces / wall film.

Analysis of Wall Wetting Regimes, Kettmann (2017)

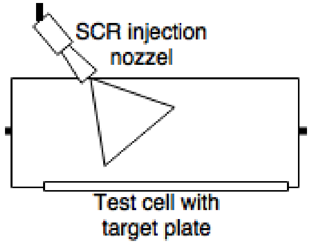


Spray parameter
- Pressure-swirl atomizer
- 1Hz pulse-width modulation
- D_{v90} = 95µm



- Three regimes w/ pulsed spray
  - **Dry Wall**
    → No liquid deposition
  - **Temporary Wall Wetting**
    → Complete evaporation during one injection period
  - **Permanent Wall Wetting**
    → Accumulation of liquid
- Correlation of regime and wall temperature
- Deposit potential expected only in liquid wall film feed

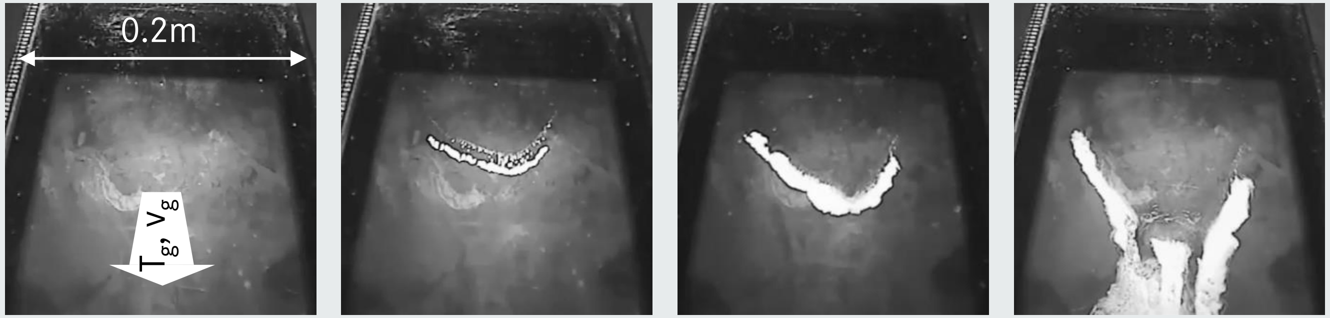
Deposit Growth
Impingement Overload and Temporal Evolution



Angled top view, gas velocity 20m/s

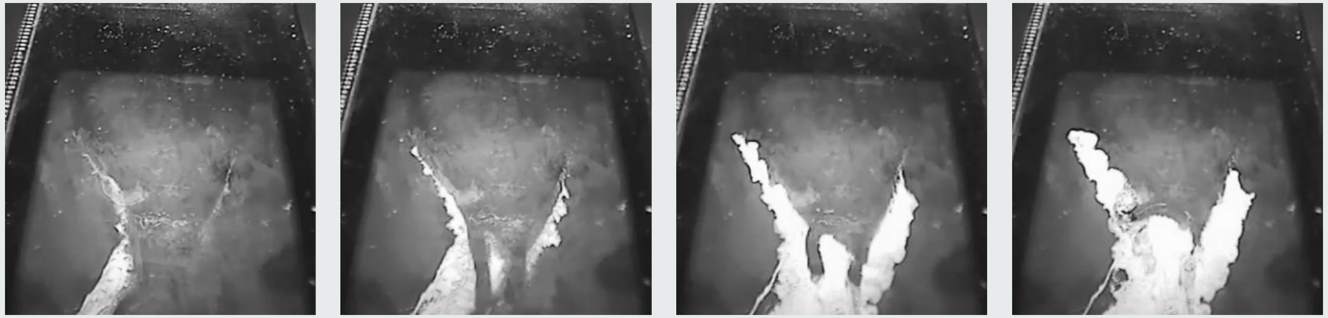
30min

$\dot{m}_{uws\_TWW}$ | +200g/h | +400g/h | +600g/h



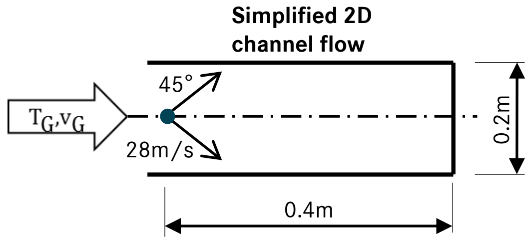
$\dot{m}_{uws\_TWW}$ + 600g/h

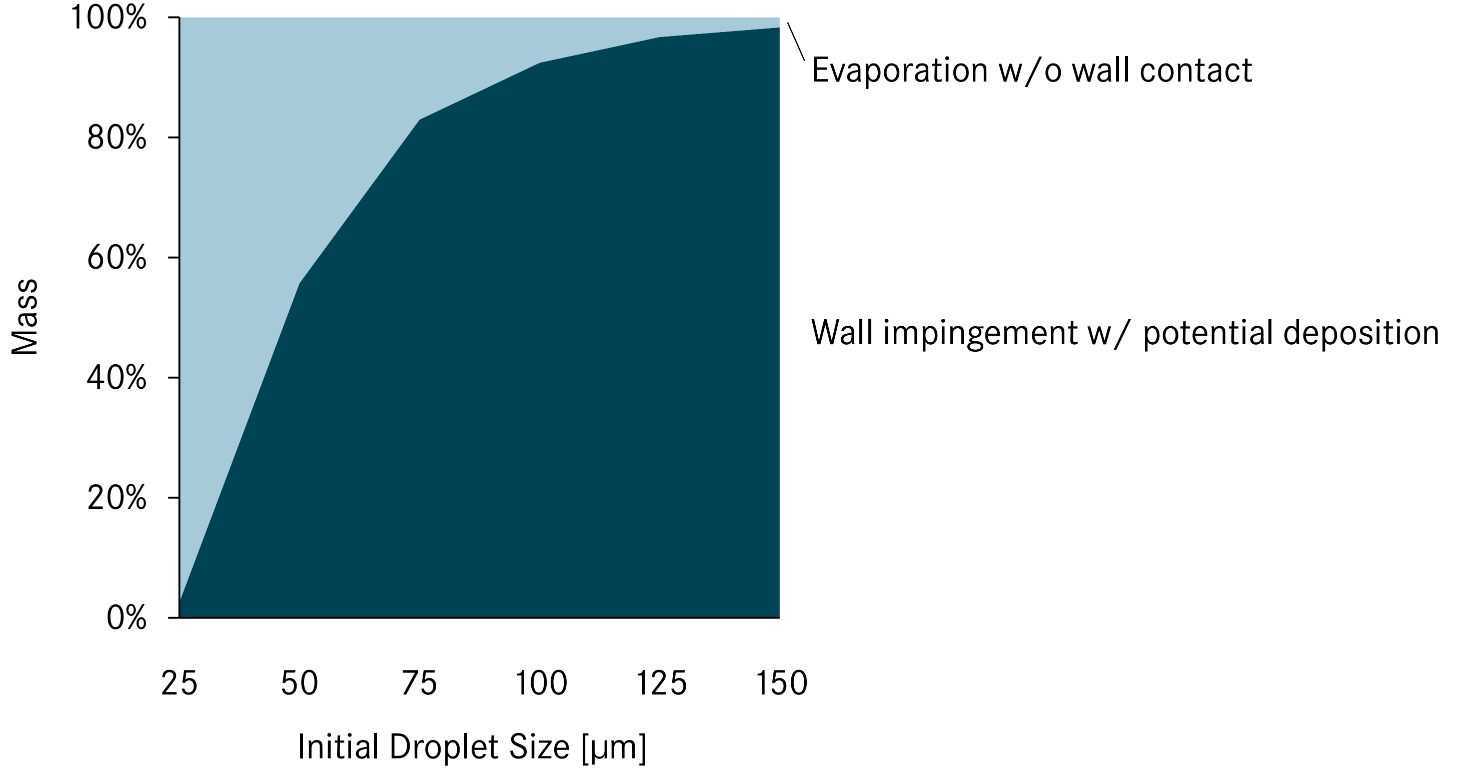
5min | 10min | 30min | 60min



- Deposit growth correlates to impingement overload
- For moderate overload deposit located near the wall film rim
- For strong overload streamlets break through
- Over time growth appears initially planar, then layered and shifted upstream

Spray Evaporation
Impact of Droplet Size on Wall Impingement

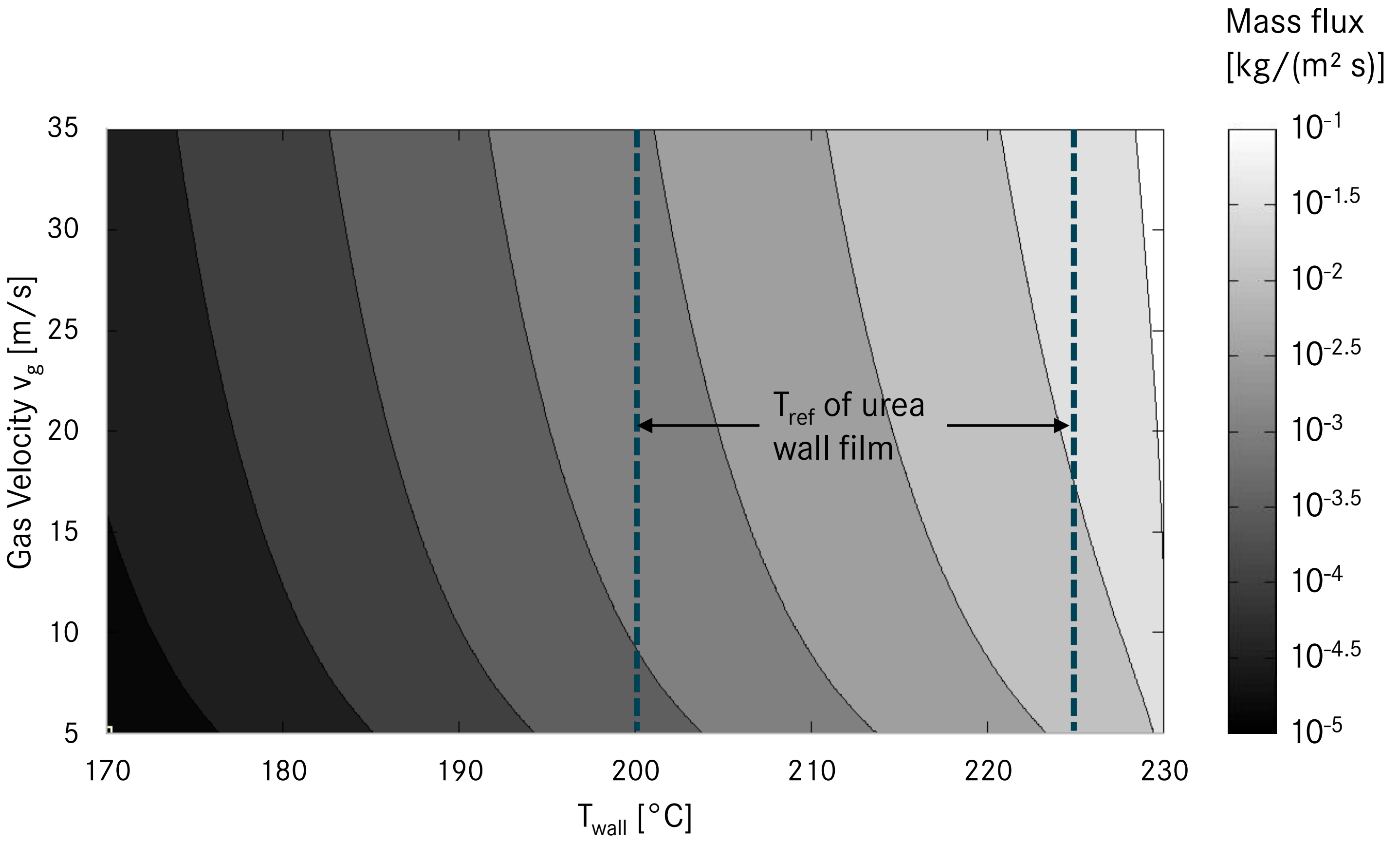




2D laminar flow 20m/s at 573K

- Mass hitting the wall calculated for single droplets
- Typically 30…80% impinged at wall in average
- Evaporation improved and deposit potential lowered w/ sizes below 50µm significantly
- Additional trade-offs determined by packaging and uniformity

Wall Film Evaporation
Mass Flux for Typical Boundaries

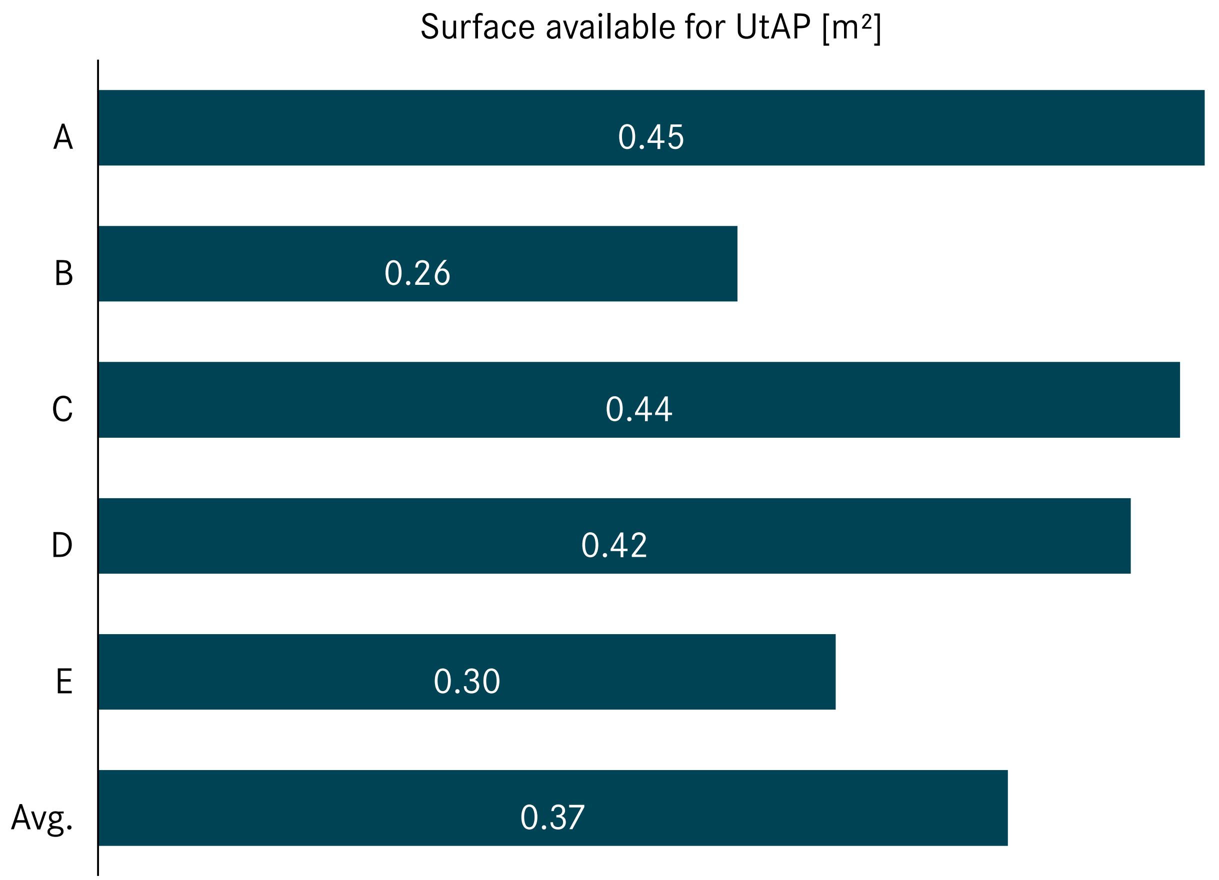


Calculation neglecting water content

$$\frac{\dot{m}_{evap}}{A} = \frac{\alpha}{c_{p,g} \cdot Le^{2/3}} \cdot \ln(1+B_M) \quad \text{with} \quad B_M = f(p_{sat,u})$$

- Evaporation depends mainly on dynamic of urea vapor pressure
- Velocities determined by layout of mixing section and driving profile
- Wall temperatures and gas velocities correspond to typical boundaries in application
- Evaporation mass flux spanned from $7 \cdot 10^{-4}$ to $5 \cdot 10^{-2}$ kg/(m² s)

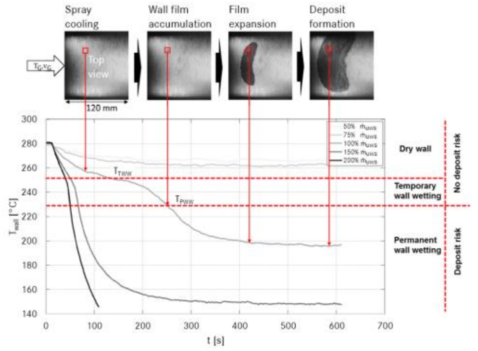
Current Heavy Duty Aftertreatment-Systems in Comparison
Surface Area of the Mixing Section



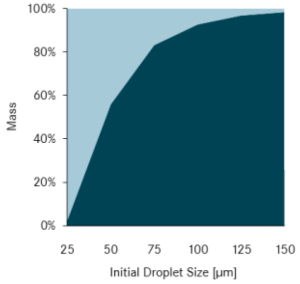
- Overall available surface for preparation estimated geometrically as indicator
- Mixing sections in today‘s aftertreatment applications equipped w/ surface around 0.37m^2 in average
- Trend for future applications expected to include increased surface up to 0.5m^2 in average

Summary

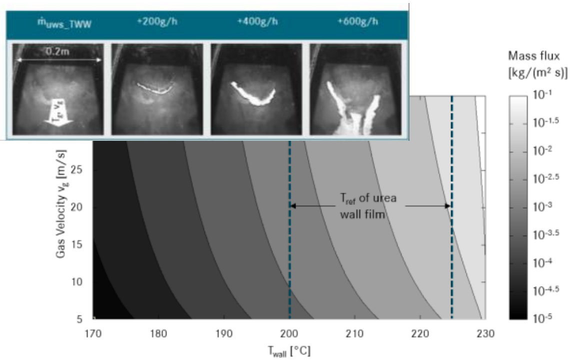
- The system's capability for preparation is a product of
  - thermal conditions due to exhaust gas temperatures / flow field,



  - spray evaporation w/o wall contact due to droplet sizes and



  - balances between wall film evaporation and impingement load / large surface area.



- Aggregate trade-offs between uniformity, backpressure and overall cost need to be fulfilled
- Injection rates corresponding to raw-NO_x emission level expected to go up
- For better preparation the adjustments between the shown factors demanded

Thank You for the Attention!

Source: Daimler| 2016_07_2584377_2016_07_28_Company_charts.pptx

Back Up

Wall Film Evaporation
Main Equations

$$\frac{\dot{m}_{evap}}{A} = \beta \cdot \rho_g \cdot \ln\left(1 + B_M\right)$$

$$p_{sat,u} = e^{-\frac{24238.62}{T} + 59.69}$$

$$\frac{\dot{m}_{evap}}{A} = \frac{\alpha}{c_{p,g} \cdot Le^{2/3}} \cdot \ln\left(1 + B_M\right)$$