Challenge in Urea Mixing Design

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General Motors

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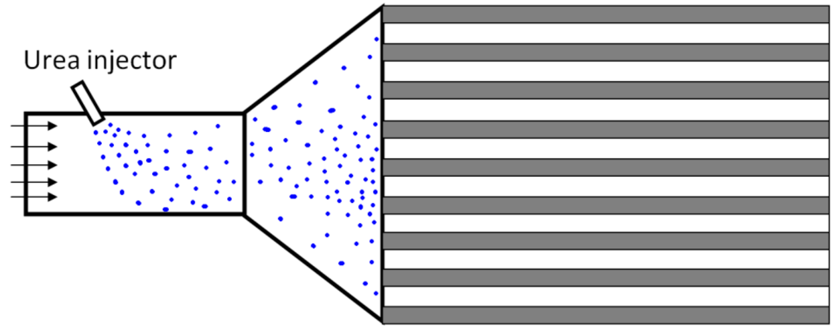
Introduction

- Urea SCR System
  - Liquid urea is introduced into exhaust flow
  - Urea droplet goes through vaporization, hydrolysis reactions to form ammonia gas
  - Ammonia adsorbs on catalyst first then reacts with NOx

  <u>(it is pre-stored ammonia to have SCR reaction, but not instant injected urea)</u>



$$(NH_2)_2CO\ (l) \dashrightarrow (NH_2)_2CO\ (g)$$

$$NH_3(g) + * \dashrightarrow NH_3*$$
$$NH_3* + O_2 \dashrightarrow H_2O + N_2$$
$$NH_3* + NO_x \dashrightarrow H_2O + N_2$$

$$(NH_2)_2CO\ (g) \dashrightarrow HCNO\ (g) + NH_3(g)$$
$$HCNO\ (g) + H_2O \dashrightarrow CO_2 + NH_3(g)$$

Introduction

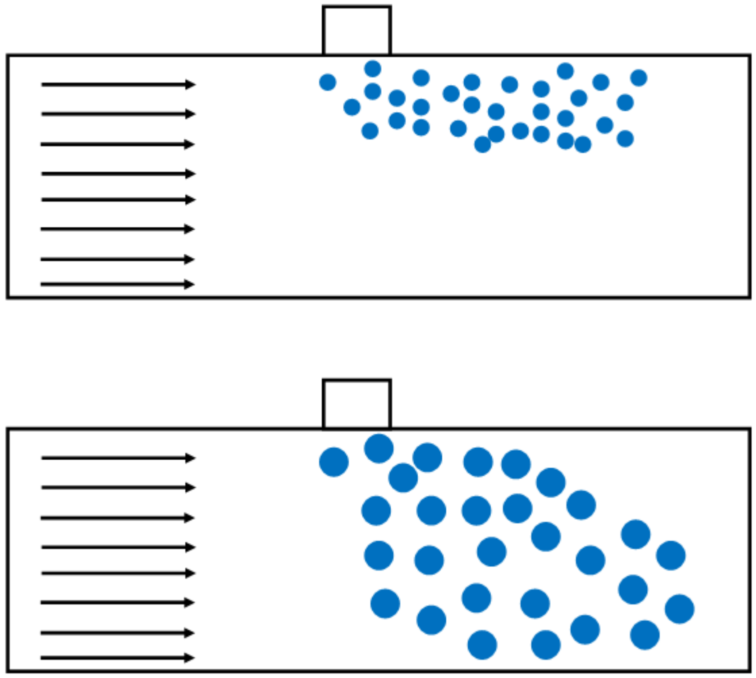
- Urea Mixing
  - Why we need mixing/mixer?
    - Vehicle packaging constrain
    - Cold-start emission
  - How mixing/mixer works?
    - Droplet breakup
    - Surface for vaporization
    - Turbulent generator
  - What conditions have poor mixing?
    - Low temperature
    - Low residue time
  - How to measure mixing result?
    - No direct method available
    - Overall SCR efficiency (NOx conversion rate)
    - Uniformity index for ***local mass flow rate ratio*** (NH3 to NOx), not urea/NH3 concentration

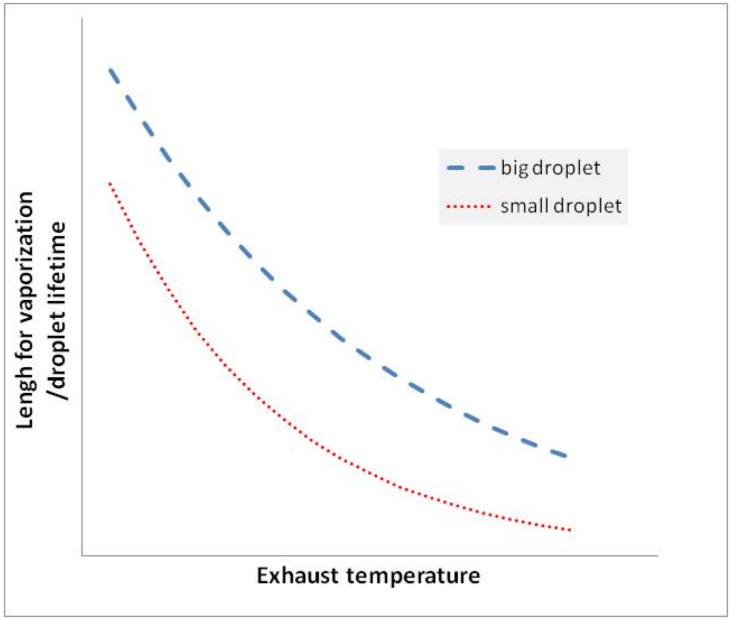
Spray

- Droplet size, small or large?
  - Vaporization rate/droplet life time

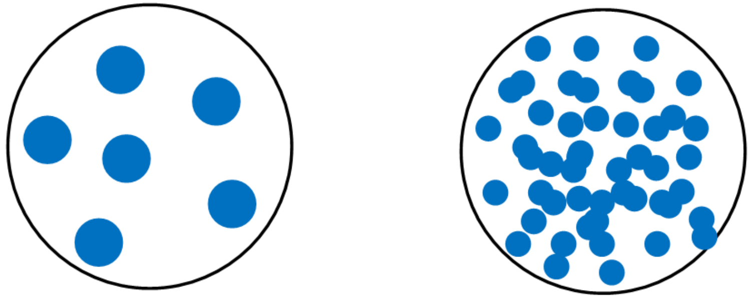
    (smaller is better)
  - Droplet number density

    (smaller is better)
  - Flow impact



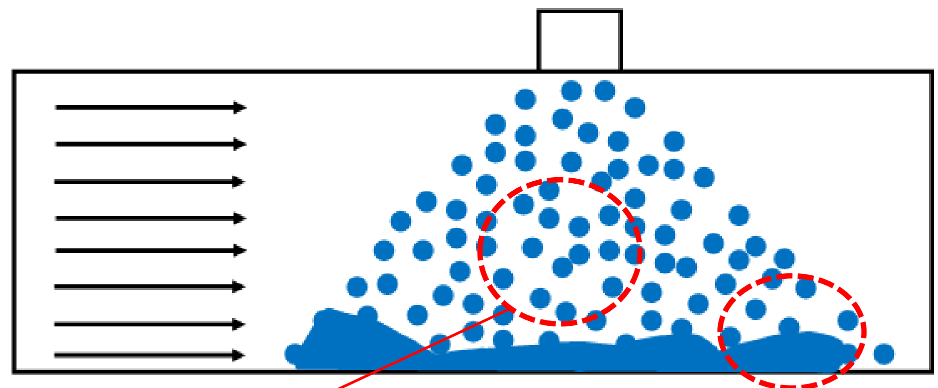


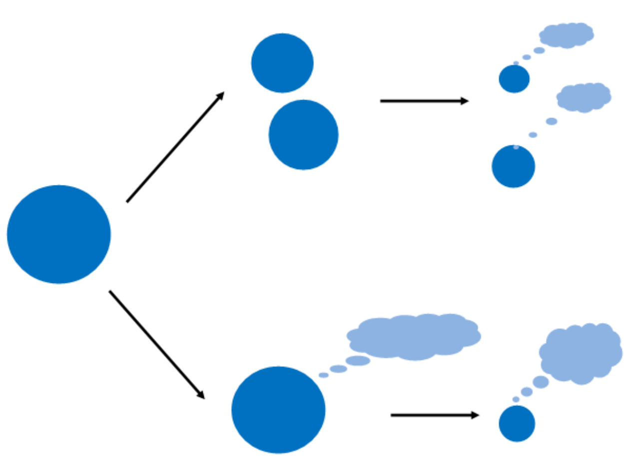
For same volume of total injected fluid, reduce droplet size by half can increase number of droplet by 8 times (2^3)

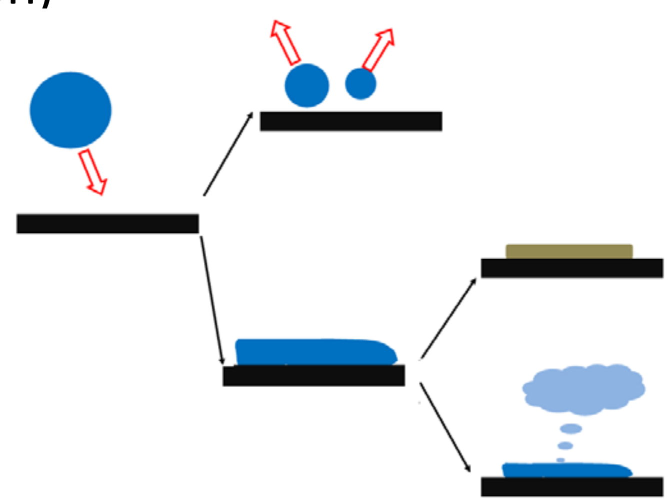


Spray

- Droplet Behavior
  - In gas phase
    - Breakup by shear stress
    - Vaporization
  - On Surface
    - Breakup by impingement
    - Liquid film
      - Vaporization
      - deposit (under certain condition)

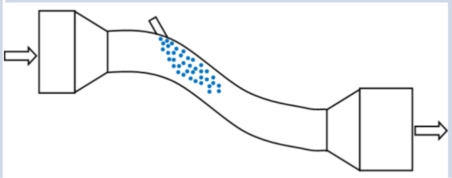
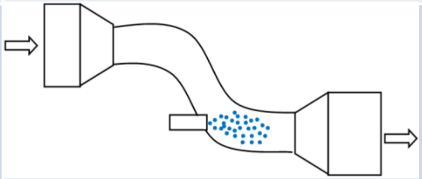






Spray

- Where to inject?
  - Side Injection
  - Center Injection
  - Elbow Injection

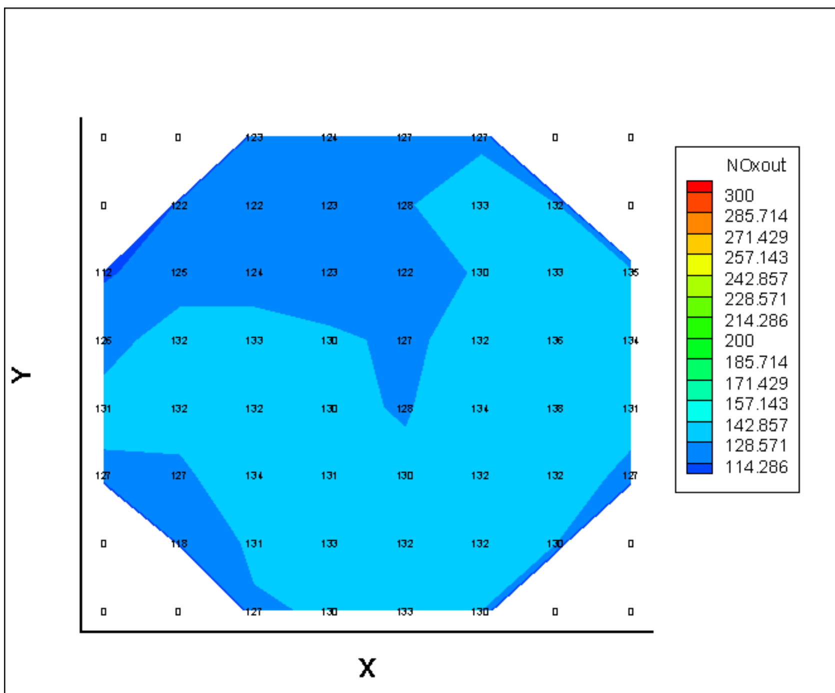
Injection Location	Diagram	Pros	Cons
Side		1. Easy for packaging	1. Poor mixing 2. Wall wetting (deposit)
Center		1. Good mixing	1 difficult for injector packaging
Elbow		1 relative good mixing and packaging	1.Back pressure 2. Flow impact

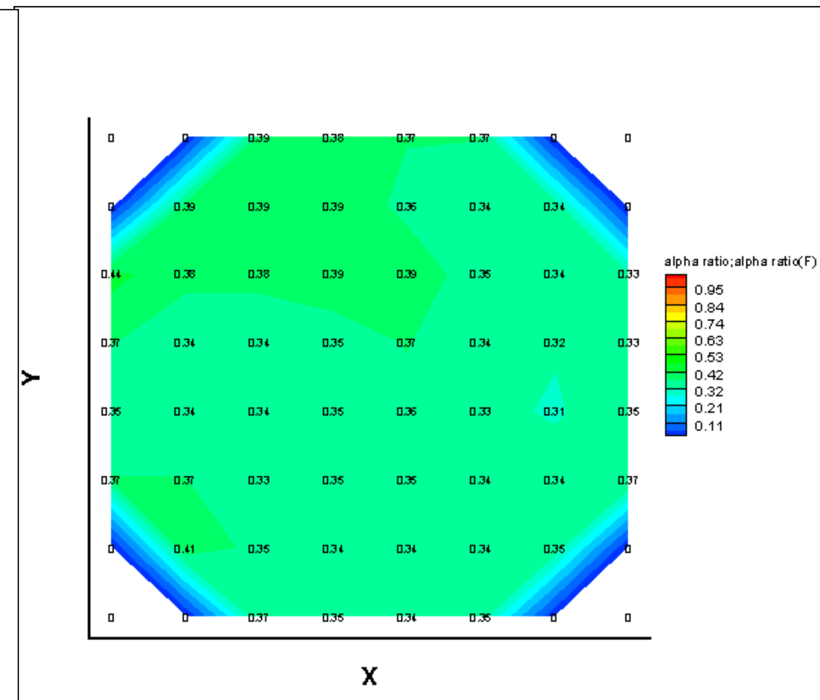
Spray

- Vaporization Rate, Does It Matter?
  - High vaporization rate can help to have good mixing of urea/NH3, however, it is not critical if the droplet size is small and uniformly distributed.

Test Condition: 180C, SV 100000/hr, inlet NO = 400ppm, alpha ratio = 0.5

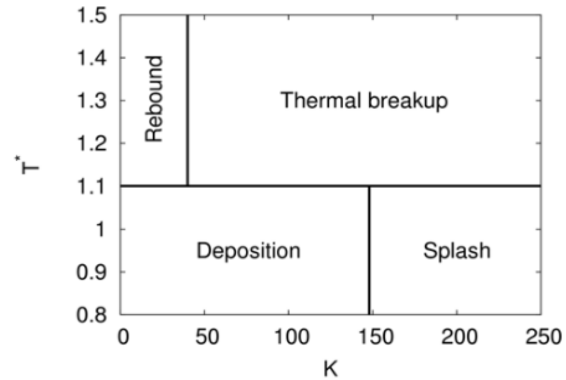
Uniformity Index > 0.9 within 7 inches mixing length (high efficient mixer installed)





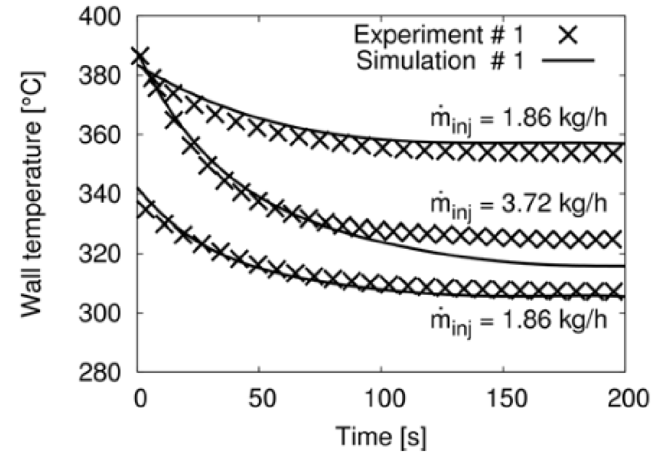
Mixer Design

- Droplet Breakup
  - Impingement (on surface)
  - Shear stress (downstream mixer)
- Liquid Vaporization
  - Surface for heat transfer (between surface and liquid, and between surface and exhaust)
  - Temperature difference between exhaust and surface
- Mixing Enhancement
  - flow turns to turbulent after the mixer , which helps transport in cross stream direction



$$T^* = \frac{T_w}{T_{sat}} \quad K = \frac{(\rho\, D)_d^{3/4} u_d^{5/4}}{\sigma_d^{1/2} \mu_d^{1/4}} = Ca^{5/4} La^{3/4}$$

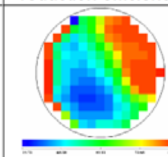
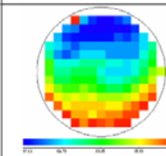
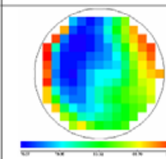
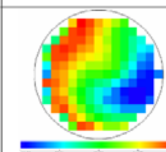
Kuhnke, PhD thesis, University Darmstadt 2004



Birkhold SAE paper 2006-01-0643

Mixer Design

- Trade-off between mixing effect and pressure drop
- Trade-off between mixing effect and cost
- Future mixer may require different structure if new injector with finer droplet or NH_3 gas dosing is applied (mixing enhancement will be more important than droplet breakup and liquid vaporization)

	Distribution of NOx reduction efficiency	OP2 Feed ratio: 1
No mixer		UI: 0.87 Pressure drop 0 KPa NOx reduction efficiency due to Urea: 0.69
Cone mixer 45 degree		UI: 0.99 Pressure drop 28.8 KPa NOx reduction efficiency due to Urea: 0.843
Cone mixer 60 degree		UI: 0.98 Pressure drop 8.5 KPa NOx reduction efficiency due to Urea: 0.837
Cone mixer 75 degree		UI: 0.95 Pressure drop 4.5 KPa NOx reduction efficiency due to Urea: 0.829

Zheng SAE paper 2009-01-2879

Deposit Formation

- Key Factors for Deposit Formation
  - Temperature
  - Exhaust gas flow rate
  - Urea dosing rate
- Correlation for Deposit Formation
  - Root cause is surface temperature
  - Based on heat transfer balance

$$m_{urea}\Delta h_{fg} = hA\left(T^g - T^s\right)$$

$$\Rightarrow T^s = T^g - \frac{m_{urea}\Delta h_{fg}}{hA}\begin{cases} T^s > T^* & no\ deposit \\ T^s < T^* & deposit\ formed \end{cases}$$

h : convective heat transfer coefficient

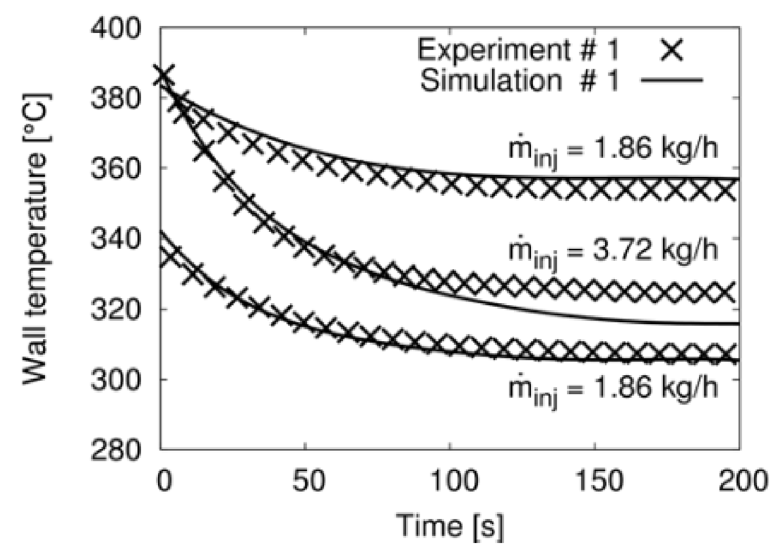
(a function of flow rate for turbulent flow)

m_{urea} :surafe vaporization rate of urea ($\leq$injection rate)

Maximum injection rate without causing wall-wetting or deposits.

Gas Temperature (C)	Exhaust Mass Flow Rate					
	200 Kg/hr	300 Kg/hr	400 Kg/hr	500 Kg/hr	600 Kg/hr	700 Kg/hr
200	0	0	0			
250	0	0	0.15	0.5	1.5+	
300		0.2	0.7	1.1	1.5+	1.5+
350			1.5	1.5+	1.5+	1.5+
400					2.0+	3.0+

Zheng SAE paper 2010-01-1941



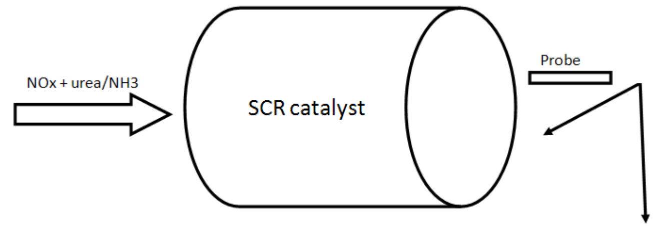
Birkhold SAE paper 2006-01-0643

Conditions for Mixing Measurement

- Test Setup
  - NOx and NH3 are measured at SCR outlet
  - NH3 Distribution at SCR inlet is estimated with outlet information and mass balance

NH3_inlet =

NH3_outlet + (NOx_inlet – NOx_outelt)



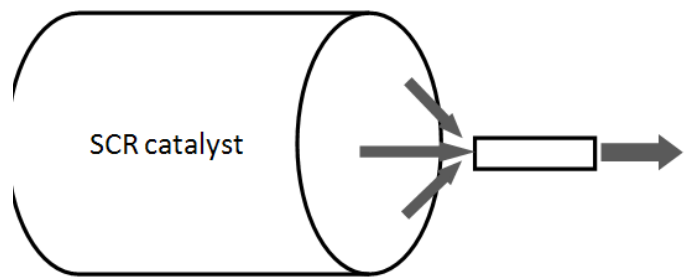
- Suitable Test Condition
  - Temperature < 400C to minimize NH3 oxidation reaction
  - Temperature higher than T(?) to avoid deposit formation and NH3 storage upstream SCR(*)
  - NH3 to NOx ratio <1 to eliminate NH3 storage effect
  - NO2 concentration as low as possible (slow SCR reaction has non 1:1 reaction ratio for NH3 and NO2)
  - Sampling gas flow rate should match the local exhaust flow rate.
  - Sampling pipe location should be close the catalyst brick.

$$4NH_3 + 3O_2 \longrightarrow 2N_2 + 6H_2O$$

$$4NH_3 + 4NO + O_2 \longrightarrow 4N_2 + 6H_2O$$

$$4NH_3 + 2NO + 2NO_2 \longrightarrow 4N_2 + 6H_2O$$

$$\underline{8NH_3 + 6NO_2} \longrightarrow 7N_2 + 12H_2O$$



<u>Is there a more accurate and directly way to measure urea/NH3 distribution in front of SCR?</u>

CFD vs. Test

- CFD model
  - Simplified spray model
  - Preciously defined initial and boundary condition
  - Instant picture of distribution
  - Clear reactions
  - True steady-state
- Test Setup
  - Complicated spray
  - Ambiguous initial and boundary condition
  - Time averaged measurement
  - Complicated reactions
  - State with small variations

- The difference in nature makes it difficult to match CFD result with test result, however, correct CFD model should predict similar distribution pattern as test result.
- Because of the local and time averaging effect, test seems to show higher uniformity than CFD prediction.
- Low temperature test (< 300C) always has urea/NH3 mass balance error (calculated urea/NH3 at SCR inlet is less (10%+) than actually dosed urea (maybe due to NH3 adsorption?), which leads the question how should we distribute the unaccounted NH3 to the measured distribution to get the accurate map of inlet.

Summary

- Urea mixing is critical to meet more stringent emission standard
- Effective urea mixing design should be based on the nature of the selected injector (spray)
- It is challenge to measure the real distribution of urea/NH3
- People should be aware of the difference of measured and simulated mixing result.