PREDICTIONS OF UREA DEPOSIT FORMATION WITH CFD USING AUTONOMOUS MESHING AND DETAILED UREA DECOMPOSITION

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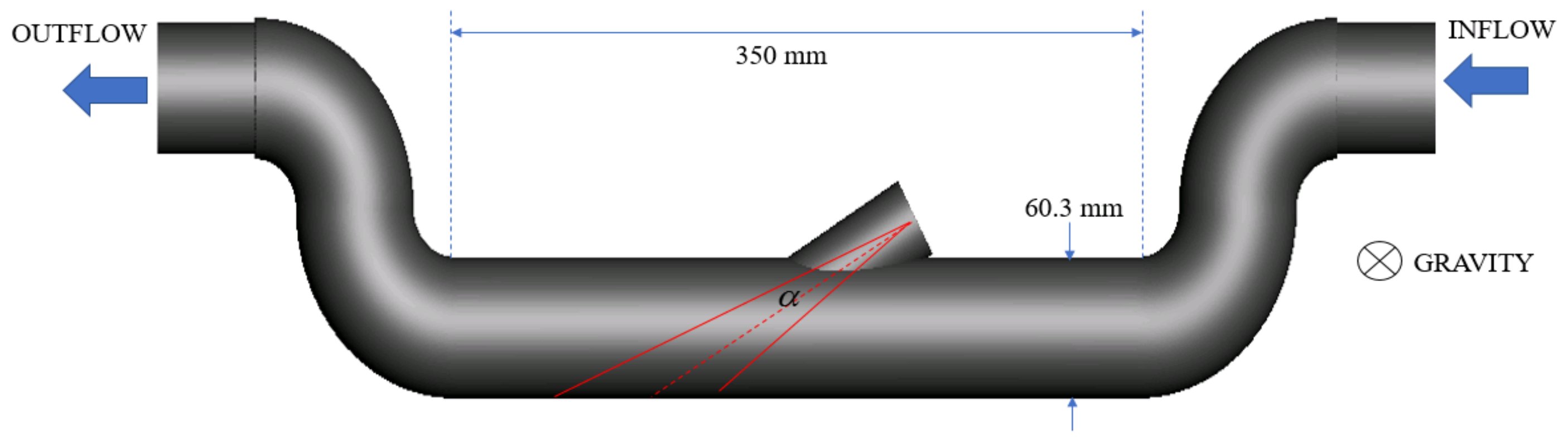
MOTIVATION and BACKGROUND

- Urea-water solution (UWS) injection combined with Selective Catalytic Reduction (SCR) has developed as an effective method of meeting EPA and EURO NOx emissions regulations for diesel engines.
- One key challenge faced by modern urea/SCR systems is the formation of solid deposits of urea decomposition by-products that are difficult to remove.
- Urea deposits only form in a narrow range of wall temperatures and take many minutes to hours to form, which poses a challenge to conventional CFD tools.
- The autonomous CFD meshing code, CONVERGE, used in this study incorporates a detailed urea decomposition mechanism with Conjugate Heat Transfer (CHT) and spray-wall interaction models to predict wall temperatures with filming. The CFD code also takes advantage of a fixed flow approach and CHT super-cycling to dramatically accelerate the flow and spray simulation to reach the time scale required for appreciable deposit formation [1].
- The prediction approach is applied to a practical exhaust system urea deposit test bench published by Brack et al, 2016 [2] .

APPROACH

CFD Geometry and Boundary Conditions



O.P.	Inflow Gas Temperature [K]	Inflow Gas Mass Flow Rate [kg/h]	UWS Dosing Rate [mg/s]	Spray Cone Angle [◦]	Duty Cycle	Outer Wall Radiation Emissivity
1	488	100	44	16	5%	0.9
2	573	200	86	10	10%	0.9
3	713	300	88	16	10%	0.9

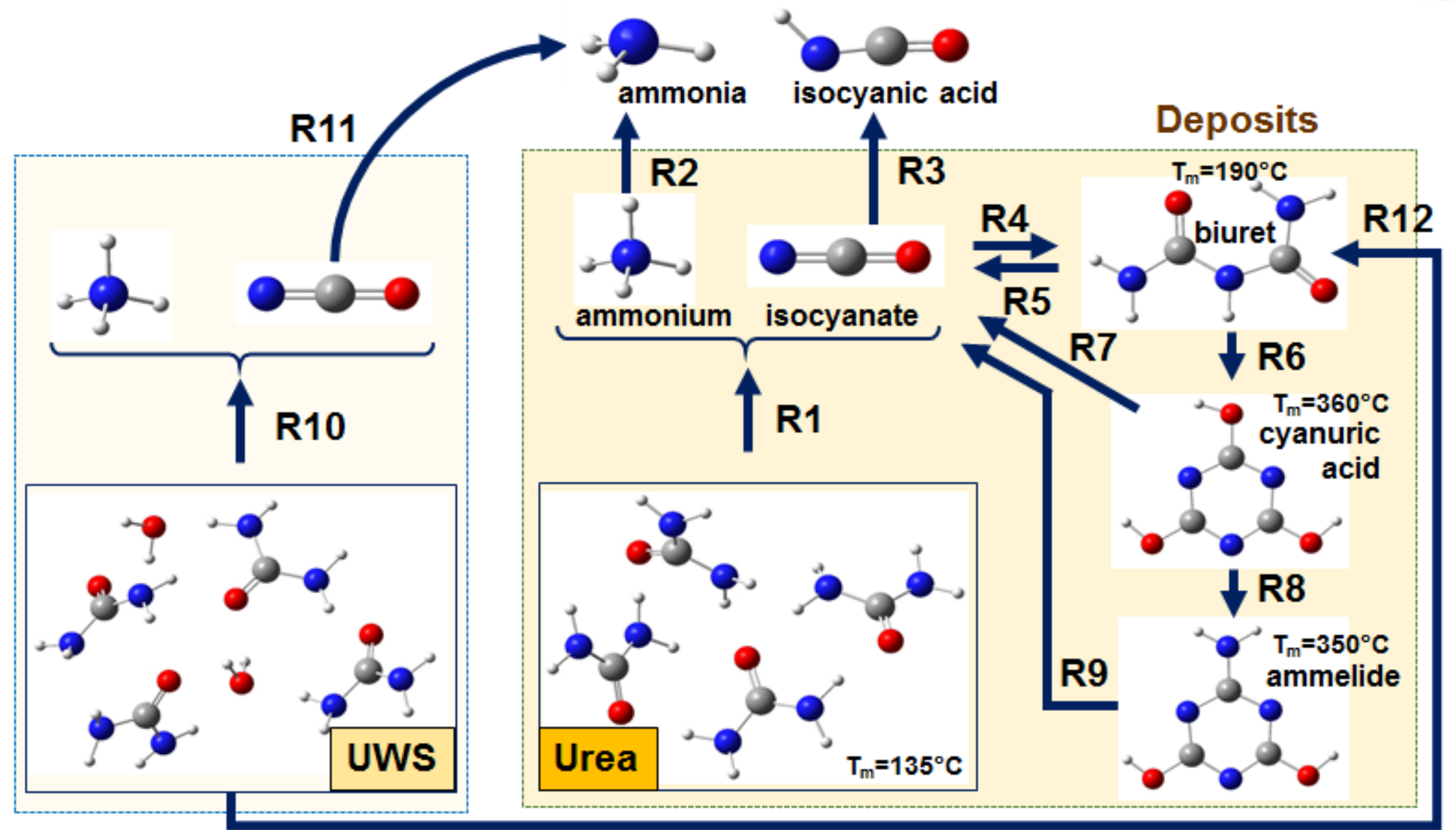
Injector	Spray Cone Angle [◦]	SMD [um]	Dv90 [um]	Rosin-Rammler q	Injection Velocity [m/s]
Bosch_1	10	173	346	2.61	24
Bosch_2	16	91	238	2.61	24

Autonomous Meshing

- The CFD code automatically generates a body-fitted volume mesh at runtime using a Cartesian cut-cell technique.
- A base grid of 4 mm is defined. Fixed embedding is applied on the pipe boundaries and near the injector. Solid wall regions have two levels of fixed embedding.
- Grid scaling feature is used to conduct a mesh sensitivity study.

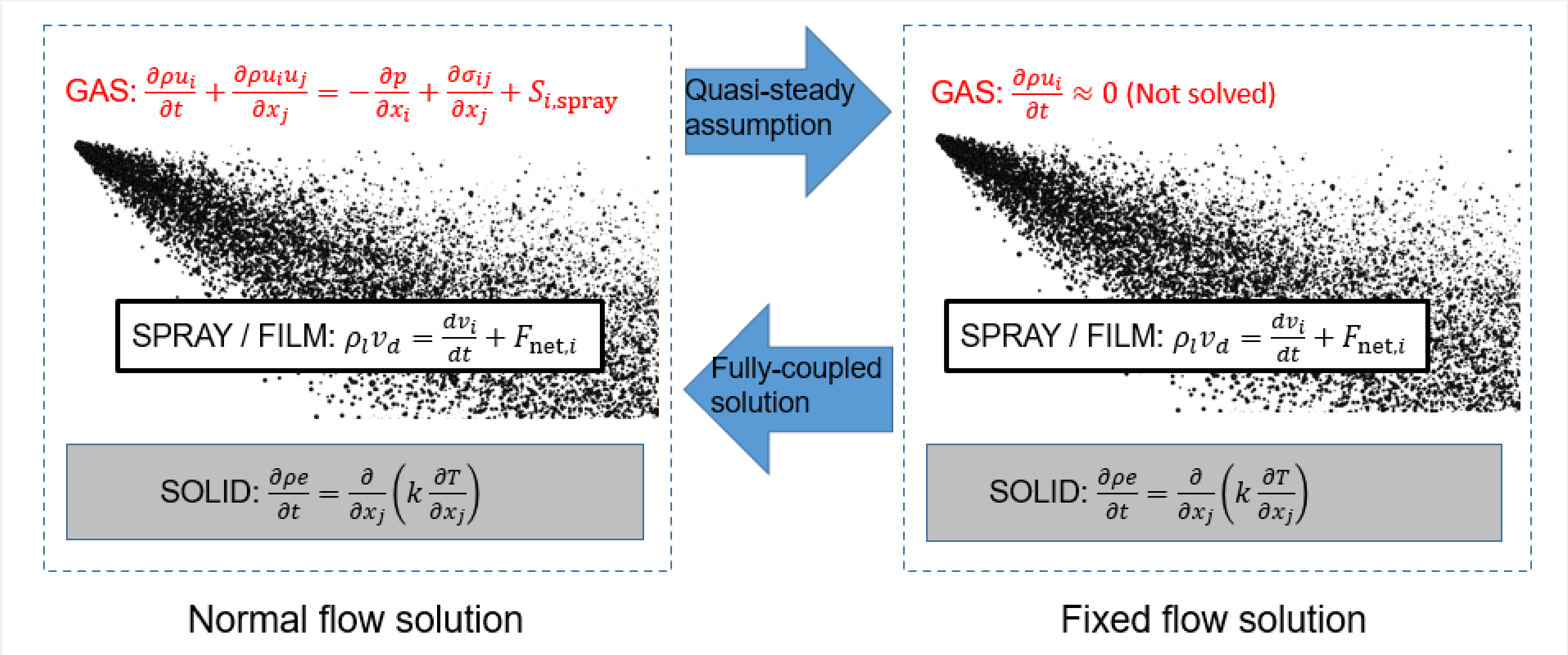
APPROACH

Urea Detailed Decomposition Model



- A 12-step chemical kinetics [3,4] is adopted to model the urea decomposition and deposit formation.
- Compared to the classic molten solid urea decomposition model, where the urea thermolysis is modeled by a single chemical reaction, the urea detailed decomposition model itemizes each step during the urea thermolysis process and is able to predict reaction rate of various urea decomposition by-products (biuret, CYA, ammelide, etc.).
- The urea deposit formation only occurs within a narrow temperature range and is sensitive to temperature change.
- The Kuhnke splash model is used to model the spray/wall interaction. The Wruck heat transfer model is turned on for spray dry wall heat transfer prediction.

Fixed Flow Model and CHT Super-cycling



Normal flow solution

Fixed flow solution

- For most aftertreatment cases, quasi one-way coupling between exhaust flow and spray can be assumed.
- For a pulsed spray, the flow field can be frozen periodically. The solver stops solving the continuity, momentum and species equations when the flow is fixed. Only spray parcel tracking continues. The fixed flow model can speed up aftertreatment filming and deposit modeling substantially [5].
- Within each super-cycle of the wall CHT, the solver gathers the heat transfer coefficient data and calculates the wall temperature in a steady-state manner at the end of the cycle. This feature allows the wall to reach thermal equilibrium at a much faster pace without tuning the solid heat capacity.

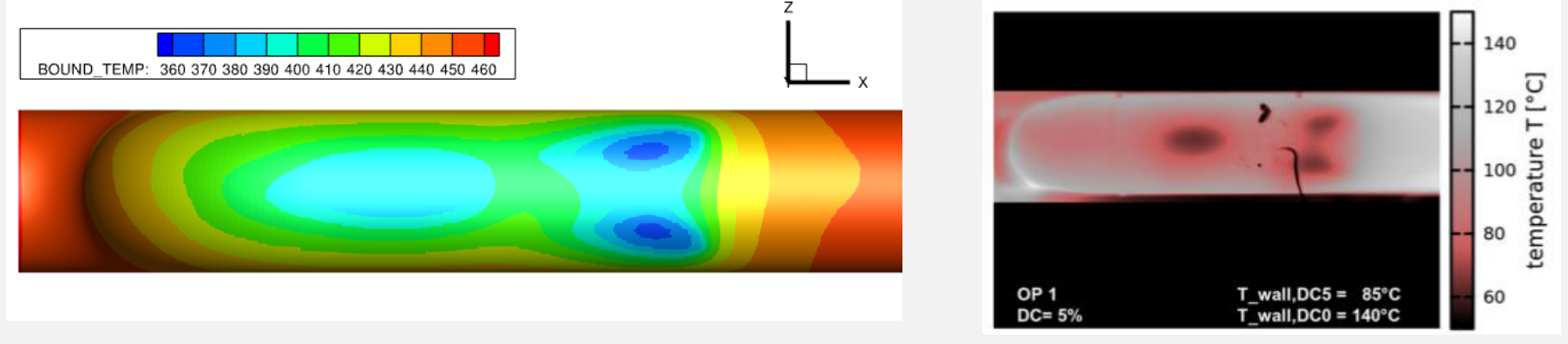
Cooldown Simulation

- A cooldown simulation is conducted to account for the cooldown period in the experiments before retrieving the deposit sample.
- Urea deposit data is mapped in the cooldown simulation from the pre-cooldown run.
- Spray is turned off along with the inflow. Wall temperature is allowed to cool down eventually to the room temperature. With a fixed CFL, the cooldown simulation can run extremely fast.

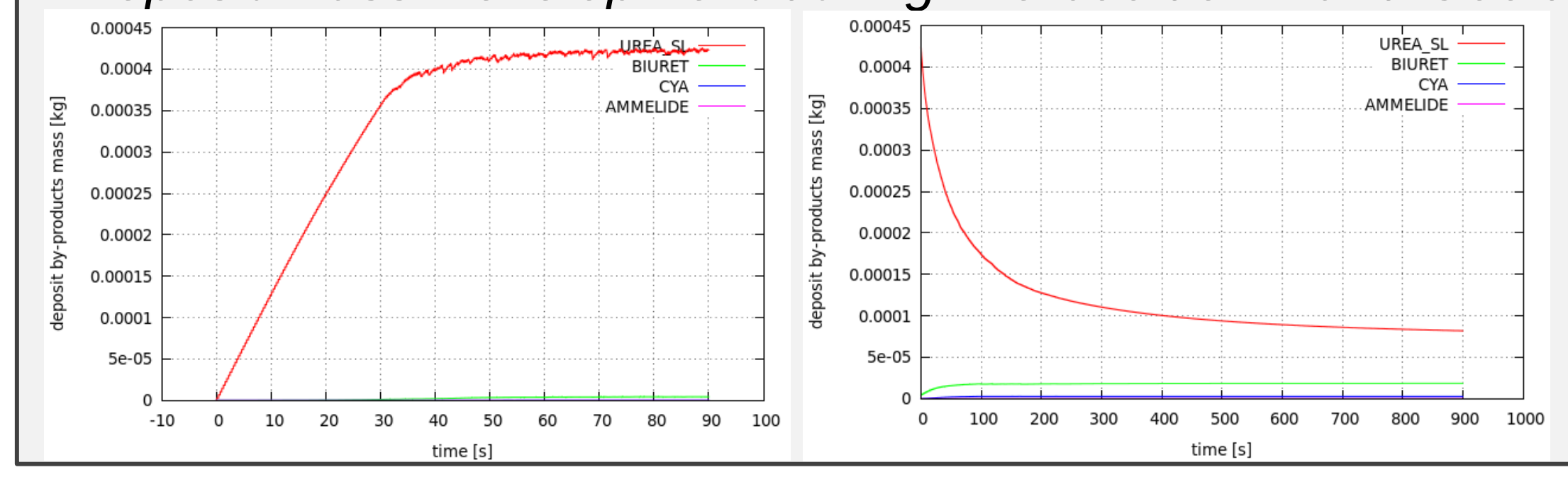
RESULTS

O.P. 1

Pipe Wall Temperature Field at Steady State



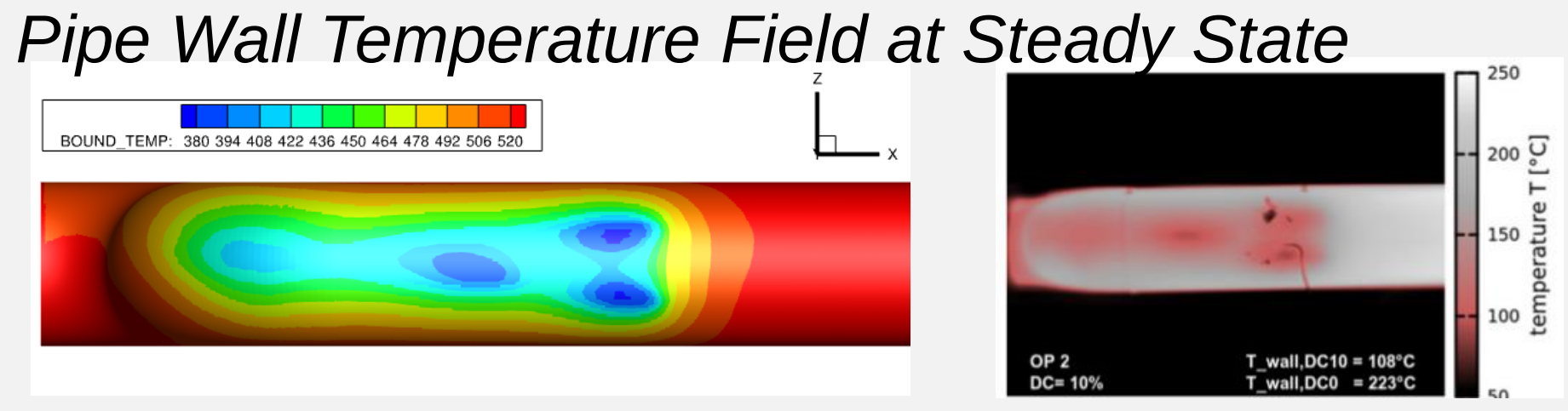
Deposit Mass Development during Pre-cooldown and Cooldown Simulation



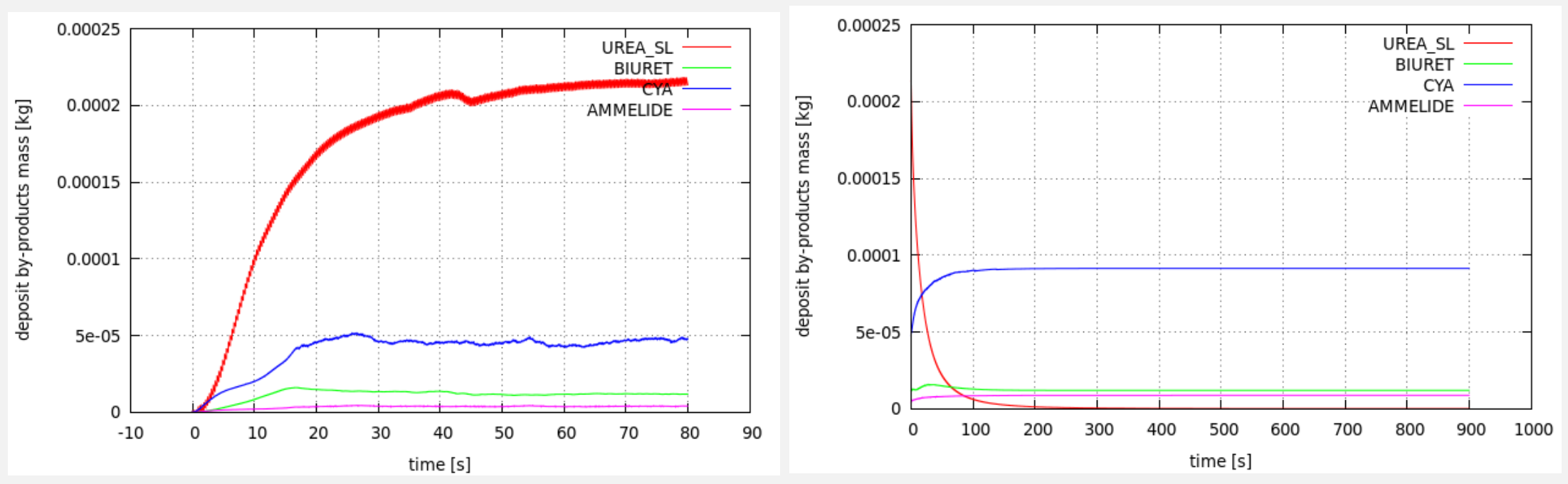
Deposit By-products	Mass [kg]	Mass Fraction	Experiment
UREA_SL	8.5e-5	80%	94.3%
BIURET	1.8e-5	17%	7.3%
CYA	3e-6	3%	0%
AMMELIDE	0	~0%	0%
Total	1.06e-4	100%	101.6%

O.P. 2

Pipe Wall Temperature Field at Steady State



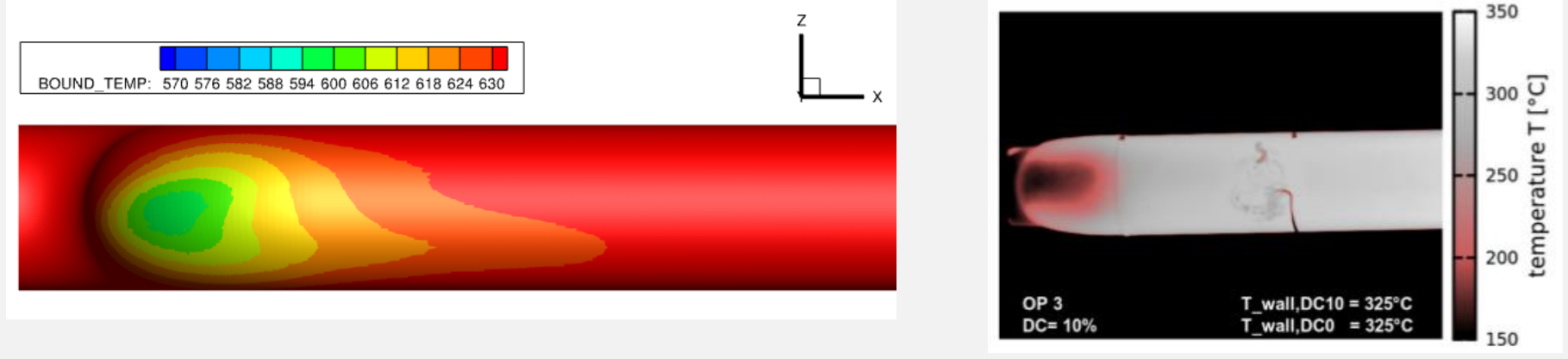
Deposit Mass Development during Pre-cooldown and Cooldown Simulation



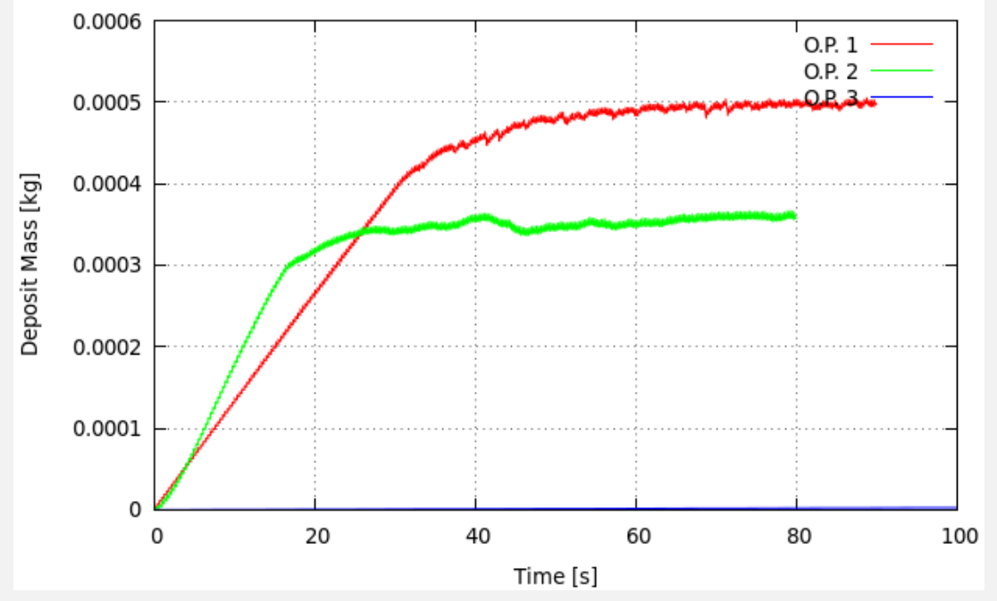
Deposit By-products	Mass [kg]	Mass Fraction	Experiment
UREA_SL	0	0%	0.8%
BIURET	1.1e-5	9.9%	0.5%
CYA	9.2e-5	82.9%	80.3%
AMMELIDE	8e-6	7.2%	18.2%
Total	1.11e-4	100%	99.8%

O.P. 3

Pipe Wall Temperature Field at Steady State



Deposit Mass Development during Pre-cooldown Simulation



Deposit By-products	Mass [kg]	Mass Fraction	Experiment
UREA_SL	0	0%	0%
BIURET	0	0%	0%
CYA	~0	0%	0%
AMMELIDE	~0	0%	0%
Total	~0	0%	0%

Simulation Runtime

- The fixed flow and CHT super-cycling model substantially speeds up the urea deposit simulations.
- O.P. 2 simulation including pre-cooldown and cooldown can be completed within several days.

	Cell Count	Core Count	Convection CFL	Spray CFL	Runtime
Pre-Cooldown	0.75 M	96	10	10	26 s/day
Cooldown	0.56 M	96	10	100	512 s/day

REFERENCES

[1] Richards, K., Senecal, P., and Pomraning, E., “CONVERGE (Version 3.0) Manual,” (Madison, Convergent Science, Inc., 2020)
[2]Brack, W., Heine, B, Birkhold, F., Kruse, M. and Deutschmann, O., “Formation of Urea-Based Deposits in an Exhaust System: Numerical Predictions and Experimental Observations on a Hot Gas Test Bench,” Emission Control Science and Technology (2016) 2:115–123
[3] Sun, Y., Sharma, S., Vernham, B., Shibata, K. and Drennan, S., “Urea Deposit Predictions on a Practical Mid/Heavy Duty Vehicle After-Treatment System,” SAE Technical Paper 2018-01-0960, 2018, doi:10.4271/2018-01-0690.
[4] Habchi, C., Quan, S., Drennan, S., and Bohbot, J., “Towards Quantitative Prediction of Urea Thermo-Hydrolysis and Deposits Formation in Exhaust Selective Catalytic Reduction (SCR) Systems,” SAE Technical Paper 2019-01-0992, 2019, doi:10.4271/2019-01-0992.
[5] Maciejewski, D., Sukheswalla, P., Wang, C., Drennan, S.A. and Chai, X., “Accelerating Accurate Urea/SCR Film Temperature Simulations to Time-Scales Needed for Urea Deposit Predictions,” SAE Technical Paper 2019-01-0982, 2019, doi:10.4271/2019-01-0982.

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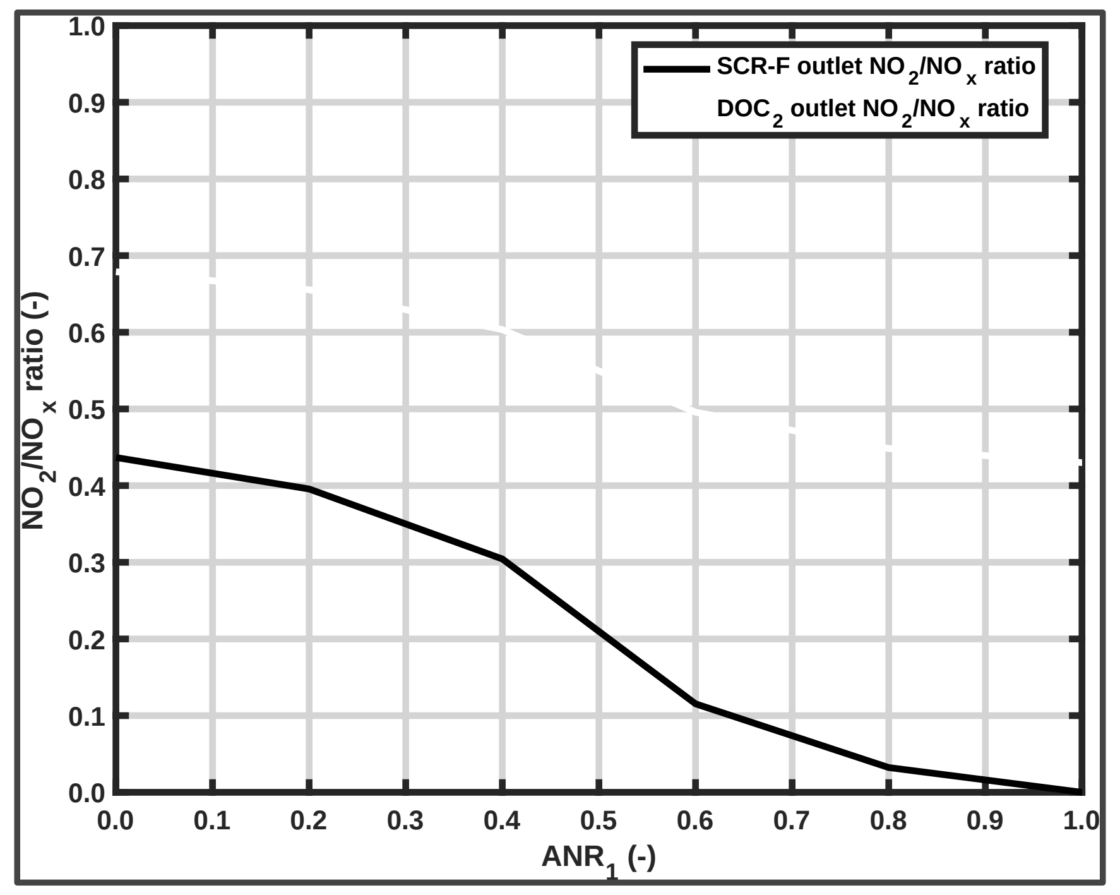
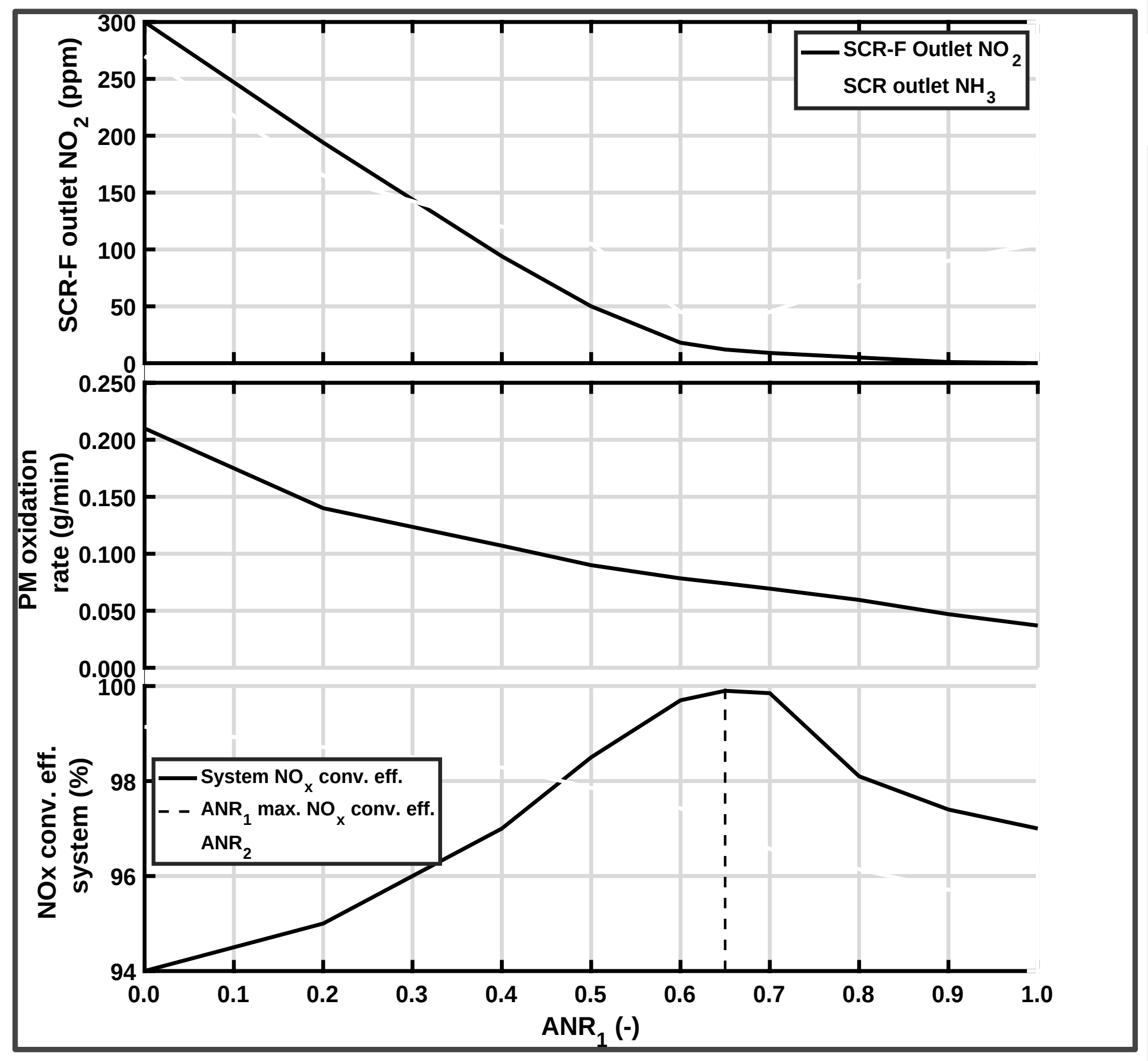


SCR-F outlet NO$_2$/NO$_x$ ratio
DOC$_2$ outlet NO$_2$/NO$_x$ ratio
NO$_2$/NO$_x$ ratio (-)
ANR$_1$ (-)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

[illegible]



SCR-F Outlet NO$_2$
SCR outlet NH$_3$
SCR-F outlet NO$_2$ (ppm)
300
250
200
150
100
50
0
PM oxidation rate (g/min)
0.250
0.200
0.150
0.100
0.050
0.000
System NO$_x$ conv. eff.
ANR$_1$ max. NO$_x$ conv. eff.
ANR$_2$
NOx conv. eff. system (%)
100
98
96
94
ANR$_1$ (-)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

[illegible]