

Improving Design of SCR Systems with CFD Modeling

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Reaction Engineering International

Project Objective

- **Demonstrate value of CFD in SCR design and tuning**
 - **Improved insight of flue gas properties through AIG, SCR catalyst, and ductwork**
 - **Impact of flue gas profiles and flow rates on SCR performance**
 - **Guidance for matching AIG flows with flue gas profiles and resulting impact of AIG tuning**



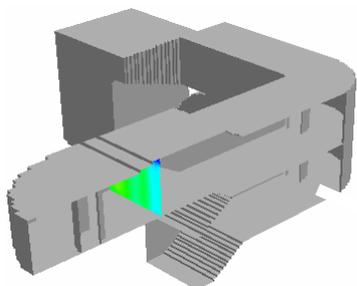
Project Approach

- **Use CFD and 1-D reactor modeling to predict flow properties and NO reduction in 550 MW coal-fired boiler SCR system**
 - **Flow patterns and velocity profiles**
 - **Overall pressure drop through duct work**
 - **Temperature distribution**
 - **NH₃ distribution from ammonia injection grid (AIG)**
 - **NO reduction through SCR catalyst**
 - **Ammonia slip after catalyst**
 - **NO reduction sensitivities**



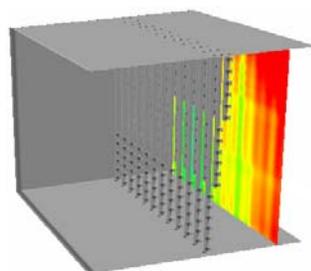
Modeling Approach

Duct Flow Model



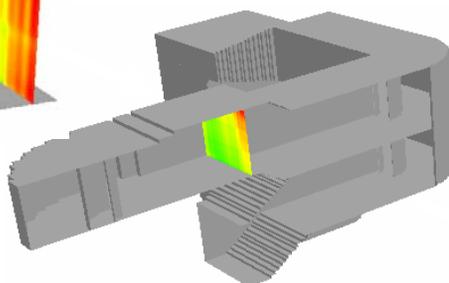
- ΔP
- Flow distribution

Detailed AIG Model



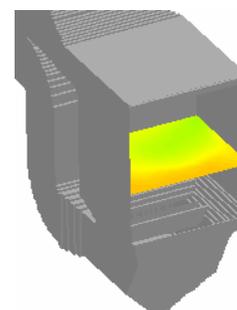
- NH_3 distribution

Duct Flow Model



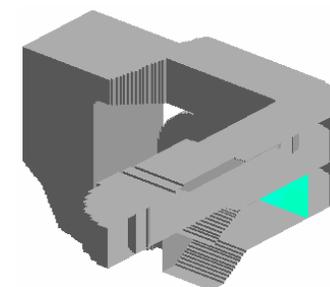
- SCR model inlet properties
 - NH_3 distribution
 - NO distribution
 - Flow distribution

SCR Reactor



- NO reduction
- NH_3 slip

Duct Flow Model



- ΔP
- Flow field
- NH_3 slip distribution
- NO distribution

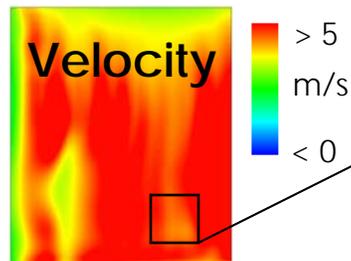
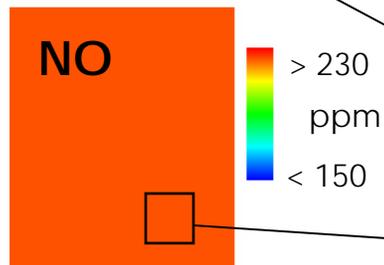
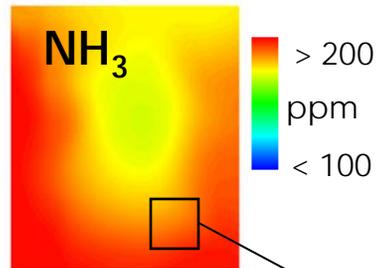
- **Three model components:**

- Duct flow model
- Ammonia Injection Grid (AIG) submodel
- SCR catalyst submodel

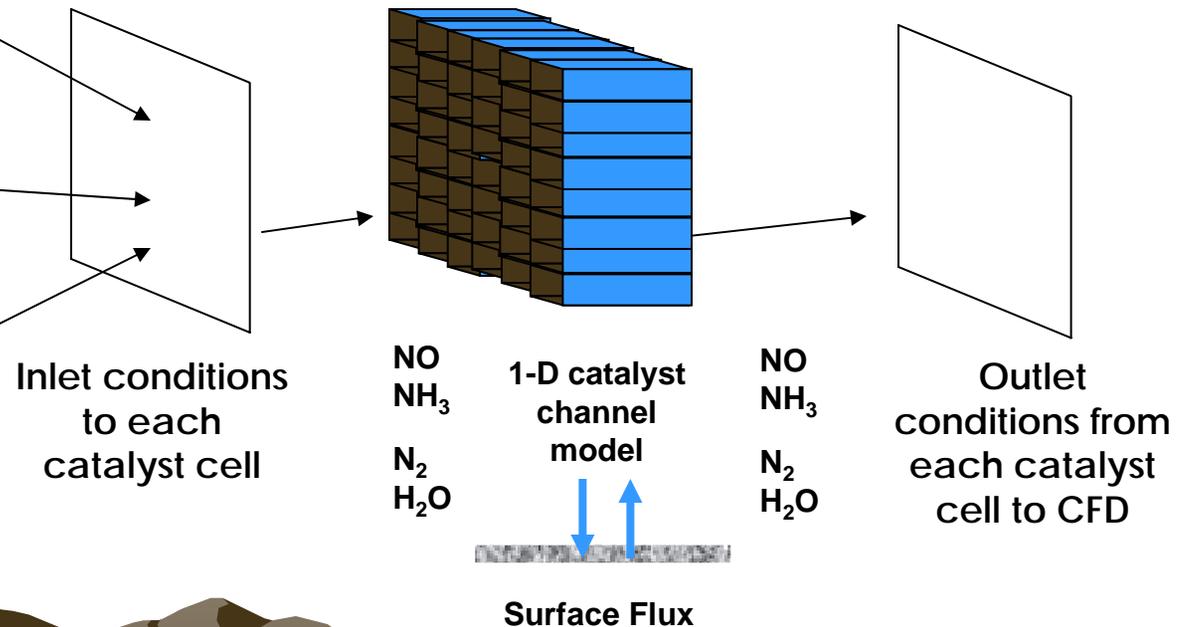


SCR Model – Implementation

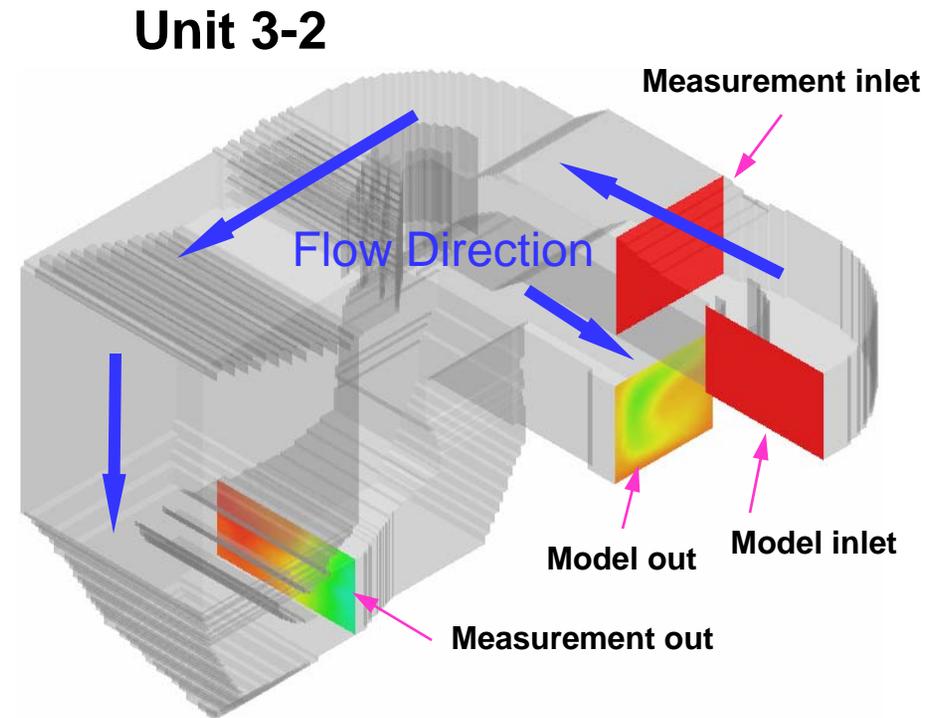
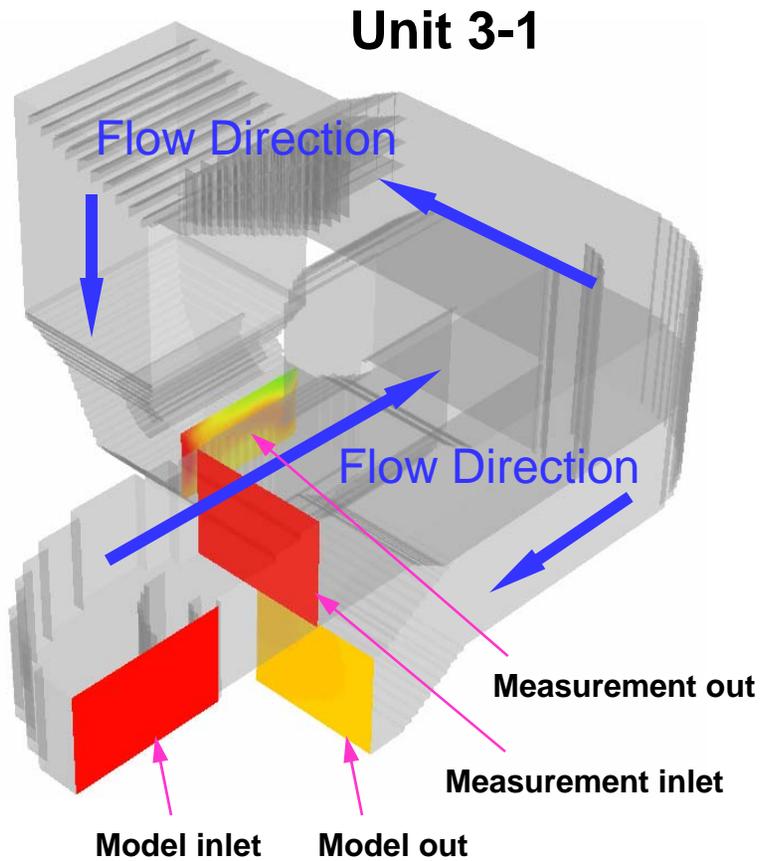
Results at SCR Inlet



- 1-D plug flow model with heterogeneous kinetics for NO reduction by NH₃ over vanadia/titania catalysts
- Solves gas transport and surface reactions along catalyst
- Number of “active sites” for reaction calibrated with design data
- Predicts dependencies of NH₃/NO ratio, temperature, residence time and flue gas composition



SCR Geometries

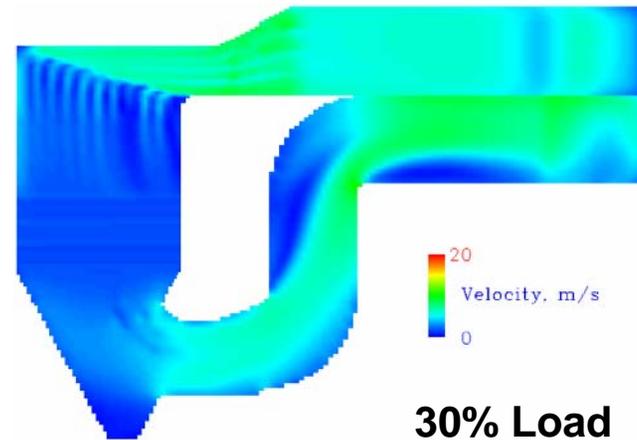
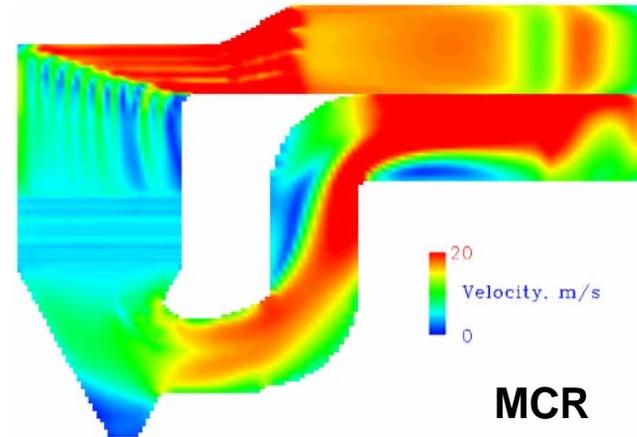
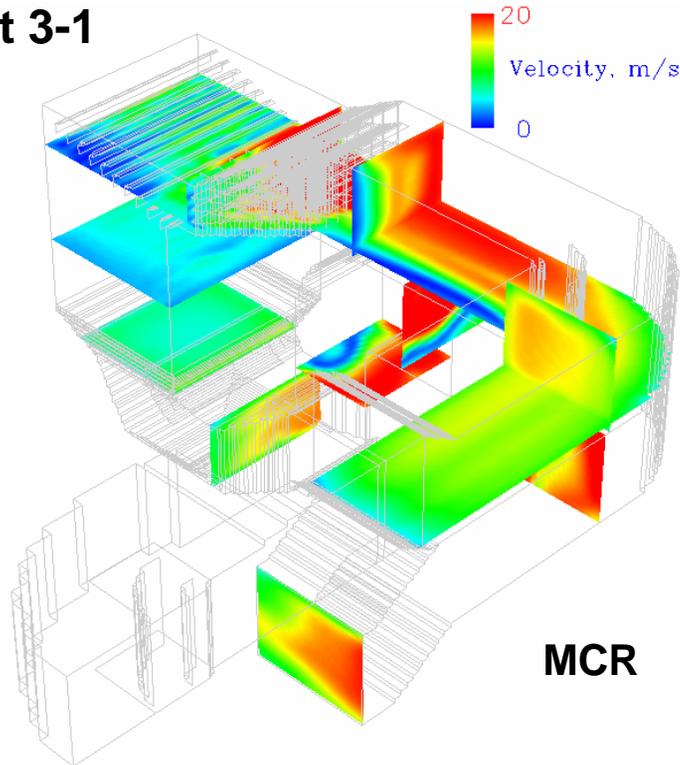


Unit 3-2 has shorter run length between turn and AIG and shorter run length between AIG, turn, and guide vanes



Gas Velocity Profile

Unit 3-1

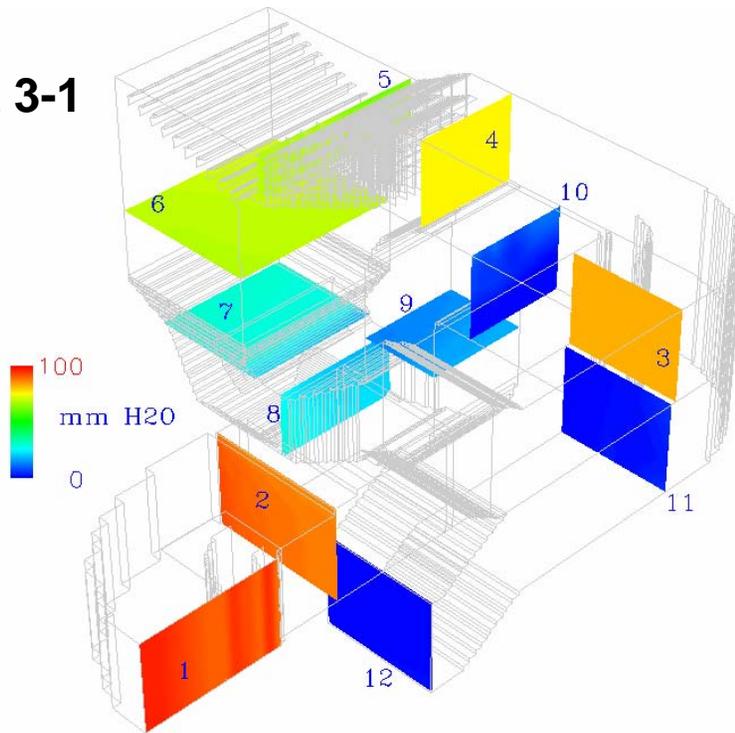


Velocity profiles can suggest improvements to guide vane design

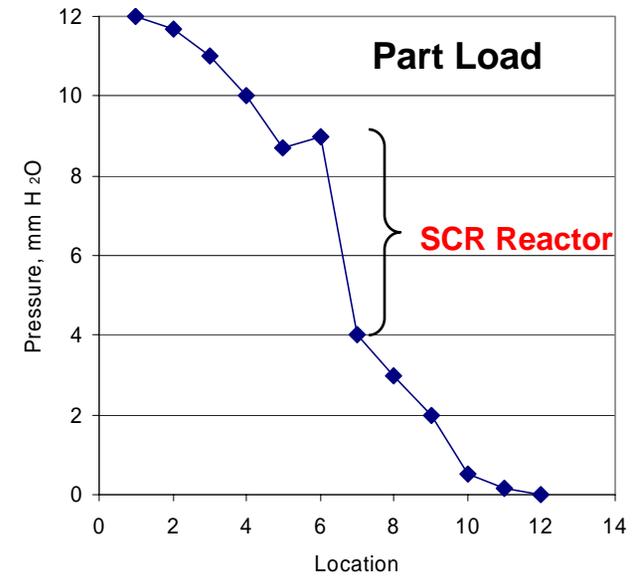
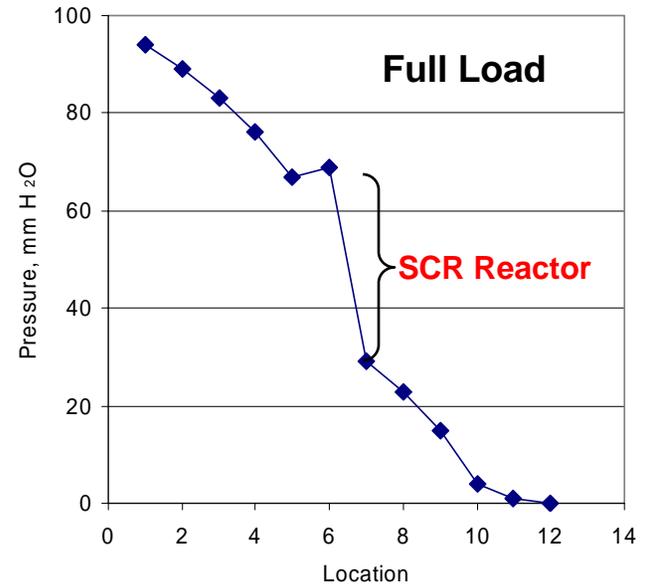


Pressure Drop

Unit 3-1



Profiles identify specific contributors as well as total system pressure drop



Flow Comparisons

			Unit 3-1	Unit 3-2	Total
MCR		Flow, 10 ³ kg/hr	1128.5	1128.5	2257.0
		ΔP (mm H ₂ O, SCR)	40.0	37.5	-
		ΔP (mm H ₂ O, N1 to N3 or N4 to N6)	89.1	79.2	-
		Total ΔP (mm H ₂ O)	94.0	84.0	-
Model	30% Load (July 17, 2004)	Flow, 10 ³ kg/hr	-	694.2	-
		ΔP (mm H ₂ O, SCR)	-	13.1	-
		ΔP (mm H ₂ O, N1 to N3 or N4 to N6)	-	27.7	-
		Total ΔP (mm H ₂ O)	-	29.0	-
30% Load (design)		Flow, 10 ³ kg/hr	431.5	431.5	863.0
		ΔP (mm H ₂ O, SCR)	5.0	4.9	-
		ΔP (mm H ₂ O, N1 to N3 or N4 to N6)	11.7	10.4	-
		Total ΔP (mm H ₂ O)	12.0	10.8	-
Measured	MCR (July 16, 2004)	Flow, 10 ³ Nm ³ /hr	948.3	871.0	1819.2
		Flow, 10 ³ kg/hr	1260.8	1158.0	2418.9
		Design SCR ΔP (mm H ₂ O)	39.8	37.3	-
		ΔP (mm H ₂ O, N1 to N3 or N4 to N6)	98.4	73.7	-
30% Load (July 17, 2004)		Flow, 10 ³ Nm ³ /hr	576.2	522.1	1098.3
		Flow, 10 ³ kg/hr	766.1	694.2	1460.3
		ΔP (mm H ₂ O, N1 to N3 or N4 to N6)	44.1	34.1	-

- Predictions consistent with the measured data
- Differences likely due to:
 - Inlet flow profile
 - Different flow rates
 - Measurement locations/grid
 - Model accuracy



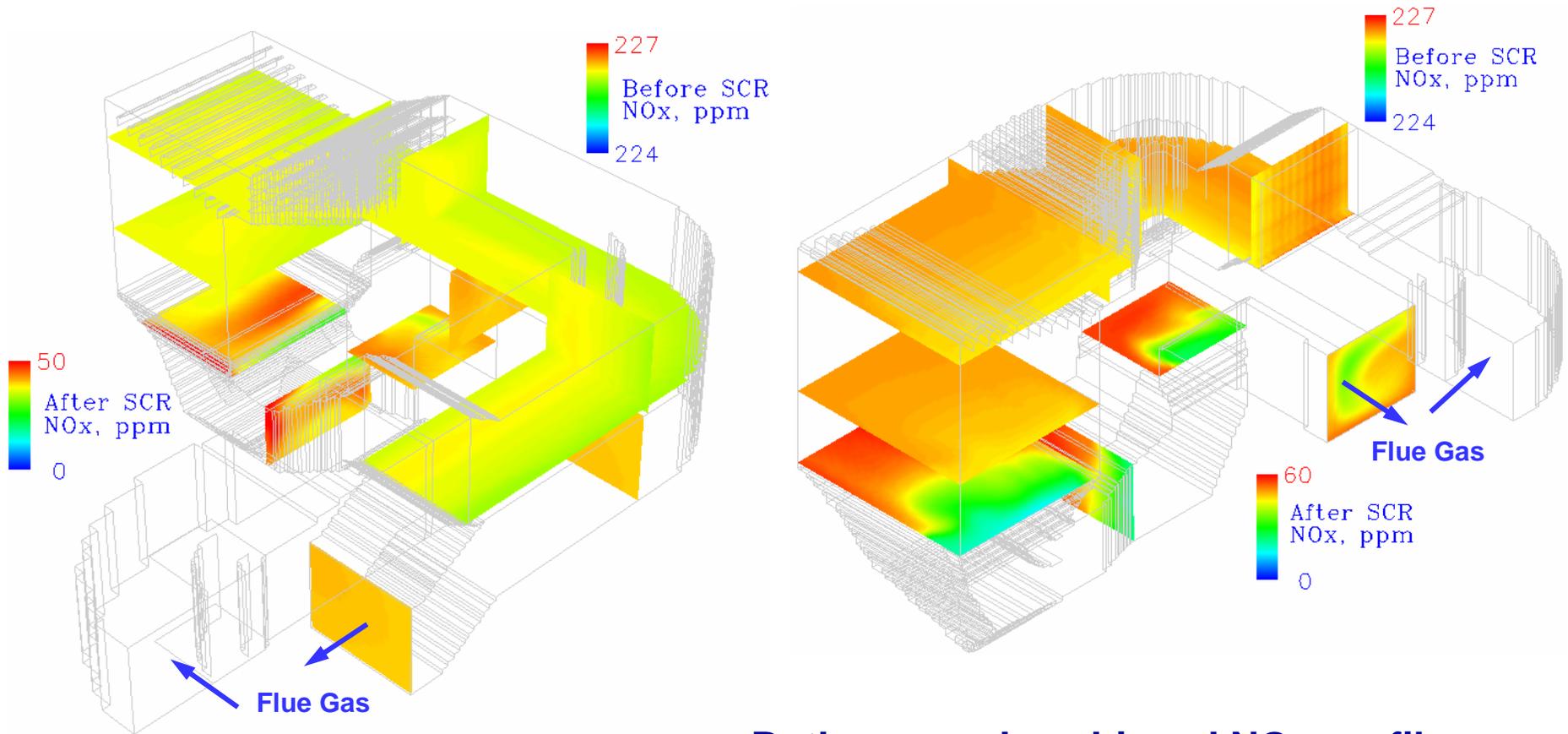
NO Reduction Dependencies

- **NO reduction depends on:**
 - **NH₃/NO ratio – insufficient ammonia (ratio<1.0) will not reduce all available NO (NO remaining)**
 - **Residence time – insufficient residence time will not allow NH₃ enough time to react with NO (NO and NH₃ remaining)**
- **NH₃ slip depends on:**
 - **NH₃/NO ratio – too much ammonia (ratio>1.0) will reduce all NO (NH₃ remaining)**
 - **Residence time – insufficient residence time will not allow NH₃ enough time to react with NO (NO and NH₃ remaining)**



NO Concentration Profile

Unit 3-1 vs 3-2 at MCR

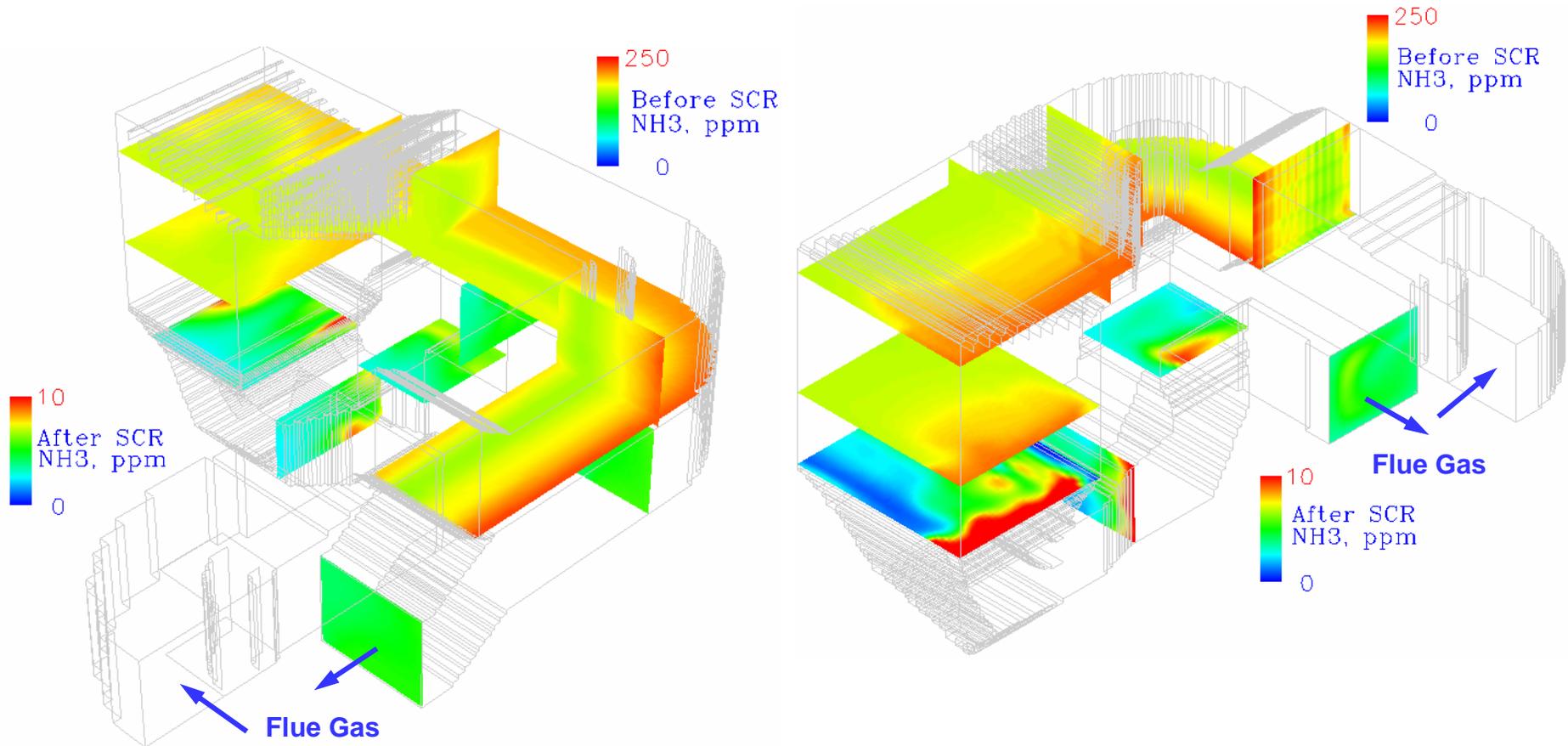


Both cases show biased NOx profiles



NH₃ Concentration Profile

Unit 3-1 vs 3-2 at MCR



Both cases show biased NH₃ profiles



SCR Model Predictions

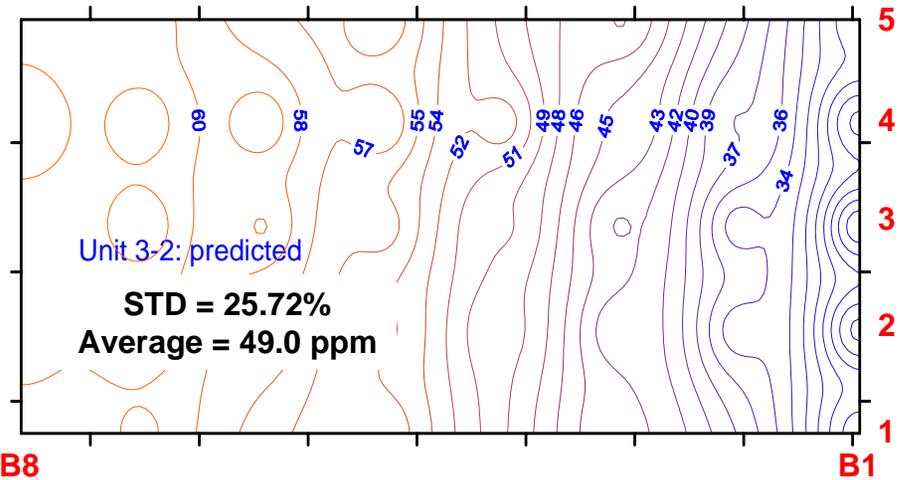
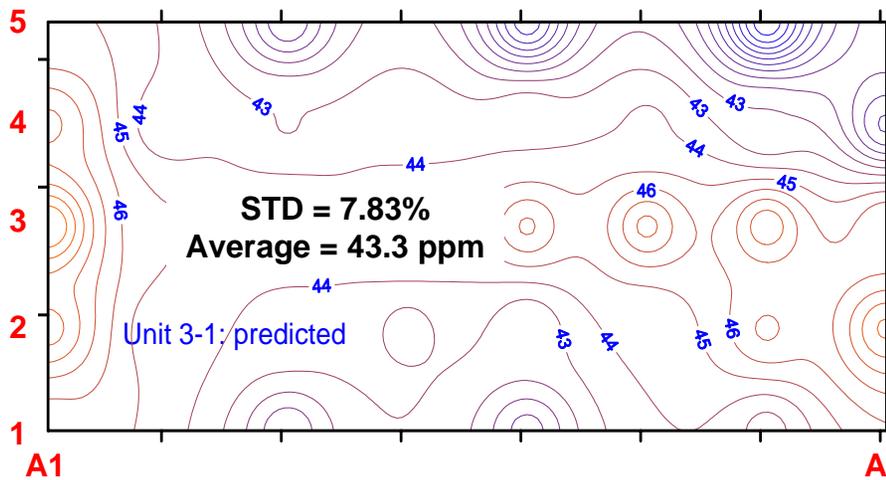
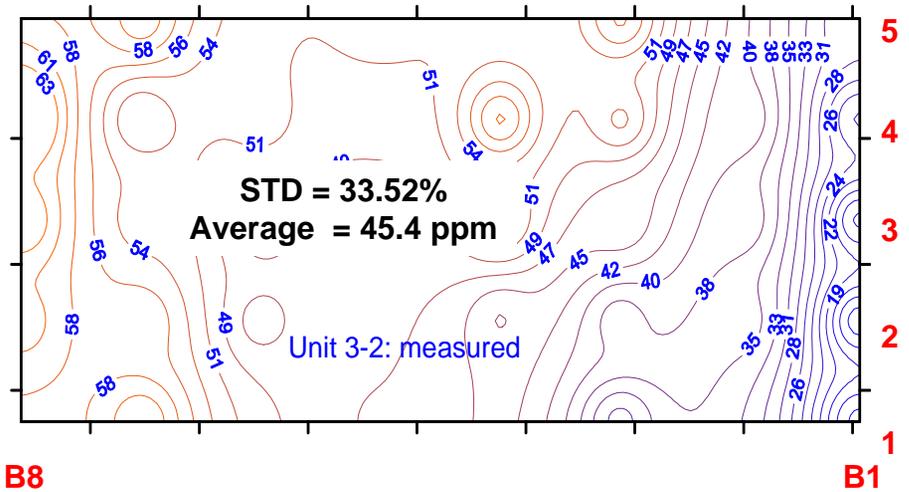
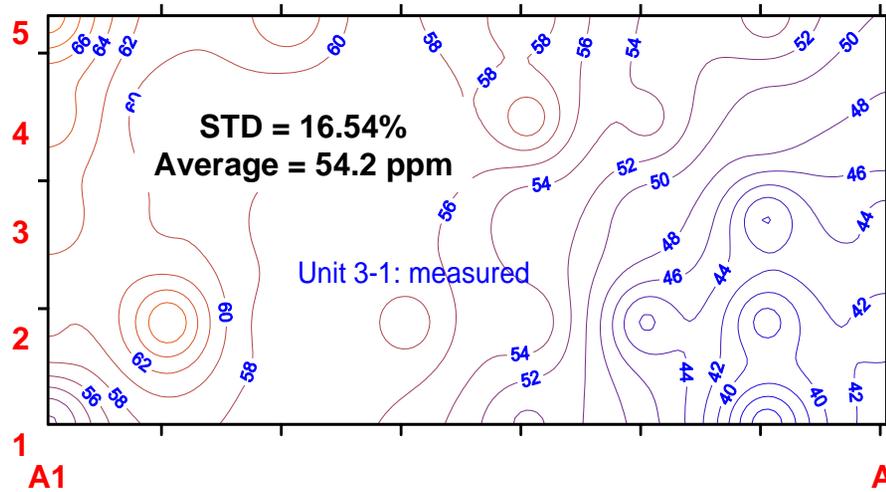
		Unit 3-1		Unit 3-2	
		INLET	OUTLET	INLET	OUTLET
MCR, Fully Open AIG	NH ₃ , ppm @ 6%O ₂ Dry	171	4.0	171	4.2
	NO, ppm @ 6%O ₂ Dry	210	42.7	210	43.0
	NO Reduction, %	-	79.6	-	79.5
30% load, Fully Open AIG	NH ₃ , ppm @ 6%O ₂ Dry	171	0.0	171	0.2
	NO, ppm @ 6%O ₂ Dry	210	38.8	210	38.9
	NO Reduction, %	-	81.4	-	81.4
30% load with higher O₂ Fully Open AIG	NH ₃ , ppm @ 6%O ₂ Dry	-	-	171	1.5
	NO, ppm @ 6%O ₂ Dry	-	-	210	40.2
	NO Reduction, %	-	-	-	80.8

- Ammonia slip likely due to higher than design velocities in catalyst (lack of residence time)
- Limited residence time also reduces NO reduction
- Will more uniform NH₃/NO profiles improve performance?

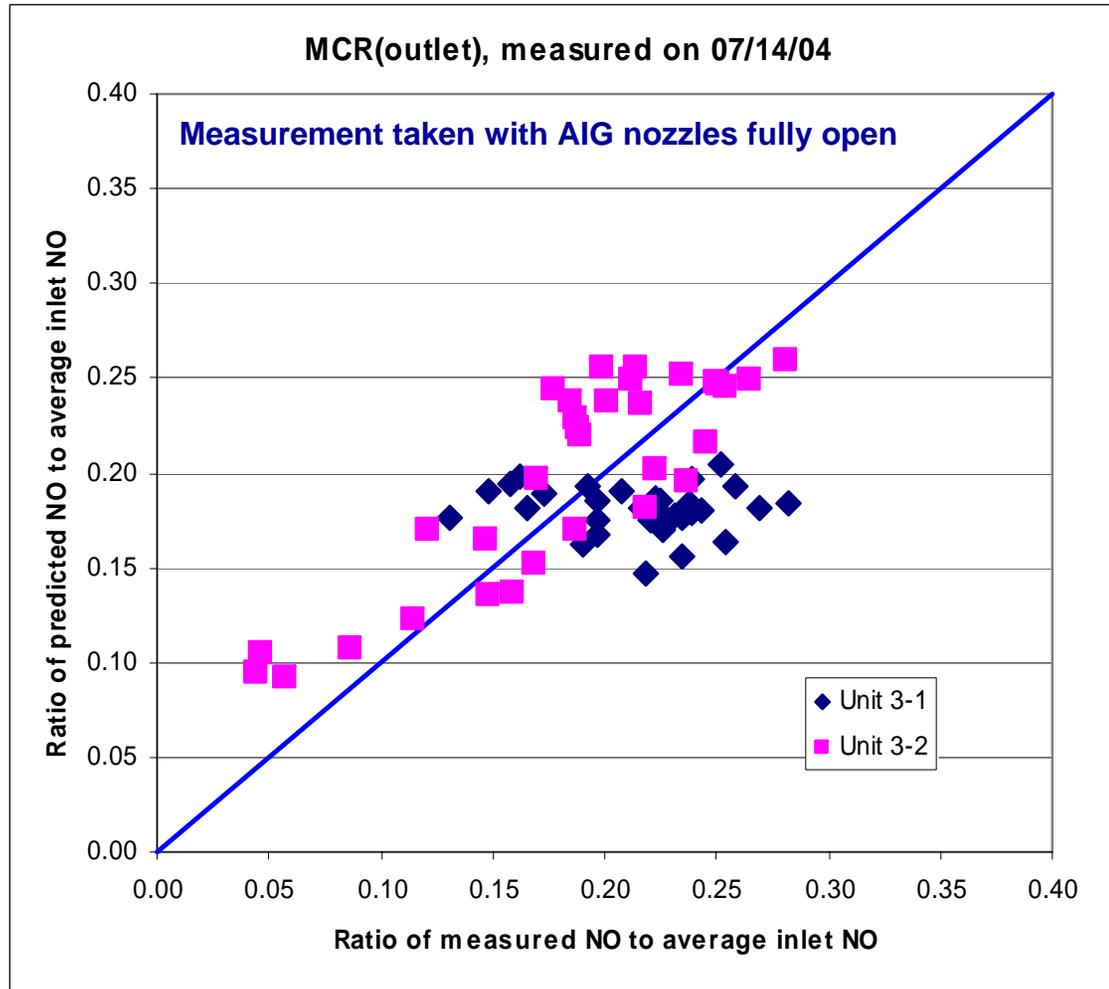


Outlet NO Profile at MCR

Measurement taken with fully open AIG nozzles (NO ppm, dry)



NO Exit Profile Results

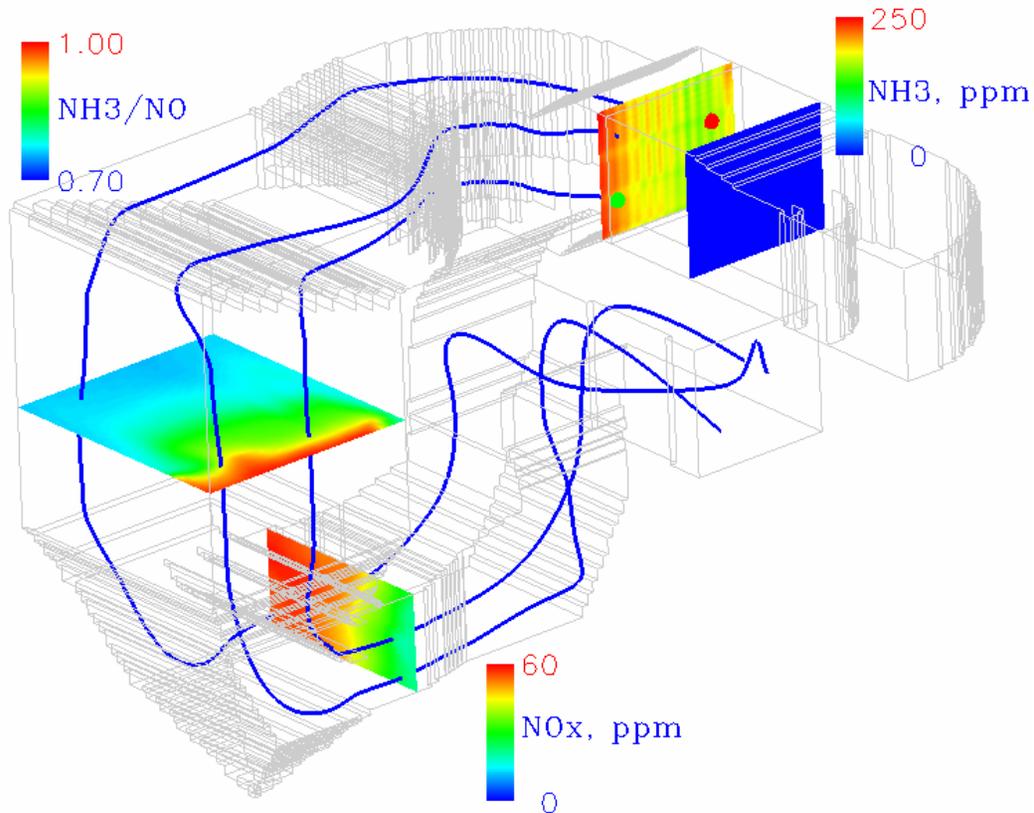


AIG Tuning

- ***Background:*** Modeling results with fully open AIG nozzles indicate a bias in the flue gas flow in the AIG region, leading to NH_3 biasing at the catalyst inlet
- ***Objective:*** Use CFD modeling to simulate AIG tuning and show how CFD can be used to guide AIG in the SCR duct (Unit 3-2)
- ***Approach:*** Use zonal AIG biasing to achieve more uniform NH_3/NO ratio (0.814)



Using CFD For Tuning

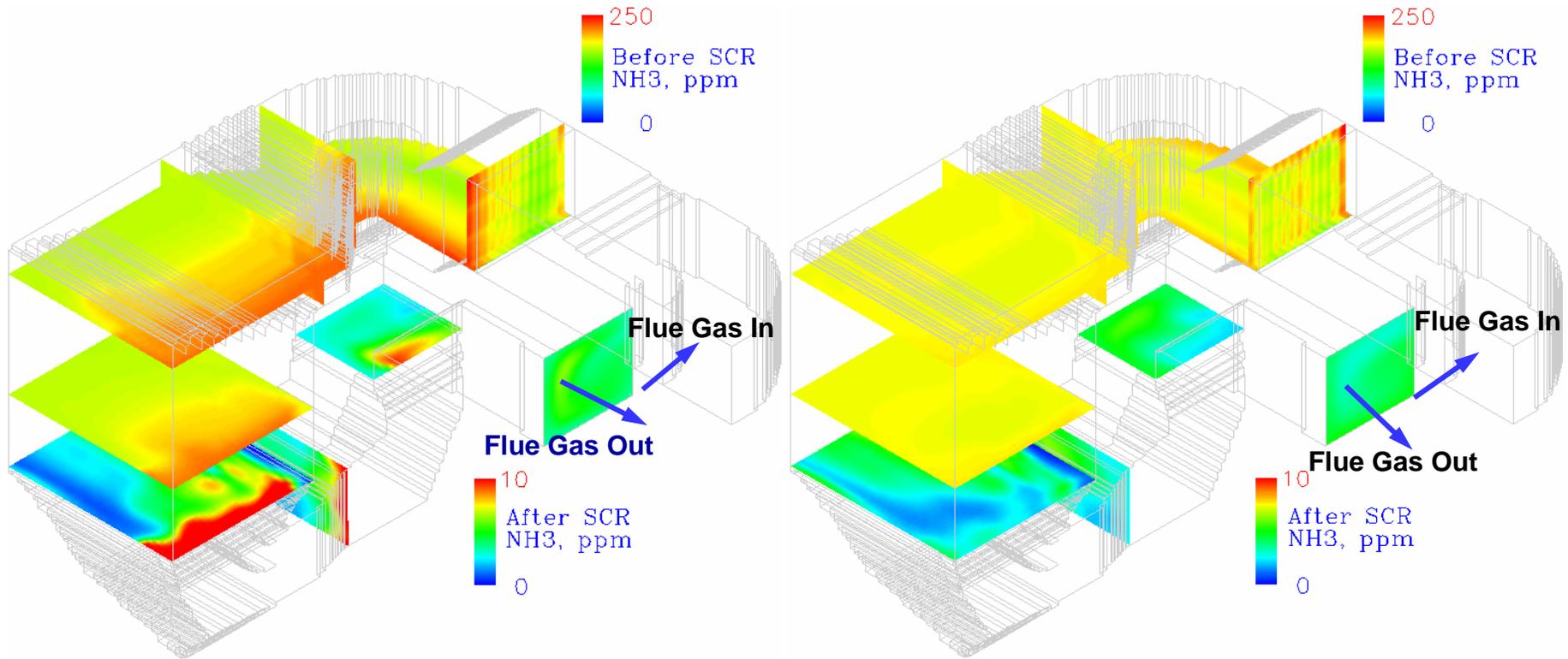


- CFD can show profiles through system
- CFD can be used to trace source of profile
- Streamlines correlate local NO at outlet with corresponding NH₃/NO entering the catalyst, and ultimately with the corresponding AIG nozzles



NH₃ Concentration Profile

Unit 3-2 at MCR



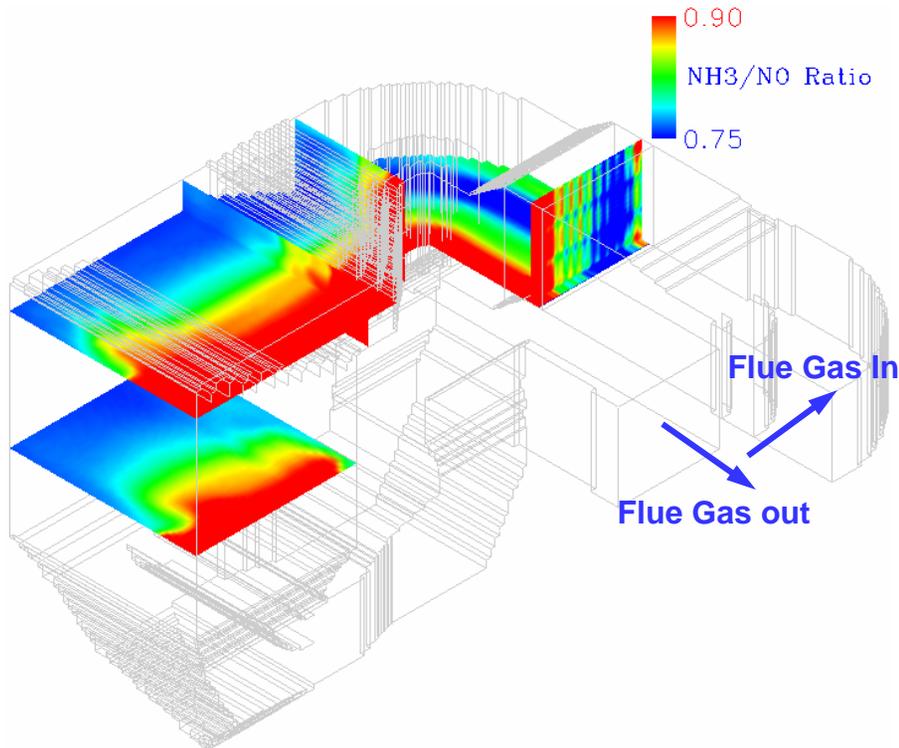
**Fully Open AIG Nozzles
(Uniform NH₃ injection)**

**AIG Tuning
(Biased NH₃ injection)**

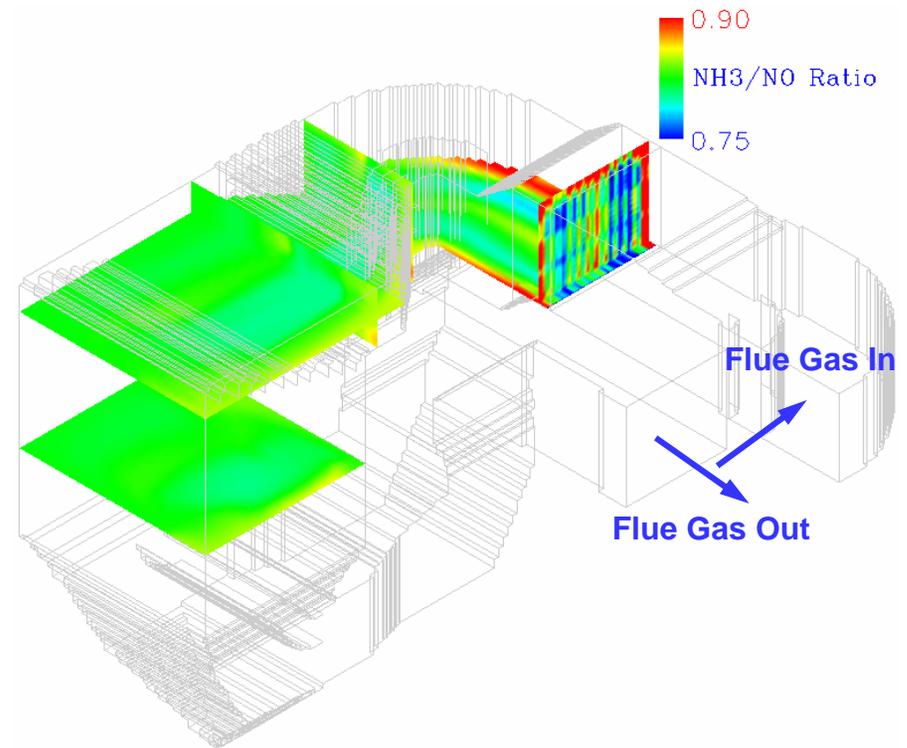


NH₃/NO Ratio Profile

Unit 3-2 at MCR



**Fully Open AIG Nozzles
(Uniform NH₃ injection)**

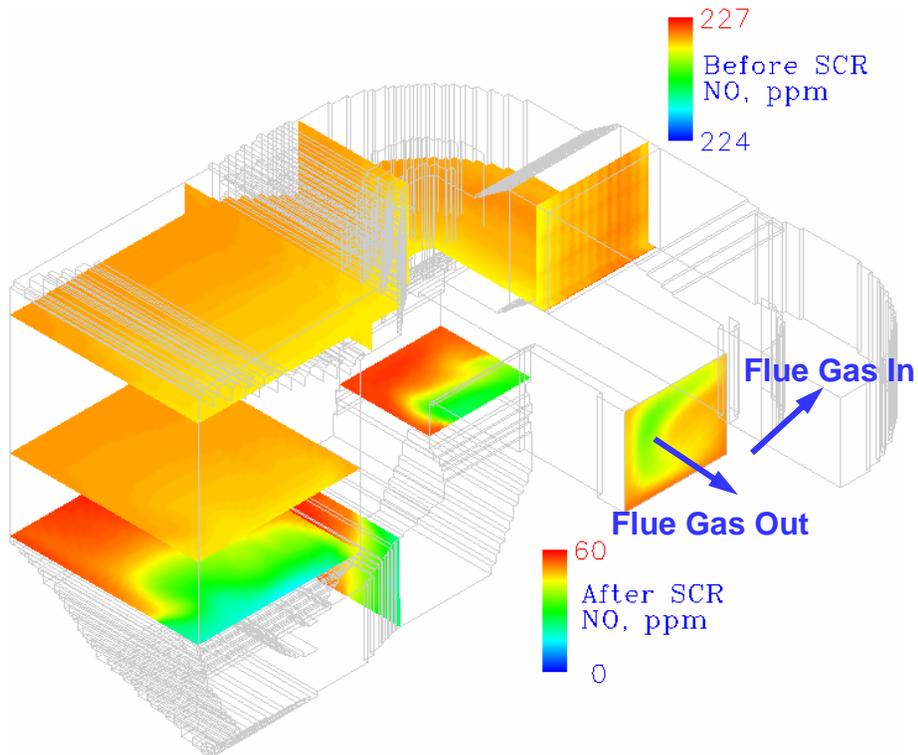


**AIG Tuning
(Biased NH₃ injection)**

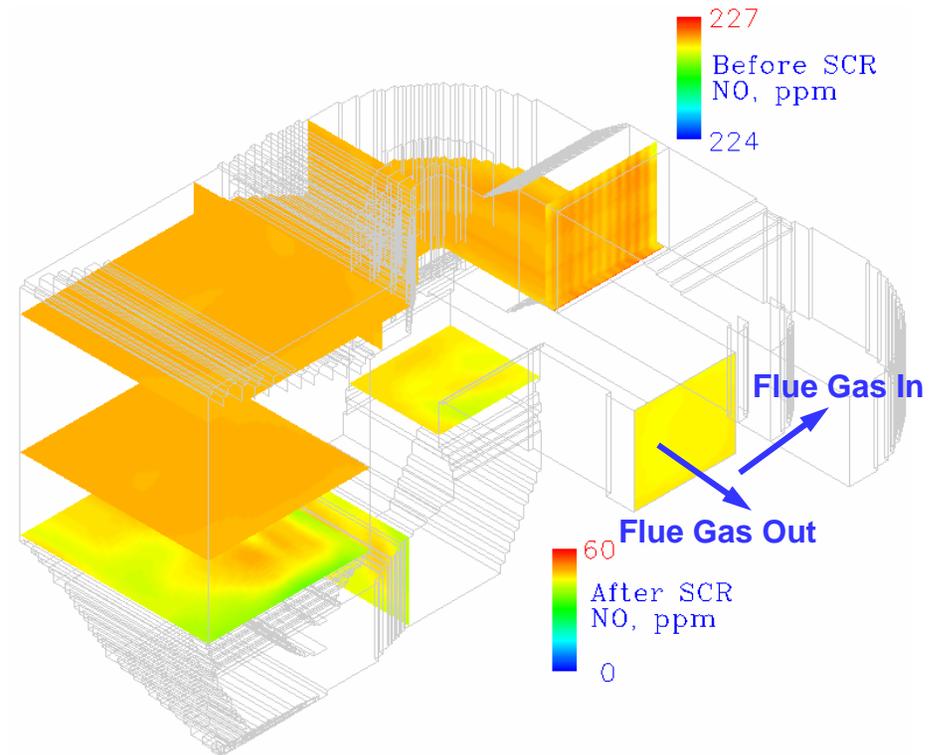


NO Concentration Profile

Unit 3-2 at MCR



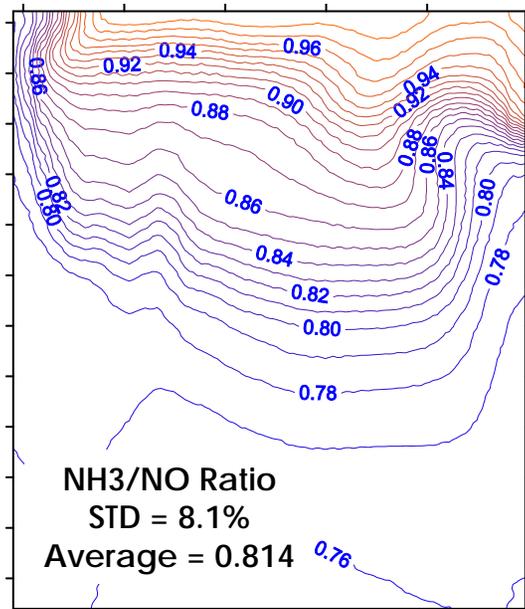
**Fully Open AIG Nozzles
(Uniform NH₃ injection)**



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(Biased NH₃ injection)**

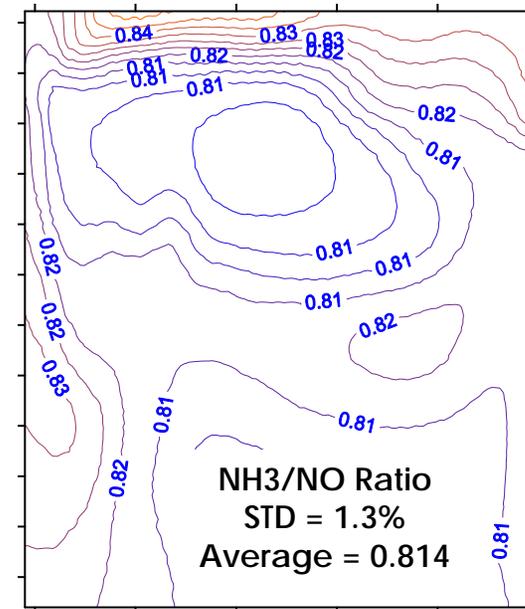


Predicted Effects of AIG Tuning



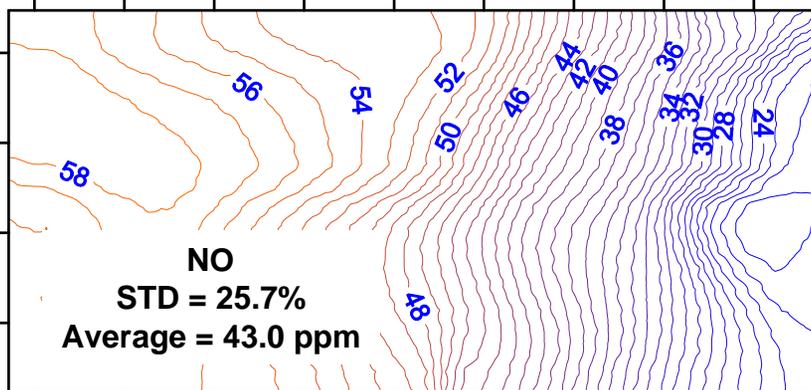
Uniform
NH₃+Air Flow

Catalyst Inlet

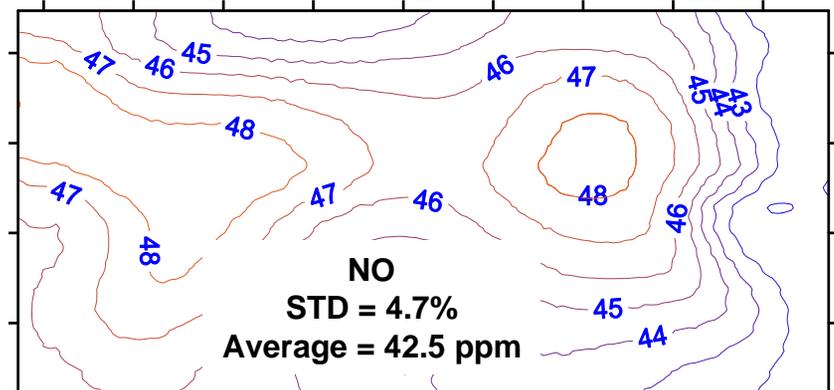


Biased
NH₃+Air Flow

Measurement



Outlet
Dry, 6% O₂



SCR Model Predictions

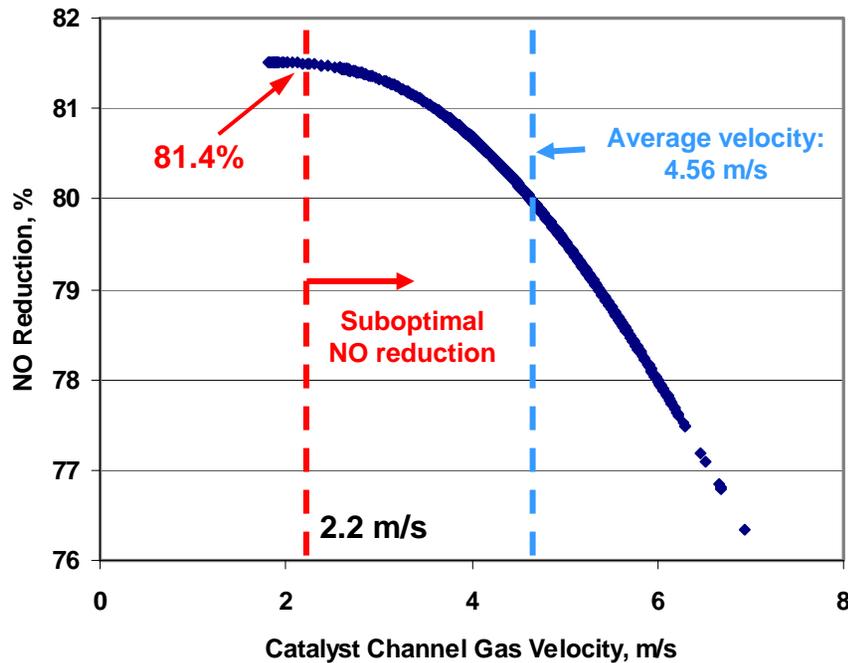
AIG Conditions	Unit 3-2: MCR			
	Uniform		Tuning	
	INLET	OUTLET	INLET	OUTLET
NH ₃ , ppm @ 6%O ₂ Dry	171	4.2	171	3.8
NO, ppm @ 6%O ₂ Dry	210	43.0	210	42.5
SCR Inlet NH ₃ /NO Mole Ratio	0.814		0.814	
NO Red, %	79.50		79.71	
NH ₃ Slip, ppm @ 6%O ₂ Dry	4.2		3.8	

- **Why didn't the NO reduction improve with a more uniform NH₃/NO ratio at the SCR reactor inlet?**
 - **More uniform NH₃/NO ratio improved reduction in low ratio regions, but decreased reduction in high ratio regions**
 - **Average residence time unchanged, still too short to allow full conversion to 81.4%**
 - **Both results were close to the optimal reduction specified in the catalyst design for this load, NH₃/NO ratio, and catalyst size (80%)**

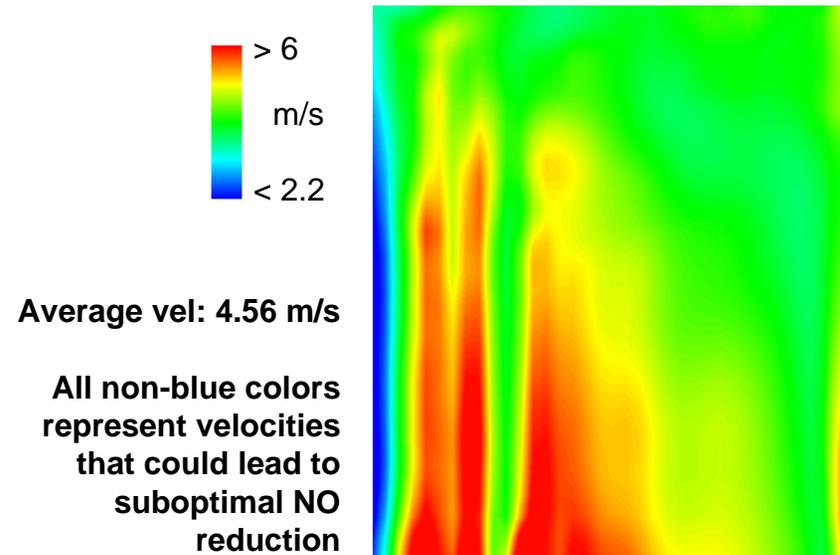


SCR Model: Effect of Gas Velocity on NO Reduction

Velocities plotted are from actual duct velocities



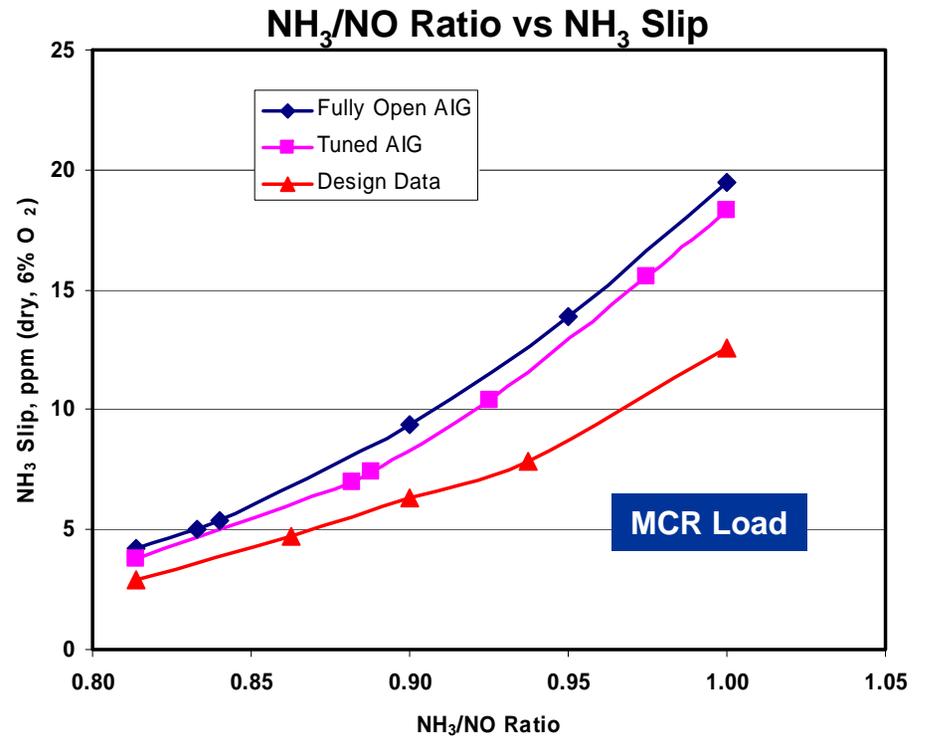
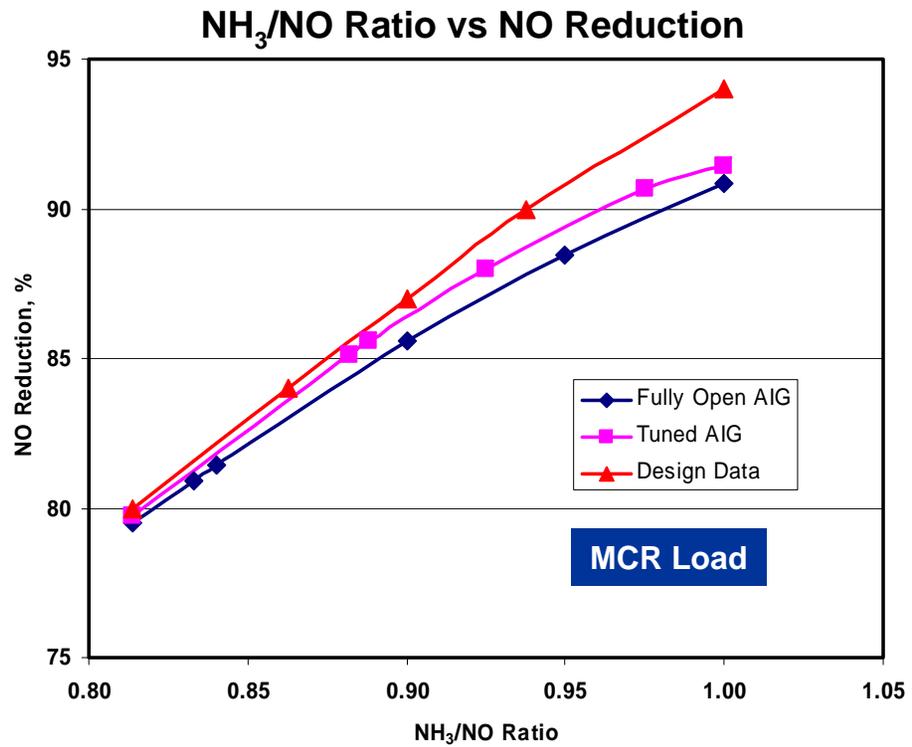
Velocity profile at SCR catalyst inlet



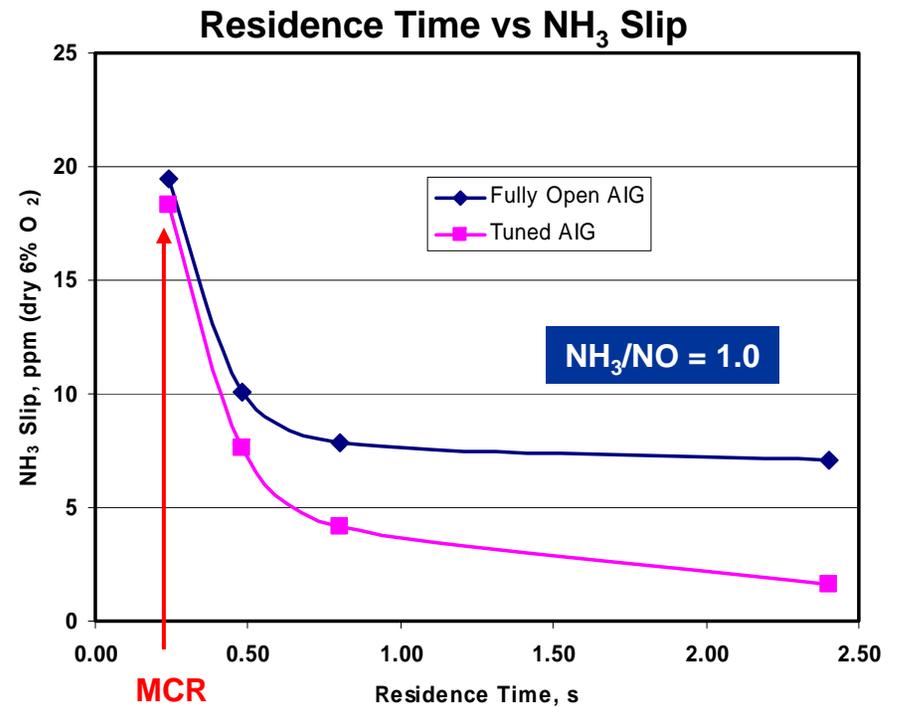
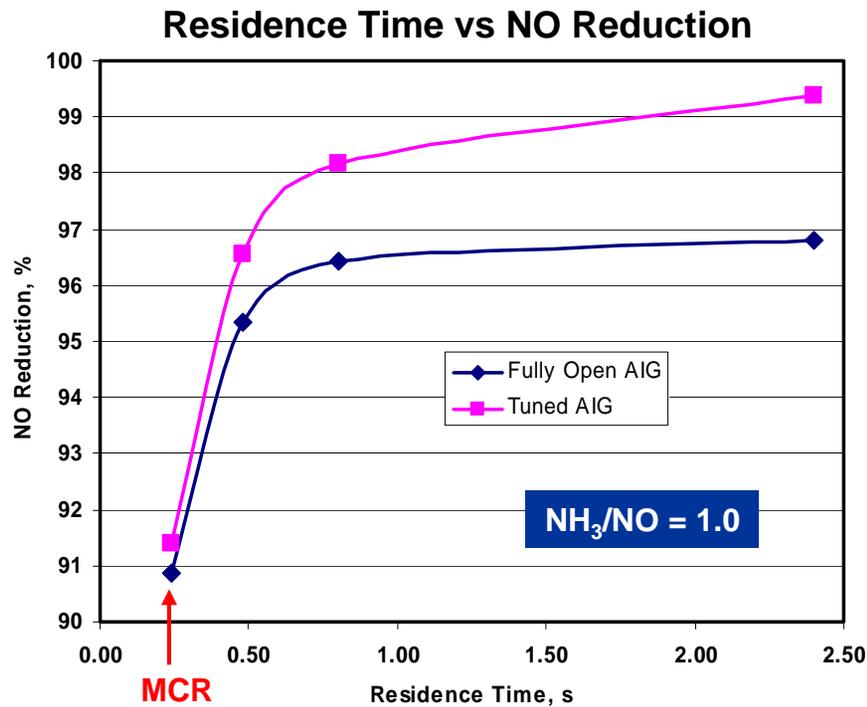
At MCR, catalyst design does not allow sufficient residence time to react all NH_3 with NO , even with optimal NH_3/NO ratio



Predictions at Higher NH_3/NO Ratios



Predictions at Higher Residence Times



What Can Model Do

- **Predict performance and identify potential design problems before design/installation**
 - Predict NO reduction and ammonia slip (measurements verify accuracy for the same NH_3/NO ratio, load, catalyst design)
 - Guide how much NH_3 needed to reach NO reduction goal
 - Guide amount of catalyst needed for NO reduction goal
 - Suggest duct designs to provide more uniform flow
- **Aid tuning and troubleshooting**
 - Illustrate tuning impacts
 - Guidance on how to tune AIG injection
 - Determine if tuning worthwhile for a particular design
 - **Identify measurement locations for testing and/or analyzer**



Thank You

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