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Recent Advances and Future Challenges in the Modeling and Simulations of the injection of Urea-Water-Solution for Automotive SCR Systems

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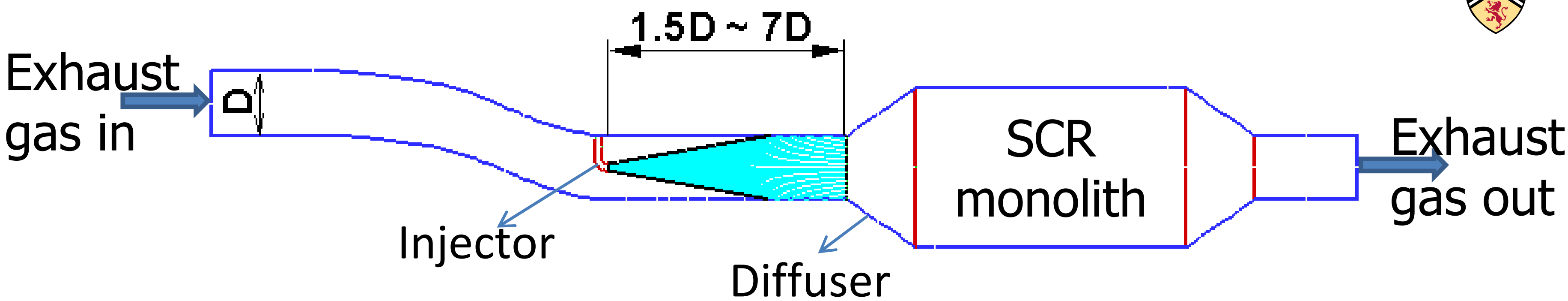
Urea-SCR System



Urea Decomposition

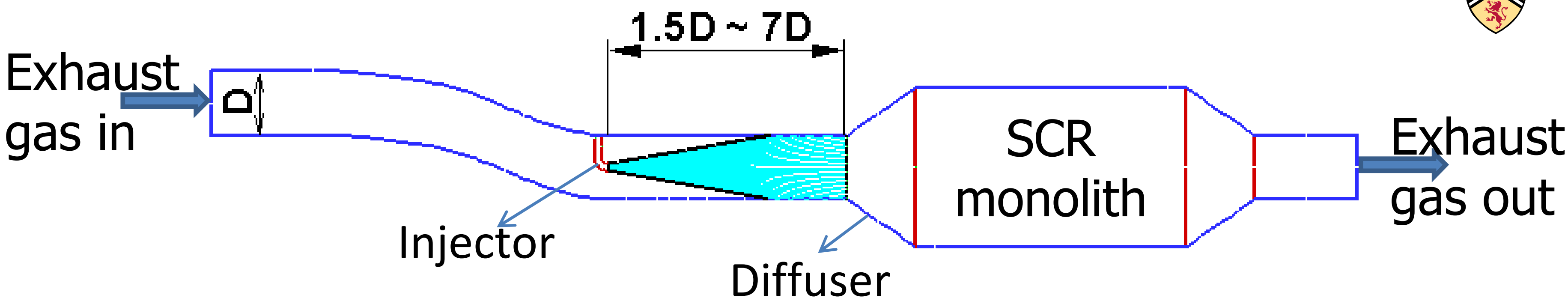
Evaporation $(NH)_2CO(aq) \rightarrow (NH)_2CO(s\,or\,l) + 6.9H_2O$

Thermolysis Tu> 405K $(NH)_2CO(s\,or\,l) \rightarrow NH_3(g) + HNCO(g)$

Hydrolysis $HNCO(g) + H_2O(g) \rightarrow NH_3(g) + CO_2(g)$

Tu> 573K, Second decomposition stage leading to the formation of melamine

Urea-SCR System



NOx Reduction Mechanism

Standard $$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O$$

Fast $$4NH_3 + 2NO + 2NO_2 \rightarrow 4N_2 + 6H_2O$$

System Requirements & Challenges

- Homogenous gas mixture at the catalyst entrance with $NH_3/NOx = 1$
  - Efficient decomposition and spatial distribution of the reducing agent
- Minimization of Urea deposition on the exhaust pipe upstream of the catalyst
- Challenges
  - Short residence time ($\approx$ 0.09) $\rightarrow$ incomplete urea decomposition[1]
  - Varying operating conditions

1. M. Koebel et al, Catal. Today 59 (2000) 335

Design Criteria

Optimization of the UWS injection/dosing system to maximize the decomposition efficiency while minimizing wall depositions at varying operating conditions

CFD Role

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- Validated CFD model is required for fast, efficient optimization of the UWS injection and decomposition processes
- Model requirements
  - Predict the interaction between the exhaust gas and UWS spray
  - Account for the interaction between the spray and exhaust walls
  - Accurately simulate the UWS decomposition process

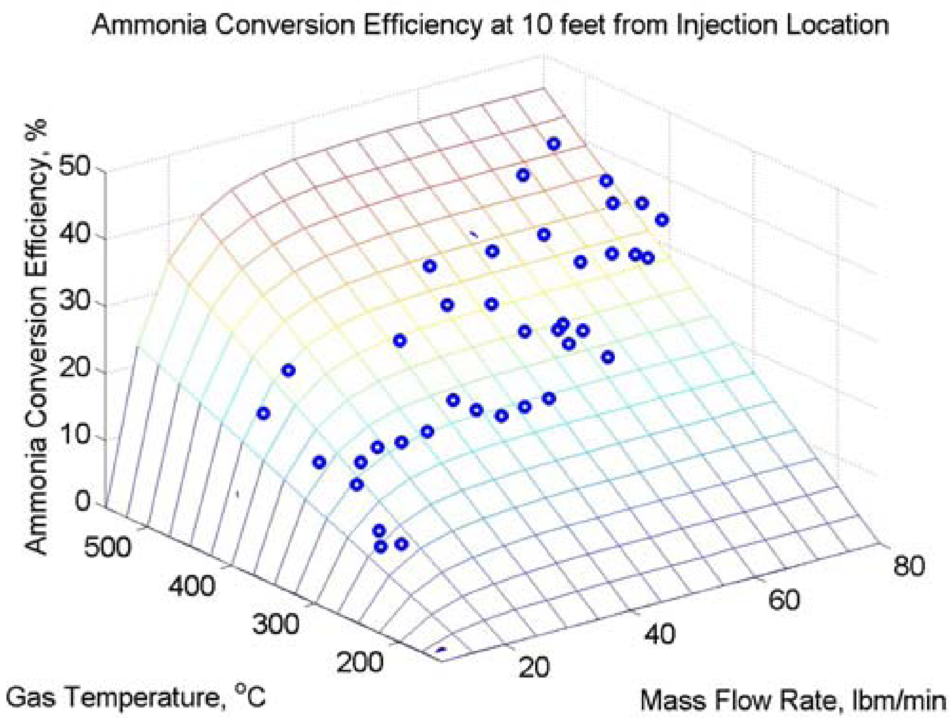
Developing such a CFD model is the main objective of this work

General Modeling Guidelines

- Eulerian-Lagrangian approach
- Continuous phase (Exhasut Gas)
  - RNG k-ε model
- Dispersed phase (UWS droplets)
  - Necessary forces: Drag and buoyancy forces
  - Dynamic drag model
  - Taylor Analogy Breakup (TAB) model
  - Turbulent dispersion: Stochastic particle tracking
- Two-way coupling between droplets and gas phase
  - Sensitive to the quality of the turbulence model
- Regime map for spray/wall interaction

Decomposition Modeling Techniques 1

- Empirical conversion efficiency factor[1]
  - No spray/system interaction
  - Reliability at lower gas temperatures
  - Adequate for validation purposes



1. J.N. Chi, H.F.M. DaCosta, SAE Technical Paper 2005-01-0966

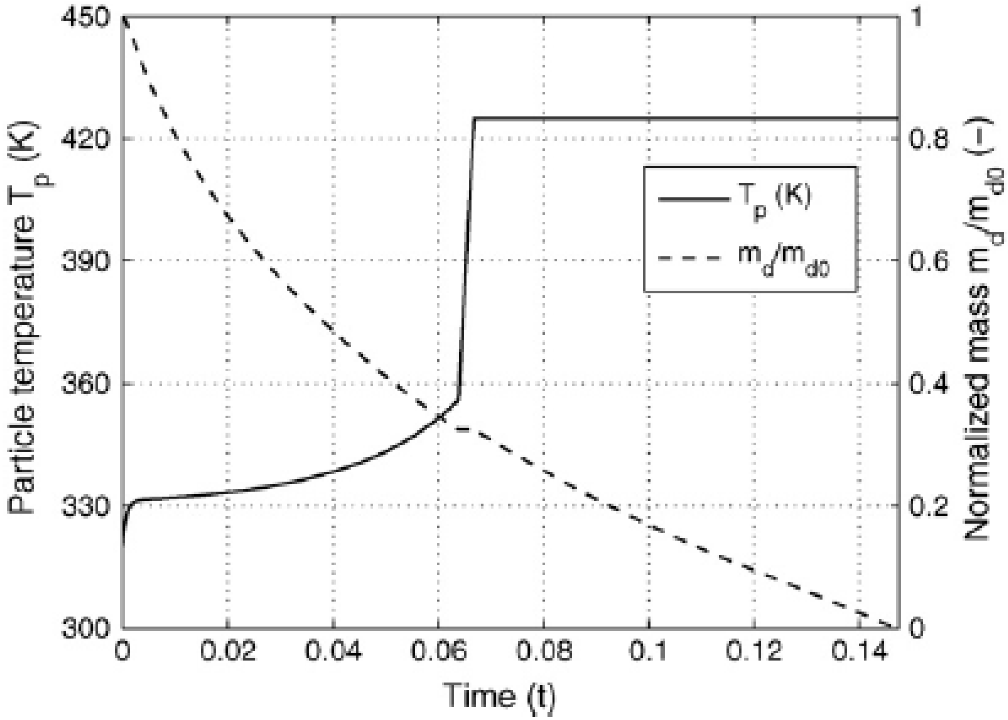
Decomposition Modeling Techniques 2

- Controlled by turbulent mixing (Eddy-Dissipation Model)[1,2]
  - Overestimates the conversion efficiency
  - Lacks validity assessment
  - Limited to steady state conditions
  - Sensitive to the quality of turbulence model's prediction
  - Relatively fast and inexpensive

1. S.J. Jeong et al., Environ. Eng. Sci. 25 (2008) 1017
2. M. Chen, S. Williams, SAE Technical Paper 2005-01-0969

Decomposition Modeling Techniques 3

- Heat transfer limited process at T_d = 425K



- Neglects hydrolysis and the second stage of urea decomposition

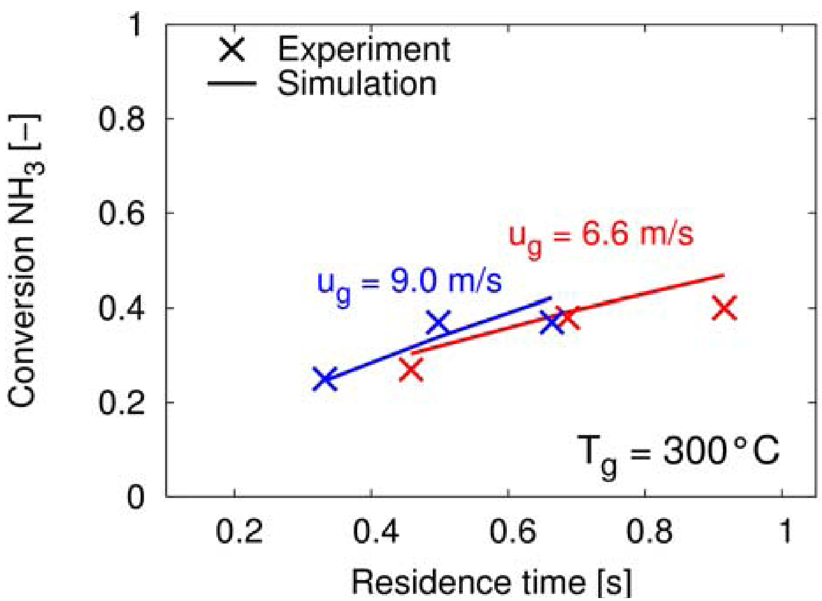
1. H. Ström et al., Chem. Eng. J. 150 (2009) 69.

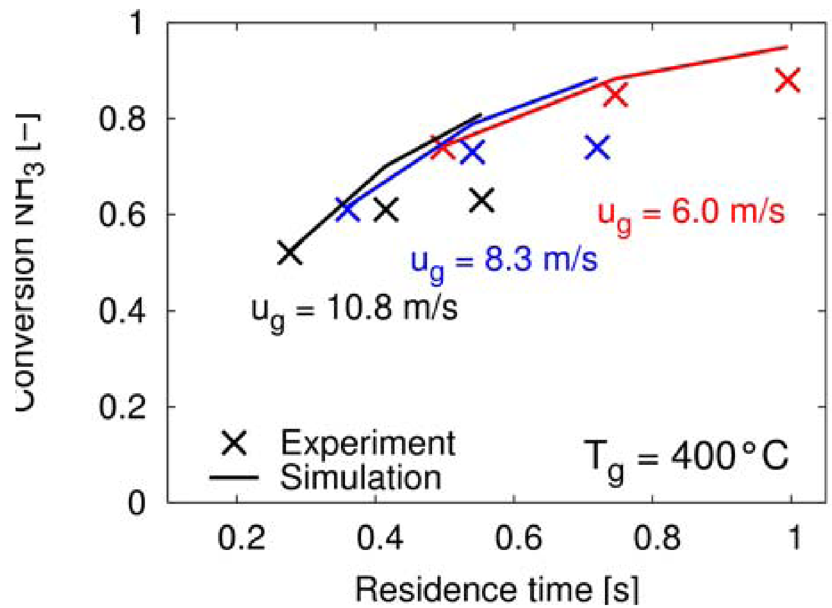
Decomposition Modeling Techniques 4

- Empirical saturation pressure curve[1]

$$p_u = e^{12.06 - 3992/T_d}$$

  - Hydrolyses is incorporated by Arrhenius expression
  - Incorporates spray/wall interaction



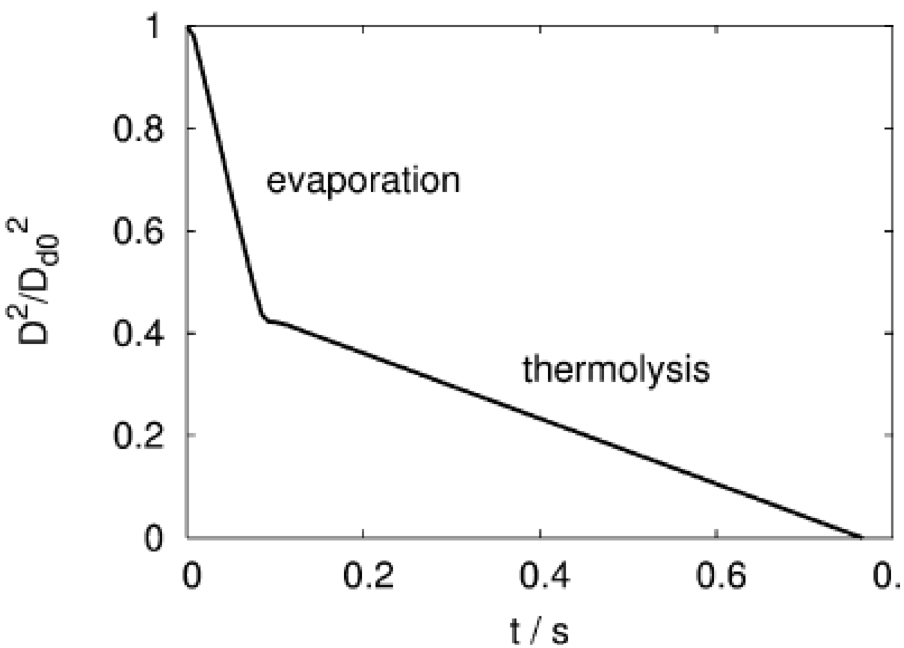


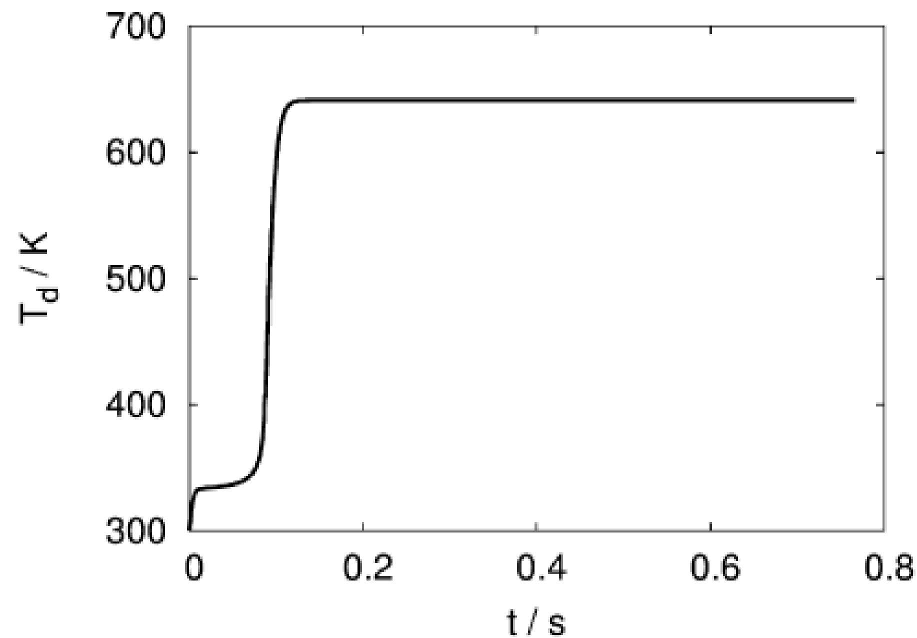
1. Birkhold et al., SAE Technical Paper 2006-01-0643

Decomposition Modeling Techniques 5

- Thermolysis is modeled by Extended Arrhenius expression[1]

$$\frac{dm_u}{dt} = -\pi D_d A e^{\left(-E/RT_d\right)}$$

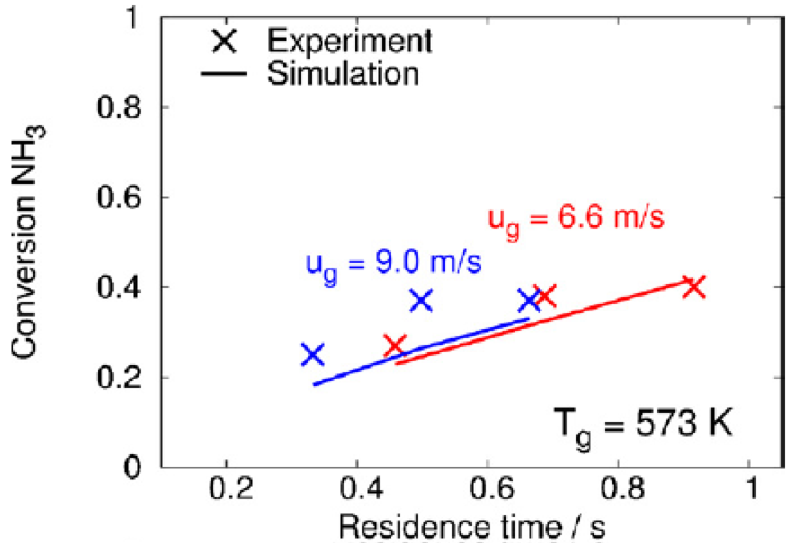


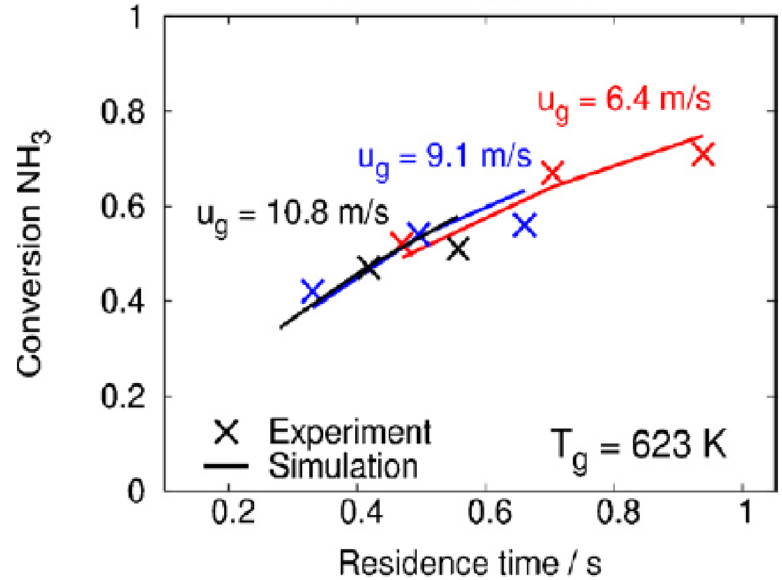


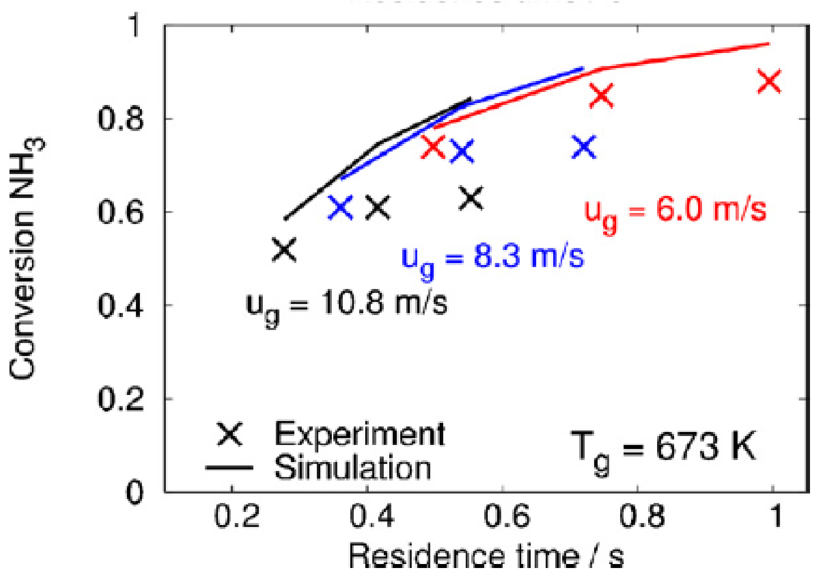
- Overpredicts the upper limit for decomposition temperature

1. F. Birkhold et al., Catal. B: Environ. 70 (2007) 119.

Decomposition Modeling Techniques 5







Comparison between Birkhold et al[1] calculated NH_3 and experimental data at different gas velocities and temperatures

1. F. Birkhold et al., Catal. B: Environ. 70 (2007) 119

Decomposition Modeling Techniques 5

- Deviation may be attributed to uncertainties in reaction description

	A (Kg/sm)	E_a (J/mol)
Yim et al.[1]	4.9	5505
Birkhold et al.[2]	0.42	6.9×10^4

$$(NH)_2CO(s\ or\ l) \rightarrow (NH)_2CO(g), \qquad \Delta H = 87.4kJ/mol$$

$$(NH)_2CO(g) \rightarrow NH_3(g) + HNCO(g), \qquad \Delta H = 98.1kJ/mol$$

1. S.D. Yim et al., Ind. Eng. Chem. Res. 43 (2004) 4863
2. F. Birkhold et al., Catal. B: Environ. 70 (2007) 119

Summary & Recommendations

- The role of CFD modeling to optimize UWS injection and decomposition was presented
- Results sensitivity to the accuracy of turbulence modeling was reported
- Various modeling techniques for UWS decomposition process was discussed
- Modifications proposed (currently under investigations)
  - The use of two layer wall treatment
  - Implementation of the two-step thermolysis process combined with the Arrhenius expression

Acknowledgment

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Thank You for Your Attention