Modeling of UREA Sprays in SCR Aftertreatment

Mario F. Trujillo

Graduate Students: Doug Ryddner and Suraj Deshpande

Engine Research Center
Mechanical Engineering
University of Wisconsin

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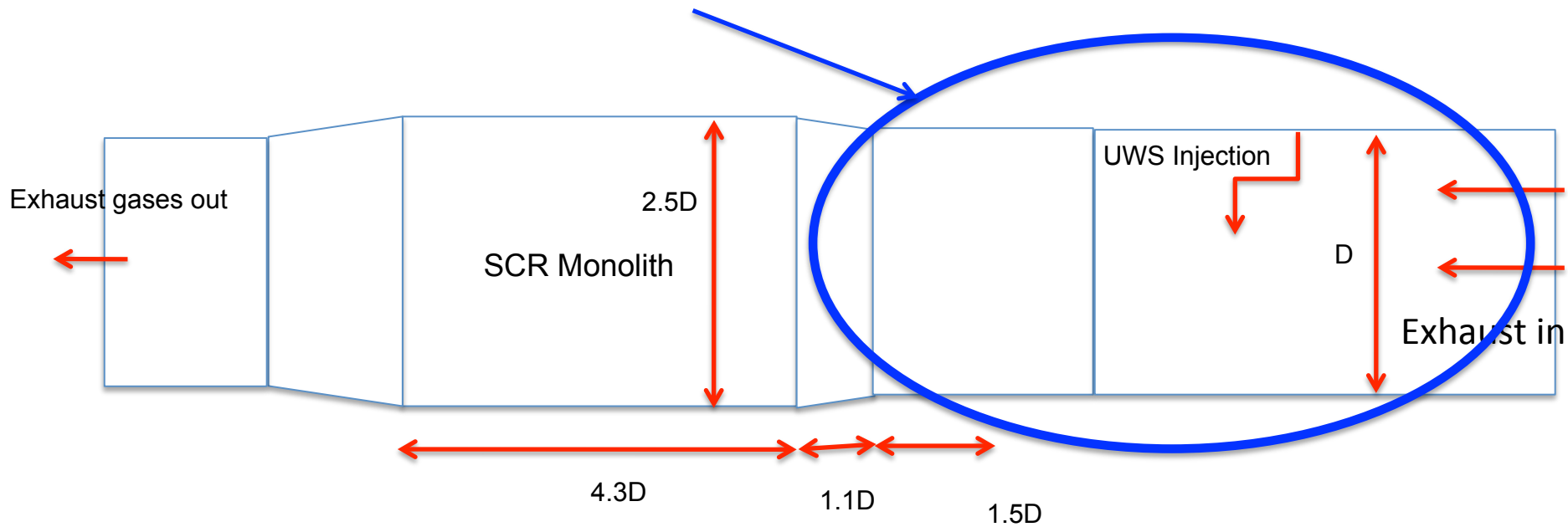
Objectives

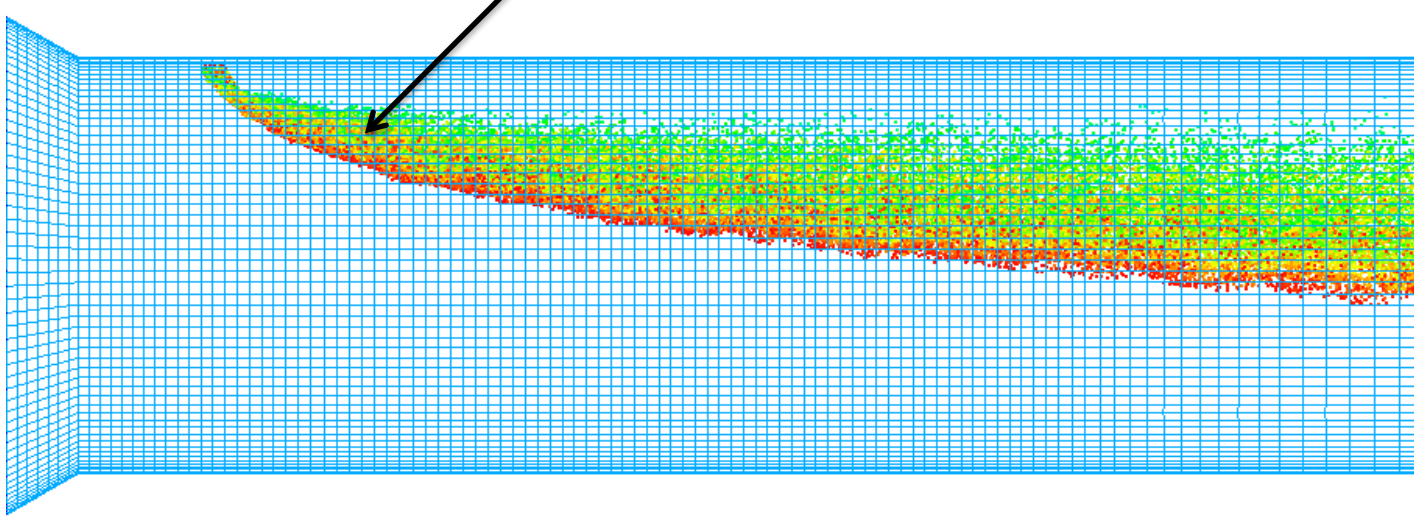
- Detailed simulations
  - UWS Spray/gaseous interactions
  - Chemical species turbulent mixing
  - Thermal mixing and its effect on UREA particle thermal decomposition
- Focus is the chamber upstream of the hydrolysis catalyst



UWS Spray Modeling with OpenFoam[1]

- OpenFoam is <u>not</u> a code ➔ C++ libraries for mechanics problems; various solvers available
  - Urea spray solver used is a modified version existing spray solver in openfoam

Lagrangian-Eulerian approach based
on standard parcel representation of particle field



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UWS Spray Modeling with OpenFoam[1]

- Gas phase Equations:

spray source terms

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{u}) = \dot{\rho}_s$$

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \bullet (\rho \mathbf{u} Y_i) - \nabla \bullet (D_{Eff} \nabla Y_i) = \dot{Y}_{i,Evap} + \boxed{\dot{Y}_{i,Chem}}$$

$$\frac{\partial \rho h}{\partial t} + \nabla \bullet (\rho \mathbf{u} h) - \nabla \bullet (\alpha_{Eff} \nabla h) = \frac{\partial p}{\partial t} + \nabla \bullet (\mathbf{u} p) + \dot{H}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \bullet (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla \bullet \left(\mu_{Eff} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \left[\frac{2}{3} \mathrm{tr}\left((\nabla \mathbf{u})^T \right) \right] I \right) \right) + \rho \mathbf{g} + \dot{\mathbf{M}}$$

$$\frac{\partial \rho k}{\partial t} + \nabla \bullet (\rho \mathbf{u} k) - \nabla \bullet (D_{kEff} \nabla k) = G - \frac{2}{3} \rho (\nabla \bullet \mathbf{u}) k - C_e \rho \frac{k^{3/2}}{\Delta}$$

(subgrid kinetic energy)

$$\left(D_{Eff}, \mu_{Eff} \right) = \mu_{sgs} + \mu;$$

$$\mu_{sgs} = C_k \rho \Delta \sqrt{k}$$

Δ is the filter size

In addition to the LES treatment, RANS with k-ε is also exercised

UWS Spray Modeling with OpenFoam[1]

- Urea-Water-Solution spray droplets

- Water vaporization[1] ($T \leq 100\ ^{o}\mathrm{C}$) (by D^2 – Law behavior)

$$H_2N-CO-NH_2\ (\mathrm{aq}) \rightarrow H_2N-CO-NH_2\ (\mathrm{l\ or\ g}) + xH_2O\ (\mathrm{g})$$

$$\frac{dM_{H20}}{dt} = -M_{H20}\frac{6D_v Sh\ \rho_g}{\rho_l D^2}\ln\left(1+\frac{X_{S,i}-X_{\infty,i}}{1-X_{S,i}}\right)$$

- After water vaporization[2]

$$m_{urea,s}C_{urea,s}\frac{dT_{urea,s}}{dt} = Nu\ \pi\ k\ D\ (T_g - T_{urea,s}) \quad \text{for} \quad T \in (\sim 373,425)\,K$$

$$\frac{dm_{urea,s}}{dt}H_{vap,fus} = Nu\ \pi\ k\ D\ (T_g - T_{urea,s}) \quad \text{for} \quad T \text{ remains constant at } 425\ K$$

$$\left(H_{vap,fus} = 185.5\ \mathrm{KJ/mol,\ includes\ both\ fusion\ \&\ vaporization}\right)$$

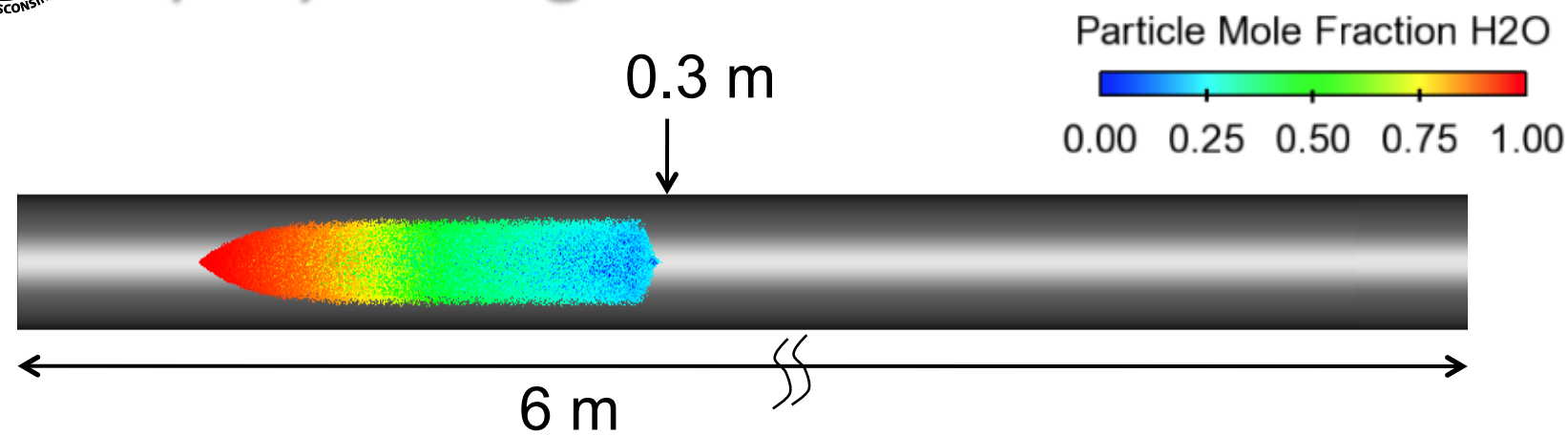
- Thermal decomposition[1]

$$H_2N-CO-NH_2\ (\mathrm{g}) \rightarrow \mathrm{NH_3}\ (\mathrm{g}) + \mathrm{HNCO}\ (\mathrm{g})$$

Arrhenius equation with $k = 4.9\times10^3 \exp\left(\frac{-5505}{RT}\right)$ (NO hydrolisis of $HNCO$ at the moment)

[1] Yim et al. (Ind. Eng. Chem. Res., 2004) ; [2] somewhat following Schaber et al. (Thermochimica Acta, 2004)

Spray Configuration



Air:
U : variable
P : 1 atm
T : variable

<u>Composition</u>
<u>(Mass fractions)</u>
N_2 : 0.9461
O_2 : 0.0534
NO: 0.0005

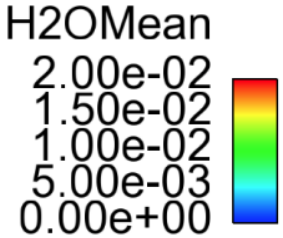
Spray:
U : 11.8 m/s
$\dot{m}$: 0.00036 kg/s
D_{inj} = 44 micron
T= 303 K
# nozzles : 1

<u>Composition</u>
<u>(Mass fractions)</u>
Urea : 0.4
H_2O : 0.6

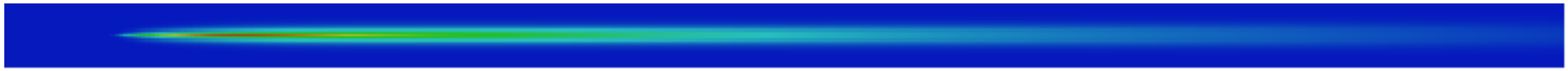
Results

Mass fraction contours of H_20 vapor

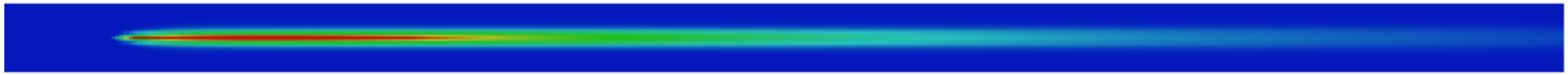
View above flow



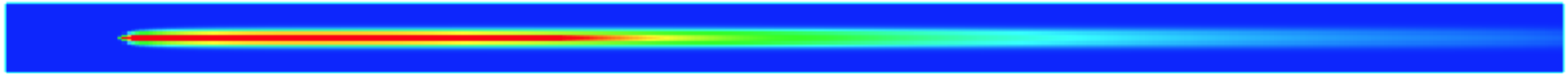
U_{air} = 6 m/s with LES
T = 523 K



U_{air} = 6 m/s with LES
T = 723 K



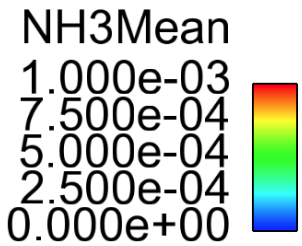
U_{air} = 6 m/s with LES
T = 1150 K



Results

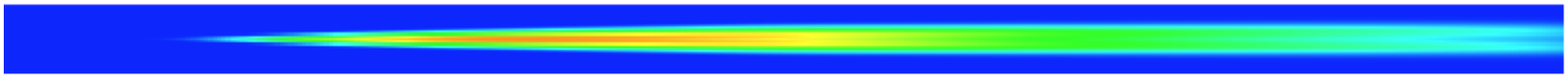
Mass fraction contours of NH_3 vapor

View above flow



U_{air} = 6 m/s with LES
T = 523 K

U_{air} = 6 m/s with LES
T = 723 K

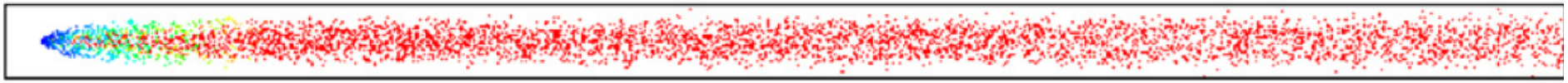


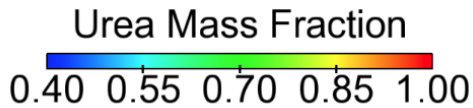
U_{air} = 6 m/s with LES
T = 1150 K

Comparison to Literature findings[1]

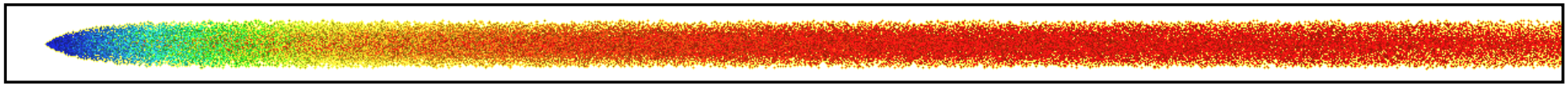
Mass fraction urea in droplet field

Data from [1]



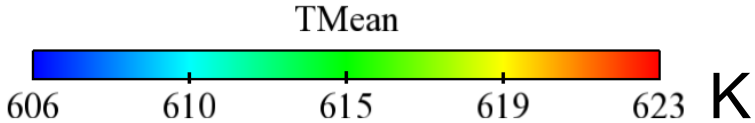


Current Model with RANS



Temperature field

Data from [1]



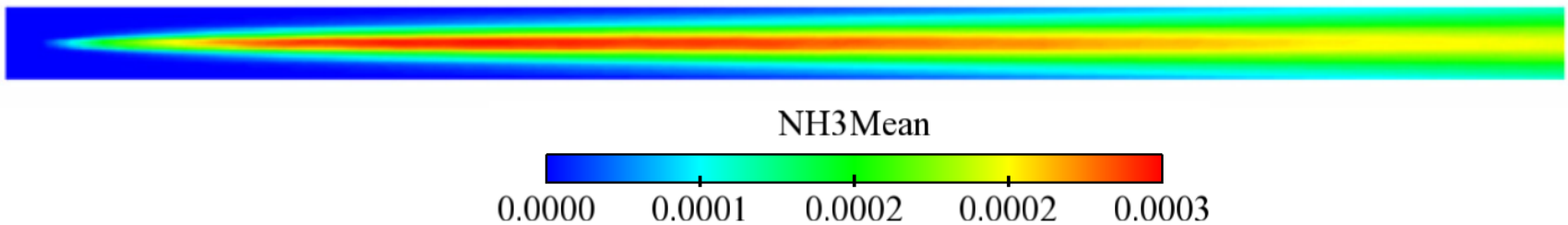
Current Model with RANS

[1] Birkhold et al. (Applied Catalysis B: Environmental 2007); same conditions Uin=9.08 m/s, T=623 K

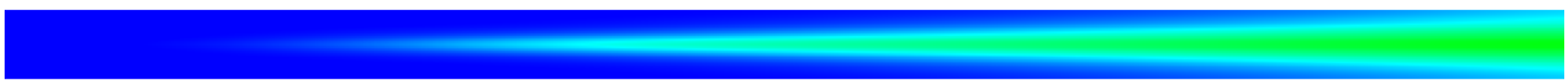
Comparison to Literature findings[1]

Mass fraction NH_3

Data from [1]



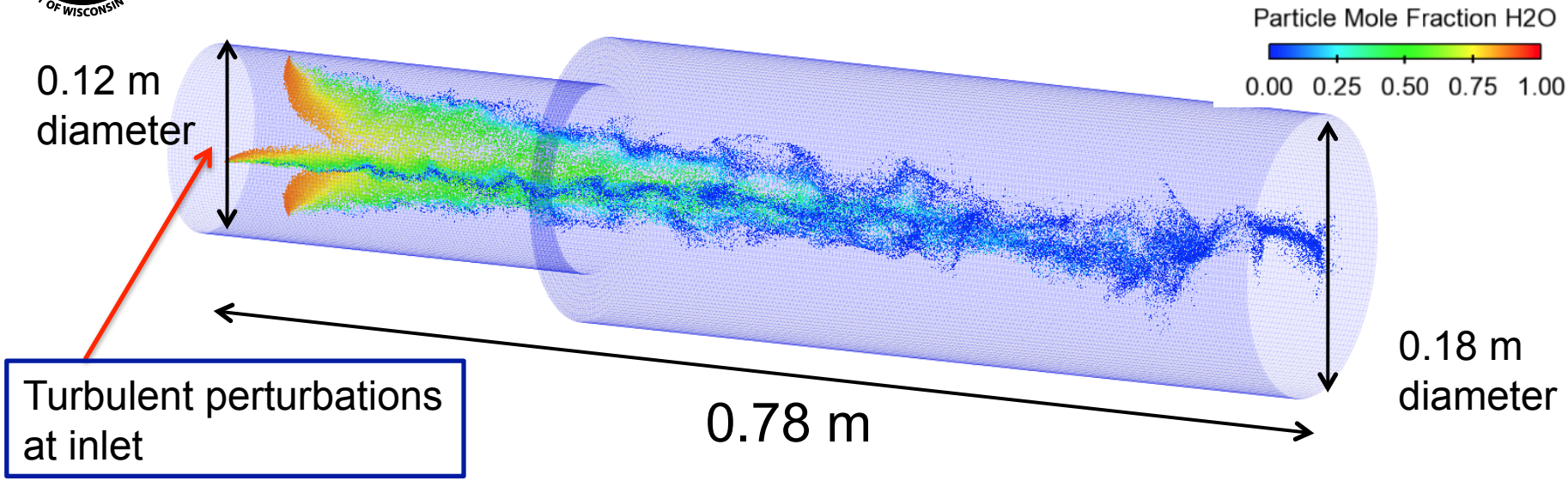
Current Model with RANS



Note: differences in thermal decomposition treatment and values of Arrhenius constants

[1] Birkhold et al. (Applied Catalysis B: Environmental 2007); same conditions Uin=9.08 m/s, T=623 K

A Second Spray Configuration



Air:
U : 12.06 m/s
P : 1 atm
T : 1100 K

<u>Composition (Mass fractions)</u>
N_2 : 0.9461
O_2 : 0.0534
NO: 0.0005

Spray:
(injected in crossflow)
U : 10.4896 m/s
$\dot{m}$: 0.00018 kg/s
D_{inj} = 50 micron (mean) RR (exponent=3)
T= 303 K
# nozzles : 3

<u>Composition (Mass fractions)</u>
Urea : 0.325
H2O : 0.675

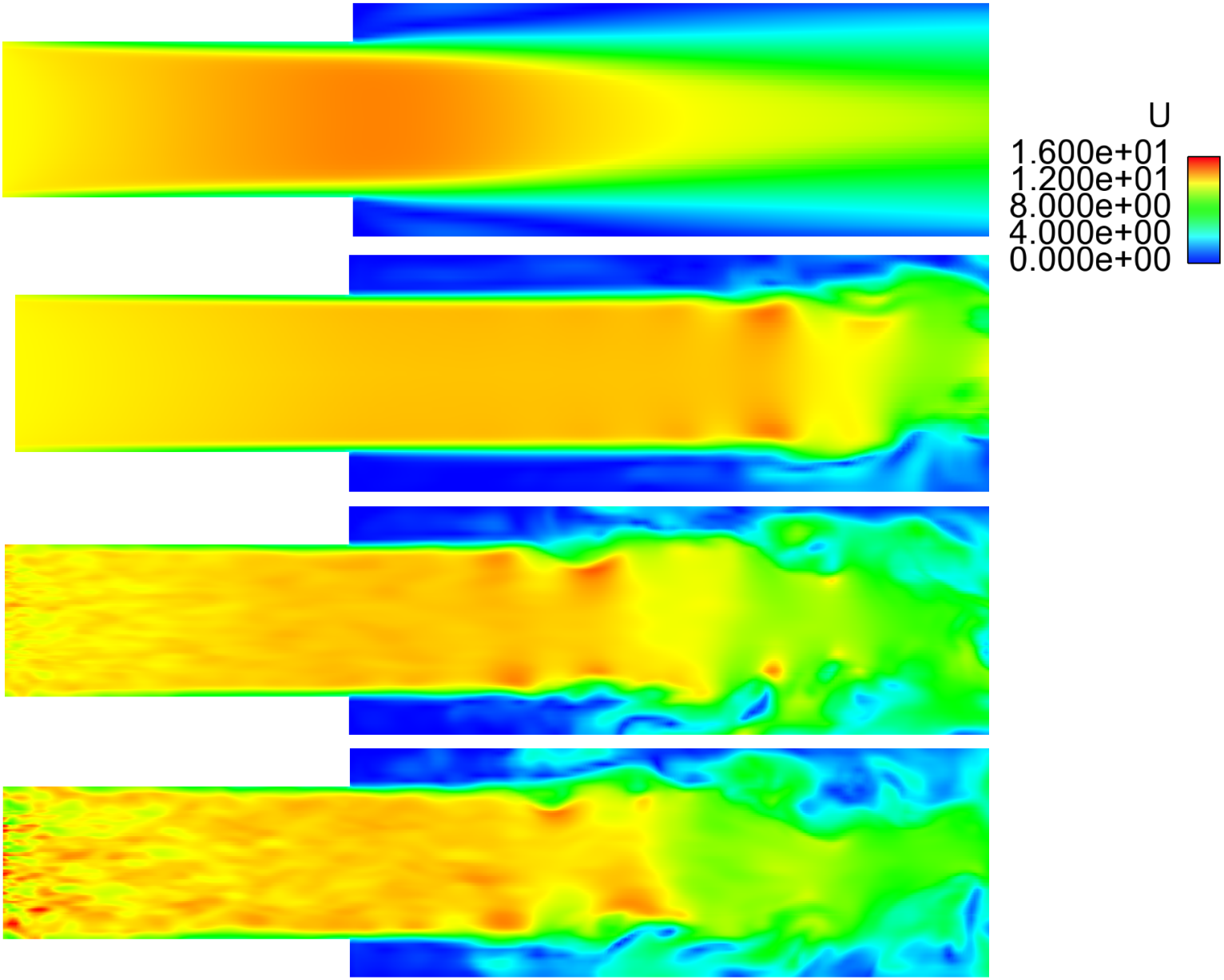
Instantaneous Velocity Field

0% turb
RANS

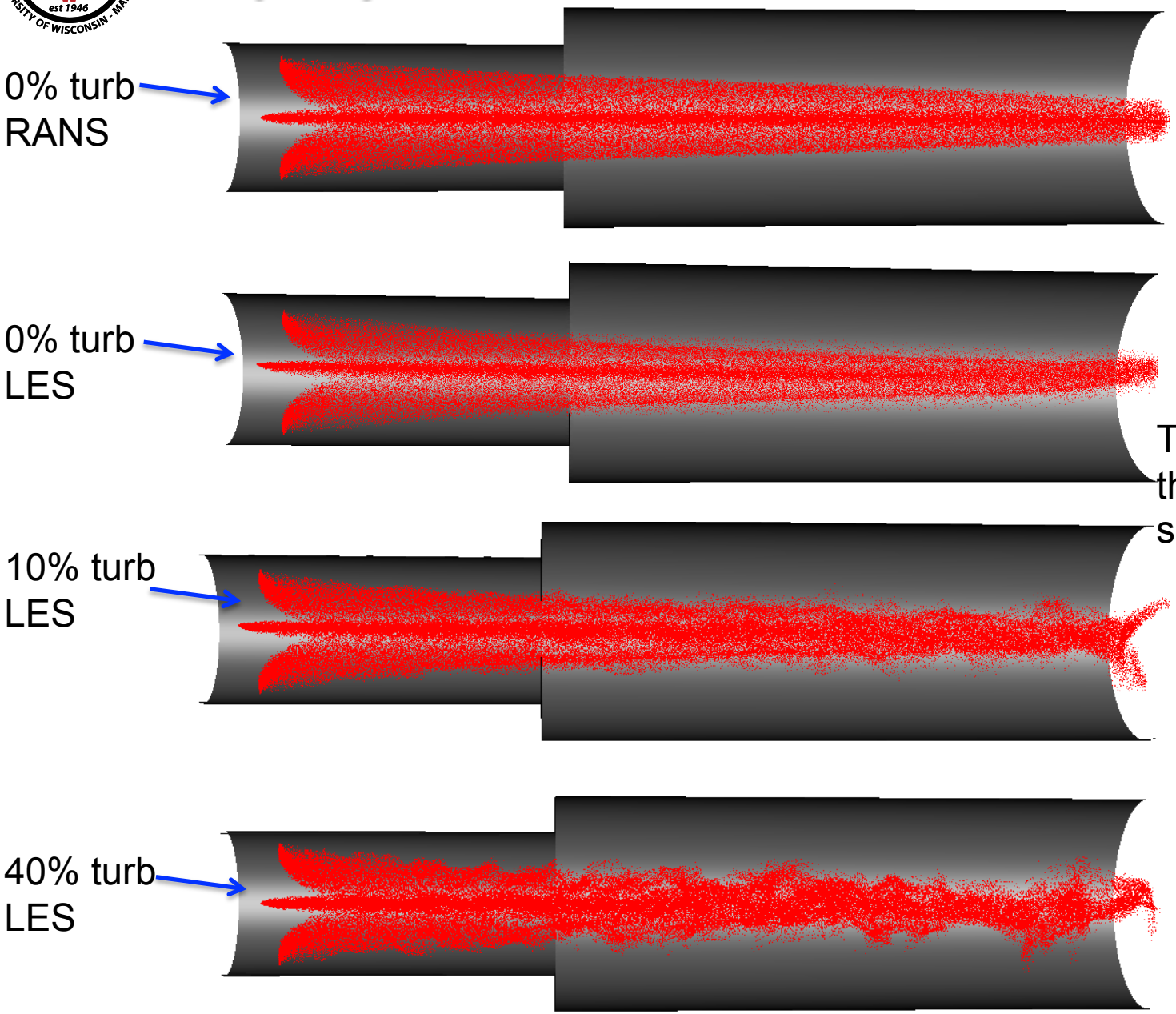
0% turb
LES

10% turb
LES

40% turb
LES

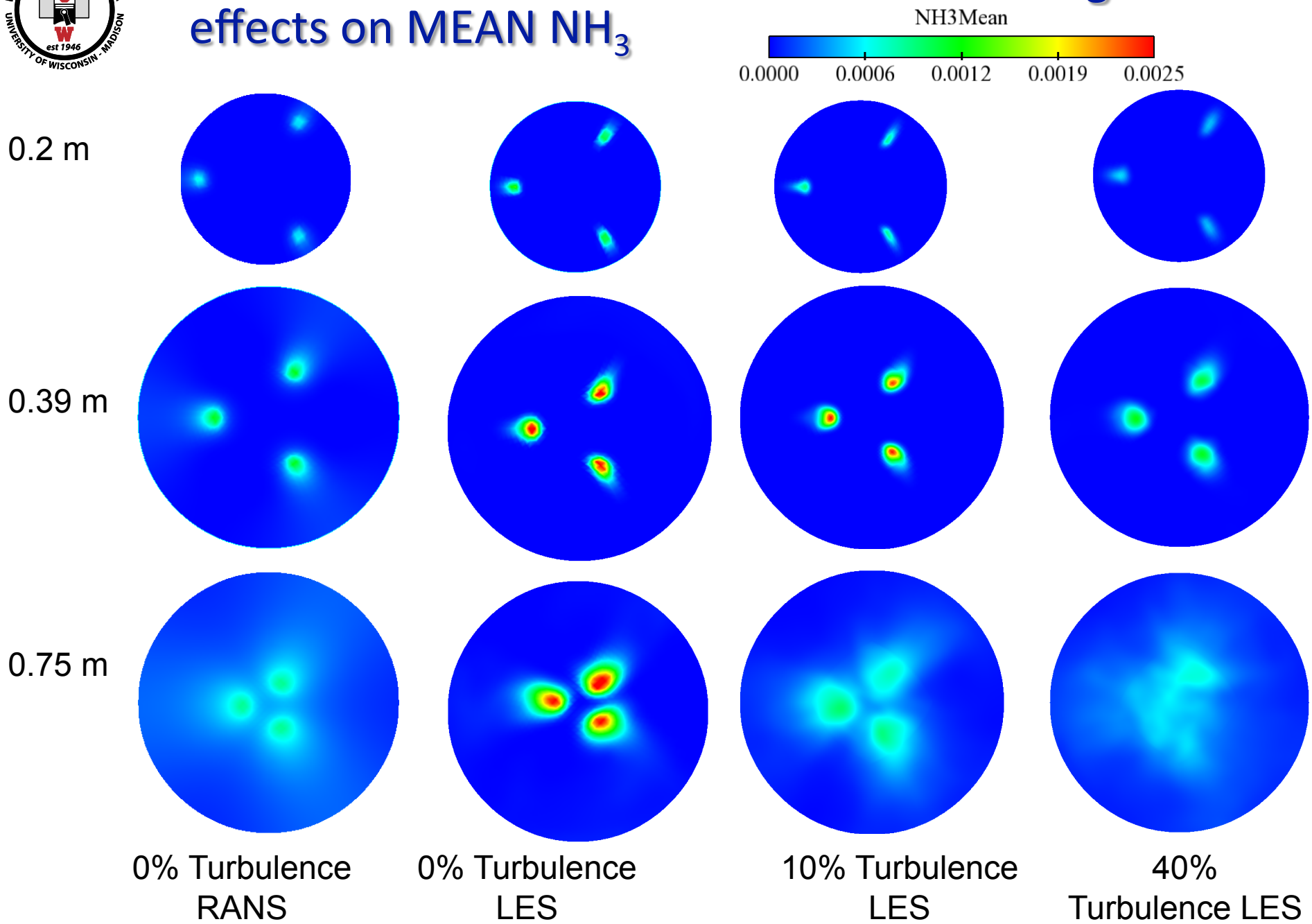


Spray structure



Turbulence causes the spray to deflect significantly.

Turbulence effects and turbulence modeling effects on MEAN NH_3



Summary & Future Work

- Both turbulence effects and their modeling have a significant effect on local temp➔NH_3 production➔NH_3 and NO mixing
- Degree of uncertainty in the thermal decomposition process remains high
- More validation data for UWS spray is needed
  - turbulence conditions at inlet
  - A more complete characterization of spray
  - Temperature, NH_3, NO, and HNCO contour maps
- Full resolution of urea droplets will provide insight into the dominant heat/mass transfer players
  - Will employ to advance UWS spray treatment
- (Not discussed) Fully resolved heat transfer from multiple droplet impingement on liquid films