Nitrogen Oxides Emissions in the Wood Dust Burners Preliminary Results

Energy and Environmental Combustion Laboratory
Department of Mechanical Engineering
University of Washington
Seattle, Washington
98195-2600

Modeling Approaches

- **Computation Fluid Dynamics (CFD)**

Solves set of Navier-Stokes Equations (usually time averaged) coupled with Energy and Species Transport Equations.

- **Chemical Reactor Modeling (CRM)**

Solves the Energy and Species Transport Equations decoupled from the Fluid mechanics

CFD approach

- **Benefits:**

Might give valuable insight information -- computes the flow field

Gives spatial and temporal information

- **Issues:**

NSEs have more unknowns than equations, closure model required

Reynolds Averaging wipes out some information

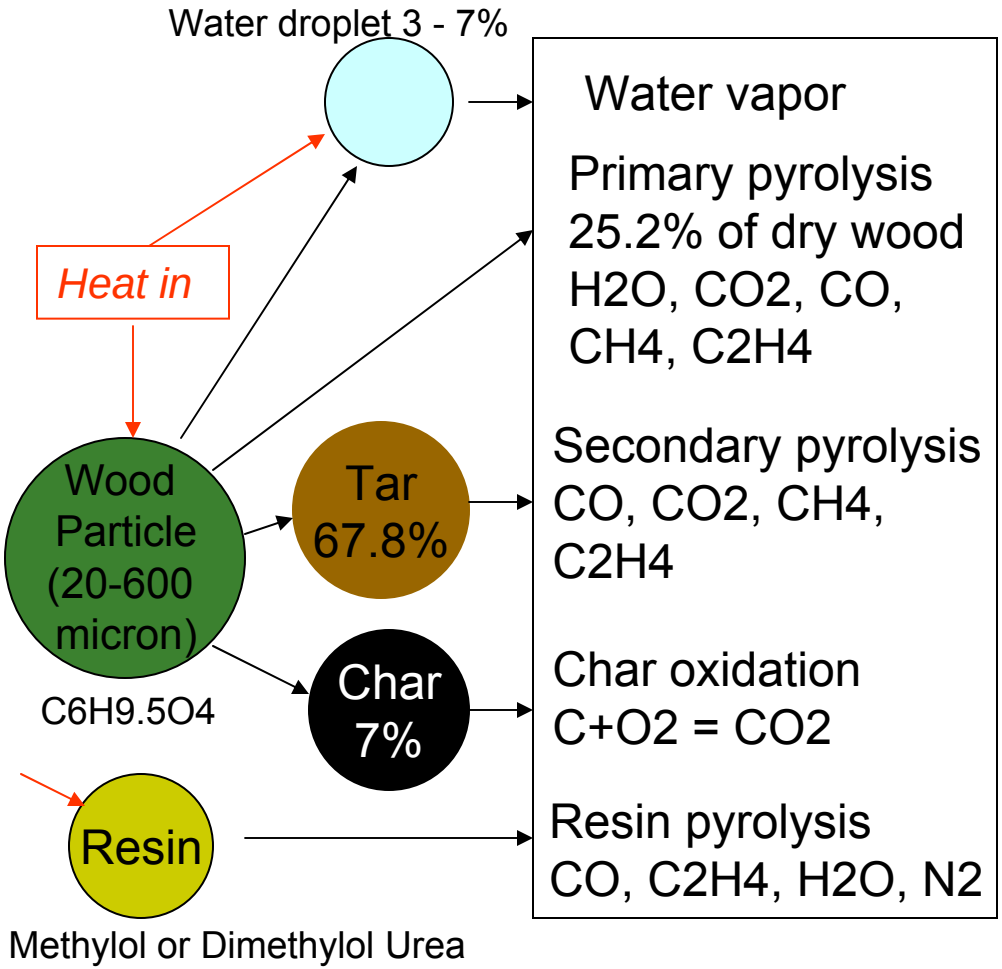
Full chemical kinetic mechanism is difficult to implement in complex geometry

Takes long time to converge

Flame modeling in CFD

- Eddy Break-Up Model
- Flamelets modeling, Bray-Moss-Libby (BML) model based on the progress variable
- G-equation based on non-reacting scalar. This scalar describes the flame surface area in the given volume of the flame zone
- PDF approach to solve for the reacting species mass fractions

Particle interaction with the flow



- Flow and species fields solved in Eulerian system
- Particle receives heat from the mean flow
- Volatiles evaporate and burn, give heat back to the mean flow
- Char burns and gives heat to the mean flow

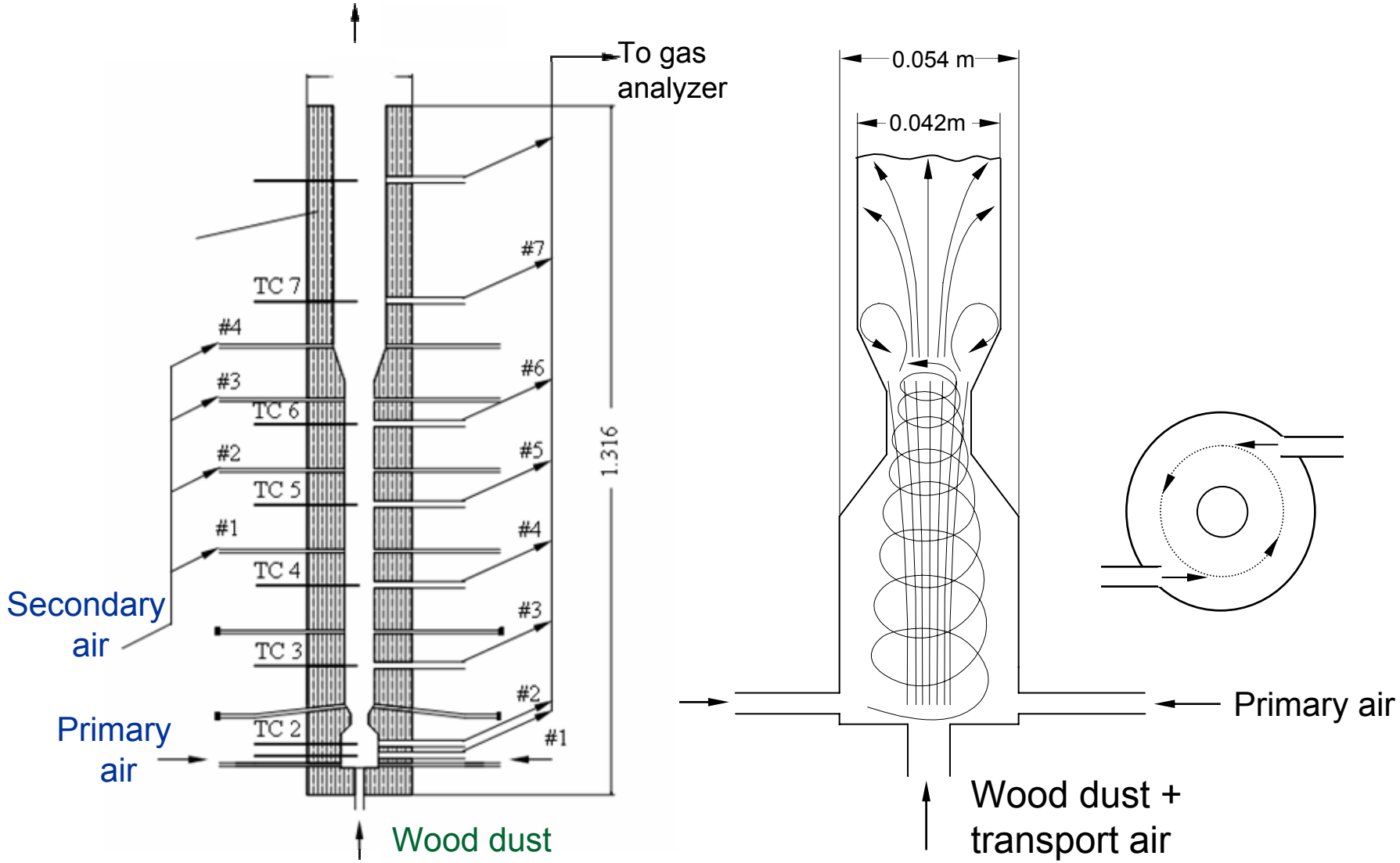
Chemical Kinetic Mechanism

- Detailed kinetic mechanism describes elementary reactions (50+ species, 300+ reactions): GRI3.0. Mechanism not used directly in CFD.
- Global mechanism: few reactions, does not calculate radicals, can be applied in CFD relatively easy, however accuracy requires testing and calibration.

Global Mechanism for Wood Volatiles and Resin Oxidation

- Reaction 1 Wood Volatiles $\rightarrow$ Tar+CO+CH4+C2H4+H2O+CO2
- Reaction 2 Tar $\rightarrow$ CO+CH4+C2H4+CO2
- Reaction 3 Resin Volatiles $\rightarrow$ CO+CH4+H2O+N2
- Reaction 4 CH4+1.5O2 $\rightarrow$ CO+2H2O
- Reaction 5 C2H4+2O2 $\rightarrow$ 2CO+2H2O
- Reaction 6 CO+0.5$\times$O2 $\rightarrow$ CO2
- Reaction 7 CO2 $\rightarrow$ CO+0.5$\times$O2

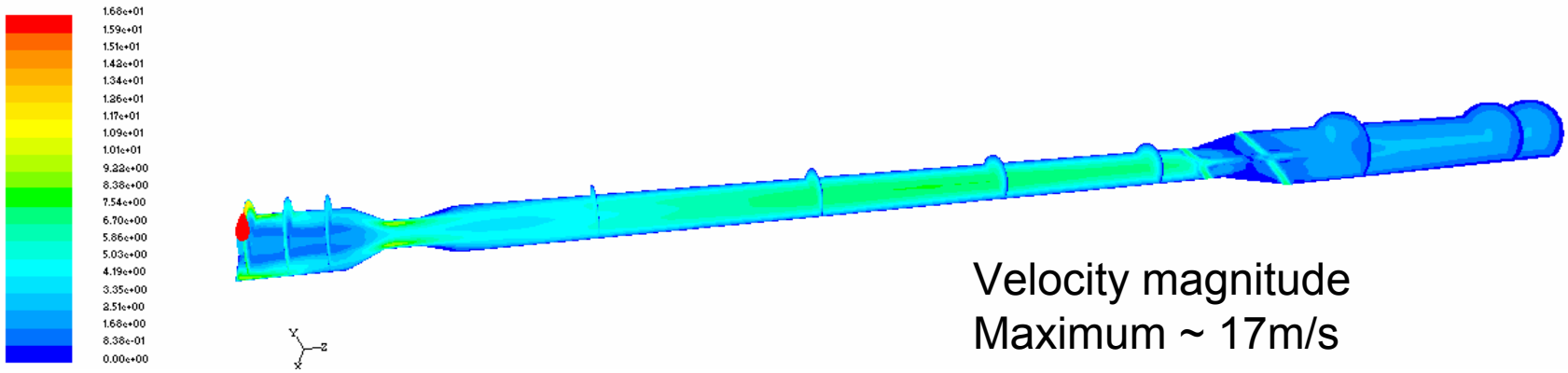
UW wood dust burner



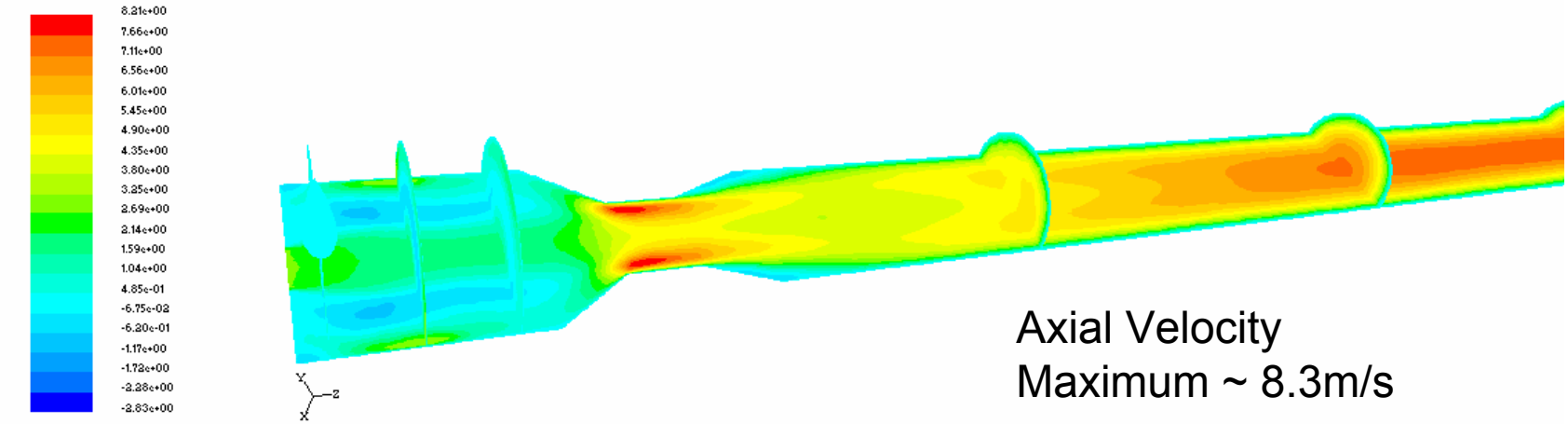
CFD model of the wood dust burner

- Domain 750 000 grid cells
- Reynolds Stress turbulence closure model
- Discrete Ordinates heat transfer model
- EBU / Kinetic limited reaction rates
- Global Chemical Kinetic mechanism optimized for 1 atm, near stoichiometric conditions
- Lagrangian Particle tracking couple with heat transfer

CFD Results

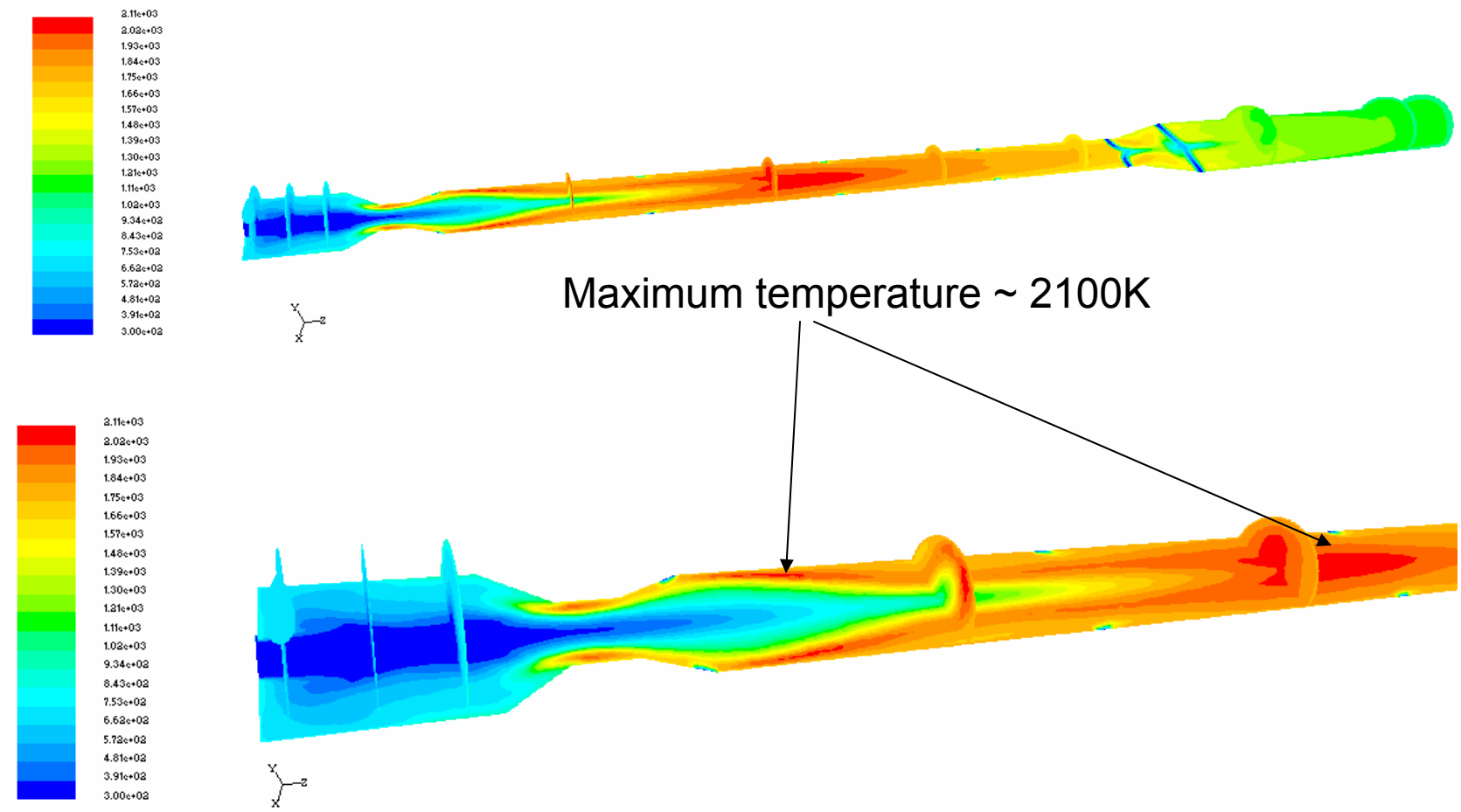


Velocity magnitude
Maximum ~ 17m/s

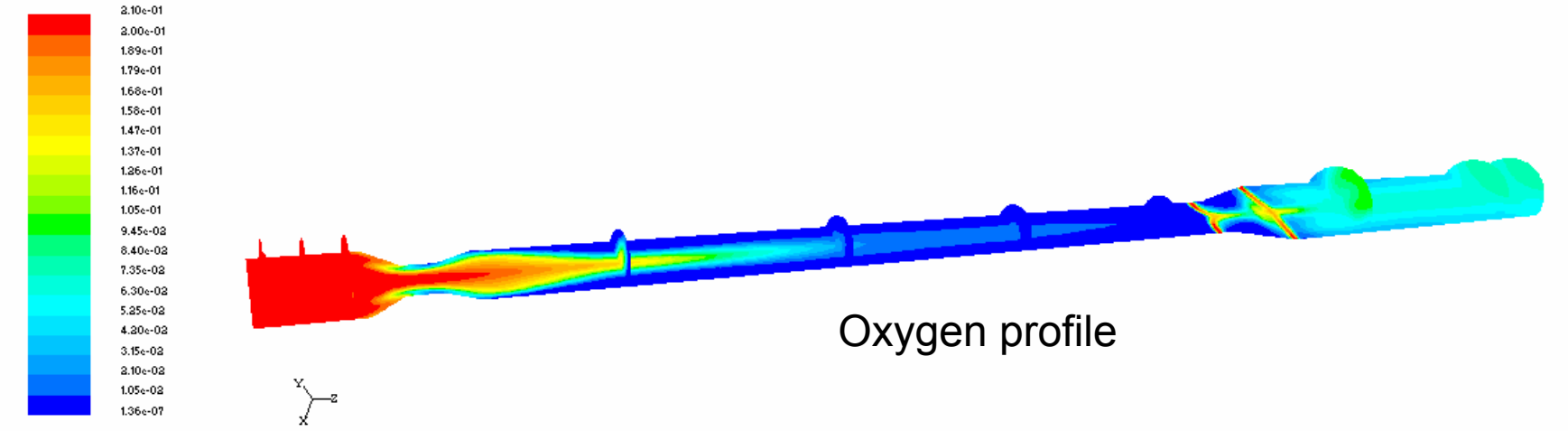


Axial Velocity
Maximum ~ 8.3m/s

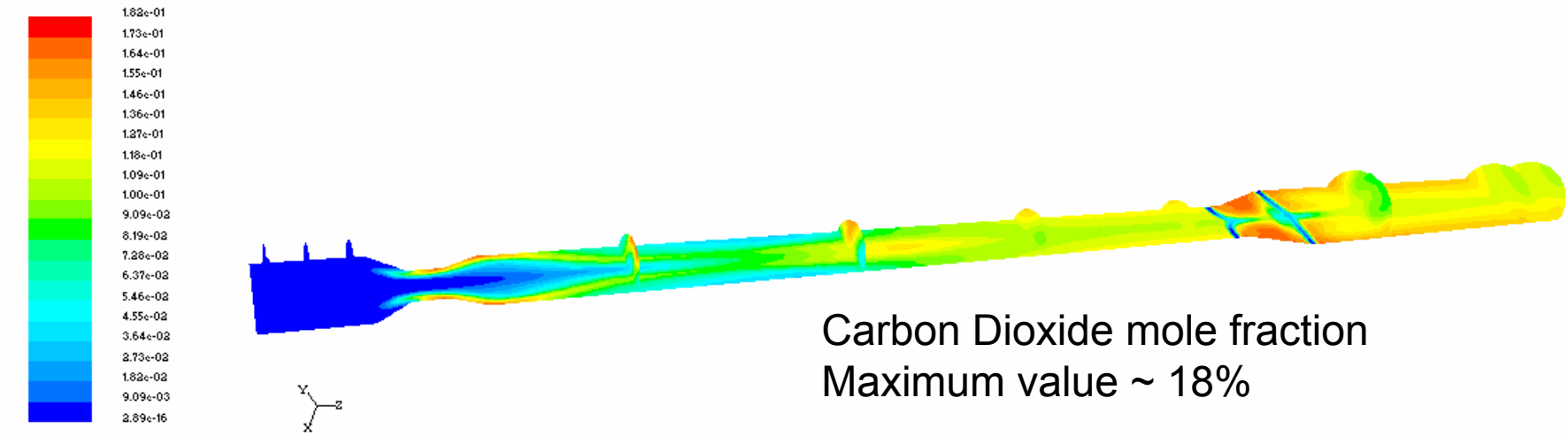
Temperature profile



Species profiles I

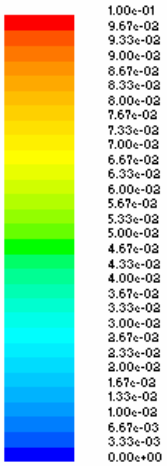


Oxygen profile



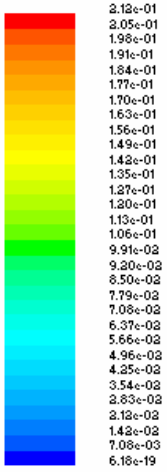
Carbon Dioxide mole fraction
Maximum value ~ 18%

Species profiles II

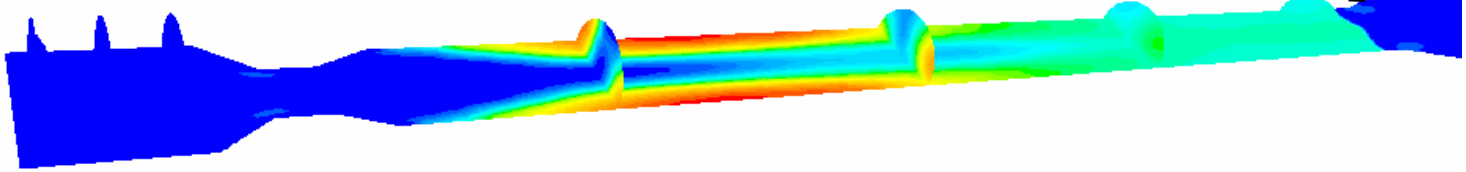


Particles trapped near throat entry

Volatiles mole fraction
Maximum value ~12%

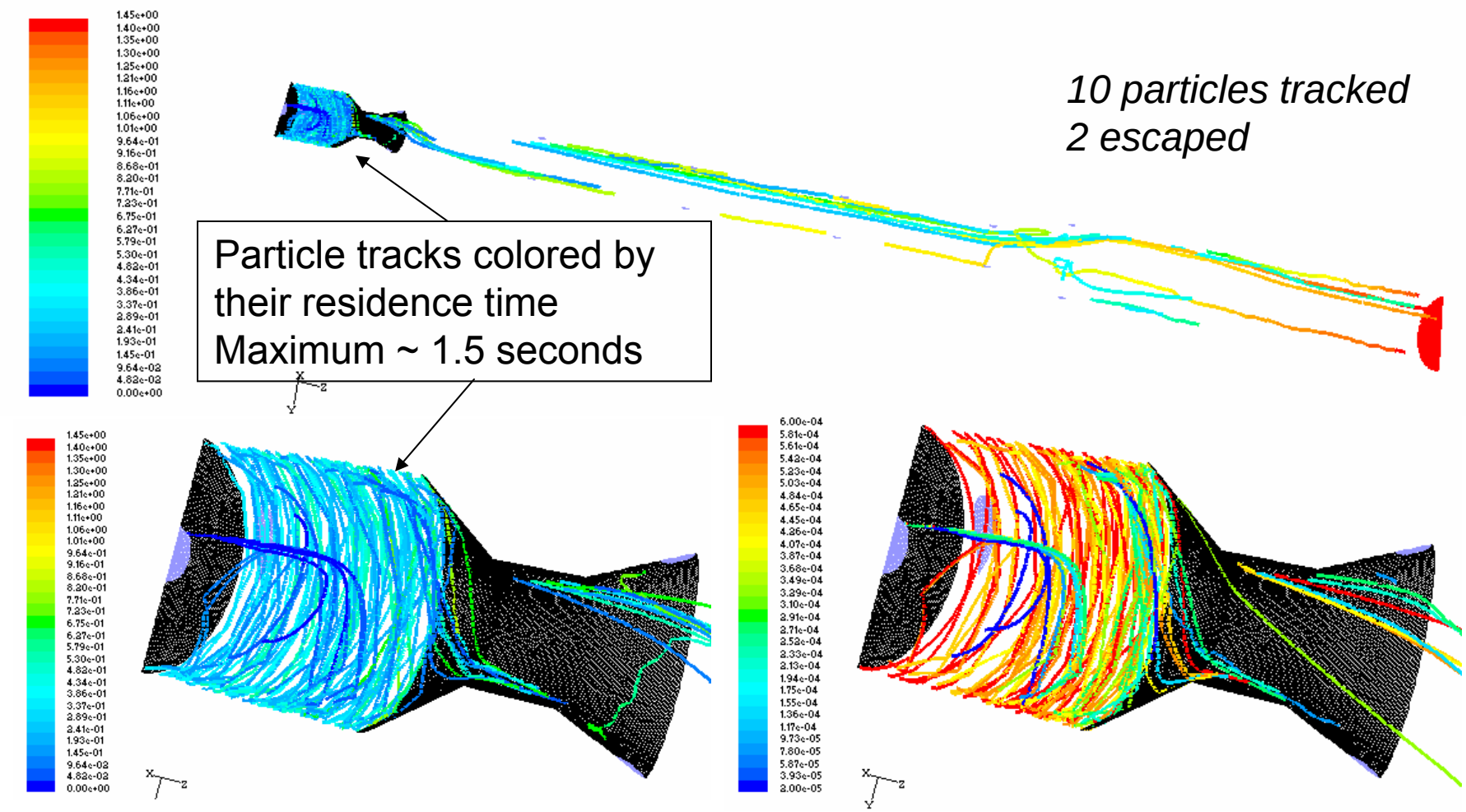


Secondary air inlets



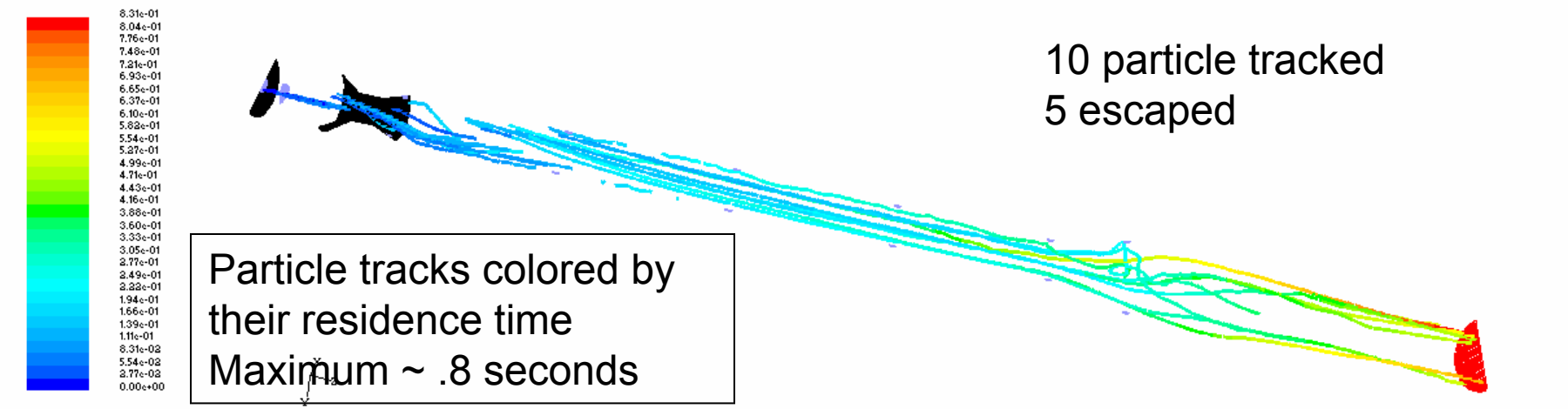
Carbon Monoxide mole fraction
Maximum value ~ 21%

Particle tracks near the edge of the jet



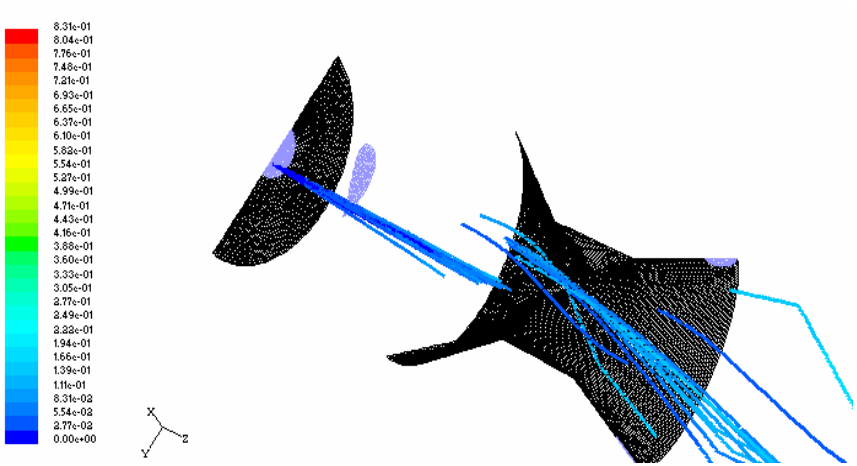
End of the particle track indicates that particle burned out

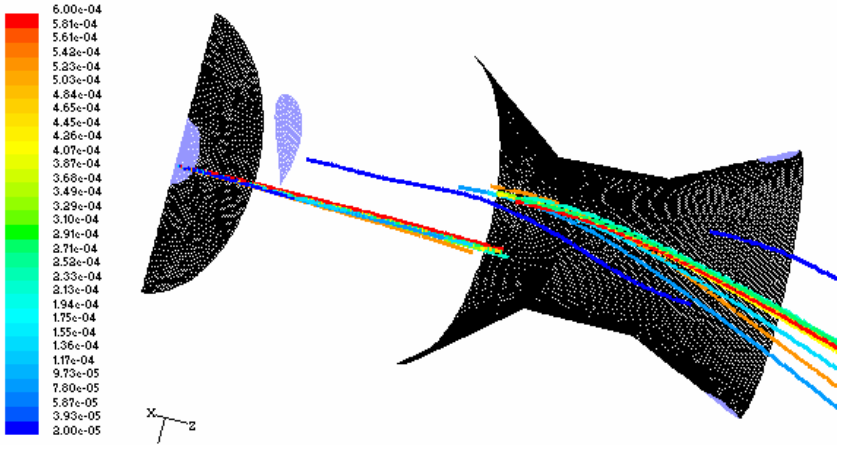
Particle near the center of the jet



10 particle tracked
5 escaped

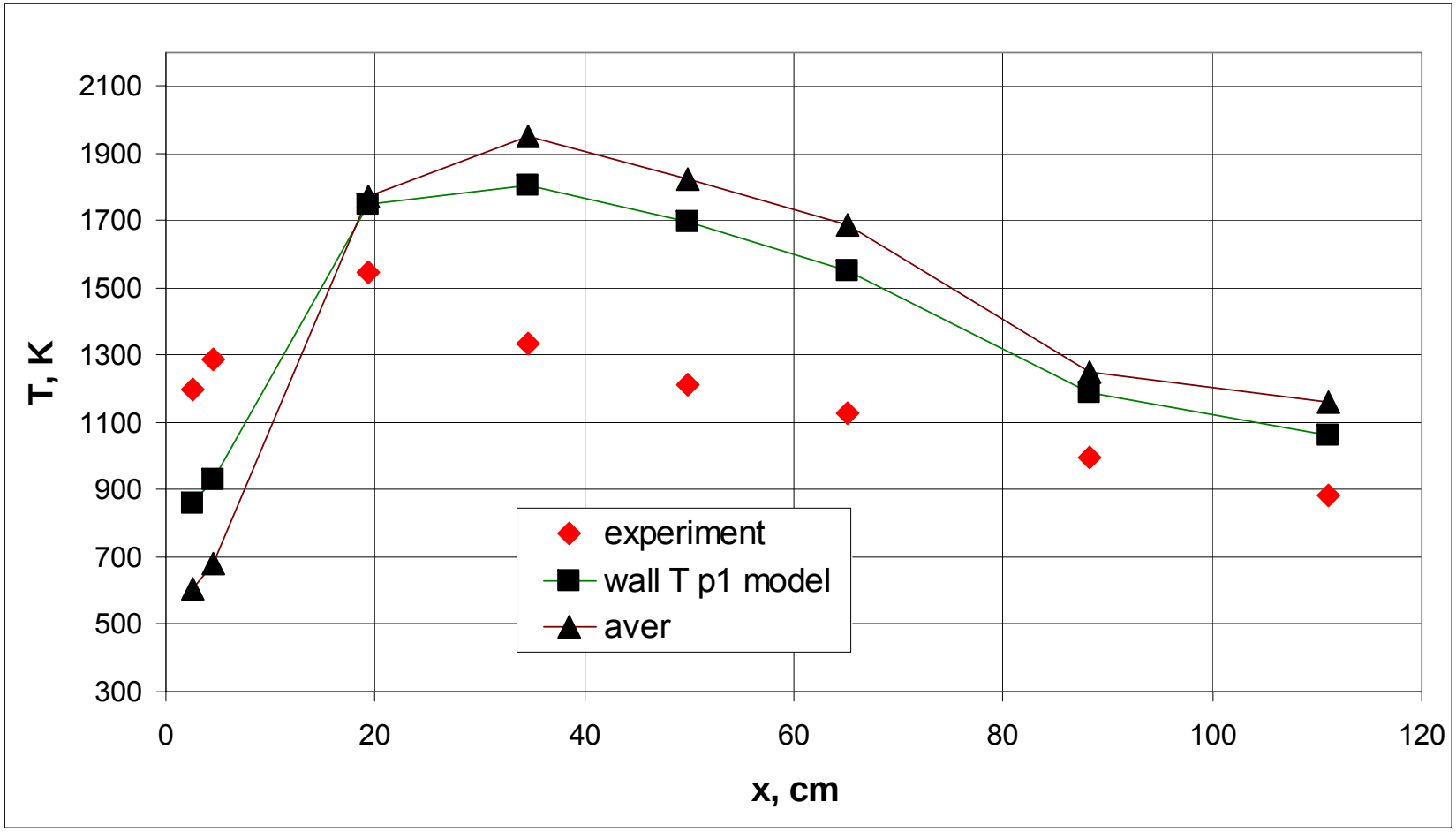
Particle tracks colored by their residence time
Maximum ~ .8 seconds



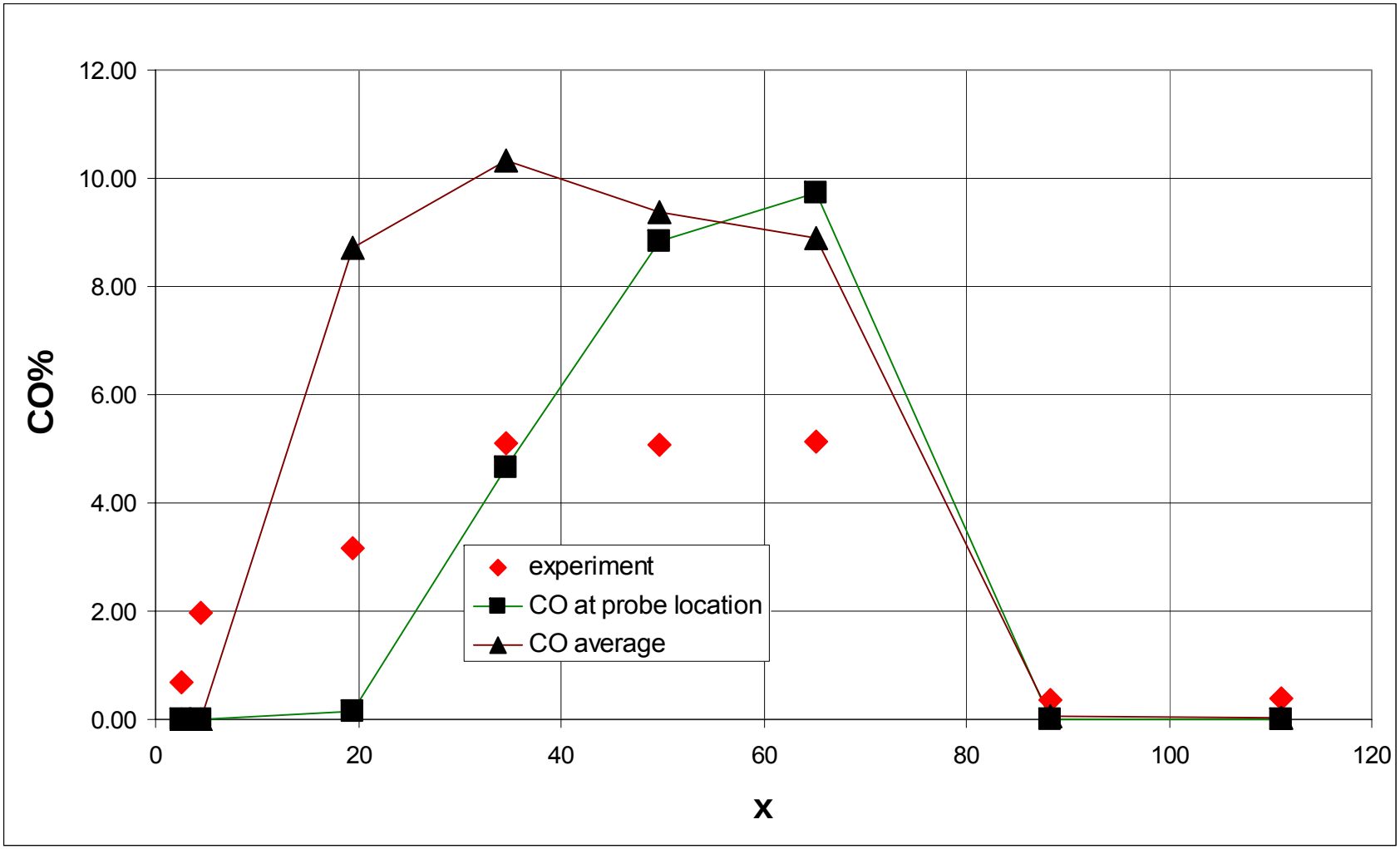


Colored by particle diameter

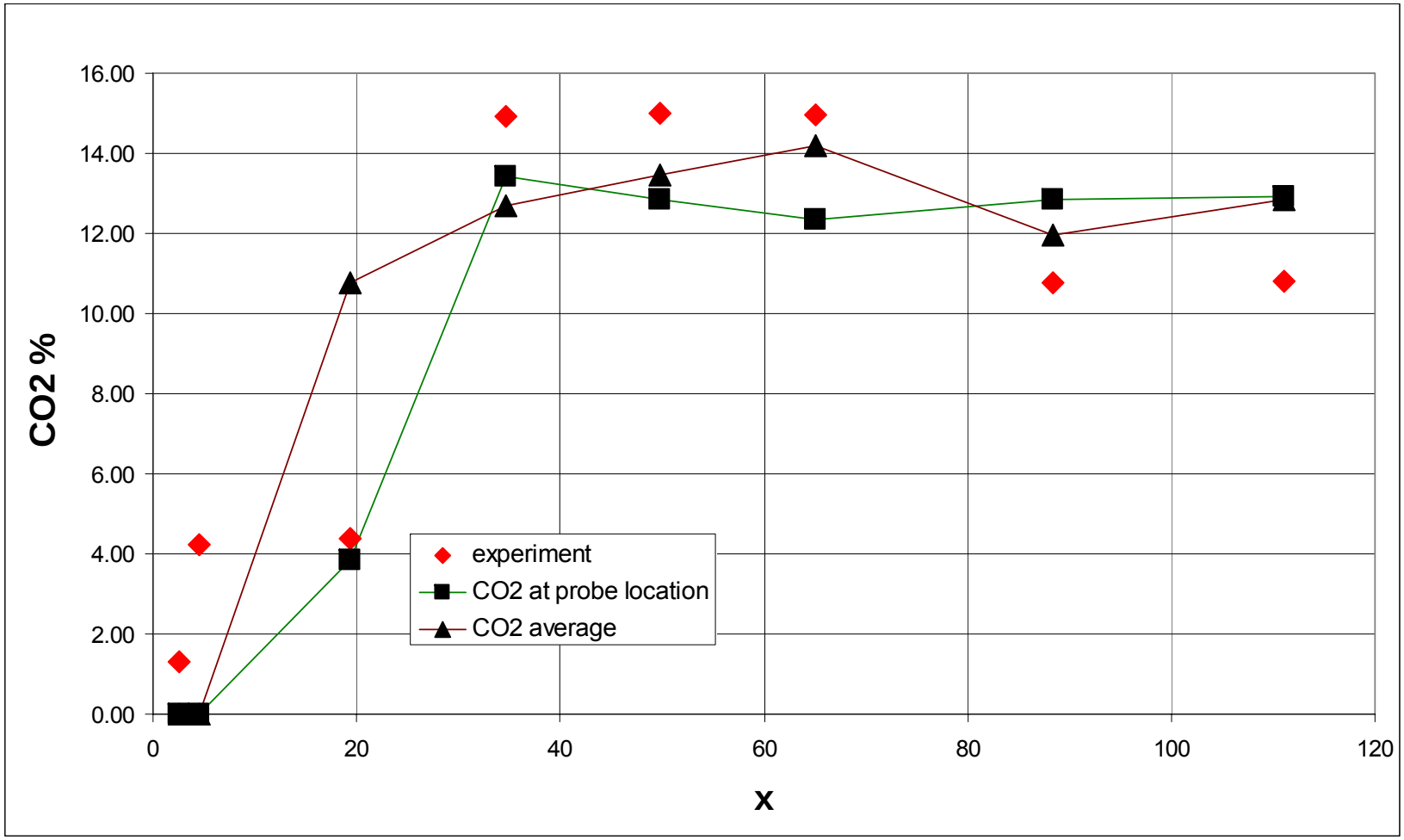
Axial Temperature profile



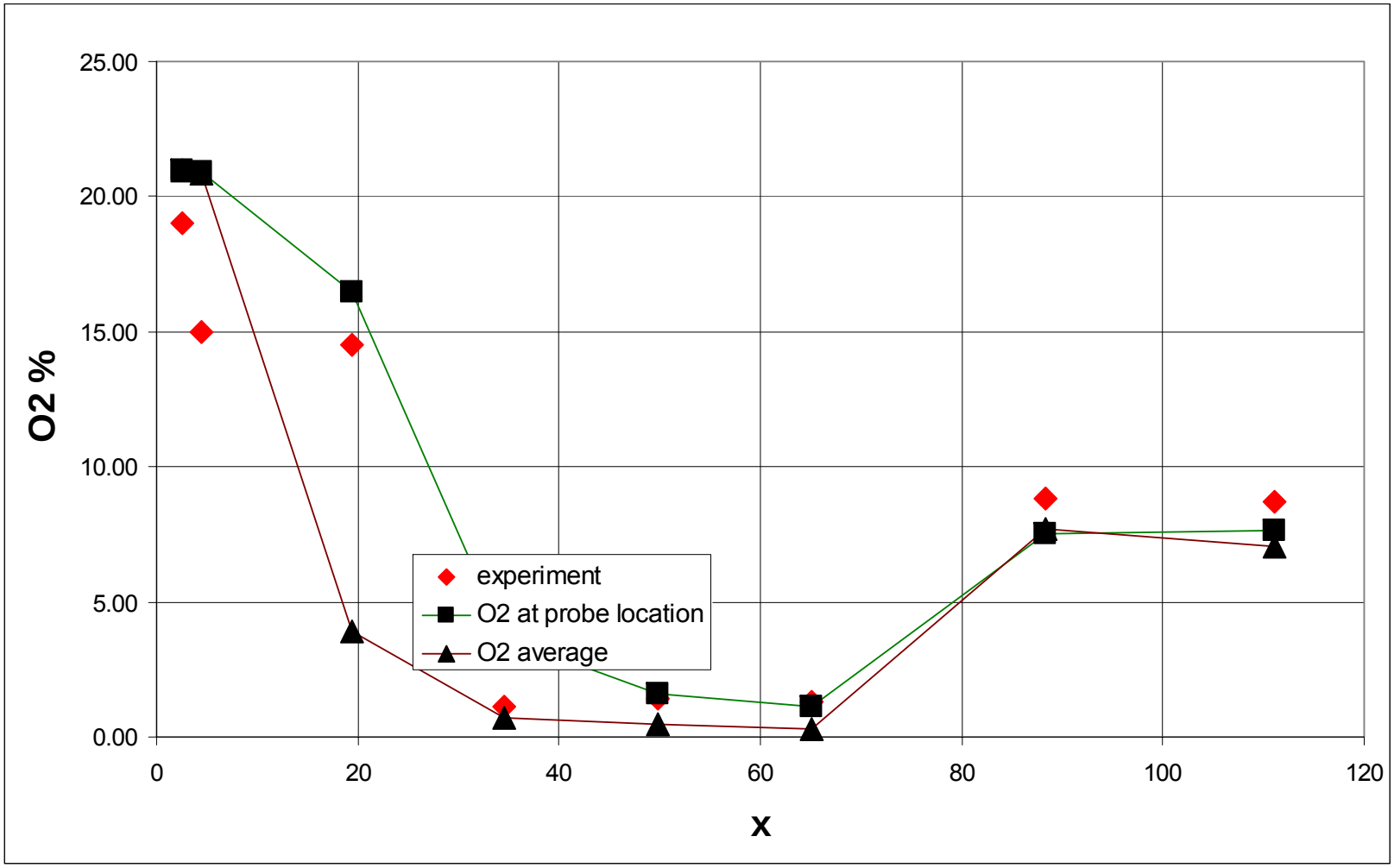
CO axial profile



Carbon Dioxide axial profile

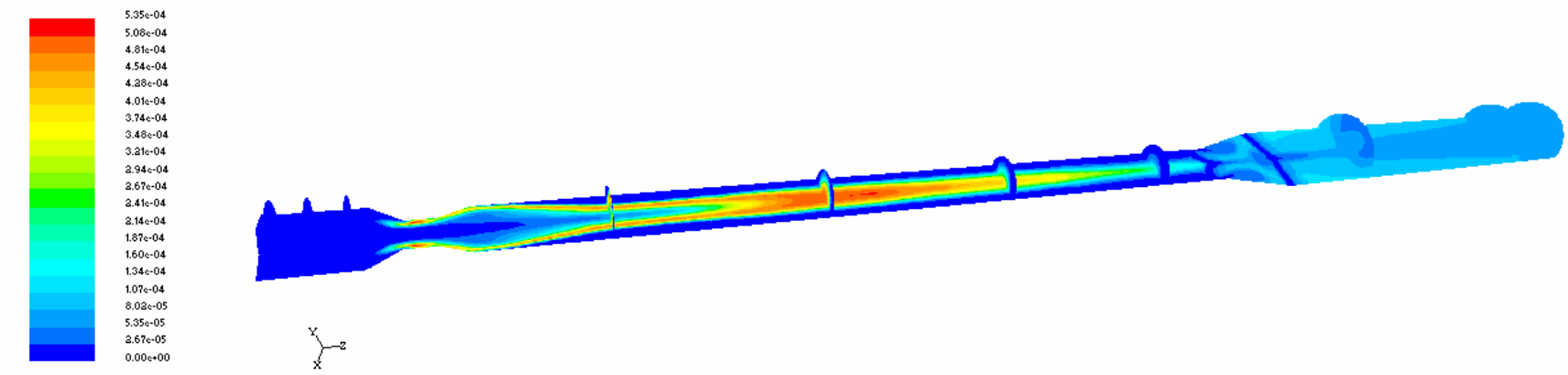


Oxygen axial profile

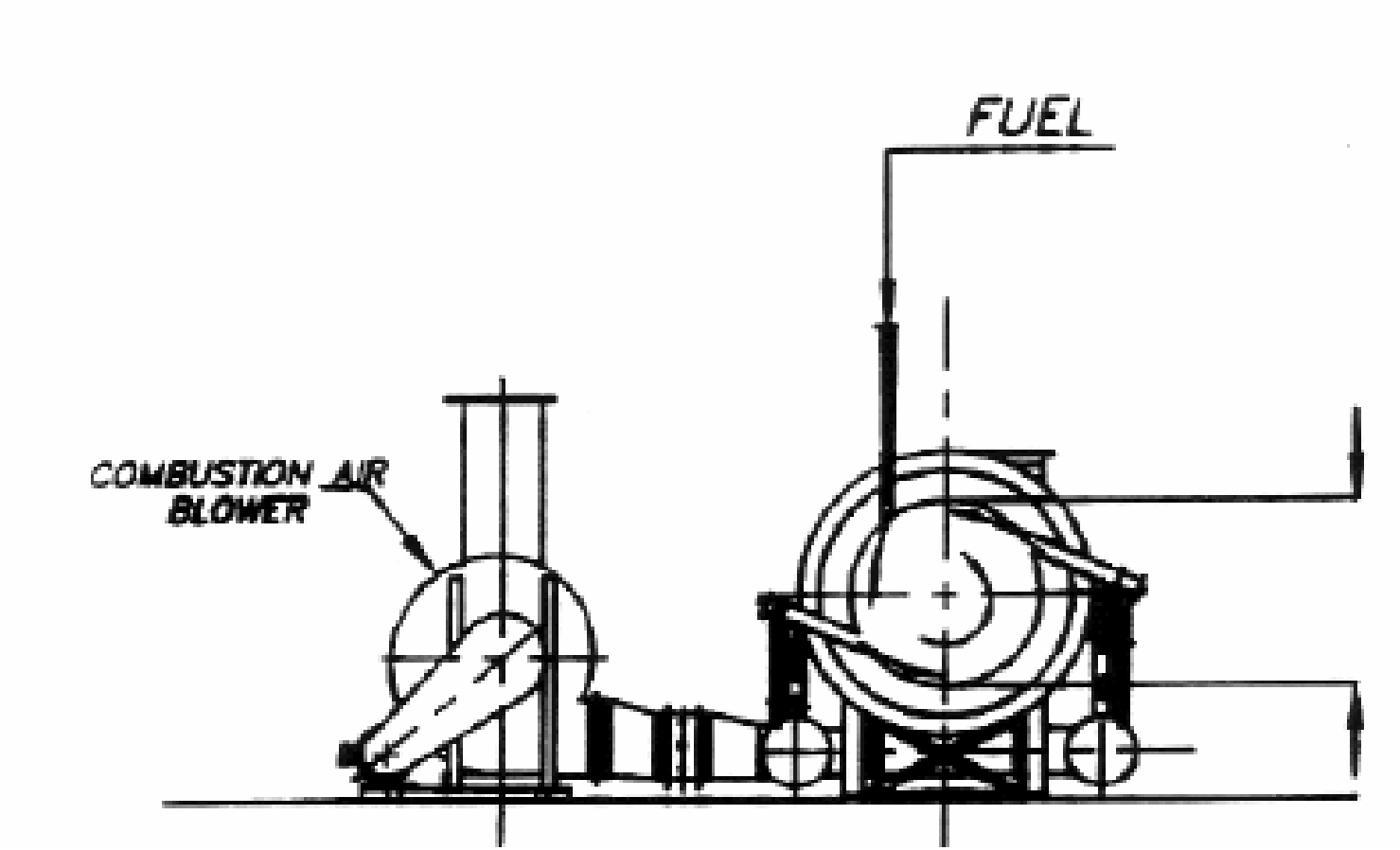


NOx formation

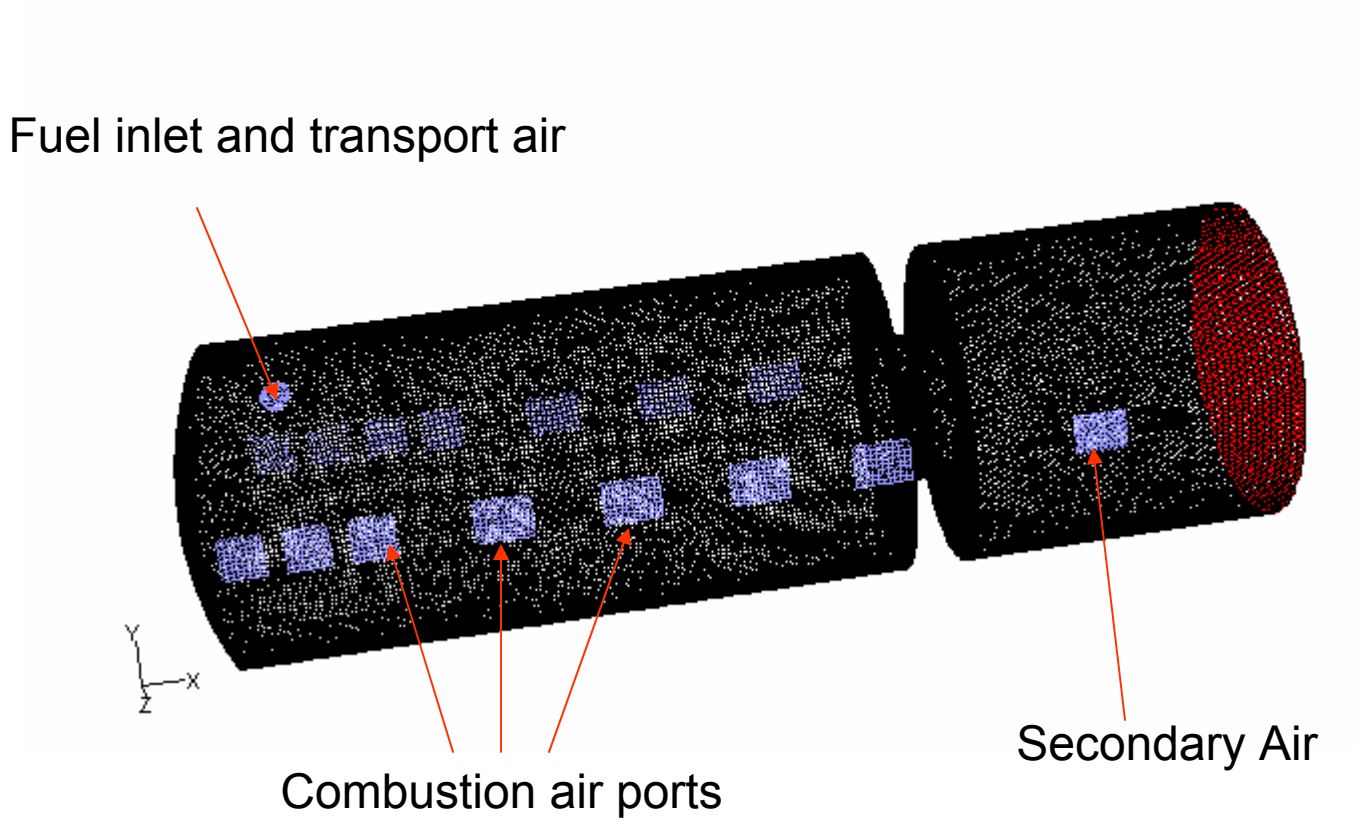
- Fuel NOx – Fuel may contain up to 6% (high resin wood dust)
- Thermal NOx – temperatures higher than 1800K will contribute due to high O, OH radical equilibrium concentration
- Prompt NOx – CH and NNH radicals
- Nitrous Oxide Mechanism



MacConnell wood burner



McConnell Wood burner grid



CRM approach

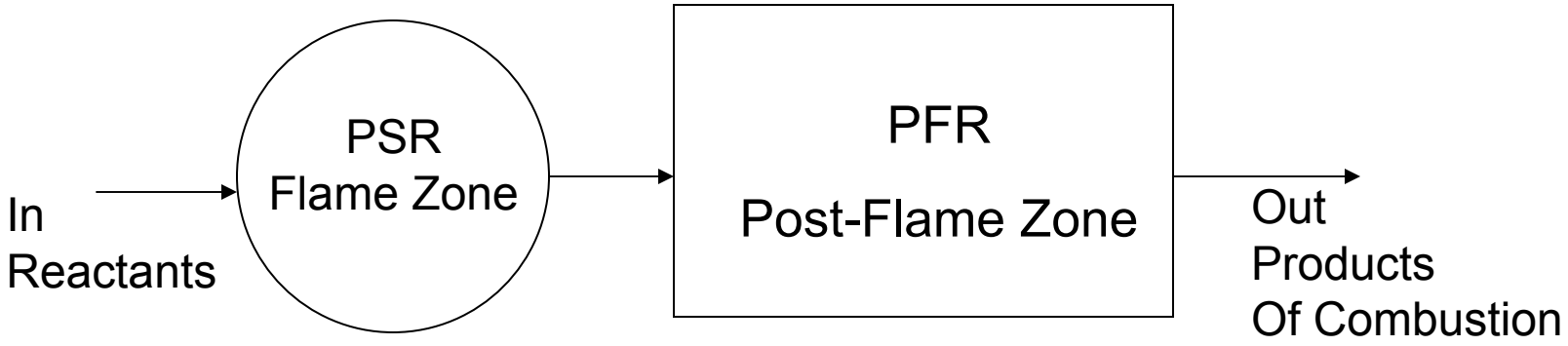
- Uses the arrangement of Perfectly Stirred Reactors (PSR) and Plug Flow Reactors (PFR)
- Detailed kinetic mechanism can be used
- Flow field information is required as input to the code – this information has to be obtained from the experiment or CFD simulation
- Turbulent parameters needed to estimate mixing times (lengths)

UW Chemical Reactor Model

- Solves the system of non-linear partial differential equations at stationary time step
- Jacobi-Newton (Diagonalized Newton-Raphson) scheme
- Initial guess values from adiabatic equilibrium for the given conditions

Generic Flame Model in CRN

Arrangement of PSR and PFR configuration can give a good representation chemical reactions in a flame

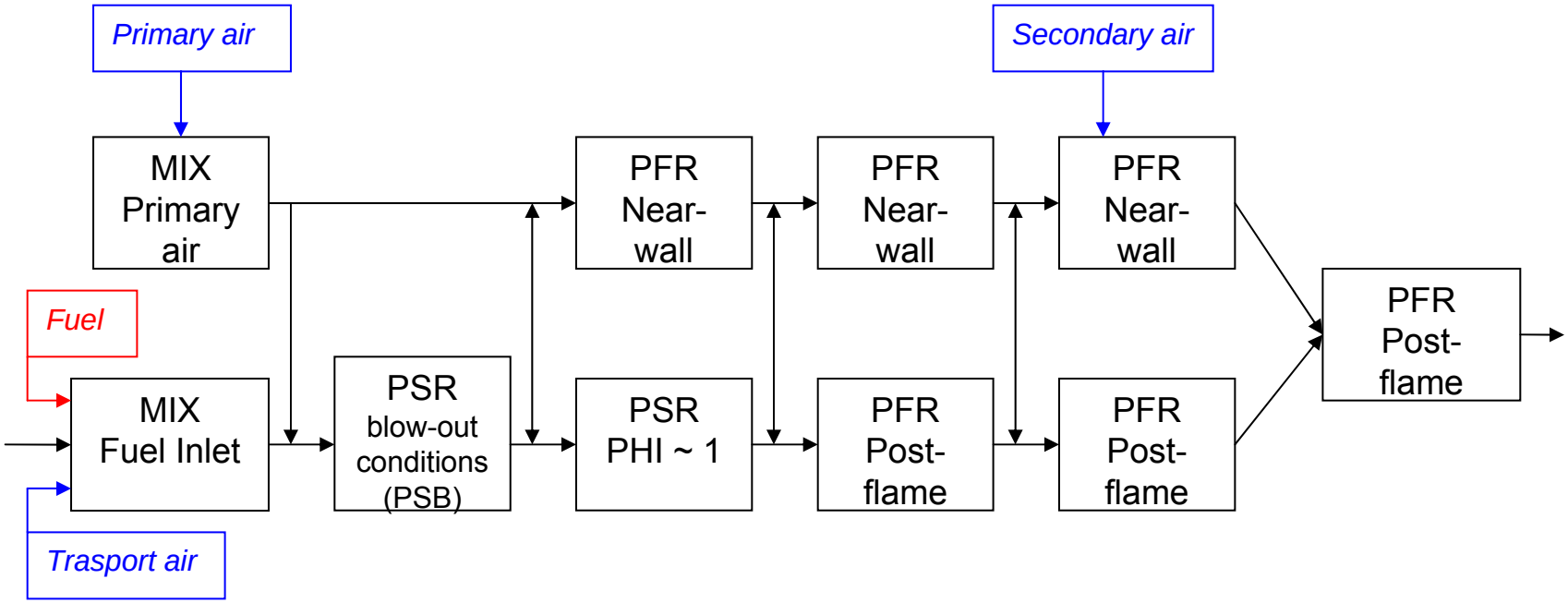


Often ore complicated models are needed to account for the complex flow field in the combustor

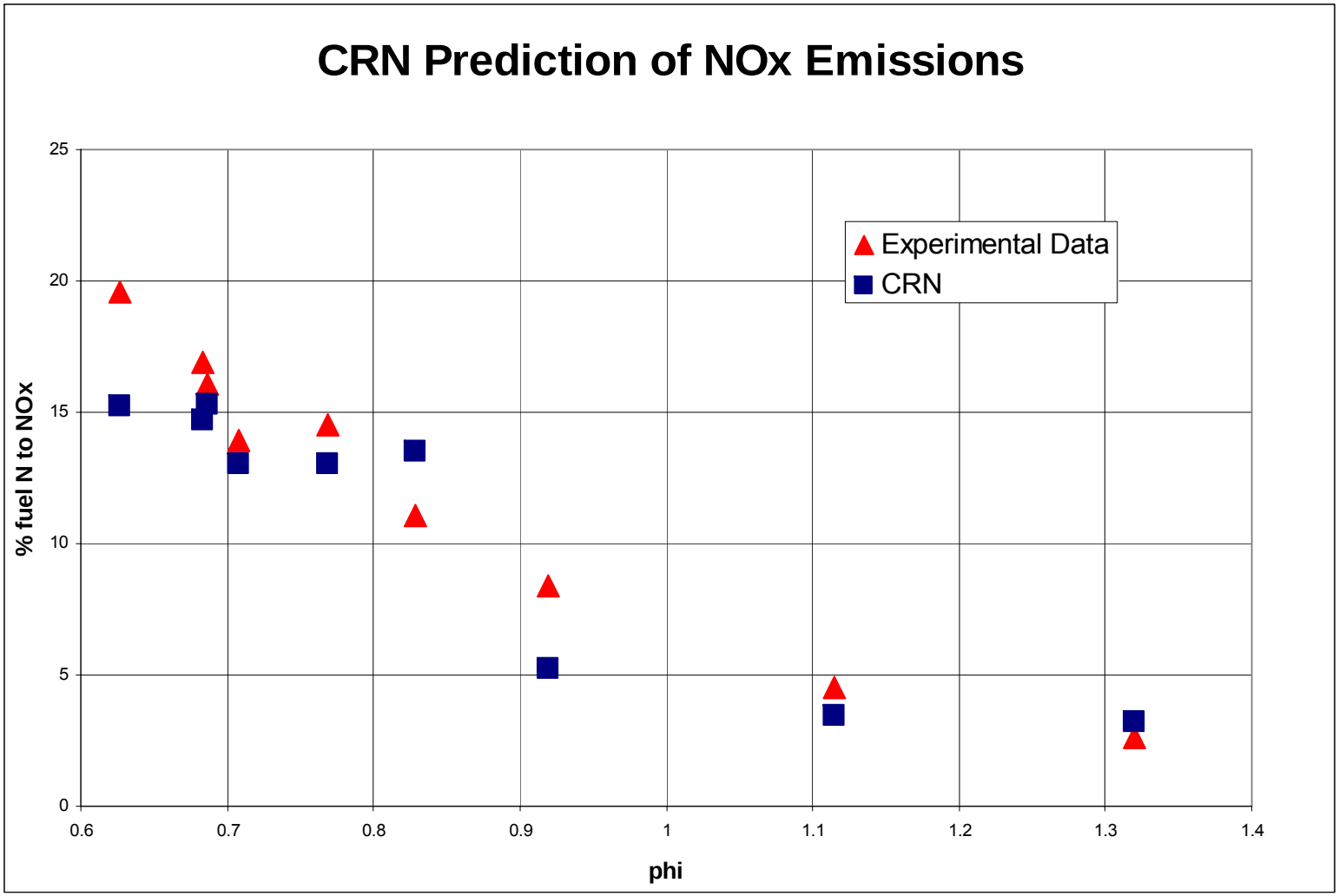
What CRM needs from CFD

- Flow field (flow rates and flow splits for the reactor elements)
- Temperature field (residence time in the reactor elements)
- Species concentrations: (type of the element and residence time)
- Turbulent information: A_{EBU}, k, ε, T`, $[Y_i]$`

Simplified Chemical Kinetic Model for UW Wood Dust Burner



Fuel Nitrogen Conversion to NOx



Future work

- Completing CFD modeling for UW wood dust burner with updated wood chemistry
- Developing reliable CRN for UW wood burner
- Completing CFD modeling for McConnell industrial wood dust burner using global chemistry and PDF methods
- Developing CRN for McConnell industrial wood dust burner

Zeldovich mechanism

- $O+N2 \rightarrow NO+N$
- $N+O2 \rightarrow NO+O$

Often the third reaction is added to the to the mechanism:

- $N+OH \rightarrow NO+H$

Nitrous oxide

- $O + N2 + M \leftrightarrow N2O + M$
- $N2O + H \rightarrow N2 + OH$
- $N2O + O \rightarrow N2 + O2$
- $N2O + O \rightarrow NO + NO$

- $N2O + H \leftrightarrow NH + NO$
- $O + H2 + M \leftrightarrow H2O + M$

NNH mechanism and CH mechanism

- **NNH mechanism**
- $NNH+O \rightarrow NH+NO$
- $NH+O2 \rightarrow NO+OH$
- $NH+O \rightarrow NO+H$
- **CH mechanism**
- $CH+N2 \rightarrow HCN+N$
- $C2+N2 \rightarrow 2\times CN$
- The N-atom, when colliding with diatomic oxygen follows the Zeldovich pathway:
- $N+OH \rightarrow NO+H$
- $N+O2 \rightarrow NO+O$
- Nitrogen oxide can be formed from HCN via the following reactions:
- $HCN+O \rightarrow NCO+H$
- $NCO+H \rightarrow NH+CO$
- $NH+(H, OH) \rightarrow N+(H2, H2O)$
- $N+OH \rightarrow NO+H$
- $N+O2 \rightarrow NO+O$
- $NH+O2 \rightarrow NO+OH$
- $NH+O \rightarrow NO+H$

Fuel NOx formation and reduction