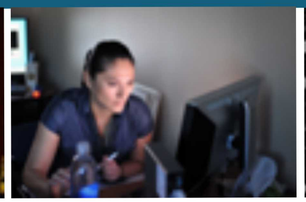
This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

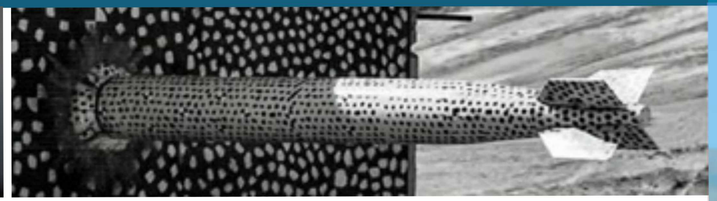
SAND2019-12302C

Sandia National Laboratories

CONSTRUCTING AND ACCESSING TABULATED CHEMISTRY FOR FIRE SCENARIOS

SAND#





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U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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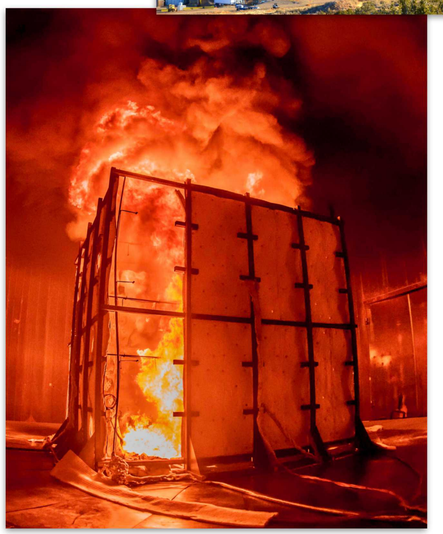
10/14/2019

Non-adiabatic flamelet chemistry tabulation with LES/RANS enables simulation of sooting, turbulent fires at engineering scales of interest

- Tabulation techniques aid in making fire simulations computationally feasible
- We were seeing over-predictions in soot and unstable simulations in some cases…
- Want to explore different ways of constructing/accessing chemistry tables

SIERRA/Fuego

SNL's Thermal Test Complex



<u>How chemistry tabulation works:</u>

Get data
- DNS
- ODT
- Flamelet
- Experiments

→ **Tabulate properties** (temperature, fluid properties, soot source terms…) over reduced set of coordinates

→ **Fuego (CFD): transport reduced coordinates**

<u>Options for the reduced set of coordinates:</u> (for strongly sooting and radiating fires)

<u>1 dimension:</u> mixture fraction (Z)
Equilibrium, Burke-Schumann

composition

<u>2 dimensions:</u> Z, scalar dissipation rate (χ)
Steady Laminar Flamelet Model (SLFM)

composition, strain

<u>3 dimensions:</u> Z, χ, enthalpy (h) or enthalpy deficit ($\gamma = h - h_{ad}$)
Non-adiabatic Flamelet Model

composition, strain, heat loss

Non-adiabatic flamelet chemistry tabulation with LES/RANS enables simulation of sooting, turbulent fires at engineering scales of interest

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composition

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Equilibrium, Burke-Schumann

composition, strain

2 dimensions: Z, scalar dissipation rate (χ)
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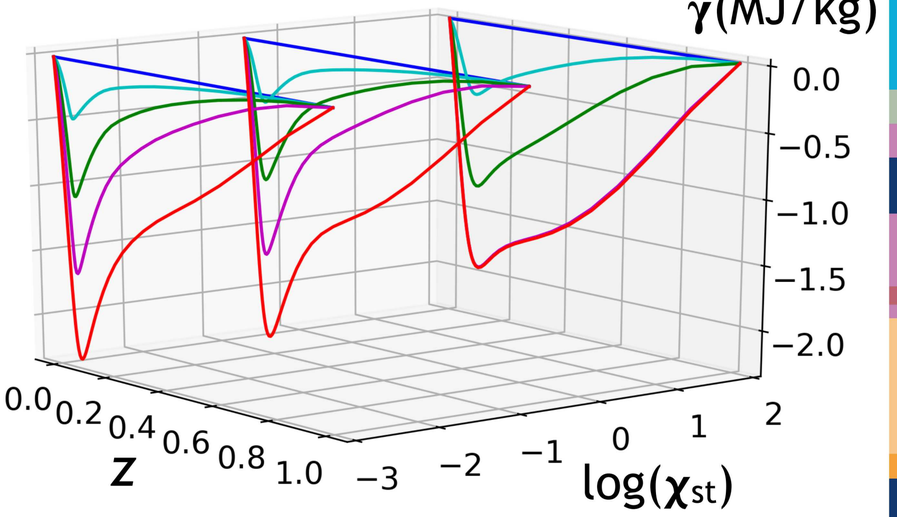
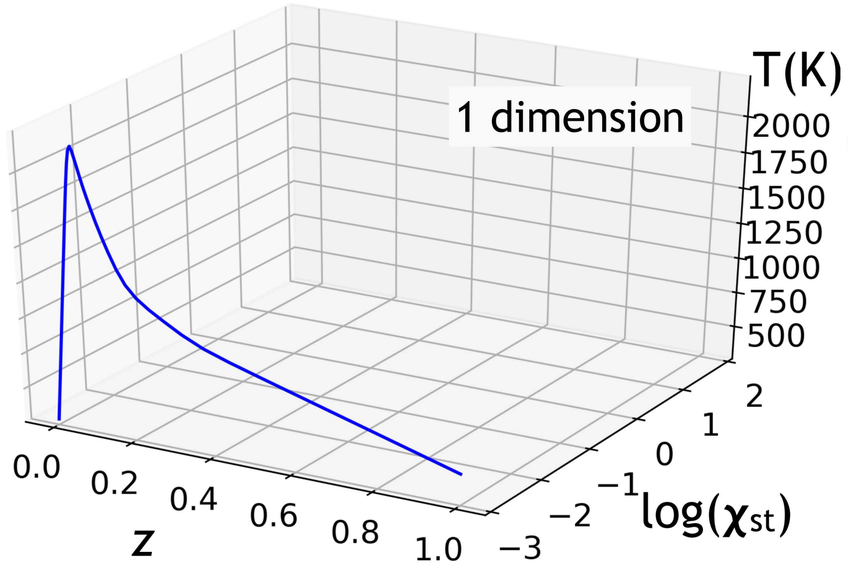
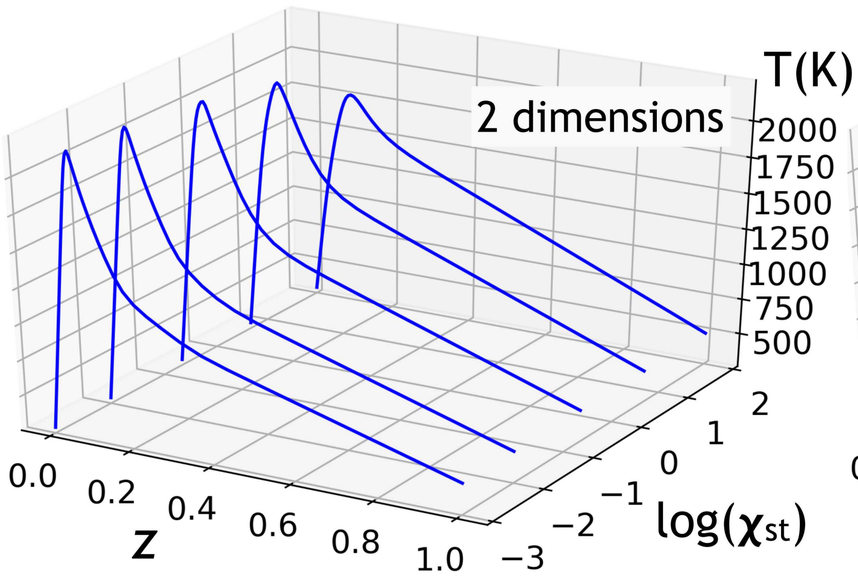
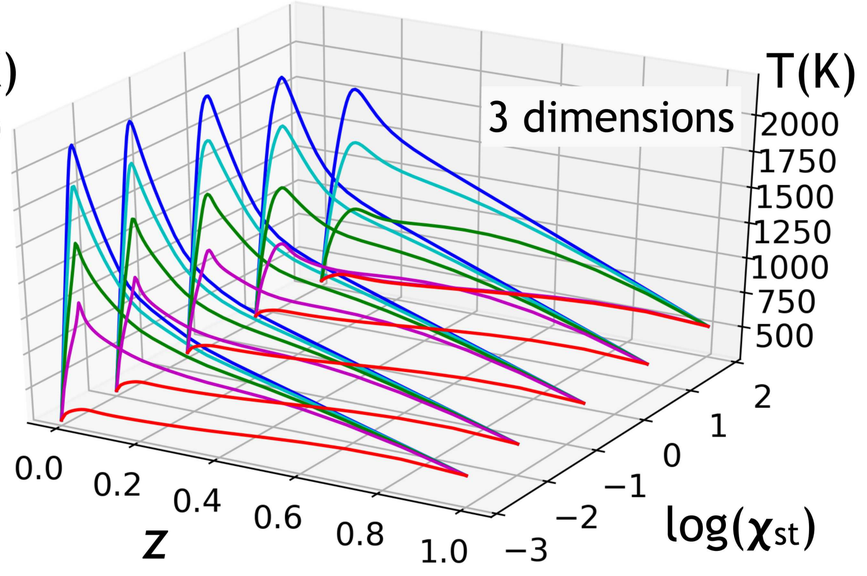
Non-adiabatic Flamelet Model





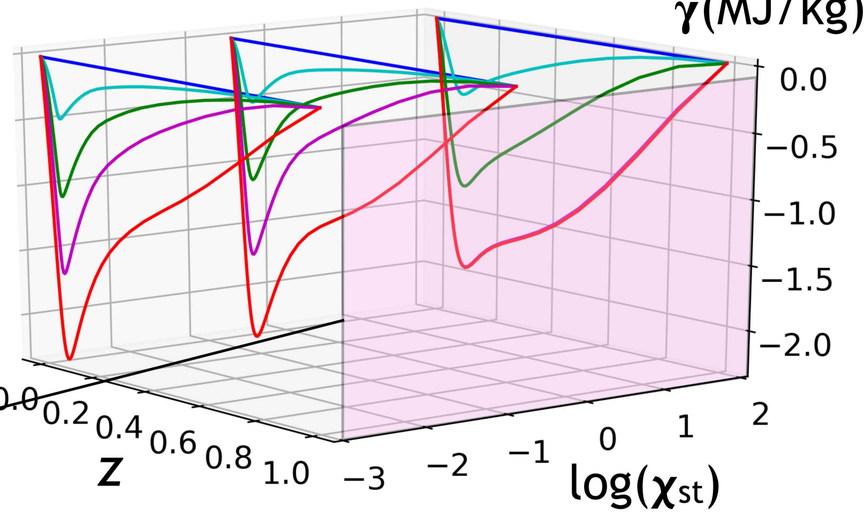




Unstructured non-adiabatic flamelet data over (Z, χ, γ)

Interpolation onto structured grid (for speed)

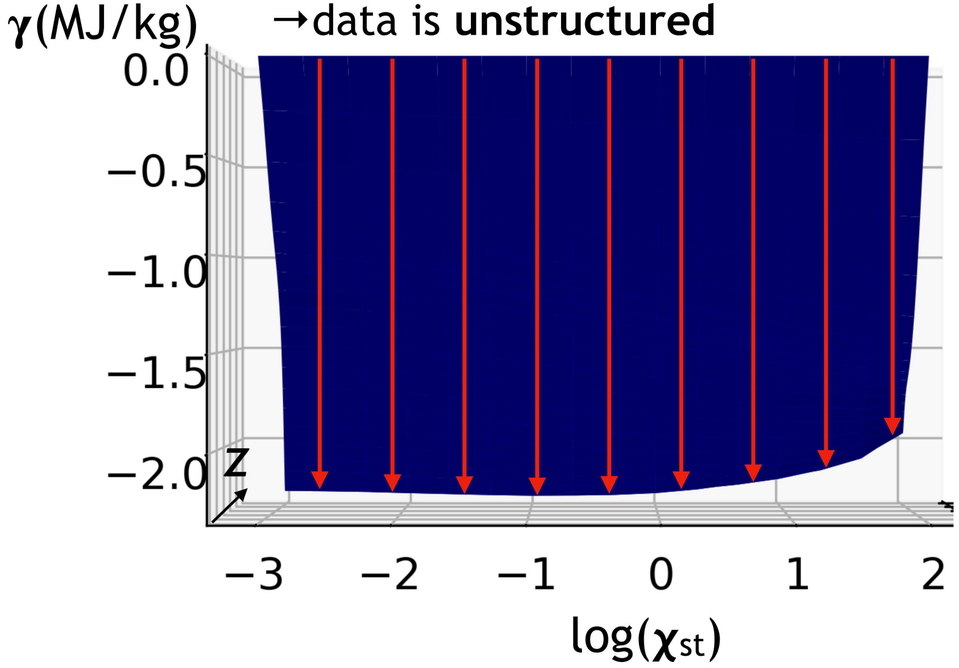
Structured Table

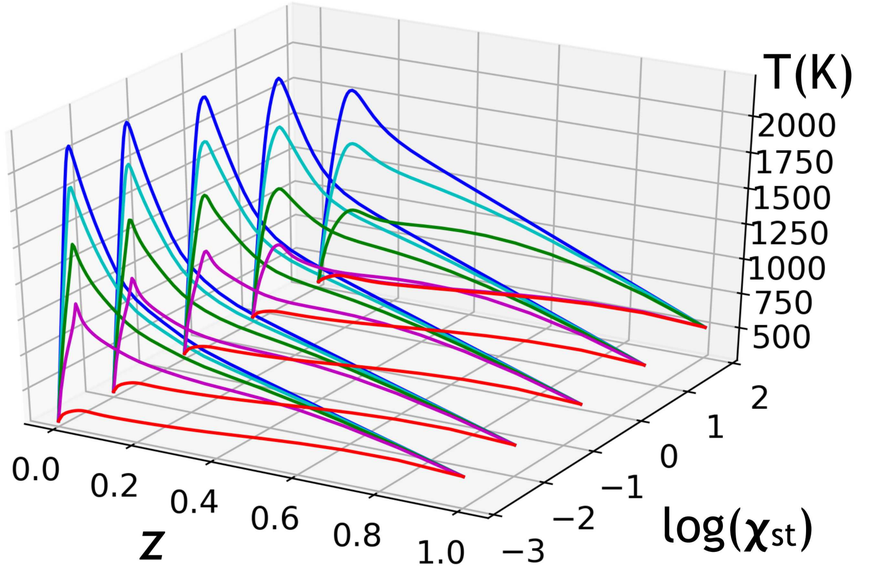


Viewing this plane

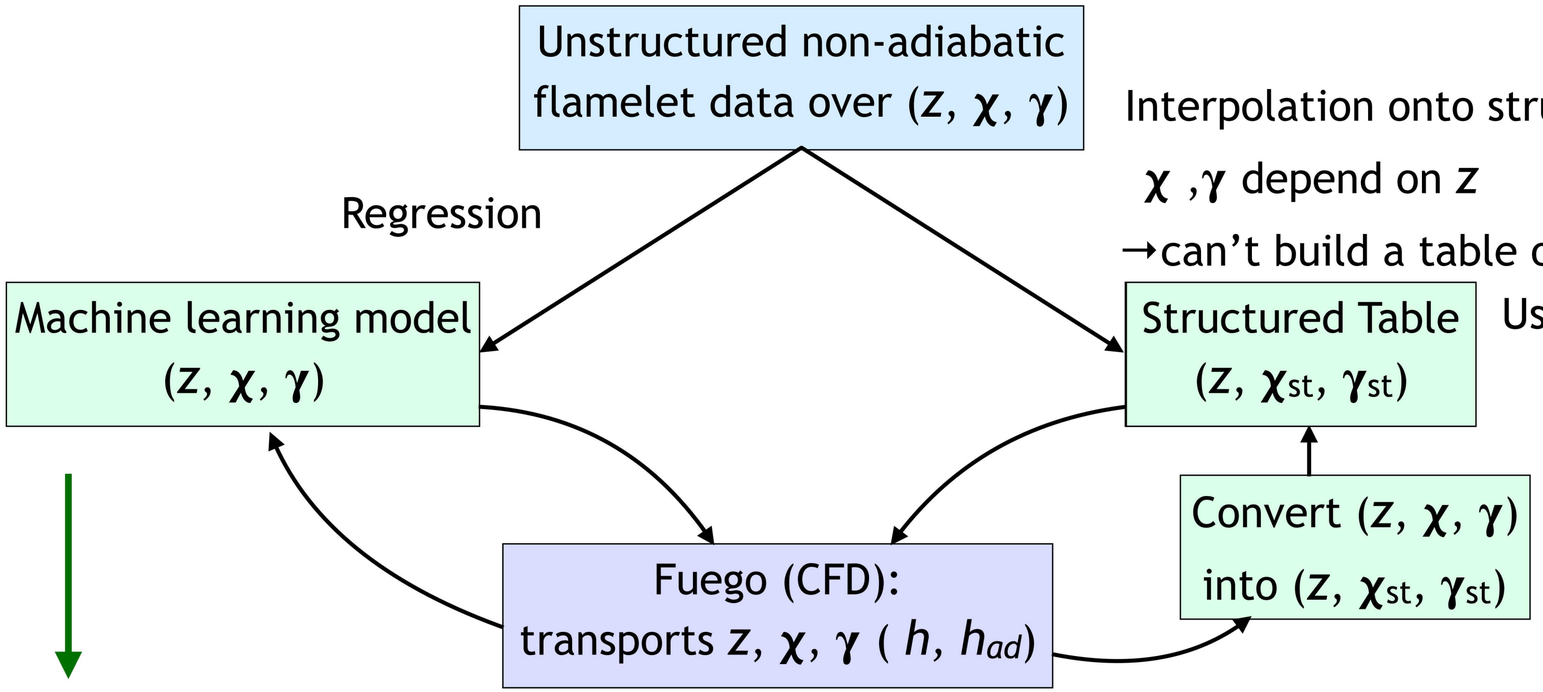
Different ranges in γ for each χ_{st}

→data is **unstructured**





There are challenges in constructing and accessing tabulated/modeled chemistry



Interpolation onto structured grid (for speed)

χ ,γ depend on Z

→can't build a table over (Z, χ, γ) directly

Use reference (stoichiometric) values

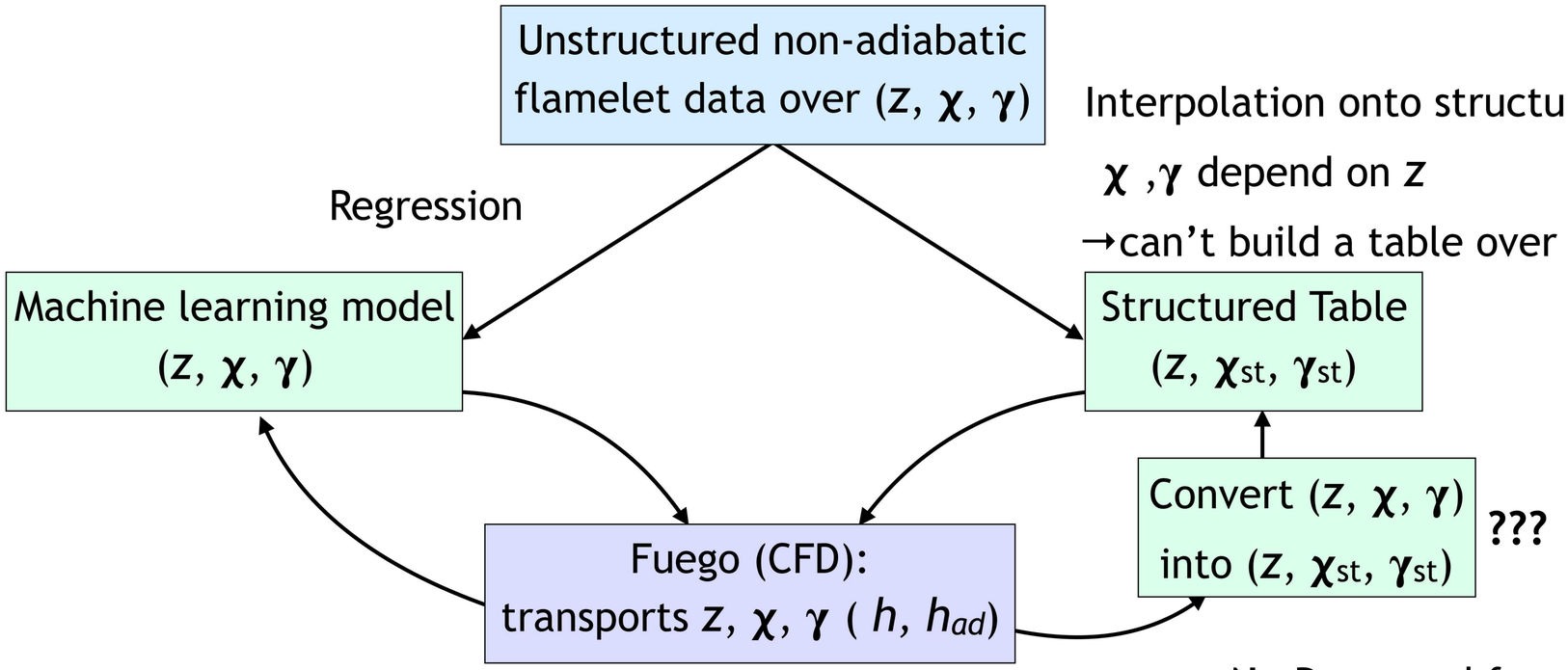
Advantages:

- Simulation variables are the model inputs
- Smaller memory requirements
- Higher dimensional models

Disadvantages:

- Challenges associated with finding "optimal" networks
- Difficult to determine error bounds
- More expensive to query a neural network than interpolant

There are challenges in constructing and accessing tabulated/modeled chemistry



Interpolation onto structured grid (for speed)

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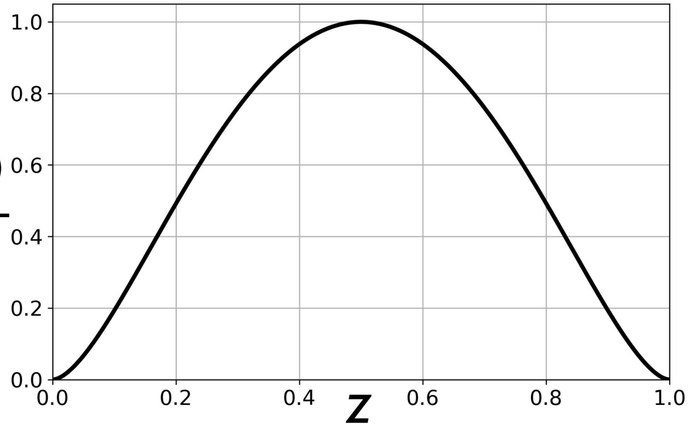
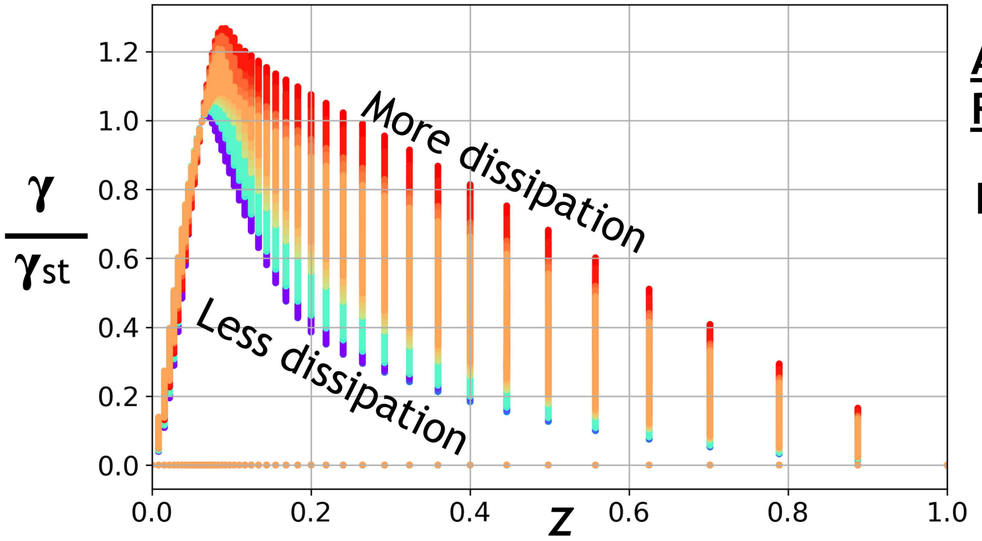
Presumed form for χ

$$F_\chi(Z) = \frac{\chi F_\chi(Z_{st})}{\chi_{st}}$$



No Presumed form for γ



Consistent Enthalpy Reconstruction (CER)

- Find the correct γ_{st} in the table using a (Newton-based) root finding method

$$\gamma_{\text{table}}(Z, \chi_{st}, \gamma_{st}) = \gamma_{\text{CFD}}$$

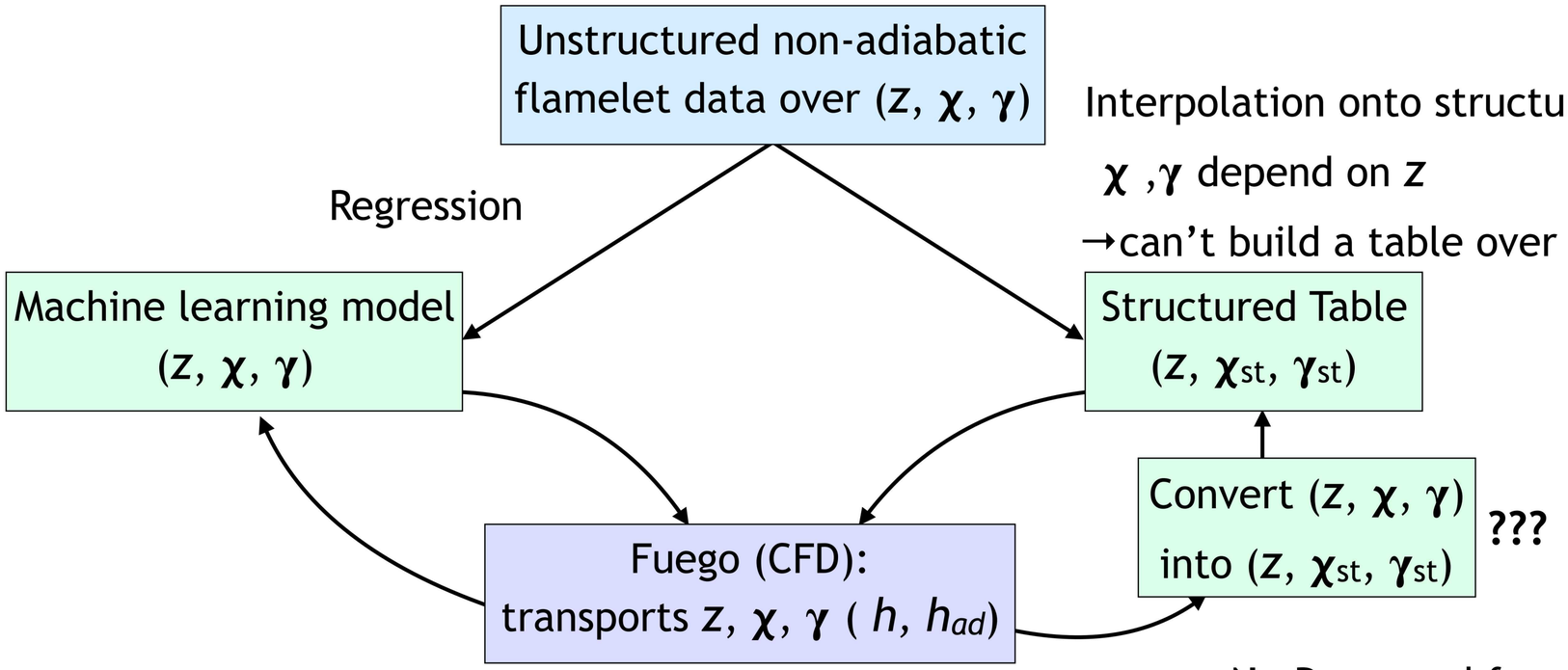
- Requires have γ in the property table
- More accurate
- More expensive

Approximate Enthalpy Reconstruction (AER)

Presume a functional form for $\gamma(Z;\gamma_{st})$

$$\gamma = F_\gamma(Z)\gamma_{st}$$

There are challenges in constructing and accessing tabulated/modeled chemistry



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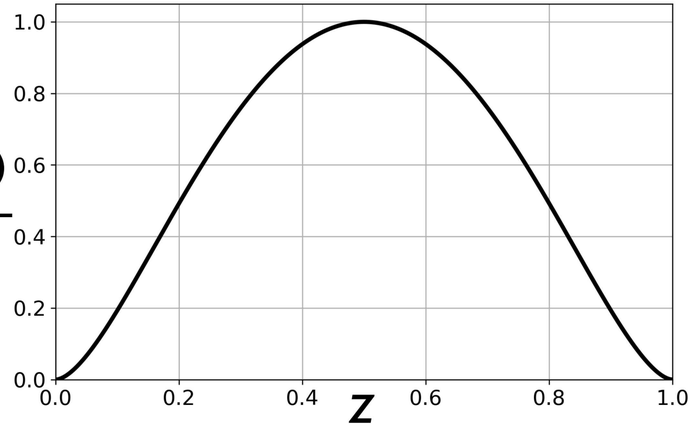

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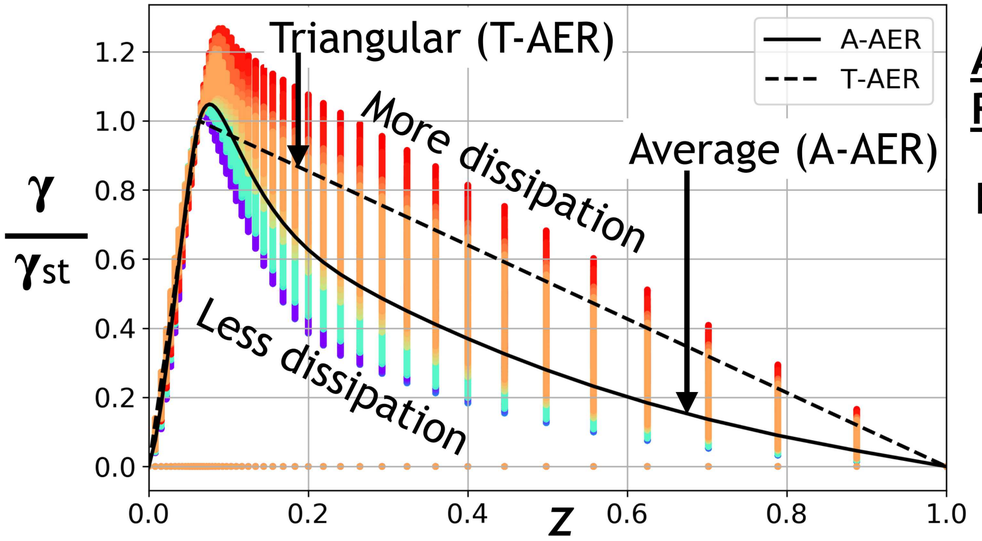

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Approximate Enthalpy Reconstruction (AER)

Presume a functional form for $\gamma(Z;\gamma_{st})$

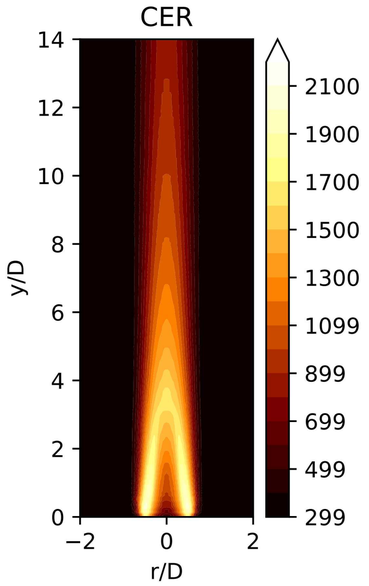
$$\gamma = F_\gamma(Z)\gamma_{st}$$

The AER methods lead to substantial errors in scenarios with high heat loss

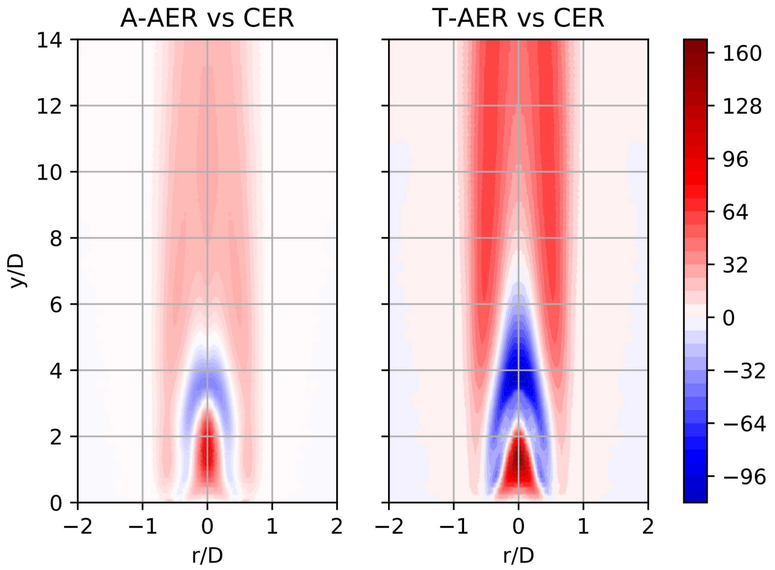
Ethylene laminar coflow, sooting jet steady state
- 11 mm diameter (D) jet
- Simple radiation model ($4\sigma T_{\text{ref}}^4$)
- 2-equation soot model

- Non-linear trend in temperature errors moving up centerline
  - Largest errors in rich regions near inlet, O(100 K)
- Persistent errors (errors remain in steady state)
- 10% over-prediction in soot for T-AER than CER
  - Emitting more smoke
  - 2% over-prediction in soot for A-AER than CER
- Overall less error in A-AER method compared to T-AER
- Little to no errors in pure streams and near adiabatic
- Observed similar trends in the errors for heptane and for a participating media radiation model
- The CER simulation was 2x slower than the T-AER simulation
  - Currently performing Newton solve for every property table
  - Optimal redesign should result in only 5-10% more time for CER

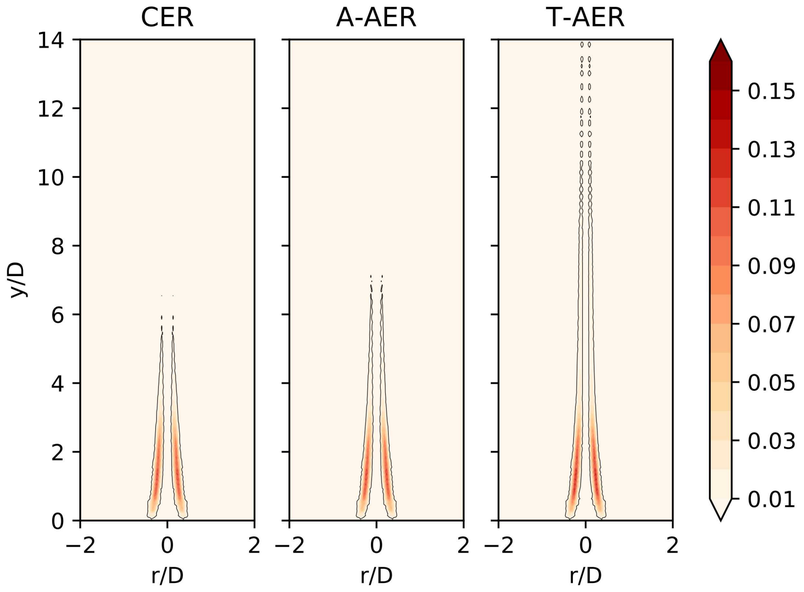
temperature (K)



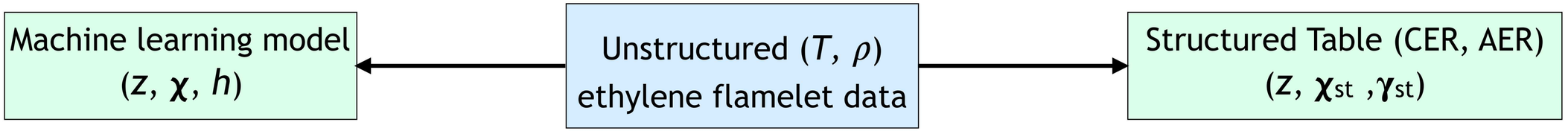
temperature error (K)



soot mass fraction

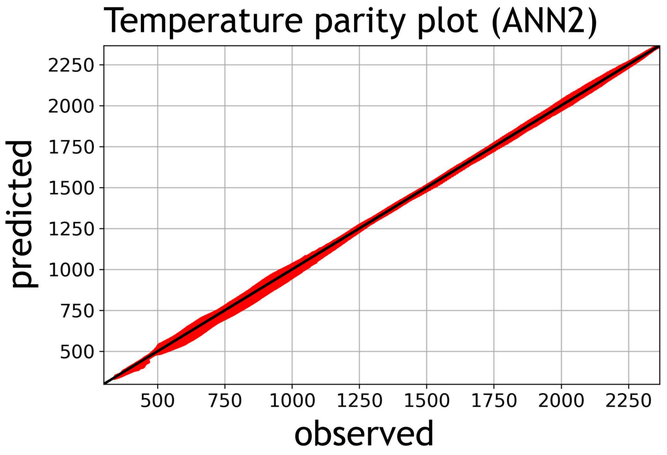


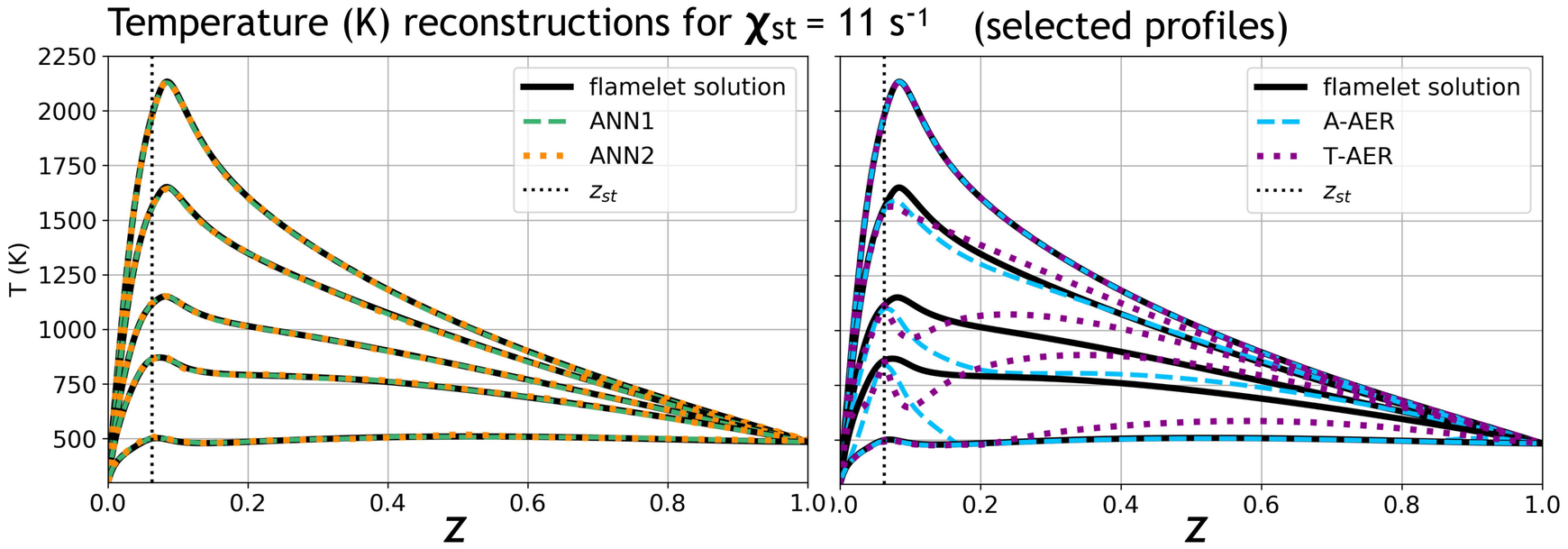
Machine learning is a promising alternative to structured chemistry tabulation



ANN1: trained on whole unstructured flamelet dataset

ANN2: trained on every other point in dataset



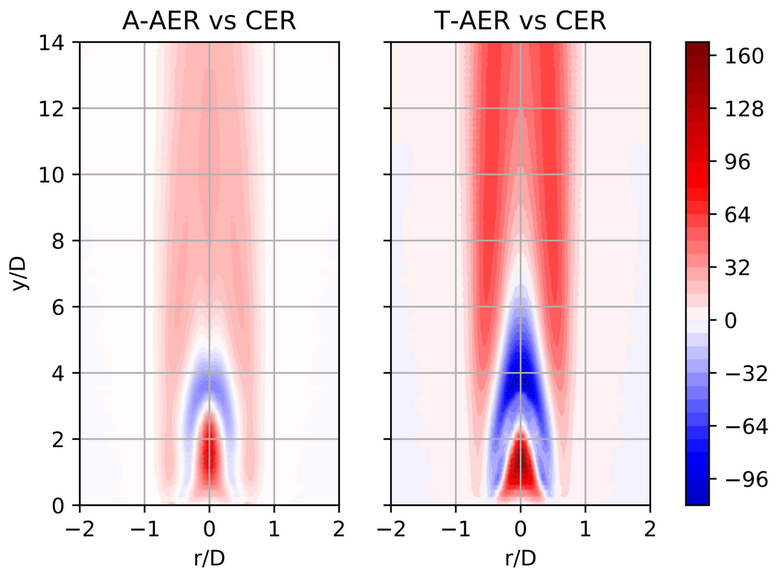


- The ANNs have **more** error than CER, but **less** error than AER methods
- ANNs trained on coarsened datasets show good accuracy
- ANNs are only 1 MB compared to 28 MB for a structured table build using (T, ρ, γ)
  - Structured tables can reach around a few GB large for actual turbulent simulations

Conclusions

- AER methods lead to substantial errors in scenarios with high heat loss
  - Up to 10% over-prediction in steady state soot mass fraction for T-AER compared to CER for the laminar sooting ethylene jet flame studied here
  - Improved approximations can be constructed (A-AER), but are not generally accurate
- The CER method offers more accuracy for high heat loss scenarios
  - Should only be 5-10% more expensive than AER when optimized
- Replacing structured tabulation with ANNs shows promise
  - May dramatically reduce memory ~30x
  - May enable higher dimensional models
  - Shows accuracy between AER and CER

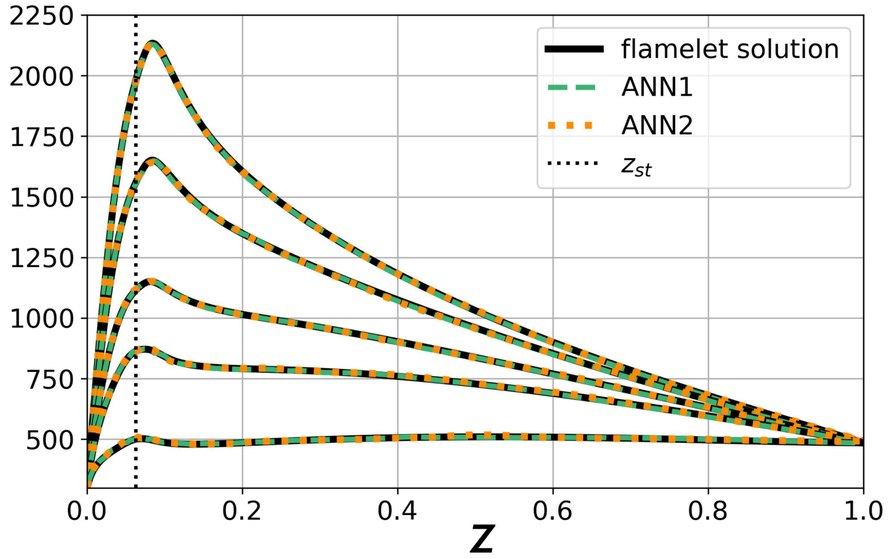
temperature error (K)



Future Work

- Explore optimal ANNs and run *in situ* for flame calculations
- Study optimized interpolants to improve CER
- Perform more detailed cost analysis between CER and ANN approaches
- Test in turbulent simulations at scale

Temperature (K) reconstructions for χ_{st} = 11 s^{-1}



Acknowledgements

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John C. Hewson	Research Staff (SNL)
James C. Sutherland	Professor of Chemical Engineering (Univ. Of Utah)

Supplemental Slides

A transient non-adiabatic flamelet approach enables a large enough range of states accessed in sooting, turbulent fire simulations

$$\frac{\partial Y_i}{\partial t} = \frac{\chi}{2}\frac{\partial^2 Y_i}{\partial Z^2} + \frac{\omega_i}{\rho}$$

$$\frac{\partial T}{\partial t} = \frac{\chi}{2}\frac{\partial^2 T}{\partial Z^2} - \frac{1}{\rho c_p}\sum_{i=1}^{n}\omega_i h_i - \frac{H\chi_{\max}}{\rho c_p}\frac{1-Z_{\mathrm{st}}}{Z_{\mathrm{st}}}\frac{T-T_\infty}{T_{\max}-T_\infty}$$

adiabatic formulation

non-adiabatic formulation

provide cooling for flames with higher mixing rates

related to heat released, hydrocarbons $O(10^7\,\mathrm{J/m^3})$

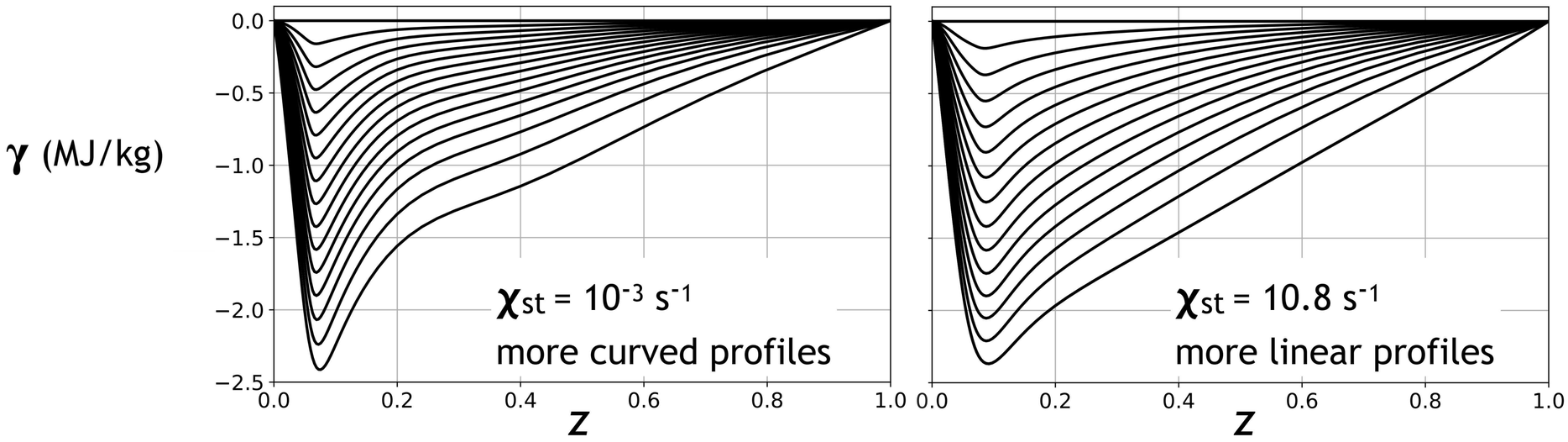
more uniform heat loss during transient heat-loss driven extinction

linear background temperature

avoid increase in stoichiometric enthalpy from reactant mixing

Integrate equations until T comes within 5% of max(T_∞)

Solved using Spitfire
(soon to be open-sourced)

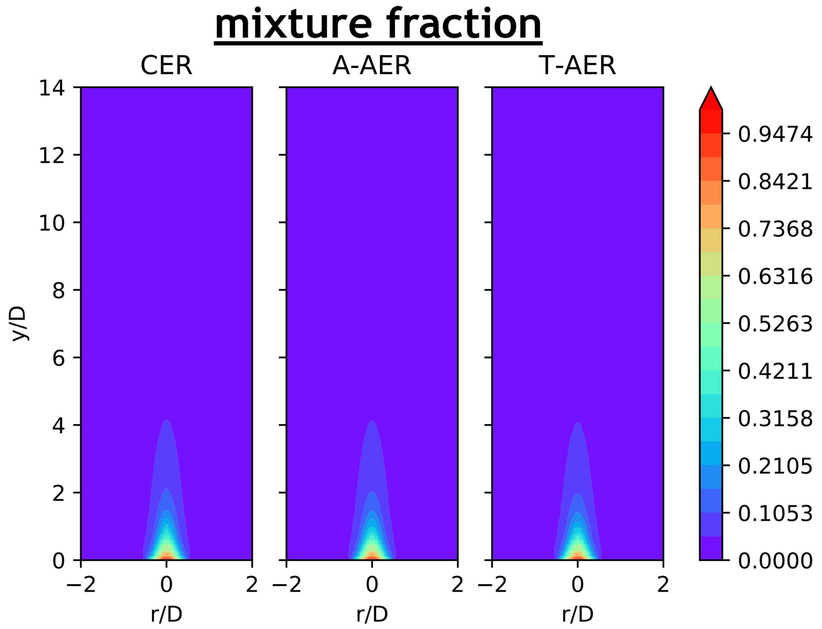


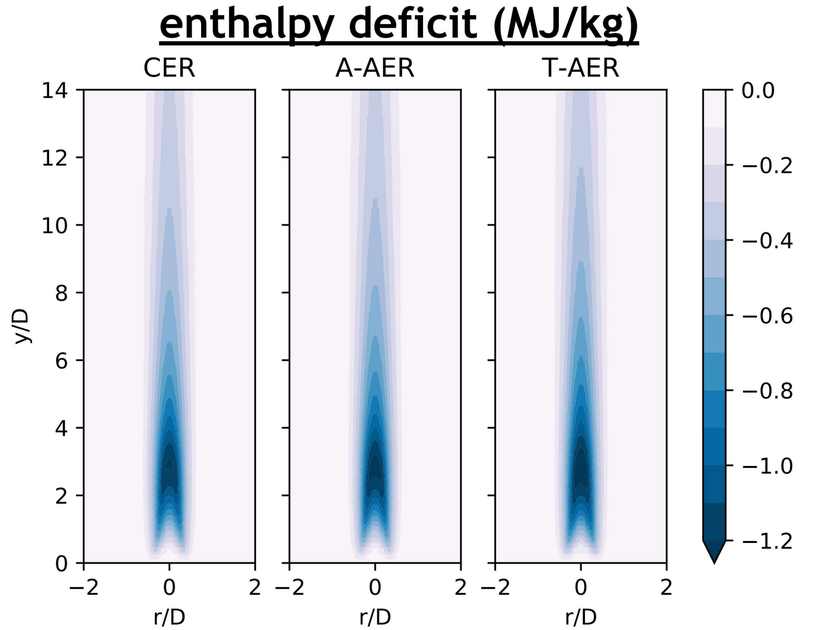
Qualitative differences are observed between the methods for a steady laminar ethylene sooting jet flame

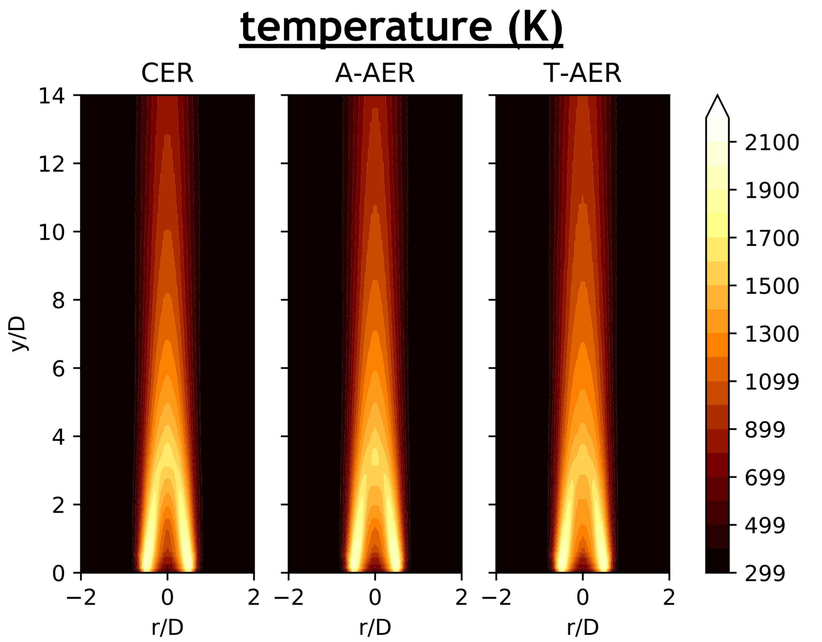
Steady state profiles for an ethylene laminar coflow, sooting jet with 11 mm diameter (D)

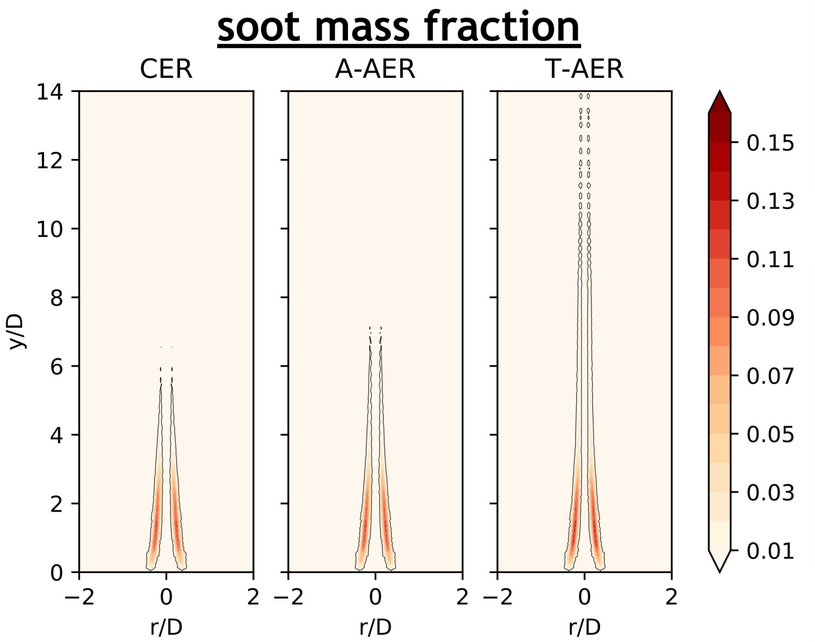
Simple radiation $(4\sigma T_{\text{ref}}^4)$

- Largest qualitative difference in soot mass fraction
- T-AER has the largest areas of heat loss for a given contour





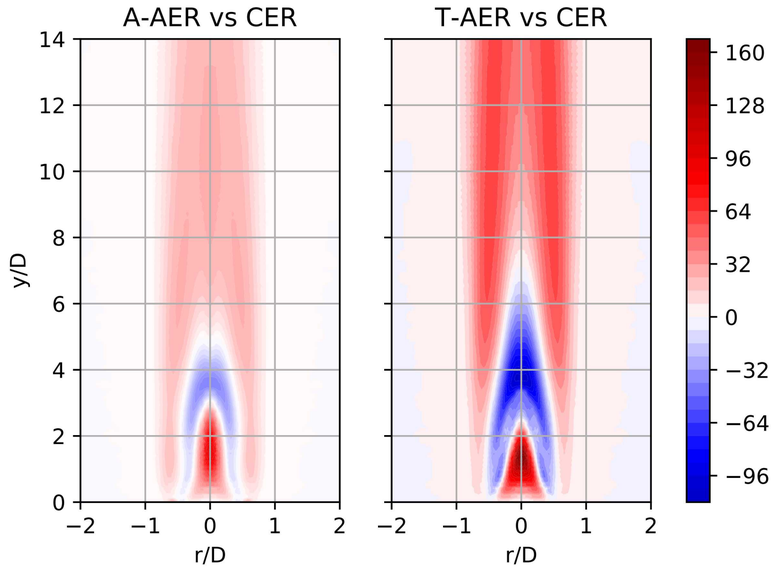




AER methods have less error in scenarios with less heat loss

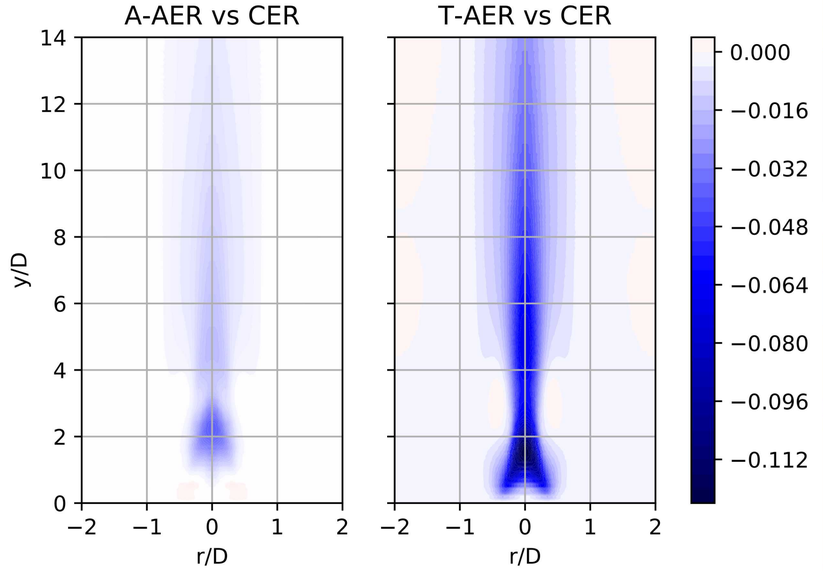
Computed from table queries

temperature error (K)

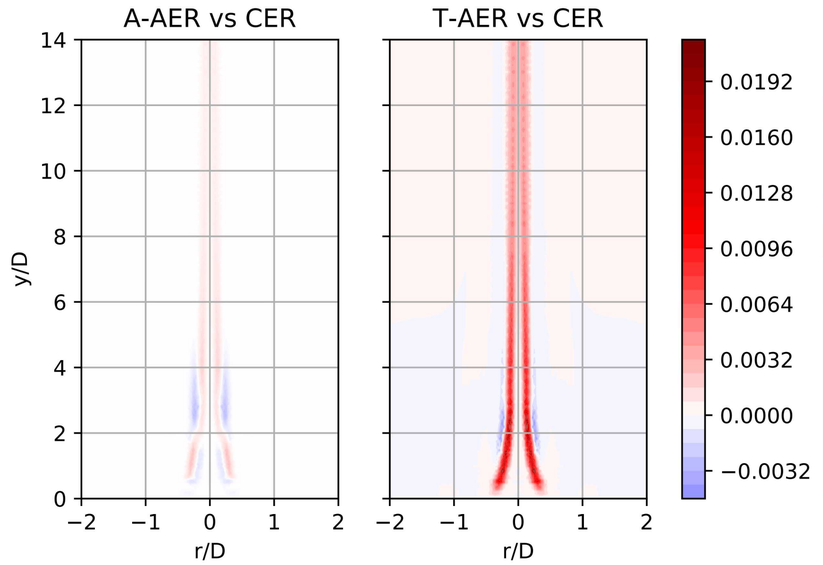


Transported in simulation

enthalpy deficit error (MJ/kg)



soot mass fraction error



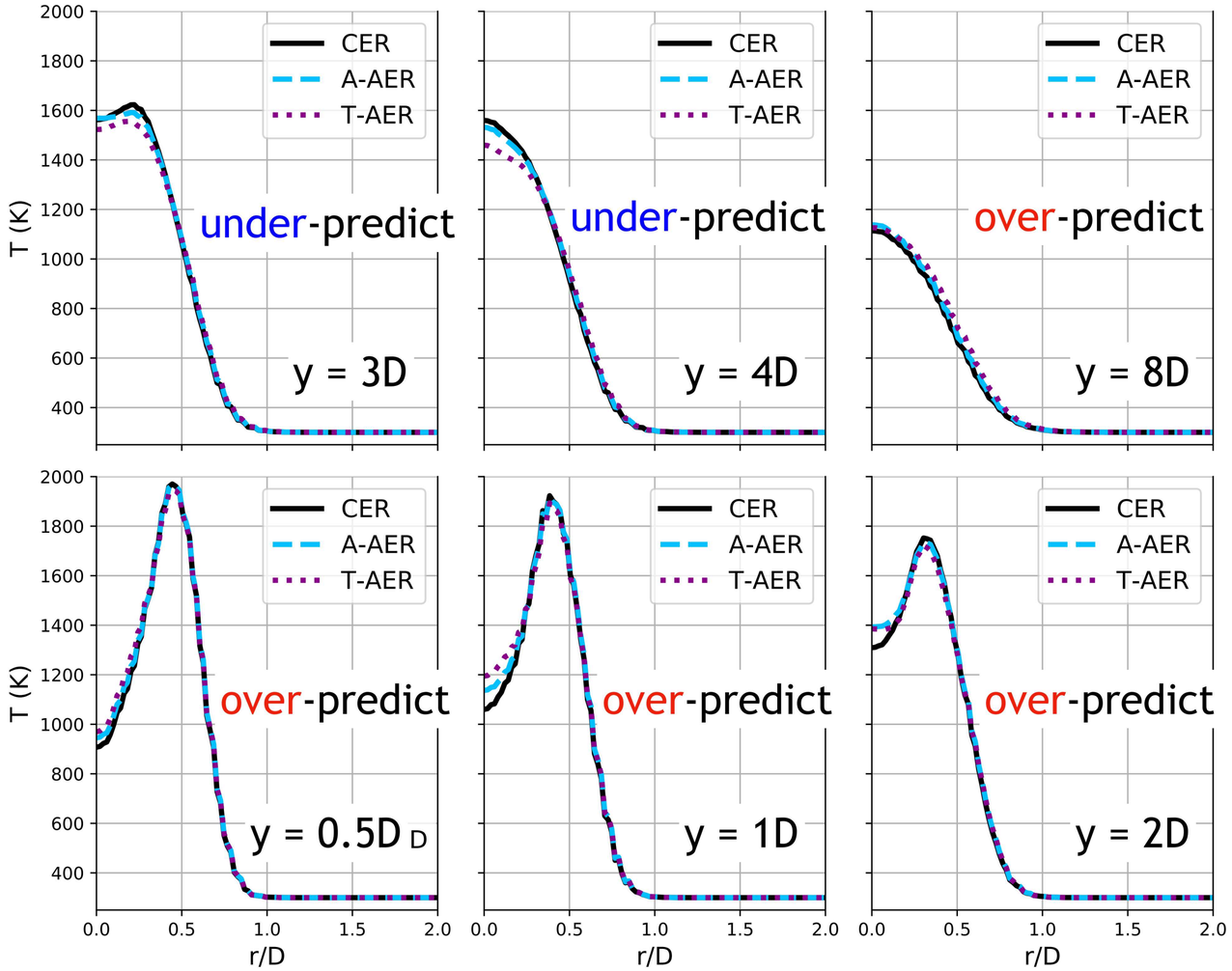
Qualitative differences are observed between the methods for a steady laminar ethylene sooting jet flame

Steady state profiles for an ethylene laminar coflow, sooting jet with 11 mm diameter (D)

Simple radiation $(4\sigma T_{\text{ref}}^4)$

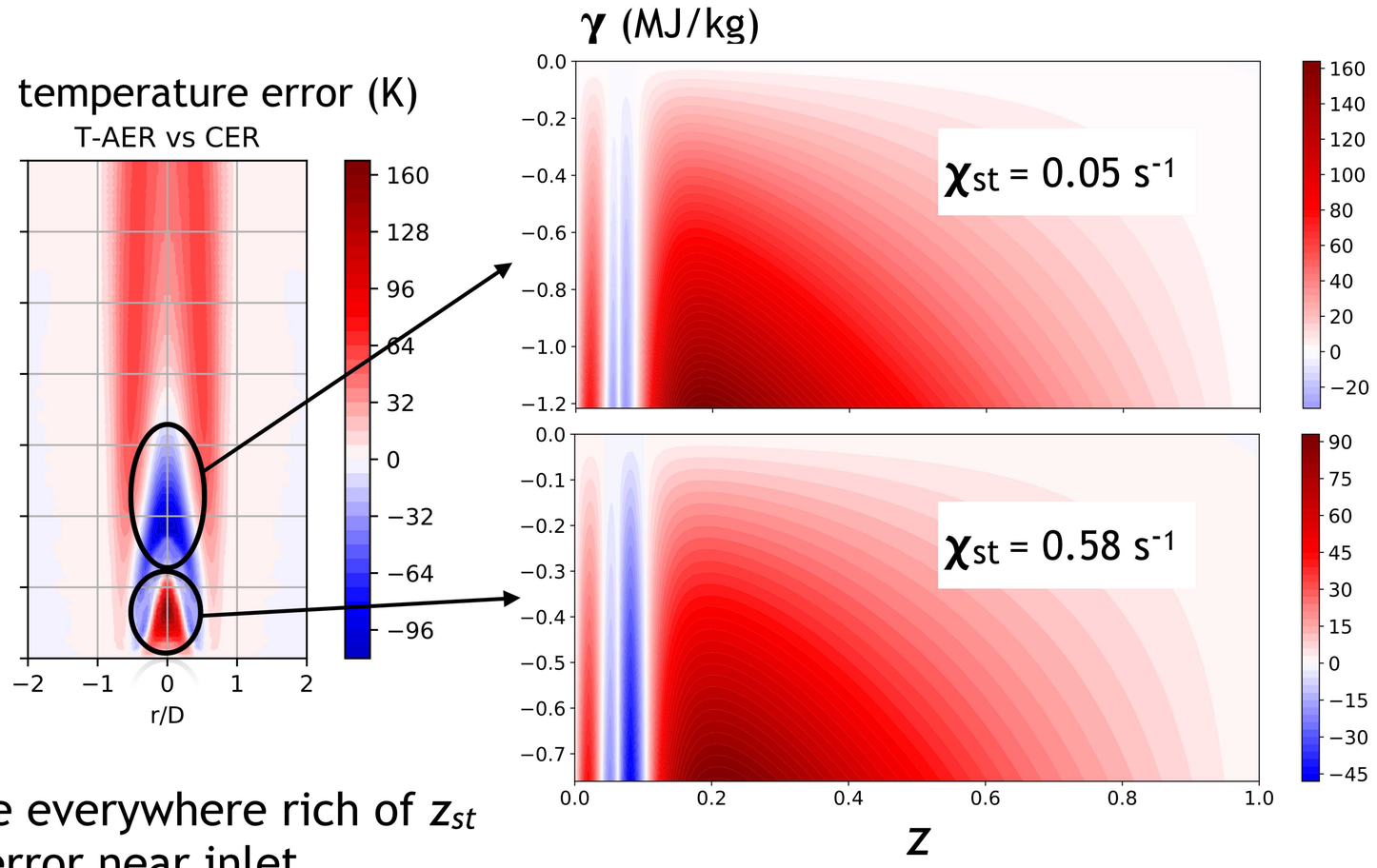
- A-AER results are closer to CER than T-AER results
- AER methods show a non-linear pattern of over-under-predictions in temperature moving up the domain at the centerline

temperature (K) at different heights in the flame



We can explain errors in the steady state profiles through *a priori* error analysis

Under-predicting temperature around z_{st}
Smaller magnitude of error in this region compared to rich regions at 0.58 s^{-1}

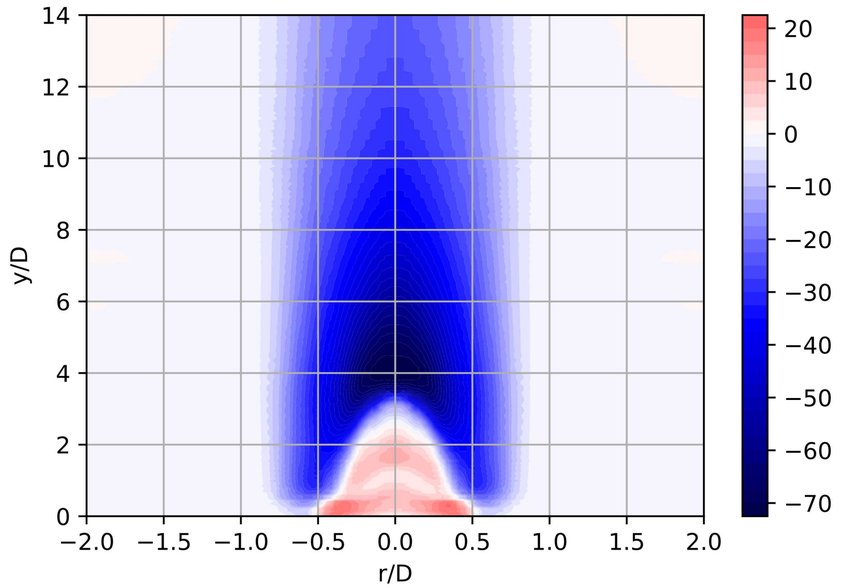


Over-predicting temperature everywhere rich of z_{st}
Matches observations for T error near inlet

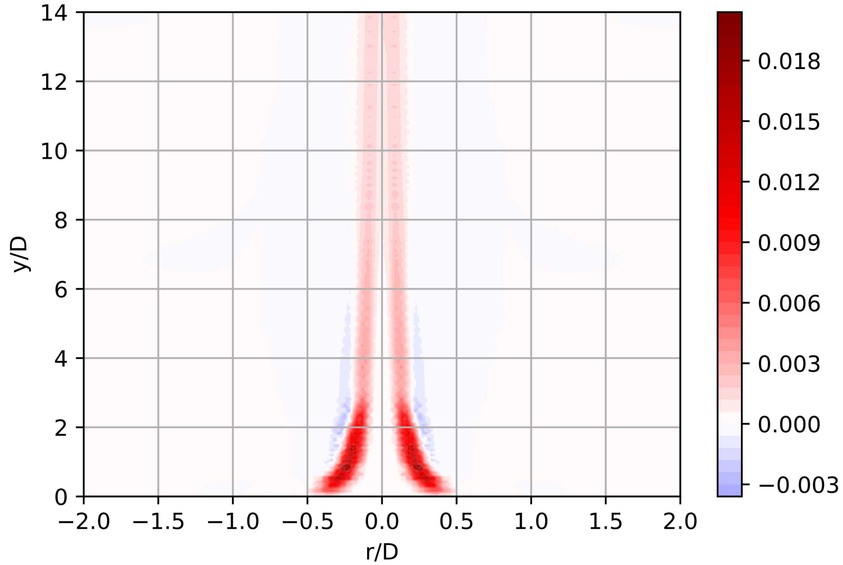
The analysis remains applicable for radiation modeled with PMR

participating media radiation (PMR) - simple radiation for CER

Temperature difference (K)



Soot mass fraction difference

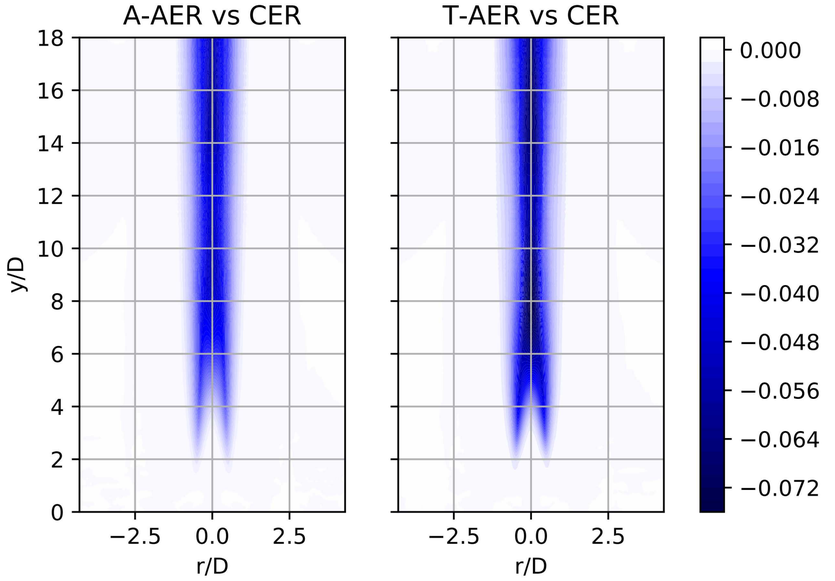


- Near the inlet, the temperature is higher for PMR than SR, which corresponds to a larger soot mass fraction
- At most a 5% difference in temperature, but an 11% higher maximum observed soot mass fraction for PMR compared to simple radiation
  - any differences in temperature can be amplified in the soot production due to sensitivities
  - soot production more coupled to PMR
- PMR changed the overall quantities of the steady state properties compared to simple radiation, but did not change the relative differences between the CER, T-AER, and A-AER

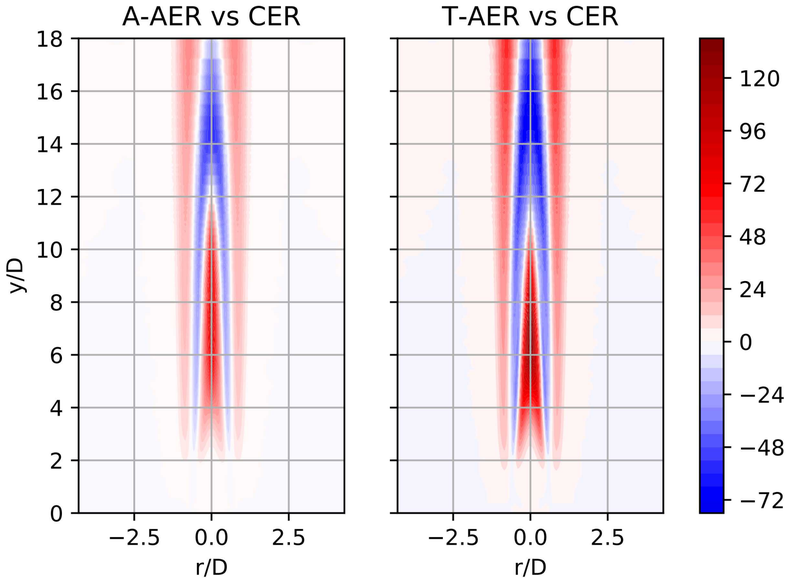
The analysis remains applicable for heptane

- See same trends in results as saw with ethylene
- However, with heptane there is only about a 5% over-prediction of the maximum soot mass fraction by T-AER compared to CER
- The heptane case also has less heat loss overall compared to ethylene
  - AER methods have less error in scenarios with less heat loss
  - have the benefit of being less expensive in these scenarios

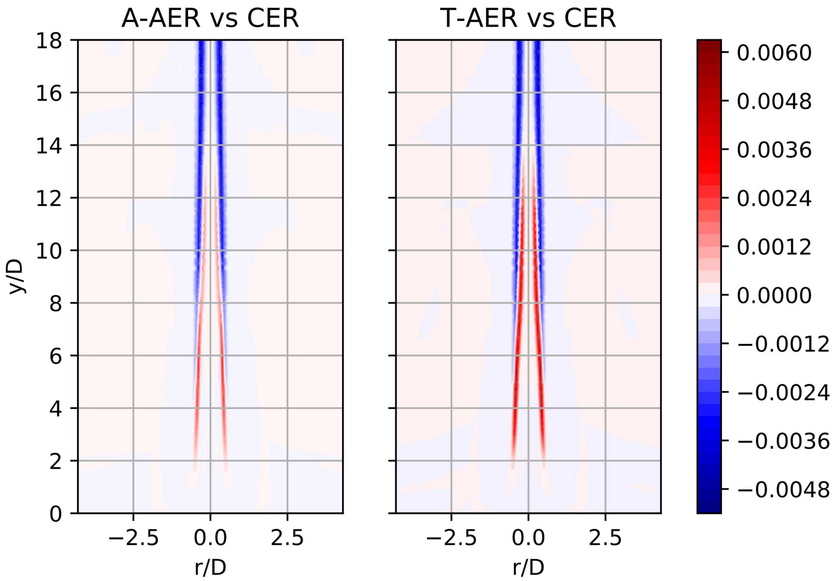
enthalpy deficit error (MJ/kg)



temperature error (K)



soot mass fraction error



The equations we solve

- Thermochemical states are typically calculated using the steady laminar flamelet model (SLFM)

$$\frac{\partial Y_i}{\partial t} = \frac{\chi}{2}\frac{\partial^2 Y_i}{\partial Z^2} + \frac{\omega_i}{\rho}$$

$$\frac{\partial T}{\partial t} = \underbrace{-\frac{1}{\rho c_p}\sum_{i=1}^{n}\omega_i h_i + \frac{\chi}{2}\frac{\partial^2 T}{\partial Z^2}}_{\text{classical flamelet equations}} + \underbrace{\frac{\chi}{2}\frac{1}{c_p}\frac{\partial T}{\partial Z}\frac{\partial c_p}{\partial Z}}_{\text{variable } c_p} + \underbrace{\frac{\chi}{2}\frac{\partial T}{\partial Z}\sum_{i=1}^{n}\frac{c_{p,i}}{c_p}\frac{\partial Y_i}{\partial Z}}_{\text{distinct } c_{p,i}}$$