Advanced Model Development for Large Eddy Simulation of Oxy-Combustion and Supercritical CO$_2$ Power Cycles

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Project objective

- Development and validation of predictive models for treatment of direct sCO$_2$ power cycles through a synergistic combination of computational and experimental research
  - Multiphysics model development using DNS/LES (Oefelein/Connolly/Andrews)
    - Detailed treatment of high-pressure (supercritical) flow processes inherent to oxy-fueled combustion
    - Progression from canonical laboratory-scale studies to device-scale conditions and geometries (e.g., 1500 K, 30 MPa turbine inlet conditions)
  - Experiments for model validation using a combination of laser and optical measurement techniques (Steinberg/Ranjan/White)
    - Mixing layer dynamics in sCO$_2$ loop at Georgia Tech (i.e., Density measurements using 2D burst-mode Raman scattering)
    - 1 MW sCO$_2$ combustor at Southwest Research Institute (i.e., Chemiluminescence imaging of H$_2$O and post-flame CO$_2$)
Supercritical fluids pose unique additional modeling challenges due to highly nonlinear property variations.
Tasks/milestones

• Task 1.0: Project Management and Planning

• Task 2.0: Multiphysics Model Development
  – Subtask 2.1: Unit physics model evaluation and verification studies
  – Subtask 2.2: Treatment of turbulent multiscalar mixing processes
  – Subtask 2.3: Treatment of turbulence-chemistry interactions

• Task 3.0: Benchmark Large Eddy Simulations
  – Subtask 3.1: Model validation (Georgia Tech sCO2 Loop)
  – Subtask 3.2: Model validation (SwRI 1 MW Oxy-Fueled sCO2 Combustor)
  – Subtask 3.3: Parametric Analysis

• Task 4.0: Experiments for Model Validation
  – Subtask 4.1: Non-reacting density and velocity measurements in redesigned test section
  – Subtask 4.2: Preliminary IR measurements in 1 MW oxy-fueled sCO2 combustor
  – Subtask 4.3: Complete IR measurements in 1 MW oxy-fueled sCO2 combustor

Current focal points
Detailed analysis and model development enabled using RAPTOR code suite designed for DNS/LES

- **Theoretical framework (Comprehensive)**
  - Fully-coupled, compressible conservation equations
  - Nonideal gas/liquid equation of state (high-pressure phenomena)
  - Detailed thermodynamics, transport with finite-rate chemistry
  - Multiphase flow with interface tracking (LS-GFM), spray (Lagrangian-Eulerian)
  - Dynamic subfilter modeling (no tuned constants)
  - Fully-integrated CHT and FSI (in progress)

- **Numerical framework (High-quality)**
  - Kinetic-energy/entropy preserving (non-dissipative, discretely conservative)
  - All-Mach-number (dual-time stepping with generalized preconditioning)
  - Complex geometry and BC’s

- **Massively-parallel (Highly-scalable)**

Project selected to receive 2020-2021 ASCR Leadership Computing Challenge (ALCC) award
Detailed analysis and model development enabled using RAPTOR code suite designed for DNS/LES

Initial focus on turbulent scalar mixing processes

Current focus on both mixing and combustion
Simulations performed using completely general treatment EOS, thermodynamic, and transport properties

- State-of-the-art formulation for EOS, thermodynamics, transport, and interfacial properties based on NIST expertise over decades
  - Real-fluid mixture properties obtained using Extended Corresponding States model
  - Multicomponent formulation using Cubic (e.g., SRK, PR), BWR, or Helmholtz EOS
  - Generalized to treat wide range of hydrocarbon mixtures (Fuel/Oxidizer/Products)
- Custom stand-alone software designed to run efficiently on HPC platforms

Focus on property variations at $p = 80$ bar and $308 \leq T \leq 318$ K
Georgia Tech \(\text{sCO}_2\) loop designed to provide insights into supercritical fluid mixing \((80\ \text{bar},\ 308 \leq T \leq 318\ \text{K})\)

<table>
<thead>
<tr>
<th></th>
<th>Pressure [MPa / psi]</th>
<th>Temperature [K / F]</th>
<th>Re</th>
<th>Density [kg/m(^3)]</th>
<th>Velocity [m/s]</th>
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</thead>
<tbody>
<tr>
<td><strong>Upper Stream</strong></td>
<td>8 / 1160</td>
<td>308 / 94.7</td>
<td>1.26e5</td>
<td>419.08</td>
<td>0.55</td>
</tr>
<tr>
<td><strong>Lower Stream</strong></td>
<td>8 / 1160</td>
<td>318 / 113</td>
<td>4.48e4</td>
<td>241.04</td>
<td>0.11</td>
</tr>
</tbody>
</table>
Test section is designed to give full optical access across the entire axial span of the mixing layer.
Detailed analysis supported via progression of 2D/3D DNS and LES

Goal: Facilitate analysis required to understand basic physics and model injection/mixing/combustion processes unique to high-pressure (supercritical) power and propulsion systems
Computational domain and grid match experiment (WRLES completed, full DNS in progress)

Time-dependent turbulent inflow fluctuations imposed using Synthetic Eddy Method

\[ U = 0.55 \text{ m/s} \quad T = 308 \text{ K} \quad Re_h = 126,000 \]

\[ U = 0.11 \text{ m/s} \quad T = 318 \text{ K} \quad Re_h = 44,800 \]

\[ \delta_{ref} = 1 \text{ mm (Splitter Plate Thickness)} \]

\[ p = 8 \text{ MPa} \]
How do nonlinear property variations affect flow and what are the implications with respect to modeling?

- Heat capacity of the fluid increases dramatically (e.g., more than an order of magnitude between 1 bar and 80 bar over the interval 308 ≤ T ≤ 318 K)

- Similarly, significant increases in the Prandtl number are induced (e.g., more than an order of magnitude between 1 bar and 80 bar over the interval 308 ≤ T ≤ 318 K)
How do nonlinear property variations affect flow and what are the implications with respect to modeling?

- Two forms of compressibility must be considered
  - Isothermal compressibility … change in volume due to change in pressure at constant temperature
  - Coefficient of thermal expansion … change in volume due to change in temperature at constant pressure
Rate of change in pressure and temperature can be significantly modulated by these nonlinearities

\[
\frac{\partial p}{\partial t} = -\frac{c^2}{\rho C_p} \left\{ \rho_T h + \rho C_p - \sum_{i=1}^{N-1} (\rho_T h_{Y_i} - \rho_{Y_i} C_p) Y_i \right\} \nabla \cdot (\rho u) \text{ Mass} + \rho_T \left( \frac{u \cdot \nabla p + M^2 \tau : \nabla u - \nabla \cdot (\rho h u) + \nabla \cdot q_e}{\text{Momentum Total Energy}} \right) + \sum_{i=1}^{N-1} (\rho_T h_{Y_i} - \rho_{Y_i} C_p) \left( \nabla \cdot (\rho_{Y_i} u) - \nabla \cdot q_i - \omega_i \right) \right\} \text{ Species}
\]

\[
\frac{\partial T}{\partial t} = \frac{c^2}{\rho C_p} \left\{ \rho_p h + \rho_T \frac{T}{\rho} - \sum_{i=1}^{N-1} \left( \rho_p h_{Y_i} - \rho_{Y_i} \rho_T \frac{T}{\rho^3} \right) Y_i \right\} \nabla \cdot (\rho u) \text{ Mass} + \rho_p \left( \frac{u \cdot \nabla p + M^2 \tau : \nabla u - \nabla \cdot (\rho h u) + \nabla \cdot q_e}{\text{Momentum Total Energy}} \right) + \sum_{i=1}^{N-1} \left( \rho_p h_{Y_i} - \rho_{Y_i} \rho_T \frac{T}{\rho^3} \right) \left( \nabla \cdot (\rho_{Y_i} u) - \nabla \cdot q_i - \omega_i \right) \right\} \text{ Species}
\]

where

\[
\frac{c^2}{\rho C_p} = \frac{1}{\rho_p \rho C_p + \rho_T (1 - \rho h_p)} = \frac{1}{\rho} \left[ \frac{1}{\alpha \rho C_p - \beta (1 - \rho h_p)} \right] = \frac{1}{\rho} \left[ \frac{1}{\alpha \rho C_p - \beta^2 T} \right]
\]
Variation of isothermal compressibility across three-dimensional mixing layer

\[ \alpha = \frac{1}{\rho} \left( \frac{\partial \rho}{\partial p} \right)_{T, Y_1, \ldots, Y_N} \]
Isosurface showing threshold where the coefficient of thermal expansion is 0.15

\[ \beta = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_{p, Y_1, \ldots, Y_N} \]
Ratio of $c^2/\rho C_p$ also modulates observables in highly nonlinear manner

$C_p = 20000 \text{ J/kg} \cdot \text{K}$

$\gamma = 2$

$\nu = 7.1 \times 10^{-8} \text{ m}^2/\text{s}$

Transport properties exhibit similar behavior
“Interim” summary and observations …

- Thermodynamic nonidealities and transport anomalies impose additional nonlinearities that modulate both broadband turbulence characteristics and observables (e.g., multiscalar mixing)

- Alters both the instantaneous and filtered equations for LES identically*
  - i.e., they premultiply convective/diffusive operators and source terms in both sets of equations and thus modulate these terms in the same way
  - *Additional focus needs to be placed on filtering nonlinear EOS and related properties (in progress)

- Chemical source term Jacobians and related eigenvalues also involve \( \rho_p \) and \( \rho_T \)
  - i.e., compressibility and thermodynamic nonidealities also affect finite-rate chemical kinetics and related stiffness in chemistry

- Nonequilibrium turbulence, baroclinic torque, etc., also significant factors

- Analysis of results is ongoing

\[
c^2 = \frac{\rho h_T}{\rho \rho_p h_T + \rho_T (1 - \rho h_p)}
\]
Reacting flow studies ...

Non-reacting supercritical LOX-CH4 mixing layer

Reacting supercritical LOX-CH4 mixing layer

Supercritical mixing at 100 bar (density field)

Non-reacting supercritical LOX-CH4 mixing layer

Temperature (K)

\[
\begin{align*}
T &= 300 \text{ K} \\
p &= 10 \text{ MPa} \\
\rho &= 74 \text{ kg/m}^3 \\
u &= 60 \text{ m/s} \\
\delta &= 0.3 \text{ mm} \\
T &= 120 \text{ K} \\
\rho &= 1003 \text{ kg/m}^3 \\
u &= 10 \text{ m/s}
\end{align*}
\]
Many additional terms arise as consequence of filtering compressible multicomponent conservation equations

- Filtered Mass:
  \[
  \frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u}) = 0.
  \] (1)

- Filtered Momentum:
  \[
  \frac{\partial (\bar{\rho} \bar{u})}{\partial t} + \nabla \cdot \left( \bar{\rho} \bar{u} \otimes \bar{u} + \frac{\bar{p}}{M^2} I \right) = \nabla \cdot \bar{\tau} - \nabla \cdot \mathbf{T},
  \] (2)
  where
  \[
  \bar{\tau} = \frac{\mu}{Re} \left[ -\frac{2}{3} (\nabla \cdot \mathbf{u}) I + (\nabla \mathbf{u} + (\nabla \mathbf{u})^T ) \right].
  \]

- Filtered Species:
  \[
  \frac{\partial (\bar{\rho} \bar{Y}_i)}{\partial t} + \nabla \cdot (\bar{\rho} \bar{Y}_i \bar{u}) = \nabla \cdot \bar{q}_i - \nabla \cdot \bar{S}_i + \bar{\omega}_i \quad i = 1, \ldots, N - 1,
  \] (3)
  where
  \[
  \bar{q}_i = \frac{\mu}{Sc_i Re} \nabla Y_i.
  \]
e.g., Variances of viscous stress tensor and diffusion fluxes can be significant depending on filter width

Filter size 10x larger relative to DNS ($\Delta_{LES}/\Delta_{DNS} = 10$)
Filtered total energy equation

- Filtered Total Energy:

\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{e}_t) + \nabla \cdot (\bar{\rho} \bar{u}_t + \bar{\rho} \bar{u}) = \nabla \cdot (\bar{\mathbf{q}}_e + M^2 (\bar{\tau} \cdot \bar{\mathbf{u}})) - \nabla \cdot (\bar{Q}_e + M^2 (\bar{T} \cdot \bar{\mathbf{u}})) - \nabla \cdot \left[ \frac{M^2}{2} \text{tr} (\bar{T} \bar{u}''') \right] + \nabla \cdot \left( M^2 (\bar{\tau} \cdot \bar{u}'') \right) + \bar{Q}_e, \tag{4}
\]

where

\[
\bar{e}_t = \bar{e} + \frac{M^2}{2} \bar{\mathbf{u}} \cdot \bar{\mathbf{u}} + \frac{M^2 \text{tr} (\bar{T})}{2 \bar{\rho}},
\]

\[
\bar{e} = \sum_{i=1}^{N} \bar{h}_i \bar{Y}_i - \frac{\bar{p}}{\bar{\rho}} + \sum_{i=1}^{N} \left[ (\bar{\bar{h}}_i \bar{Y}_i - \bar{h}_i \bar{Y}_i) + (\bar{h}_i \bar{Y}_i'' + \bar{h}_i'' \bar{Y}_i) + \bar{h}_i'' \bar{Y}_i'' \right],
\]

\[
\bar{Q}_e = - \sum_{i=1}^{N} \bar{\omega}_i \bar{h}_i^o, \quad \text{and} \quad \bar{q}_e = \frac{\mu C_p}{Pr Re} \nabla T + \sum_{i=1}^{N} \bar{h}_i \bar{q}_i.
\]
Consistent modeling of SFS variances/covariances rare, enthalpy/EOS must also be filtered and require closures

- Turbulent Momentum, Energy, and Species Fluxes:

\[
T = \bar{\rho}(\bar{\hat{u}} \otimes \hat{\bar{u}} - \hat{u} \otimes \bar{\hat{u}}) + \bar{\rho}(\bar{u} \otimes \hat{u}' + \hat{u}' \otimes \bar{u}) + \bar{\rho u}'' \otimes \hat{u}''
\]

\[
Q = \bar{\rho}(\bar{\hat{h}} \bar{u} - \hat{h} \bar{u}) + \bar{\rho}(\bar{h} u'' + h'' \bar{u}) + \bar{\rho h'' u}''
\]

\[
S_i = \bar{\rho}(\bar{\hat{Y}_i} \bar{u} - \hat{Y}_i \bar{u}) + \bar{\rho}(\bar{Y}_i \bar{u}'' + Y_i'' \bar{u}) + \bar{\rho Y_i'' u}''
\]

- Enthalpy:

\[
\bar{\rho e} + \bar{p} = \bar{\rho} \sum_{i=1}^{N} \bar{h}_i \bar{Y}_i + \bar{\rho} \sum_{i=1}^{N} \left[ (\bar{h}_i \bar{Y}_i - \hat{h}_i \bar{Y}_i) + (\bar{h}_i Y_i'' + h_i'' Y_i + h_i'' Y_i) \right]
\]

- Equation of State:

\[
\bar{p} = \bar{\rho} R_u \sum_{i=1}^{N} \left( \frac{\bar{T}Y_i}{W_i} + \frac{(\bar{T}Y_i - \bar{T}Y_i) + (\bar{T}Y_i'' + T'' Y_i) + T'' Y_i}{W_i} \right)
\]

- Filtered Viscous Stress Tensor, and Filtered Energy and Mass Diffusion Fluxes
“Mixed” Dynamic Smagorinsky (DMM) model shown below is consistent, DSM in not since it neglects terms

- Eddy Viscosity:

\[ \mu_t = \bar{\rho} C_R \Delta^2 \Pi_S^{1/2} \quad \Pi_S = \tilde{S} : \tilde{S} \quad \tilde{S} = \frac{1}{2} (\nabla \tilde{u} + \nabla \tilde{u}^T) \]

- Stress Tensor:

\[ \tilde{T} = (\tilde{\tau} - \tilde{T}) = (\mu_t + \mu) \frac{1}{Re} \left[ -\frac{2}{3} (\nabla \cdot \tilde{u}) I + (\nabla \tilde{u} + \nabla \tilde{u}^T) \right] - \tilde{\rho} \left( \tilde{u} \otimes \tilde{u} - \tilde{\tilde{u}} \otimes \tilde{\tilde{u}} \right) - \frac{1}{3} \tilde{\rho}q_{sfs}^2 I \]

- Energy Flux:

\[ \tilde{Q}_e = (\tilde{\bar{\alpha}}_e - \tilde{Q}) = \left( \frac{\mu_t}{Pr_t} + \frac{\mu}{Pr} \right) \frac{1}{Re} \nabla \tilde{h} + \sum_{i=1}^{N} \tilde{h}_i \tilde{S}_i - \tilde{\rho} \left( \tilde{h} \tilde{u} - \tilde{\tilde{h}} \tilde{\tilde{u}} \right) \]

- Mass Flux:

\[ \tilde{S}_i = (\tilde{\bar{\alpha}}_i - \tilde{S}_i) = \left( \frac{\mu_t}{Sc_{t_i}} + \frac{\mu}{Sc_i} \right) \frac{1}{Re} \nabla \tilde{Y}_i - \tilde{\rho} \left( \tilde{Y}_i \tilde{u} - \tilde{\tilde{Y}}_i \tilde{\tilde{u}} \right) \]

Coefficients $C_R$, $Pr_t$, and $Sc_{t_i}$ evaluated dynamically as functions of space and time.
A priori assessment of Dynamic Smagorinsky Model versus Dynamic Mixed Model

\( \tilde{\eta u} - \tilde{\eta \eta} \)

\( \tilde{\eta \nu} - \tilde{\eta \nu} \)

\( \tilde{\nu \nu} - \tilde{\nu \nu} \)

\( \Delta_{\text{LES}}/\Delta_{\text{DNS}} = 5 \)
A priori assessment of Dynamic Smagorinsky (DSM) versus Mixed Dynamic Smagorinsky (DMM)

<table>
<thead>
<tr>
<th>Covariance</th>
<th>Dynamic Smagorinsky</th>
<th>Mixed Dynamic Smagorinsky</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(\overline{uu})_{sfs}$</td>
<td>65.7 %</td>
<td>82.8 %</td>
</tr>
<tr>
<td>$(\overline{uv})_{sfs}$</td>
<td>84.2 %</td>
<td>89.8 %</td>
</tr>
<tr>
<td>$(\overline{vv})_{sfs}$</td>
<td>53.0 %</td>
<td>90.7 %</td>
</tr>
<tr>
<td>$(\overline{uT})_{sfs}$</td>
<td>69.8 %</td>
<td>92.2 %</td>
</tr>
<tr>
<td>$(\overline{vT})_{sfs}$</td>
<td>74.8 %</td>
<td>91.0 %</td>
</tr>
<tr>
<td>$(\overline{uY})_{sfs}$</td>
<td>68.0 %</td>
<td>74.6 %</td>
</tr>
<tr>
<td>$(\overline{vY})_{sfs}$</td>
<td>61.6 %</td>
<td>92.7 %</td>
</tr>
</tbody>
</table>

Filter size 5x larger relative to DNS ($\Delta = 5$).
**A priori assessment of Dynamic Smagorinsky (DSM) versus Mixed Dynamic Smagorinsky (DMM)**

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<th>Covariance</th>
<th>Dynamic Smagorinsky</th>
<th>Mixed Dynamic Smagorinsky</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(\widetilde{uv})_{sfs}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Delta = 5$</td>
<td>84.2 %</td>
<td>89.8 %</td>
</tr>
<tr>
<td>$\Delta = 10$</td>
<td>17.2 %</td>
<td>60.9 %</td>
</tr>
<tr>
<td>$(\widetilde{uT})_{sfs}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Delta = 5$</td>
<td>69.8 %</td>
<td>92.2 %</td>
</tr>
<tr>
<td>$\Delta = 10$</td>
<td>9.3 %</td>
<td>33.5 %</td>
</tr>
<tr>
<td>$(\widetilde{vY})_{sfs}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Delta = 5$</td>
<td>61.6 %</td>
<td>92.7 %</td>
</tr>
<tr>
<td>$\Delta = 10$</td>
<td>18.8 %</td>
<td>58.9 %</td>
</tr>
</tbody>
</table>
Concurrent work … collaborations initiated with SwRI on simulations of direct fired supercritical oxy-combustion

- High-resolution first-principles LES that identically matches geometry and operating conditions combined with close collaborations with SwRI CFD group
- Analysis of sub-model accuracy and performance in a complex geometric environment; e.g.,
  - Turbulent velocity and multiscalar mixing
  - Turbulent mixed-mode combustion
  - Finite-rate chemical kinetics
  - Best practices for model implementation
Concurrent work … collaborations initiated with SwRI on simulations of direct fired supercritical oxy-combustion

\[
\bar{\omega}_i(x, t) = \int_{t}^{t+\Delta t} \left\{ \int_{V(\tau)} \int \mathcal{G}(y-x, \tau-t; \delta y, \delta \tau) \, \hat{\omega}_i(\phi_1, \phi_2, \ldots ; y, \tau) \, dV \right\} d\tau
\]

\[
\phi_i(x, t) = \hat{\phi}_i(x, t) + \phi''_i(x, t)
\]

- Currently investigating the merits of a new combustion closure based on space-time filtering
- Hypothesis … space-time filtering can be used to close the filtered chemical source terms directly
  - Apply approximate deconvolution model with assumed scalar spectrum to calculate subfilter variance/covariance matrix
  - Variance/covariance matrix used as input to generate correlated scalar fluctuations on subfilter scales in time
  - Use modeled instantaneous signal to evaluate filtered chemical source terms directly
- Benefits … 1) conceptually regime independent, 2) minimizes assumptions required for closure, 3) approaches correct behavior in limit of DNS (i.e., facilitates hybrid-DNS/LES approach)

![Diagram](image_url)

\( \Delta t_{LES} \)

**n-dodecane**

- e.g., Modeled instantaneous fluctuations of fuel-air mixture on centerline at 100 diameters downstream of injection
e.g., Modeled instantaneous fluctuations facilitate formation of ignition kernels on subfilter time scales

Volume rendered fuel mass fraction
- Highlighting mixing

Volume rendered temperature
- Highlighting ignition kernel development
Major goal is to tightly couple simulations to complex companion experiments (i.e., SwRI rig)

- First kernel, diameter ≈ 500 μm (too small to be optically detected)
  Location: tip of the jet, off-axis

- Independent kernels appear, diameter ≈ 500μm to 2mm (still very small for optical detection)
  Location: tip of the jet, off-axis

- Many small kernels present in the “jet edge” region, what is the impact on Schlieren?

- Single flame structure with upstream independent kernels, flame expands through dilatation and autoignition

- Main flame region at the jet extremity, autoignition locations observed ahead of main front

- Schlieren images by Skeen et al., PCI, 2015

- 200 μs
- 250 μs
- 270 μs
- 300 μs
- 380 μs

- 250 μs
- 220 μs
- 380 μs

- Red Isocontour = 1000 K

- 3D high-repetition flow-flame interactions, dynamics of scalar-dissipation and its effects on chemical kinetics

- Converting simulation data to modeled signals produced via laser diagnostics for enhanced analysis in complex environments

- e.g., Enable unique analysis of processes that can’t be measured at conditions that match experiments
Summary

• Details related to fundamental physics and modeling for LES for compressible flows and supercritical fluids
  – Numerous additional terms appear in the filtered conservation equations as a result of the filtering process
    • Compressibility effects and nonequilibrium turbulence apply to all compressible flows
    • Scalar-scalar variance/covariances associated with filtered total energy equation, EOS, enthalpy
    • Viscous stress tensor, energy diffusion, and mass diffusion fluxes
  – Terms need to be treated through combination of consistency, modeling, and quantified resolution requirements
    • Demonstrated process for establishing resolution requirements related to scalar mixing
    • Mixed Dynamic Smagorinsky (DMM) model is consistent and thus more accurate as function of resolution
    • Dynamic Smagorinsky model is not consistent since it neglects terms
  – Future work will incorporate treatment of scalar-scalar variances and the filtered mass, momentum, energy diffusion fluxes (e.g., what can we control via resolution constraints, what needs to be modeled)

• Anomalies associated with multiscalar mixing and combustion in context of direct fired supercritical oxy-combustion LRE’s at supercritical pressures
  – Thermodynamic nonidealities and transport anomalies impose additional nonlinearities that modulate both broadband turbulence characteristics and observables (e.g., multiscalar mixing, pressure, temperature)
    • Demonstrated how nonlinearities in EOS, thermodynamics, transport can modulate local flow characteristics
    • Compressibility and thermodynamic nonlinearities also affect finite-rate chemical kinetics
  – Future work will focus on modeling filtered EOS and related thermodynamic and transport properties as well as nonequilibrium turbulence, baroclinic torque, etc., which are significant factors that require further investigation