Model portfolio
Reactive flows

- Infinitely Fast Chemistry (non-premixed)
  - EDC
  - EDC-SDT (Scalar Dissipation Timescale)
  - EDC-MTS (Multiple Timescale)
  - RANS (LES & VLES, under development)

- Finite Rate Chemistry (non-premixed)
  - Arrhenius (volumetric and surface reaction)
  - Flamelet based on Mixture Fraction, Progress Variable & Scalar Dissipation Rate
  - DQMOM (in progress)
  - RANS and LES & VLES

- Coupling with CANTERA (derived from Chemkin)
  - Evaluate thermodynamic and transport properties
  - Import Chemkin reaction mechanisms
  - Evaluate reaction rates
    - Pressure dependent reactions
    - Third body reaction
    - Surface reactions
  - Build Flamelet libraries
Catalytic Wall Reaction
Example 1: Finite rate surface reaction in tube
(Mladenov et al., 2000)

- Flow in a tube Re = 201
- Fixed wall temperature 523 K
- Inlet: Typical exhaust gas of an engine
  - Mainly N2, O2, CO2 and H2O
  - Traces of C3H6, CO, NO, NO2
- Reactions on the tube surface
- Main pathways:
  - C3H6 oxidation
  - CO oxidation
  - Reactions involving NO and NO2
Example 1: Finite rate surface reaction in tube (Mladenov et al., 2000)

Mass flow averaged gas phase species in a channel. Comparison to the reference results of Mladenov et al.

Surface absorbed species in a channel. Comparison to the reference case of Mladenov et al.
Example 2: Catalytic wall reaction in a channel (Raja et al., 2000)

- 2D channel (0.2cm; 10cm) Methane-Air mixture wall-reacting (heterogeneous) flow
- Re=200 (1 bar) & 2000 (10 bar); compressible flow conditions
- U = 5m/s; T = 600K; Tw=600-1290K : x < 0.1cm;
- 8 gas-phase species & 11 surfaces species
- Use Cantera library to extract material properties
Example 2: Catalytic wall reaction in a channel
(Raja et al., 2000)

Methane production rate
(1 vs. 10 bar pressure) →

Mass fraction of major species
Example 2: Catalytic wall reaction in a channel (Raja et al., 2000)

Surface coverage and surface species mass fractions
A square duct (section: 0.7cm; 30cm) with Hydrogen-Air mixture wall-reaction

- Using Benzene reaction chemistry
- Walls coated with platinum
- $U = 9.6\text{m/s}; T = 572\text{K}; Tw=1150\text{ K} : x < 0.1\text{cm}$
- 7 gas-phase species & 5 surfaces species
- Use Cantera library to extract material properties
Example 3: Catalytic wall reaction in a duct (Ghermay et al., 2010)
Example 3: Catalytic wall reaction in a duct (Ghermay et al., 2010): 2D results
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Example 3: Catalytic wall reaction in a duct (Ghermay et al., 2010): 3D results
Example 3: Catalytic wall reaction in a duct (Ghermay et al., 2010): 3D results
3D Simulations of flow/catalytic reaction in complex Kelvin-cells structures

(catalytic Reactors for gas exhaust in cars: Courtesy from EMPA, Switzerland)
3D Simulations of flow/catalytic reaction in complex Kelvin-cells structures

- A Kelvin cell with Hydrocarbons-Air-CO mixture wall-reaction
- Walls coated with platinum
- $U = 10$ m/s; $T = 1000$K
- Infintely fast reaction
- Heat release (exothermal reaction combined with conjugate heat transfer)
3D Simulations of flow/catalytic reaction in complex Kelvin-cells structures
3D Simulations of flow/catalytic reaction in complex Kelvin-cells structures

- Auto-generated BMR grid
- Pollutant conversion
- Multi-step reaction mechanism
- Conjugate heat transfer
- Heat release due to the reaction
3D Simulations of flow/catalytic reaction in complex Kelvin-cells structures

- catalytic reaction on the kelvin-cell walls, with conjugate heat transfer.
- Use is the made of the IST to mesh the cells, on a Cartesian grid
2D simulations of flow/catalytic reaction in a channel with washcoat

- Catalytic combustion of Methane in a thermally isolated channel
- Multi-step reaction mechanism
- Species diffusion and reaction in the washcoat
- Conduction in the washcoat
- Conjugate heat transfer
• Channel case of Mladenov et al. with washcoat model
• Multistep reaction mechanism (~ 80 reactions)
Homogeneous Combustion
Turbulent Diffusion Flames
(The Equations)

- Favre averaging procedure: \( \tilde{\psi} = \frac{\rho \psi}{\rho} \); \( \psi = \tilde{\psi} + \psi'' \)

Mass

\[
\frac{\partial \rho \tilde{u}_i}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{u}_j}{\partial x_i} = 0
\]

Momentum

\[
\frac{\partial \rho \tilde{u}_i}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{u}_j}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \tilde{\tau}_{ij} - \rho u''_i u''_j \right) - \frac{\partial p}{\partial x_i}
\]

Enthalpy

\[
\frac{\partial \rho \tilde{h}_s}{\partial t} + \frac{\partial}{\partial x_i} \rho \tilde{u}_i \tilde{h}_s = \tilde{\omega}_T + \frac{\bar{D} p}{\bar{D} t} + \frac{\partial}{\partial x_i} \left( \frac{\lambda}{\partial x_i} - \rho u''_i h''_s \right) + \frac{\tau_{ij}}{\partial x_j} - \frac{\partial}{\partial x_i} \left( \rho \sum_{k=1}^{N} V_{k,i} Y_{k} h_{s,k} \right)
\]
Turbulent Diffusion Flames
(Closure issues)

Species

\[ \frac{\partial \rho \tilde{Y}_k}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{Y}_k}{\partial x_i} = \left( \frac{\rho D_k}{\rho} \frac{\partial \tilde{Y}_k}{\partial x_i} - \rho u''_i \tilde{Y}''_k \right) + \tilde{\omega}_k \]

Unclosed terms: \( \tilde{u}'_i \tilde{Y}''_k, \tilde{u}''_i \tilde{h}_s' \Rightarrow \tilde{u}'_i \tilde{Y}''_k = -\frac{\nu_t}{Sct_{t,k}} \frac{\partial \tilde{Y}_k}{\partial x_i} \)

Unclosed terms: \( \tilde{u}''_i \tilde{u}''_j \Rightarrow \) turbulence model

- Challenge \( \Rightarrow \) modeling \( \tilde{\omega}_k \)

TransAT uses:
- Arhenius approach
- Eddy Dissipation Concept (EDC)
- Flamelet Model (basic & Peter’s formulation)
Turbulent Diffusion Flames
(EDC Closure)

- General form of the $r^{th}$ reaction
  \[ \sum_{i=1}^{N} \nu'_{i,r} M_i \Rightarrow \sum_{i=1}^{N} \nu''_{i,r} M_i \]

- The chemical kinetics are assumed to be infinitely fast
- Reaction rates are controlled by the turbulence mixing
- The net rate of production of species $i$ due to reaction $r$ is given by the smaller of the two expressions:

\[
\dot{\omega}_{k,r} = \nu'_{k,r} W_k A \rho \frac{\varepsilon_{\text{min}}}{k} \left( \frac{Y_R}{\nu'_{R,r} W_R} \right); \quad \dot{\omega}_{k,r} = \nu'_{k,r} W_k A B \rho \frac{\varepsilon}{N} \left( \sum_{i=1}^{N} \nu''_{i,r} W_i \right)
\]

- Large-eddy mixing time scale $k/\varepsilon$ governs the chemical reaction rate
Example 1: NO2 formation (Arhenius approach) (Feitelberg & Corea, 2000)

- Exhaust gas from gas turbine
- Create a plug flow reactor (1D)
- Apply NO2 formation mechanism
- Use Arrhenius model
- Use Cantera library

<table>
<thead>
<tr>
<th>REACTION</th>
<th>$A$</th>
<th>$b$</th>
<th>$E$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. CO + O + M = CO2 + M</td>
<td>$6.17 \times 10^{14}$</td>
<td>0.00</td>
<td>3000.0</td>
</tr>
<tr>
<td>2. CO + OH = CO2 + H</td>
<td>$1.51 \times 10^{17}$</td>
<td>1.30</td>
<td>$-768.0$</td>
</tr>
<tr>
<td>3. CO + O2 = CO2 + O</td>
<td>$1.60 \times 10^{13}$</td>
<td>0.00</td>
<td>41000.0</td>
</tr>
<tr>
<td>4. HO2 + CO = CO2 + OH</td>
<td>$5.60 \times 10^{13}$</td>
<td>0.00</td>
<td>22254.0</td>
</tr>
<tr>
<td>5. H2O2 + O = 2 OH</td>
<td>$1.70 \times 10^{13}$</td>
<td>0.00</td>
<td>47780.0</td>
</tr>
<tr>
<td>6. H + H2O = H2O + H</td>
<td>$1.17 \times 10^{19}$</td>
<td>1.30</td>
<td>5625.0</td>
</tr>
<tr>
<td>7. O + OH = O2 + H</td>
<td>$4.00 \times 10^{14}$</td>
<td>-0.50</td>
<td>0.0</td>
</tr>
<tr>
<td>8. O + H2 = OH + H</td>
<td>$5.06 \times 10^{14}$</td>
<td>2.67</td>
<td>6290.0</td>
</tr>
<tr>
<td>9. H + O2 + M = HO2 + M</td>
<td>$3.61 \times 10^{17}$</td>
<td>-0.72</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Enhanced third-body efficiencies: $H_2O = 18.6$, $CO_2 = 4.2$, $H_2 = 2.9$, $CO = 2.1$, $N_2 = 1.3$

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<tr>
<td>10. OH + HO2 = H2O + O2</td>
<td>$7.50 \times 10^{12}$</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>11. H + HO2 = 2 OH</td>
<td>$1.40 \times 10^{14}$</td>
<td>0.00</td>
<td>1073.0</td>
</tr>
<tr>
<td>12. O + HO2 = O2 + OH</td>
<td>$1.40 \times 10^{13}$</td>
<td>0.00</td>
<td>1073.0</td>
</tr>
<tr>
<td>13. 2 OH = O + H2O</td>
<td>$6.00 \times 10^{9}$</td>
<td>1.30</td>
<td>0.0</td>
</tr>
<tr>
<td>14. H + H2 + M = H2 + M</td>
<td>$1.00 \times 10^{18}$</td>
<td>-1.00</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Enhanced third-body efficiencies: $H_2 = 0.0$, $H_2O = 0.0$, $CO_2 = 0.0$

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<tr>
<td>15. H + OH + M = H2O + M</td>
<td>$1.60 \times 10^{22}$</td>
<td>-2.00</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Enhanced third-body efficiencies: $H_2O = 5.0$

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<tbody>
<tr>
<td>16. O + O + M = O2 + M</td>
<td>$1.89 \times 10^{13}$</td>
<td>0.00</td>
<td>-1788.0</td>
</tr>
<tr>
<td>17. H + HO2 + H = H2 + O2</td>
<td>$1.25 \times 10^{13}$</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>18. 2 HO2 = H2O2 + O2</td>
<td>$2.00 \times 10^{12}$</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>19. H2O2 + M = 2 OH + M</td>
<td>$1.30 \times 10^{17}$</td>
<td>0.00</td>
<td>45500.0</td>
</tr>
<tr>
<td>20. H2O2 + H = HO2 + H2</td>
<td>$1.60 \times 10^{13}$</td>
<td>0.00</td>
<td>3800.0</td>
</tr>
<tr>
<td>21. HO2 + OH = H2O + H</td>
<td>$1.00 \times 10^{13}$</td>
<td>0.00</td>
<td>1800.0</td>
</tr>
<tr>
<td>22. CO2 + N = NO + CO</td>
<td>$1.90 \times 10^{11}$</td>
<td>0.00</td>
<td>3400.0</td>
</tr>
<tr>
<td>23. HO2 + NO = NO2 + OH</td>
<td>$2.11 \times 10^{12}$</td>
<td>0.00</td>
<td>-479.0</td>
</tr>
<tr>
<td>24. NO2 + H = NO + OH</td>
<td>$3.50 \times 10^{14}$</td>
<td>0.00</td>
<td>1500.0</td>
</tr>
<tr>
<td>25. NO2 + O = NO + O2</td>
<td>$1.00 \times 10^{11}$</td>
<td>0.00</td>
<td>600.0</td>
</tr>
<tr>
<td>26. NO2 + M = NO + O + M</td>
<td>$1.10 \times 10^{16}$</td>
<td>0.00</td>
<td>66500.0</td>
</tr>
<tr>
<td>27. N2O + H = N2 + OH</td>
<td>$7.60 \times 10^{13}$</td>
<td>0.00</td>
<td>15200.0</td>
</tr>
<tr>
<td>28. N2O + M = N2 + O + M</td>
<td>$1.60 \times 10^{14}$</td>
<td>0.00</td>
<td>51600.0</td>
</tr>
<tr>
<td>29. N2O + O = N2 + O</td>
<td>$1.00 \times 10^{14}$</td>
<td>0.00</td>
<td>26200.0</td>
</tr>
<tr>
<td>30. N2O + O = 2 NO</td>
<td>$1.20 \times 10^{14}$</td>
<td>0.00</td>
<td>26200.0</td>
</tr>
<tr>
<td>31. N + NO = N2 + O</td>
<td>$3.27 \times 10^{12}$</td>
<td>0.30</td>
<td>0.0</td>
</tr>
<tr>
<td>32. N + O2 = NO + O</td>
<td>$6.40 \times 10^{9}$</td>
<td>1.00</td>
<td>6280.0</td>
</tr>
<tr>
<td>33. N + OH = NO + H</td>
<td>$3.80 \times 10^{13}$</td>
<td>0.00</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Note: forward rate coefficients ($k_i$) are of the form $k_i = A \cdot \exp(-E/(RT))$, where the dimensions of $A$ are mole-cm-sec-K, the units of $E$ are cal/mole, $T$ is absolute temperature, and $R$ is the ideal gas constant.
Example 1: NO2 formation (Arhenius approach) (Major species and radicals)
Example 2: H2 Non-premixed Turbulent Flame (Arhenius approach; Obieglo, Gass & Poulíkakos, 2000)

- Axisymmetric H2-Air reacting flame flow
- Axisymmetric, Re=10‘000; K-e model
- Comparisons with LDA Lab. data
- Standard EDC model
- Cantera library for material properties

Fig. 1. Scheme of the nozzle for the jet flame. The inner diameter is $D = 3.75$ mm.
Example 2: H2 Non-premixed Turbulent Flame (Arhenius approach; Obieglo, Gass & Poulakakos, 2000)
Example 3: Partially Premixed combustion (EDC Closure)

Sandia Flame D, Setup

- 2D axisymmm.
- BMR (multiblock Grid)
- 55.292 cells; 3 blocks
Example 3: Partially Premixed combustion (EDC Closure)

**Sandia Flame D, modelling & Results**

- Methane-air jet flames
- Partially premixed
- Eddy dissipation concept

![Diagram of Sandia Flame D with temperature scale]
Example 3: Partially Premixed combustion (EDC Closure)

EDC with TransAT

Figure: Radial profiles of Flame–D. EDC simulations at \( z/d = 3, z/d = 7.5, z/d = 15 \). (Top: Temperatures, Bottom: \( CO_2 \) mass fractions)
Example 3: Partially Premixed combustion (EDC Closure)

**EDC with TransAT**

Figure: Radial profiles of Flame–D. EDC simulations at $z/d = 30$, $z/d = 45$, $z/d = 60$. (Top: Temperatures, Bottom: $CO_2$ mass fractions