Overview of Reacting Flow
Various Applications
Overview of available reacting flow models
Latest additions
Example Cases
Summary
Reacting Flows Applications in STAR-CCM+

- Chemical Process Industry (liquid-liquid reactions)
  - Finite-rate chemistry model with a flexibility to modify EOS
  - EMP inter/intra-phase reactions
  - Moment methods
  - Surface Chemistry
- Rocket Engines (Solid, Liquid, and Hybrid)
  - Particle Reactions in Lagrangian
  - Real–Gas model with all Combustion Models
  - Coupled Solver
- High-speed jet engines (Ramjet, Scramjet)
  - Coupled solver with combustion models
- Oil and Gas
  - Multiple-Phase reactions (intraphase and interphase)
Ever-Expanding application coverage

- Gas turbine, process heaters, burners, and furnaces
  - Partially-premixed combustion models
  - LES
  - Soot and Nox models
- Chemical Vapor Deposition
  - Detailed/Global Surface chemistry
  - multi-component diffusion
- Aftertreatment (Automotive)
  - Detailed/Global Surface chemistry
  - Coupled with liquid film and porous media
- Energy Industry (Coal and Biomass combustion)
  - Multiple Coal Types and cofiring with gas-fuel
Reacting Flow Models in STAR-CCM+

**Non-Premixed Combustion**
- EBU
  - Standard, Hybrid, Finite-Rate
  - User Defined
- PPDF (Multi-stream)
  - Equilibrium
  - Flamelet
- PVM (Chemistry Table)

**Premixed Combustion**
- CFM (Choice for Laminar flame speed)
- PEBU
- TFC

**Partially-Premixed Combustion**
- PCFM
  - Equilibrium
  - Flamelet
- EBU
- PVM
- PTFC

**Finite-Rate Chemistry Calculation using DARS-CFD**
- EDC
- ISAT
- Dynamic Load Balancing

**Surface Reactions**
**Soot and Nox Emission Models**
Latest Additions (v 8/9)

- **Micromixing Models**
- **Surface Chemistry**
  - Global mechanisms
- **Combustion Models with Real Gases**
  - SRK and Peng-Robinson EOS
- **Soot Model**
  - MBH Model
  - Soot absorption properties
- **Eulerian Multi-phase Reaction Model**
  - Flexibility to add user defined reactions
- **Complex Chemistry Model (DARS-CFD)**
  - ISAT
  - Analytical Jacobian
  - PaSR
- **Performance**
New Micromixing Model for Liquid Reactions in 9.02

- Eddy Contact Micromixing Model (based on Froney and Nafia, Chem Eng Sc, 2000) for Liquid-Liquid Reactions.

- Users will have choice of three mixing scales
  - Kolmogorov (corresponds to Engulfment type of mixing)
  - Classical Scalar Mixing (considers high Sc number)
  - User Defined (ability to do user defined ff)
  - Kinetics Only (No Micromixing)

- The above four choices are available for each reaction
Micromixing Model – Eddy Contact Micromixing

Non-Premixed Combustion model...
- Eddy Break-up
- Eddy Contact Micromixing
- Homogeneous Reactor

Optional Models
- Thermal Comfort
- Passive Scalar
- Aeroacoustics
- Thin Film
- Gravity
- Mesh Deformation
- Radiation
- Turbulence Suppression
- Vorticity Confinement Model
- Axisymmetric Swirl
- Dispersed Multiphase
- Lagrangian Multiphase

Enabled Models
- High y+ Wall Treatment
- Standard K-Epsilon
- Gradients
- Axisymmetric
- Steady
- Cell Quality Remediation
- K-Epsilon Turbulence
- Reynolds-Averaged Navier-Stokes
- Turbulent
- Segregated Fluid Enthalpy
- Non-Premixed Combustion
- Reacting
- Constant Density
- Segregated Species
- Segregated Flow
- Multi-Component Liquid

Auto-select recommended models

<Optional>

<Additional model selections are required>
Eddy Contact Micromixing

Micromixing Timescale - Properties

- Select method
  - Kolmogorov Micromixing
    - Classical Scalar Dissipation
    - Kolmogorov Micromixing
    - No Micromixing (Kinetics Only)
    - User Micromixing
Validation Case – Low $Re$ flow in Coaxial Jet

The results compared to the numerical of Forney and Nafia (2000) and experimental data of Li and Toor (1986) at low high Reynolds number. Reactants A and B react in aqueous solution.
Mass Fractions of A, B, R (Desired) and S
Results (% Yield of R)

Comparison with Experimental Data

- Experiment (Li & Toor, 1986)
- Hybrid EBU
- Eddy Contact Micromixing (Kolmogorov)
- Eddy Contact Micromixing (Classical Scalar Mixing)
- Froney & Nafia Paper, 2000

- Micromixing Models predictions are much better than EBU
- Classical Scalar Mixing time scale appears to give best match
Surface Reactions

- No DARS-CFD licenses are required
- Users can add their own reactions
- Same interface for adding reactions as gas-phase reactions
Applications

**Tools**
- Porous chemistry
- Global Surface chemistry
- Detailed Surface Chemistry

**CVD Reactors**

**After-treatment devices:**
- Three-Way Catalytic Converters (TWC)
- Diesel Oxidation Catalyst (DOC)
- Diesel Particulate Filter (DPF)
- Selective Catalytic Reduction (SCR)
Results – NOx Reduction Comparison

Two-Step Model

Detailed Surface Chemistry
Real Fluid Modeling in STAR-CCM+

- Real Fluid Physics in STAR-CCM+
  - Van der Waals
  - Redlich-Kwong (RK)
  - Peng-Robinson (PR)
  - Soave-Redlich-Kwong (SRK, available in 8.02)
  - Modified Soave-Redlich-Kwong (MSRK, available in 8.02)

- All above Equation of States are Cubic

\[
P = \frac{RT}{v - b} - \frac{\Theta}{(v^2 + \delta v + \epsilon)}
\]
Real Fluid Thermodynamic Departures

**Enthalpy:**

\[ dh = C_p \, dT + \left[ v - T \left( \frac{\partial v}{\partial T} \right)_p \right] \, dP \]

**Specific Heat:**

\[ C_p = C_p^0 + T \int_{\infty}^{v} \left( \frac{\partial^2 P}{\partial T^2} \right)_v \, dv - T \left( \frac{\partial P}{\partial T} \right)_v \left( \frac{\partial P}{\partial v} \right)_T^{-1} - R \]

**Entropy:**

\[ ds = \frac{C_p}{T} \, dT - \left( \frac{\partial v}{\partial T} \right)_P \, dP \]

**Speed of Sound:**

\[ c_e^2 = -\frac{1}{\rho^2} \frac{C_p}{C_v} \left( \frac{\partial P}{\partial v} \right)_T \]
Results (Density Comparison)

PR

SRK

Ideal Gas
Transport equations are solved for two soot variables - Soot number density (N) and Soot Mass density (M)

Key physical processes are:
- Nucleation
- Coagulation
- Soot growth
- Soot oxidation
Nucleation

PAH inception

$C_2H_2, C_6H_6, C_6H_5, H_2$

Acetylene inception

$C_2H_2$

Compute from:
1. Species list
2. Empirical (non-premixed)

$$\left( \frac{DN}{Dt} \right)_{Inc.} = c_1 N_A \left( \frac{Y_{C_2H_2}}{W_{C_2H_2}} \right) e^{-\frac{21100}{T}}$$

$$\left( \frac{dM}{dt} \right)_{Inc.} = \frac{M_P}{N_A} \left( \frac{dN}{dt} \right)_{Inc.}$$
Two-equation model without radiation

Moments model with radiation

All the scaling factors for source terms are 1.0
Inter-Phase Reactions with EMP

- Following Options are Provided
  - First-order combined rate
  - Half-order combined rate
  - Second-order combined rate
  - User reaction rate
Gas phase reaction setup in STAR-CCM+

- When using the built-in reaction rate expression, input:
  - the temperature exponent
  - activation energy
  - pre-exponent, and
  - the diffusion coefficient.
General Overview of Furnace Flow

**Ore / Coke Layer**
- Falls down very slowly.

**Cohesive Zone**
- Ore layer temperature increases
- Blocked gas passage due to melted ore
- Cohesive zone of large volume

**Gas**
- Hot gas injection
- Flow upward through ore / coke layers
- Lost of heat into ore / coke layers
- Chemical reactions with ore / coke
Eulerian porous media approach

- **Gas Phase**
  - Three components: CO/CO2/N2

- **Porous media**
  - Three components: Fe/Ore/Coke

- **Boundary conditions:**
  - Outlet boundary: Pressure outlet
  - Inlet boundary:
    - Mass fraction of the gas phase: CO/N2=0.8/0.2.
    - Velocity = 15 m/s, Temperature = 2000K
Chemical reactions

- Two reactions
  - C + CO₂ → 2CO
  - Fe₂O₃ + 3CO → 2Fe + 3CO₂

- Time step: 1 sec

- The model is stable and fast:
  - 32 processors, one hour, simulated around 3000 seconds in the physical time.
Coke and Ore particle area

Solution Time 3430.5 (s)
Conversion of Ore into Fe
Eulerian multiphase: 2-phase model

- Full size furnace:
  - 25m height
  - 7.2m hearth diameter
  - 2D axisymmetric model
- Multi-component Eulerian phases:
  - Gas phase: CO, CO2, N2
  - Solid phase: Ore, Coke, Fe, Fe2O3, C
- Two reactions:
  - Fe2O3 + 3CO -> 2Fe + 3CO2
  - C + CO2 -> 2CO
Volume Fractions

Solution Time 3.1 (s)

Volume Fraction of Solid

0.61130
0.50143
0.39156
0.28168
0.17181
0.061940

Volume Fraction of Air

0.93805
0.82817
0.71829
0.60840
0.49852
0.38864
Temperatures

Temperature of Solid (K)

Solution Time 3.1 (s)

Temperature of Air (K)

Solution Time 3.1 (s)
Complex Chemistry

- Can read Chemkin format and no limit on number of species
- Online tabulation using ISAT is available
  - Factor of 2-5 speedup is commonly observed
- Dynamic load balancing is available to achieve scalability for chemistry calculation with large number of processors.
- DARS-Basic provides tool to reduce the chemistry that can be imported in STAR-CCM+ for further speedup for complex chemistry calculations.
Partially-Stirred Reactor (PaSR) in STAR-CCM+ 9.02

- PaSR representative of real turbulent combustion simulations
- Chemistry represented by a finite number of particles
- Particle composition evolves by pair-wise mixing and chemical reaction
- Can be used to test different combustion models for representing detailed chemistry
- Computationally inexpensive compared to real simulations – ideal for initial testing and setup
Analytical Jacobian for Dars-CFD

- Dars-CFD ODE integrator used for computing reaction solution
- ODE integration involves the use of Jacobian
- Computing Jacobian numerically using divided-difference is expensive and inaccurate
- Additional benefits when used with ISAT due to increased accuracy of sensitivity matrix and reduced CPU time per add
- Collaborating with Prof. Lu, University of Connecticut, to integrate use of analytical Jacobian in Dars-CFD ODE integrator
## Performance

<table>
<thead>
<tr>
<th>Test Case</th>
<th>Description</th>
</tr>
</thead>
</table>
| Baseline v8.02 | - 49 Species  
- Cp and Mw use Mixture Methods |
| Case 1 v8.06 | - 49 Species  
- Cp and Mw use Table Methods |
| Case 2 v9.01 dev | - 49 Species  
- Cp and Mw use Table Methods  
- Uniform mixture fraction spacing  
- Efficient retrieval of Table entries |
## Performance/Speed Comparison

<table>
<thead>
<tr>
<th>Test Case</th>
<th>Solver CPU Time (Serial Run) sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline v8.02</td>
<td>19078 s</td>
</tr>
<tr>
<td>Case 1 v8.06</td>
<td>13040 s</td>
</tr>
<tr>
<td></td>
<td>- 31.6% faster than Baseline</td>
</tr>
<tr>
<td>Case 2 v9.01 dev</td>
<td>8940 s</td>
</tr>
<tr>
<td></td>
<td>- 53% faster than Baseline</td>
</tr>
<tr>
<td></td>
<td>- 31% faster than Case 2</td>
</tr>
</tbody>
</table>
Performance/Speed Comparison

Speed Comparison (Flamelet Model)

<table>
<thead>
<tr>
<th>STAR-CCM+ Version</th>
<th>Solver CPU time (sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.02</td>
<td>8.06</td>
</tr>
<tr>
<td></td>
<td>9.02</td>
</tr>
</tbody>
</table>
Conclusions

- Expanding Application Coverage
- Eulerian Multi-Phase with Reactions
- LES effective but expensive
  - High fidelity calculations
- Finite-rate kinetics
  - Library-based
  - Direct chemistry coupling (no additional license requirement)
- Speedup (Detailed Chemistry)
  - Load balancing
  - Analytical Jacobian
  - ISAT
- Performance Improvement
More Examples

Note that close burner spacing in the center of the furnace leads to oxygen-starved areas up into the convection section.