Reacting flow modeling and applications in STAR-CCM+

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Better flow and mixing accuracy
Results in better prediction with PVM combustion models
\(~32.7\) million cells
\(\Delta t = 1 \times 10^{-6} \text{ s}\)

LES: Scaled Combustor

\(\text{Solution Time } 0.00611 \text{ (s)}\)

\(\text{Temperature (K)}\):
- 700.0
- 908.8
- 1117.5
- 1326.3
- 1535.1
- 1743.9
- 1952.6
- 2161.4
- 2370.2

\(\text{Mixture Fraction}\):
- 0.0
- 0.004
- 0.0085
- 0.013
- 0.017
- 0.021
- 0.025
- 0.030
- 0.034
- 0.038
- 0.042
- 0.047
- 0.051
- 0.055
LES Flare: Improved prediction of combustion efficiency

- PVM model
- ~15 million cells
- $\Delta t = 5 \times 10^{-5}$ s

More Large Eddy Simulation (LES)
- Better prediction of instantaneous flow characteristics and turbulence structures
- Computationally expensive

Include Detailed Chemistry
- Better prediction of autoignition and emissions (CO/NOx)
- Models
  - Complex chemistry model
  - Tabulated Chemistry model
**Complex Chemistry Model**

- Transport equation of chemical species

\[ \frac{\partial(\rho)\tilde{Y}_\alpha}{\partial t} + \frac{\partial(\rho)\tilde{Y}_\alpha u_i}{\partial x_i} = -\frac{\partial(\rho)\tilde{Y}_\alpha'' u''_i}{\partial x_i} - \frac{\partial\langle J^\alpha \rangle}{\partial x_i} + \langle \rho \rangle \tilde{S}_\alpha \]

- Nonlinear, stiff ordinary differential equations (ODEs)

\[ \frac{d\phi}{dt} = S_\phi(\phi, p, T) \]

**CCM**

- Computational Cost
  - Efficient ODE solver
  - Analytical Jacobian
  - Load balancing for parallel computing
  - Chemistry reduction: Offline (DRG)
  - Storage/Retrieval Scheme (ISAT)
  - Equilibrium Time Scale (Initialization)

- Turbulence-chemistry Interaction

- Eddy Dissipation Concept (EDC)

\[ \tilde{S}_\alpha(\tilde{Y}, h, \rho) \approx S_\alpha(\tilde{Y}, \tilde{h}, \tilde{\rho}) \]
Equilibrium Time Scale Model (EqTSM)

Motivation

- A better initial condition can greatly accelerate DARS-CFD

Model

- The model assumes the species composition to relax towards the local chemical equilibrium at a characteristic time scale determined based on the local flow and chemistry time scales
- Quickly provides a reasonable initial condition to DARS-CFD
- Results similar to PPDF equilibrium, but more flexible:
  - no stream limitation/no precomputed table needed/easier to set up
- Can be used as a standalone model to obtain a quick approximate solution
**Motivation**

- Detailed chemistry is important to predict autoignition and emissions (CO/NOx)
- Computationally expensive to include a full set of species

**Tabulated Detailed Chemistry for turbulent combustion**

- Precompute chemistry table and retrieve during CFD computation
  - Can use large mechanism
- Dimension reduction to chemistry
- Consider turbulence-chemistry interactions.

**Existing models**

- PPDF with equilibrium
- PPDF with laminar flamelets
- PVM (Progress variable model)
- FGM (Flamelet Generated Manifold)
FGM combustion model

Similar to the existing PVM model:
- A tabulated detailed chemistry model
- A progress variable is used to bridge the CFD side and the table

Improvements compared to the existing PVM model
- Table is from flamelet manifold
  - A turbulent flame is an ensemble of laminar flamelets
- Option of using progress variable variance
  - Presumed Beta PDF in progress variable space
- Option of considering heat loss ratio
- Flexible progress variable definition
  - Chemical enthalpy
    - Sum over all species
  - Species weights
    - Defaults: YCO+YCO2
FGM table generation in DARS-BASIC

- Generated table can be directly loaded into STAR-CCM+ for further construction
A glass furnace simulation using FGM model

- Furnace dimensions: 3.8m x 0.88m x 0.955m, fuel inlet diameter: 1.2cm
- Natural gas at 283 K at Fuel Inlet
- 10% excess air at 1373 K at Air Inlet
- Comparison with experiment at four measuring points; x= 0.6m, x = 0.9m, x =1.2m and x = 1.8m
- Illustration of approximate region of NO\textsubscript{x} formation (light blue), mixing & combustion (red)
## Boundary Conditions

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Fuel Inlet</th>
<th>Air Inlet</th>
<th>Glass Wall</th>
<th>Chamber Walls</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity (m/s)</td>
<td>125.0</td>
<td>10.0</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>283.0</td>
<td>1373.0</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Heat Flux (kW/m²)</td>
<td>-</td>
<td>-</td>
<td>90.0</td>
<td>2.0</td>
</tr>
</tbody>
</table>
Validation with IFRF glass furnace

Heat loss effect is important
Latest model additions (v 9.04-10.04)

- Include detailed chemistry with an affordable computational cost
  - Equilibrium Time Scale
  - Flamelet Generated Manifold (FGM)

- Cope with more complex configurations
  - Inert stream
  - Reacting channels

- Expand application coverages
  - Polymerization
  - Surface chemistry with multiple sites and open sites
Reaction models in STAR-CCM+

Reaction Models

- Multi-component Gas
  - Non-Premixed Combustion
  - Premixed Combustion
  - Partially-Premixed Combustion
- Multi-component Liquid
  - Emission Models (Soot/NOx/CO)
  - Eddy Contact Model (ECM)
  - Polymerization
- Lagrangian Multiphase
  - Particle Reaction
  - Coal combustion
- Eulerian Multiphase
- Interphase Reaction
- Surface Chemistry
- Reacting Channel
Combustion models for multi-component gas

Multi-component Gas Combustion

- Premixed Combustion
  - Dars-CFD
  - Premixed Eddy-Breakup (PEBU)
  - Coherent Flame Model (CFM)
  - Turbulent Flame Speed Closure (TFC)
  - Premixed PVM (PPVM)

- Non-Premixed Combustion
  - Dars-CFD
  - Eddy-Breakup (EBU)
  - Presumed PDF (PPDF)

- Partially-Premixed Combustion
  - Dars-CFD
  - Eddy-Breakup (EBU)
  - Presumed PDF (PPDF)

Emission

- SOOT
- NOx
- CO

Progress Variable Model (PVM)
Flamelet Generated Manifold (FGM)
Development objectives

- Meet all aspects of requirements from our clients
  - Wider application coverage
  - Accuracy
  - Efficiency
  - Robustness
  - Ease of use

- New model development
- Improvements to existing models
Latest model additions (v 9.04-10.04)

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Inert stream for PPDF combustion model

**Motivation**
- To reduce the PPDF table size for complex configurations where one stream, or part of the stream, is inert (negligible reactivity and sole effect is for dilution)

**Inert stream treatment**
- Only consider its dilution effects to the reacting mixture
- Compared to take it as active
  - Smaller table size
  - Faster table generation
  - Faster interpolation

**Inert stream model**
- A transport equation for the mixture fraction solved for inert stream
- Species mass fractions from reacting and inert streams
- Temperature from local total enthalpy and mean species
Reacting Channel Co-Simulation

**Application**
- Process heaters
- Cracking furnaces
- Steam reformers

**Modeling Challenges**
- Firebox side has multiple burners
- Process side has many tubes
- Full 3-D modeling is computationally intensive

**Performance Considerations**
- Uniform heat distribution
- Emissions
- Conversion rate

3-D vs 1-D
- Computationally expensive
- Computationally less expensive
Reacting Channel Co-Simulation

An elegant way to fully couple Firebox side and Process side

Gas-Phase: [FireBox Side]
- 3-D, turbulent flow
- Combustion models
- Heat transfer

Reacting Channel: [Process Side]
- 1-D Plug Flow Reactor (PFR)
- Inlet composition, temperature
- Process-side reactions
- No meshing, solving with STAR-CCM+

Coupling
- Temperature is provided to the process side
- Heat flux is returned back to firebox side
Output from Co-simulation: Process Side

Axial distribution of Temperature, Heat Flux, and Species conversions

CH4 Mass Fraction

H2 Mass Fraction

Velocity (m/s)

Boundary Heat Flux (W/m^2)
Expand our application coverage

Polymerization Process
- monomers are linked by chemical reactions to form long chains
- starts with mixing a Monomer (M) and an Initiator (I) in a Solvent (S)
- Steps involved: initiation/propagation/transfer/branching/termination
- Final product is polymers of varying lengths and structure.

Polymerization Moment Model for free radical polymerization
- Scalar Transport Equations for Moments are solved in STAR-CCM+: live/dead polymers
- source terms of the above moment transport equations depend on the sub processes of polymerization.
- Provide: total polymer concentrations, NACL/NAMW, WACL/WAMW, polydispersity index
Industrial-Scale Stirred Tank Reactor – Styrene Polymerization

- Steady (Implicit Unsteady)
- K-Epsilon Turbulence
- Realizable K-Epsilon Two-Layer
- Two-Layer All Y+ Wall Treatment
- Multi-Component Liquid
- Polymerization
- Segregated Flow
- Segregated Fluid Enthalpy
- Three Dimensional
- MRF, RBM

Polydispersity index
Multiple sites for surface chemistry

Chemical vapor deposition (CVD) reactor

Surface Bulk Growth Rate of Si(B) (m/s)
Open sites for surface chemistry

吸附反应的描述

- 原子位
  - $\text{AsH}_3(g) + \text{Ga}(s) \rightarrow \text{AsH}_3(s) + \text{Ga}(b)$
- 开放位
  - $\text{O}(s) + \text{AsH}_3(g) \rightarrow \text{AsH}_3(s)$

开放位的处理

- 被视为一种物种
- 不包含任何元素（为空）
- 在CHEMKIN动力学输入文件中命名为OPEN
Applications

- **Large Eddy Simulation (LES) with detailed chemistry**
  - Gas turbine combustors
  - Burners, Furnaces and Incinerators
  - Fires

- **High speed flows**
  - Scramjet
  - Rocket engine nozzles

- **Multiphase reactions**
  - Coal reactors: Pulverized/Fluidized bed
  - Surface chemistry (SCR/CVD)

- **Optimizations**
  - Chemistry
  - Combustor design
Applications

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Combustion Systems

**System Level**
- **Emissions**
  - UHC
  - Soot
  - Nox
  - CO
- **Fuel Flexibility, Flame Stability**
  - Flame shape
  - Flame location
  - Flash-back/ blow-off
  - Gaseous/liquid Fuels
- **Thermo-acoustic Instability**
- **Mechanical Durability**
  - Liner temperature
  - Component temperature
- **Cost**

**Unit Level**
- **Fluid Dynamics**
  - Flow and mixing
    - Swirlers
    - Bluff bodies
- **Combustion Chemistry**
  - Fuel formulation
  - Operating conditions
  - Chemical kinetics
  - Thermodynamics
- **Heat Transfer**
  - Conduction
  - Convection
  - Radiation
Liquid Droplet Combustion

Droplet Evaporation
- Quasi-steady
- User defined

Droplet Break-up
- Primary atomization
  - Linear Instability Sheet Atomization (LISA)
- Secondary break-up
  - Kelvin Helmholtz-Rayleigh Taylor (KHRT)
  - Taylor Analogy (TAB)
  - Stochastic Break-up (SSD)

Droplet Wall-impingement
- Bai-Gosman
- Satoh

Collision Detection Model
- No Time Counter (NTC)
- O’Rourke

Two-way Coupling

Turbulence Dispersion
- Random Walk Technique
Performance Improvements: Large Cases (LES)

- Flow Solver improvements in v9.04

- Combustion solver improvements in v9.02 (40-50% speedup)

- Flow and Lagrangian solver improvements in v9.04 (20-25% speedup from v9.02)
Run RANS first before attempting LES.

Need good quality mesh for LES. Keep a mesh size that gives a cut-off wavenumber within the inertial subrange.

Use bounded central differencing (BCD) with appropriate blending factor for LES runs.

The coupling frequency for Lagrangian (in the case of spray combustion) and radiation can be adjusted for faster run times.
  - Lagrangian update can be done once every time-step
  - Dynamic load balancing for Lagrangian spray helps with speed up

Set-up of monitors for means and variance in LES. Start sampling after 4-5 flow times.
Fuel/Air Ports

Bad surface mesh
Fuel ports not adequately resolved

Good surface mesh
Fuel ports well resolved

Recommended to have at least 2 prism layer cells and a total of 8 cells across the ports.
In case of swirlers, and other narrow passageways, need to make sure there are adequate cells and good prism layers to get the right velocity profile.

Pipes and tubes that are common in process heaters are required to be meshed in such a way that their curvature is retained.
Volumetric Refinement

Use volume control blending with a blending factor of 0.5 to obtain smooth transition between overlapping volumetric controls.

Note: blending factor has little or no effect on core mesh if the volumetric control is far away from the surface boundaries.
Table Based Refinement

Field function used for determining new mesh size

\[ \text{($MixtureFraction_0 > 0.5)? 2e-4 : (($MixtureFraction_0 > 0.3)? 5e-4 : (($MixtureFraction_0 > 0.1)? 0.0025 : 0))} \]

Other criterions for mesh refinement

- Temperature, temperature gradient
- Velocity, velocity gradient
- Species concentrations, their gradients
Applications

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- Multiphase reactions
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- Optimizations
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High Speed Reacting Flows

Density-based Solver
- Coupled, implicit formulation with AMG acceleration
- TVD reconstruction
  - AUSM+ or Roe inviscid flux schemes
  - MUSCL + Venkata limiter

Real gas models
- Redlich Kwong
- Soave-Redlich Kwong
- Modified Soave-Redlich Kwong
- Peng Robinson
**Advanced Initialization**
- Grid sequencing option
- Fully implicit newton-type solution algorithm
- Controllable number of coarse levels

**Continuity Convergence Accelerator (CCA)**
- Used for high speed flows where convergence for mass flow is slow
- Solves pressure correction equation using density based Riemann Flux discretization
- Overall and individual cell mass imbalances are minimized at each iteration
- Option available for Coupled Implicit Solver.
Combustion Modeling in High Speed Flows

**Global Chemistry**
- Single or multi-step
- Variants of eddy break-up model
  - Standard
  - Hybrid
  - Combined time-scale
    - Kinetics only

**Tabulated Chemistry**

**Detailed Chemistry**
- DARS-CFD stiff chemistry solver
- Use Equilibrium Time-Scale approximation for initial guess
- Then switch to finite rate chemistry
  - Laminar flame concept
  - Eddy dissipation concept
Coupled Implicit, Axisymmetric

Steady, SST K-Omega turbulence

Detailed chemistry: 11 species

DARS-CFD Approximation options:

- In-situ Adaptive Tabulation
  - Populates source terms as the simulation progresses for subsequent look-up
  - Speeds computational time once the table is populated

- Equilibrium Time-Scale
  - Quick approximate solution for detailed chemistry calculations
  - Assumes chemical composition relaxes to local equilibrium composition at time-scale determined by flow and chemistry
Supersonic Combustion

- H₂ Fueled NASA SCHOLA direct-connect Scramjet engine
- Validate against experiment and NASA VULCAN code

Mesh:
1.4M Hex-dominant
10 Prism Layers
Solver:
Density based solver
Steady, k-w SST, AUSM+FVS
Non-adiabatic PPDF
Applications

Large Eddy Simulation (LES) with detailed chemistry
- Gas turbine combustors
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- Fires

High speed flows
- Scramjet
- Rocket engine nozzles

Multiphase reactions
- Coal reactors: Pulverized/Fluidized bed
- Surface chemistry (SCR/CVD)

Optimizations
- Chemistry
- Combustor design
Coal-fired boilers and gasifiers

Coal combustors
- Pulverized
- Fluidized bed

Simulation motivations
- Particle nozzle design
- Stability
- Combustion efficiency
- New combustion technologies for low NOx/SOx

Simulation approaches
- Lagrangian particle
- Eulerian Multiphase (EMP)
- Discrete Element Method (DEM) particle
Gas phase
- Solves transport equations for mass/momentum/energy and species

Particle Momentum Transfer
- Solves equation of motion for parcels of dispersed phase
- Surface and body forces can be included
- Turbulent dispersion model available

Two-Way Coupling
- Particle Mass Transfer
  - Drying of coal
  - Release of coal volatiles
  - Oxidation of char
- Particle Heat Transfer
  - Heat up of particles
  - Radiative transfer in the presence of particles
Heterogeneous Reactions for Particles

- Raw Coal Devolatilization
  - Two-step devolatilization
  - User-defined devolatilization

- Char Oxidation
  char reaction with O2, H2O and CO2
  considers gas phase diffusion and heterogeneous reaction
  - First-order char oxidation
  - Half-order char oxidation
  - User-defined char oxidation

- SO2 reactions

NOx

- Thermal NOx – 3 step Zeldovich
- Prompt NOx – global chemistry
- Fuel NOx – source of nitrogen from volatiles and char

Gas phase reactions

- Global chemistry
Coal Combustion Validation

Model Selection:
- Coal particles
  - Moisture evaporation
  - Raw coal de-volatilization
  - Char oxidation
  - Fuel NOx + Thermal Nox
  - Particle radiation
- Gas Phase
  - 4 step global kinetics
  - Radiation
    - Participating Media
      Weighted Sum of Gray Gases

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Measured</th>
<th>Predicted</th>
<th>Dimension</th>
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<tbody>
<tr>
<td>T</td>
<td>1353</td>
<td>1347</td>
<td>Kelvins</td>
</tr>
<tr>
<td>Oxygen</td>
<td>3.0</td>
<td>3.08</td>
<td>Vol. %, dry</td>
</tr>
<tr>
<td>CO₂</td>
<td>15.6</td>
<td>15.43</td>
<td>Vol.%, dry</td>
</tr>
<tr>
<td>Burnout</td>
<td>99.4</td>
<td>100.0</td>
<td>Weight %</td>
</tr>
</tbody>
</table>

Selective Catalytic Reactions: Surface Chemistry

- Spray dynamics
- Gas chemistry & surface chemistry in the catalyst
- Turbulence mixing & heat transfer

• Main challenges/objectives in SCR design:
  Minimum dosing, maximum NOx reduction, prevention of NH$_3$ slip
Global Chemistry
- One or two step reactions
- Computationally fast
- Might need tuning of kinetic parameters

Detailed Chemistry with porous media
- DARS-CFD solver for stiff equations
- Computationally expensive
- Spatially more accurate
Results – NOx Reduction Comparison

Two-Step Model

Detailed Surface Chemistry
Application Example: SCR modelling

- Lagrangian droplets are injected into the hot exhaust flow
- The liquid droplets and gas exhaust pass through a mixing vane
- Some of the droplets impinge on the vane and form a film which boils
- The mixture of exhaust gases and boiled vapour move into the catalyst
Applications

- Large Eddy Simulation (LES) with detailed chemistry
  - Gas turbine combustors
  - Burners, Furnaces and Incinerators
  - Fires
- High speed flows
  - Scramjet
  - Rocket engine nozzles
- Multiphase reactions
  - Coal reactors: Pulverized/Fluidized bed
  - Surface chemistry (SCR/CVD)
- Optimizations
  - Chemistry
  - Combustor design
Optimization of Gas Turbine using STAR-CCM+ and Optimate+

Geometry Optimization or Operating Condition Optimization

- Match flame length and shape with experiments,
- Minimize NOx and CO emissions,
- Minimize pressure drop,
- Maximize combustion efficiency,
- Maximize homogeneity at combustor exit
Hybrid
- Blend of search strategies

Adaptive
- Adapts to design space

Efficient
- Set-up very easy
- Solution found in

Robust
- Global and local optimization at the same time

Easy to use
- One parameter: Number of runs
Generic Combustor for Optimization

❖ Combustor Type – Annular
   – Optimize geometry based on performance objectives

❖ Parameterized design features
   – Swirler twist angle
   – Liner hole radius
   – Hollow cone injector’s
     • Inner and outer cone angle
Parameter Ranges

Swirler geometry for Min (16°), Baseline (45°), Max (93°)

Hole radius for liner: Min=1mm, Baseline=2mm, Max=2.9 mm

Inner cone angle: 0 to 45 degrees. Outer cone angle: 45 to 120 degrees
Pareto Optimization – Results

Objective 1 - Total CO at outlet (kg/s)

'Pareto Front' & Baseline

Rank 1

Baseline
## Optimization Result

<table>
<thead>
<tr>
<th>Case</th>
<th>Baseline (Rank – 40)</th>
<th>Rank – 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Twist angle (°)</td>
<td>45</td>
<td>51</td>
</tr>
<tr>
<td>Liner Hole Radius (mm)</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>Inner Cone Angle (°)</td>
<td>10</td>
<td>37</td>
</tr>
<tr>
<td>Outer Cone Angle (°)</td>
<td>90</td>
<td>61</td>
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<tr>
<td>Cone Angle (°)</td>
<td>80</td>
<td>24</td>
</tr>
<tr>
<td>Volume averaged T (K)</td>
<td>1000.7</td>
<td>969.5</td>
</tr>
<tr>
<td>Total CO (kg/s)</td>
<td>9.441E-07</td>
<td>8.613E-07</td>
</tr>
<tr>
<td>Total NOx (kg/s)</td>
<td>2.697E-08</td>
<td>1.126E-08</td>
</tr>
<tr>
<td>Performance</td>
<td>-2.00</td>
<td>-1.33</td>
</tr>
</tbody>
</table>
Summary

New models added to (v 9.04-10.04)
- Include detailed chemistry with an affordable computational cost
  - Equilibrium Time Scale
  - Flamelet Generated Manifold (FGM)
- Cope with more complex configurations
  - Inert stream
  - Reacting channels
- Expand application coverages
  - Polymerization
  - Surface chemistry with multiple sites and open sites

Applications
- Large Eddy Simulation (LES) with detailed chemistry
- High speed flows
- Multiphase reactions
- Optimizations
Thank you for your attention!