ANSYS Strategy for Internal Combustion Engine Simulations

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IC Engine Products at ANSYS

- Workbench – ICE System (WB-ICE)
  ANSYS Workbench based ICE analysis

- FORTÉ
  Full 3D CFD analysis for IC engine designers

- Model Fuels Library
  Best-validated fuel models in the market (~60)

- CHEMKIN PRO
  Ignition, flame-speed tables, zonal models

- CHEMKIN-PRO REACTION WORKBENCH
  Fuel analysis and mechanism reduction
The ANSYS strategy for IC engine simulations is: FORTÉ CFD

- We are investing in the ANSYS FORTÉ solution:
  - Integrating RD Products into ANSYS Workbench and WB-ICE
  - Integrating with FLUENT for conjugate heat transfer (CHT)
  - Developing new capabilities
  - Performing extensive verification and validation tests
  - Continuing development of fuel models & fuel modeling tools

- FLUENT (with WB-ICE) remains a supported option for cold-flow and scale-resolved turbulence simulation
A brief history of FORTÉ CFD

• Partnered with Profs. Rolf Reitz and Chris Rutland
  – State of the art spray models
  – Engine design expertise
• Reaction Design
  – Combustion kinetics and kinetics solvers
• Model Fuels Consortium experience
  – 7+ year, industry-led effort
  – Comprehensive library of fuel models for engine combustion simulation
• Now part of ANSYS, Inc.!
  – Full suite of analysis tools and integration
Key advantages of FORTÉ CFD

• Set up tailored to IC Engines
• Automatic mesh generation
  – On-the-fly, dynamic mesh motion
• Well validated fuel-combustion kinetics with fast solver
  – Capture fuel effects
  – Predict ignition, emissions
  – Predict flame-front location and knocking in SI engines
• State-of-the-art spray and spray-wall models
  – Capture physics accurately and robustly
FORTÉ provides auto-generated, Cartesian immersed-boundary mesh

- Dynamic mesh from CAD:
  - CAD STL data read directly into FORTÉ
  - WB-ICE can be used to provide geometry
    - E.g., Fluent *.msh file read in => surface mesh
  - FORTÉ generates the mesh on-the-fly
    - With automated refinement around valve gaps and small features
    - Preview the mesh in the Simulation Interface

- Flexible mesh options:
  - Fully automatic Cartesian meshing
  - Body-fitted sector meshing for quick diesel design studies
    - Sector Mesh Generator included
    - ICEM-CFD can also be used
FORTÉ integration with WB-ICE allows quick geometry preparation from CAD
Advanced solution techniques allow practical turn-around with chemistry

A good chemistry mechanism is key to predicting engine combustion behavior
Example: Dual-fuel heavy-duty engine

- RCCI Simulation with 470-species for Diesel & Gasoline
- CPU time (16 CPUs): < 4 hours

CO and UHC agree with experiment

From: K. Puduppakkam, et al., SAE 2011 World Congress
Particles are used to track the initial kernel growth and flame location. The spark ignites a kernel of gas that is very small at first. The flame (typically <~0.01 mm thick) propagates through the unburned gas. Afterwards, the level-set (G-eq.) method takes over in tracking the flame front.

Flame represented by the $G=0$ iso-surface. When the flame structure grows big enough so that it can be resolved by the mesh, the particles are no longer needed.

The flame propagation responds to local turbulence conditions and chemistry is solved throughout.

FORTÉ spray model captures all the physics with reduced mesh dependence

- Even with a coarse mesh, the spray characteristics are well represented
  - Allows quick exploratory studies as well as detailed
  - Removes need to iteratively test for mesh “convergence”

From N. Abani, A. Munnannur, and R. D. Reitz, ILASS 2006
(Data from Naber and Siebers, SAE960034)
FORTÉ includes advanced spray-wall interactions

- Important to many engine simulations:
  - Cold start of PFI engines
  - Fuel/air mixing in DISI and GDI engines
  - Soot from small-bore diesel and GDI engines

- FORTÉ includes physics for:
  - Droplet stick, rebound
  - Droplet splash
  - Film spread, separation (stripping)
Work-in-progress for FORTÉ and WB-ICE

• Optional gradient-driven mesh refinement
• Multi-cylinder simulations
• Conjugate Heat Transfer coupling with Fluent
• Full automation & scripting through WB
  – Parameterization of geometry inputs
  – Optimization of geometry as well as other parameters
Summary of key capabilities in FORTÉ

• **Ease of Use**
  – Automatic mesh generation with moving boundaries
  – Workflow specifically for engine combustion simulations

• **Accuracy**
  – Detailed kinetics tied to Model Fuels Library to capture fuel effects
  – Track flame front location using level-set method, DPIK for SI engines
  – State-of-the-art spray and spray-wall models
  – Capture correct physics on practical mesh
  – Direct prediction of ignition, emissions, particle size

• **Speed**
  – Fast and accurate chemistry solver
  – Parallel (MPI) simulation using automatic domain decomposition

• **Integration with other simulation**
  – Integration with WB-ICE, ANSYS Workbench for fluid-structural interactions
Applying FORTÉ to Design Simulations: Importance of the Fuel Model
Changing engine-design requirements shift the focus to the fuel model.
Model Fuels Library (MFL)

• The MFL enables detailed fuel modeling
  – Represent complex “real” fuels with appropriate model fuels
  – Extensively validated chemistry

• Results from the MF Consortium:
  – 7 years and $7 million invested
  – Involved 20 companies

• The MFL is now continuously updated and maintained through a subscription program
  – Internal expertise adds & improves models
  – Advised by world-wide experts
A model fuel should match real fuel properties

**Desired Fuel Properties**

Set target characteristics
- Class composition
- Heating value
- Octane / Cetane #
- H/C ratio, O content
- Boiling points
- Sooting threshold index

**CHEMKIN Reaction Workbench**
- Select surrogate components
- Optimize blend to match properties

**Surrogate fuel composition**
- n-heptane: 19%
- Iso-octane: 45%
- 1-pentene: 15%
- mc-hexane: 15%
- m-xylene: 3%
- Ethanol: 1%
- m-xylene: 15%

**Model Fuel Library**
- Aromatics
- Olefins
- C-paraffins
- i-paraffins
- n-paraffins

**Fuel Model for Simulation**
A good chemistry mechanism is key to describing the fuel combustion behavior

The engine is a chemical plant:

Fuel

Chemical reactions between molecules

Air \((O_2 + N_2)\)

Horsepower
Heat release

\(CO_2, H_2O\)

\(CO, NO_x, PM\)

Unburned HC

Many other species
The Model Fuel Library is a large set of validated fuel-component mechanisms

~ 60 Validated Fuel Models

- Biodiesel Components
- Diesel and Jet-Fuel Surrogates
- Gasoline Surrogates
- Gaseous Fuels

+ Detailed Particle-based and Pseudo-gas Soot Models

- Common core chemistry
- Consistent rules for reaction rates
- Validated fuel-blending behavior
With a good fuel model, we match emissions in high-performance Diesel engines

- Detailed (7-component fuel model), 500 gas-phase species, multi-step soot model
- Combustion and emissions trends captured with no change to model or model approach

Joint publication with BMW: Puduppakkam, et al. SAE Powertrain Fuels and Lubes, 2014
Detailed kinetics also enable prediction of soot in GDI engines

SAE 2014-01-1135, Naik, et al..

7-component gasoline fuel model
230 species mechanism
Full cycle simulations using RNG k-eps

Data from IFPEN, Pires da Cruz et al.
FORTÉ can predict knocking tendency

- Detailed chemistry predicts end-gas auto-ignition
- Pressure sensor monitors, just like the test stand

Pressure sensors in FORTÉ simulation match experimental setup

- Allows exploration of trade-offs
  - Fuel effects, spark timings, higher compression ratios, boost, etc.

FORTÉ calculates Knock Intensity

SAE 2007-0Cal1-0165
Knocking can also be visualized in FORTÉ

- White/Black grid line intersections shows flame front location
- Contour plot shows temperature distribution in the engine

No knocking observed

![Flame Front](image)

Auto-ignited end gas ahead of the flame front

- Intake Pressure = 0.9bar
- Spark Timing = -32CA ATDC

Significant knocking observed

![Flame Front](image)

- Intake Pressure = 1.2bar
- Spark Timing = -32CA ATDC
Better fuel model = better predictions

- Multi-component fuel model captures knock in the engine where a single-component fuel does not

Same engine conditions

The only difference is the fuel model
Overall Summary

- ANSYS is committed to advancing IC Engine Simulation
- FORTÉ is the core of the ANSYS IC engine strategy
  - New capabilities and WB integration well underway
  - Integration with Fluent for CHT
  - Continuous improvement on performance and scalability
  - Validation and verification is an active and continuous process
- The Model Fuels Library is key to accurate combustion, and for soot and knocking predictions
- We are working closely with customers to fine-tune our long-term plan and address critical short-term needs