Numerical study & validation of a complete SCR system using 1D-3D (CFD) coupling

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Company overview

Convergent Science Inc.

- Founded in 1997, headquartered in Madison, Wisconsin, USA
- Founders are alumni of ERC (Engine Research Center, Univ of Wisconsin-Madison)
- Experts in CFD, engine analysis, combustion, spray modeling, and design optimization
- Started selling Converge in 2008
- CSI is a rapidly growing and stable organization. Offices in US, Europe, India, and distributors all over the globe

CONVERGE CFD Software was developed as a specialized tool for IC Engine Combustion CFD analyses, but now it is very much suitable for many other applications.
CONVERGE: What’s different

Traditional Approach

- Long meshing times
- Meshing by guessing
- Skewed cells
- Moving/deforming mesh
- Grid convergence?

CONVERGE Approach

- Automated meshing (no meshing time)
- Adaptive Mesh Refinement (AMR) – no more guessing
- Orthogonal cells
- Easy to perform grid convergence studies
Meshing in CONVERGE is done by the solver automatically during run-time

- **Grid Scaling**
  Scale the entire mesh up or down at pre-described times

- **Grid Embedding**
  Specify areas a-priori within the domain where you wish to have a fine mesh, and turn off when not required

- **Adaptive Mesh Refinement**
  Automatically refine the mesh based on gradients in the flow. Different variables like Temperature, Velocity, Species and Y+

All the above have time control: Permanent, Sequential and Cyclic
Almost 400 papers published!

SELECTED BIBLIOGRAPHY FOR CONVERGENT SCIENCE & CONVERGE CFD SOFTWARE

Updated August 01, 2017

Georgia Southern University

Wayne State University, University of Connecticut, Storrs

Wayne State University, Georgia Southern University, Shanghai Jiao Tong University

Georgia Southern University, Rensselaer Polytechnic Institute, University of Connecticut

Southwest Research Institute

Southwest Research Institute

Indian Institute of Technology Madras

Indian Institute of Technology Madras

University of Illinois at Chicago, Convergent Science

King Abdullah University of Science and Technology

King Abdullah University of Science and Technology

Indian Institute of Technology Bombay

Southwest Research Institute
Abidin, Z., Hoag, K., Micke, D., and Badain, N., "Port Design for Charge Motion Improvement within the Cylinder," SAE Paper 2016-01-0600, 2016. DOI:10.4271/2016-01-0600
CONVERGE & GT-Suite coupling

After-treatment modeling
CONVERGE Speeds Urea/SCR CFD Simulations

- Automatic meshing
  - No user-meshing
  - Automatic grid-scaling
  - Adaptive Mesh Refinement (AMR)
  - Mesh dependent → Grid-converged
- Superfast transient solver
  - Time-accurate
- Comprehensive set of accurate models
  - Spray/Film
  - Urea decomposition
CONVERGE Models for Urea/SCR

- Primary / Secondary liquid breakup
  - Drop collision / coalescence
  - Dynamic drop drag
- Urea decomposition in spray / films
  - Multi-component and Molten-solid
- Liquid wall interaction
  - Kuhnke, Wruck and Bai-Gosman models
  - Filming, splashing, stripping, separating
- Conjugate Heat Transfer (CHT)
- Surface chemistry
  - through link to GT-SUITE
Urea/SCR Validation Cases

Single urea-water droplet

Urea-water sprays
J.Y. Kim, et al ICEF 2004-889

Spray – wall interaction
F. Birkhold, et al. SAE 2006-01-0643

Urea/SCR system with NOx reduction
Z. Abadin, et al, SAE 13PFL-0137
SwRI Case Description

SCR-1 Mixer Case

SCR-2 No Mixer Case

Z. Abadin et al, “3D-Semi 1D Coupling for a Complete Simulation of an SCR System,” SAE 13PFL-0137
SwRI Set Up in CONVERGE

- Hollow cone spray
  - 22 µm Rosin-Rammler distribution
  - Multiple-component urea model
  - TAB secondary breakup
- Time-accurate Unsteady RANS turbulence
- Mesh Controls
  - 5mm base mesh (2 M cells)
  - AMR for Velocity (3 levels-1.25mm)
  - Fixed embedding on walls and mixer
- Porous media for SCR pressure drop
UWS Simulation Approaches in CONVERGE

Multiple-Component Approach (urea_flag = 1)
- Nozzle
- Water & Urea Evaporating → Urea decomposing (gas-phase only) → Hydrolysis of HNCO → Ammonia (NH3)
- Iso-cyanic acid (HNCO)

Molten-Solid Approach (urea_flag = 2)
- Nozzle
- Water Evaporating
- Urea decomposing (Solid to gas)
- Ammonia (NH3)
- Iso-cyanic acid (HNCO)
- Hydrolysis of HNCO

Water Evaporated
Only Urea left

Urea water multi-component parcels
Urea only
SwRI Results

SCR-1

SCR-2

Time-Averaged
Results at SCR Inlet

**SCR-1**
- Uniformity Index (UI)
  - UI = 0.74
- Ammonia NOx Ratio (ANR)

**SCR-2**
- Uniformity Index (UI)
  - UI = 0.78
- Ammonia NOx Ratio (ANR)
SwRI SCR Coupled 1-Way Results

- CONVERGE to GT-Suite Link
  - Surface chemistry in catalyst solved using 3D reactor module
- Validated GT-Suite SCR model
  - Olssen 2008
  - $12 \times 12 \times 10 = 1,440$ mesh zones
  - Pass back pressure & flow conditions at interface
Other advanced capabilities

- SAGE Detailed Chemistry Solver
- Multi-cylinder simulations
- Multi component liquid modeling
- Conjugate Heat Transfer
- Complex moving boundaries
- Gas Turbine Combustion
- Fuel injection and sprays
Summary

CONVERGE CFD Software is the most powerful CFD software because:

• **Total elimination of user meshing time!**
• **Moving boundaries can be handled very easily**
• **Adaptive Mesh Refinement**
• **Detailed Chemistry Solver (SAGE) with Multi-Zone model**
• **In-built Optimization solver (CONGO)**
THANK YOU!
CONVERGECFD.COM