





Industrial pulverized coal furnace

Advanced Chemistry in Reacting Flow Using CHEMKIN-CFD and ANSYS FLUENT Software

ANSYS, Inc. and Reaction Design[®] have partnered to provide an advanced capability for simulating detailed chemistry in multidimensional, chemically reacting flows. The resulting technology closely couples Reaction Design's CHEMKIN-CFD chemistry solver with flow simulation capabilities in ANSYS FLUENT software, facilitating highly accurate combustion and emissions analysis for automotive engine and industrial power design. The analysis can be steady state or transient, and two dimensional or three dimensional. The CHEMKIN-CFD module, licensed by Reaction Design, is available to ANSYS FLUENT licensees for free.

Chemical mechanisms are readily available that provide good simulation accuracy for many important commercial combustion and materials processes. However, many of these mechanisms can be quite large, involving thousands of reactions and hundreds of species. But detailed mechanisms are often required to achieve acceptable accuracy and trace species predictions. Employing detailed chemistry leads to:

- · Predictions of both ignition and emissions for automotive engine designs
- Predictions of emissions, stability and durability for turbine, boiler and burner combustor designs
- Increased efficiency, improved yields, and reduced manufacturing costs for materials manufacturing processes ranging from glass coatings to semiconductor devices and solar cells







IC engine flow field



Flame propagation within an IC combustion chamber



Annular gas turbine combustor

CHEMKIN-CFD brings the chemistry solving power of CHEMKIN-PRO to CFD simulations, providing remarkable solution speed and stability. CHEMKIN-CFD takes advantage of unique mathematical techniques originally developed for CHEMKIN-PRO to facilitate major improvements in the speed of calculation, as shown in Figure I. CHEMKIN-CFD now converges up to five times faster than previous versions of CHEMKIN CFD (formerly called KINetics). Other solver enhancements eliminate the exponential relationship between solution time and number of species to approximate a more linear increase. This means that the use of fully detailed or skeletal chemistry is now practical in a commercial development environment.

Selected Mechanisms Included with CHEMKIN-CFD for ANSYS FLUENT

To help jump start your efficiency, the CHEMKIN-CFD module for ANSYS FLUENT technology comes with several sample multi-step reaction mechanisms that are useful for many combustion applications. The following mechanisms are included with CHEMKIN-CFD for ANSYS FLUENT installation:

- Methane/ethane: 50-species version of GRI-Mech 3.0
- Propane: 37-species high-temperature mechanism
- Hydrogen: two mechanisms:
 - 9-species version for H₂ combustion
 - 21-species version for H₂ combustion with NO_x

System Requirements and Support

CHEMKIN-CFD for ANSYS FLUENT is included with each version of FLUENT version 6.2 or higher.

Supported OS: Windows® and Linux® (32-bit and 64-bit) or AIX® (64-bit)



More Information

Contact Reaction Design to find out more about how this advanced chemistry capability can work to your advantage. 858.550.1920 info@reactiondesign.com www.reactiondesign.com

www.ansys.com



GSA Contract Holder

ANSYS, Inc. Southpointe 275 Technology Drive Canonsburg, PA 15317 U.S.A. 724.746.3304 ansysinfo@ansys.com Toll Free U.S.A./Canada: 1.866.267.9724 Toll Free Mexico: 001.866.267.9724 Europe: 44.870.010.4456 eu.sales@ansys.com

ANNYS ANNYS Workbench, Ansoft, AUTODYN, CFX, FLUENT and any and all ANYS. Inc. brand, product, service and feature names, logos and diogans are registered trademarks or trademarks of ANSYS, Inc. or its subsidiaries in the United States or other countries. ICEM CFD is a trademark used under license. All other brand, product, service and feature names or trademarks are the property of their respective owners.

Image Credits: Some images courtesy FluidDA nv, Forschungszentrum Joülich GmbH, Heat Transfer Research, Inc., Riello SPA and iStockphoto.com

© 2009 ANSYS, Inc. All Rights Reserved. Printed in U.S.A.