ANSYS®

Combustion Modeling using Ansys CFD

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Agenda

- ✓ ANSYS & Key Technologies
- ✓ Simulation Driven Product Development
- ✓ What is CFD?
- ✓ ANSYS FLUENT
- ✓ ANSYS Solutions
  - ❖ Combustion Modeling
  - ❖ DPM & Spray Modeling
  - ❖ Pollutant/Emissions Modeling
- ✓ Application Test Case(s)
- ✓ Summary & Demo

ANSYS - Simulation Leader

FOCUSED

This is all we do.
Leading product technologies in all physics areas
Largest development team focused on simulation

TRUSTED

96 of the top 100

FORTUNE 500 Industrials
ISO 9001 and NQA-1 certified

CAPABLE

2,700+ employees

75 locations

40 countries

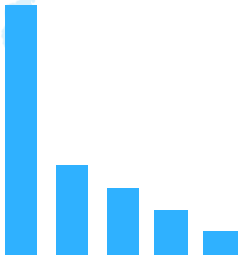
PROVEN

Recognized as one of the world's **MOST INNOVATIVE AND FASTEST-GROWING COMPANIES***

INDEPENDENT

Long-term financial stability
CAD agnostic

LARGEST



3x The size of our nearest competitor

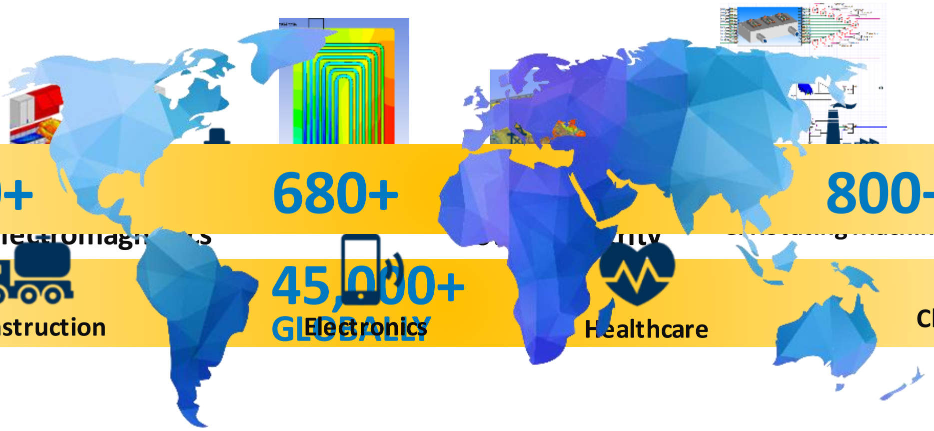
*BusinessWeek, FORTUNE

Our Industry Reach and Solution Offerings

Leading Disciplines

Industry Presence

Global Reach



PEOPLE 1,300+ 680+ 800+

2,000+ FROM CHANNEL PARTNERS

CUSTOMERS 45,000+ GLOBALLY

Fluids

Semiconductors

Aerospace & Defense

Construction

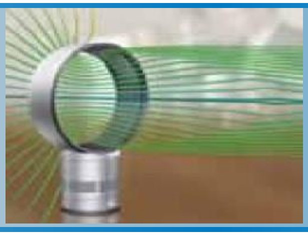
Electronics

Healthcare

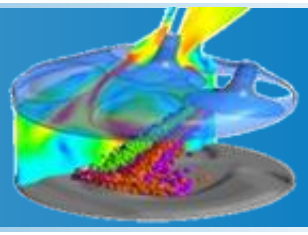
Materials & Chemical Processing

Breadth of Technologies

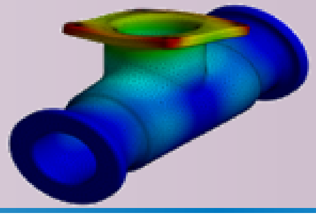
Fluid Mechanics:
From Single-Phase Flows



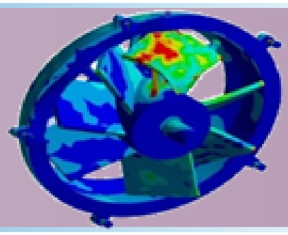
To Multiphase Combustion



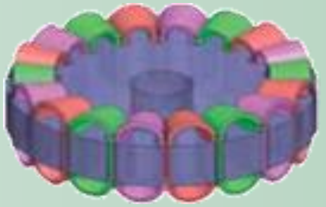
Structural Mechanics:
From Linear Statics



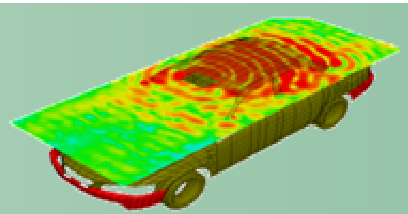
To High-Speed Impact



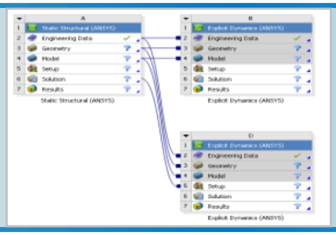
Electromagnetics: From Low-Frequency Windings



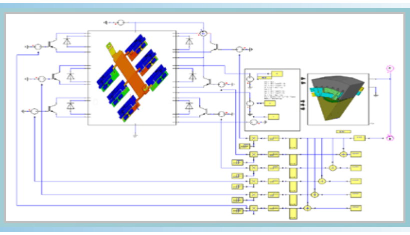
To High-Frequency Field Analysis



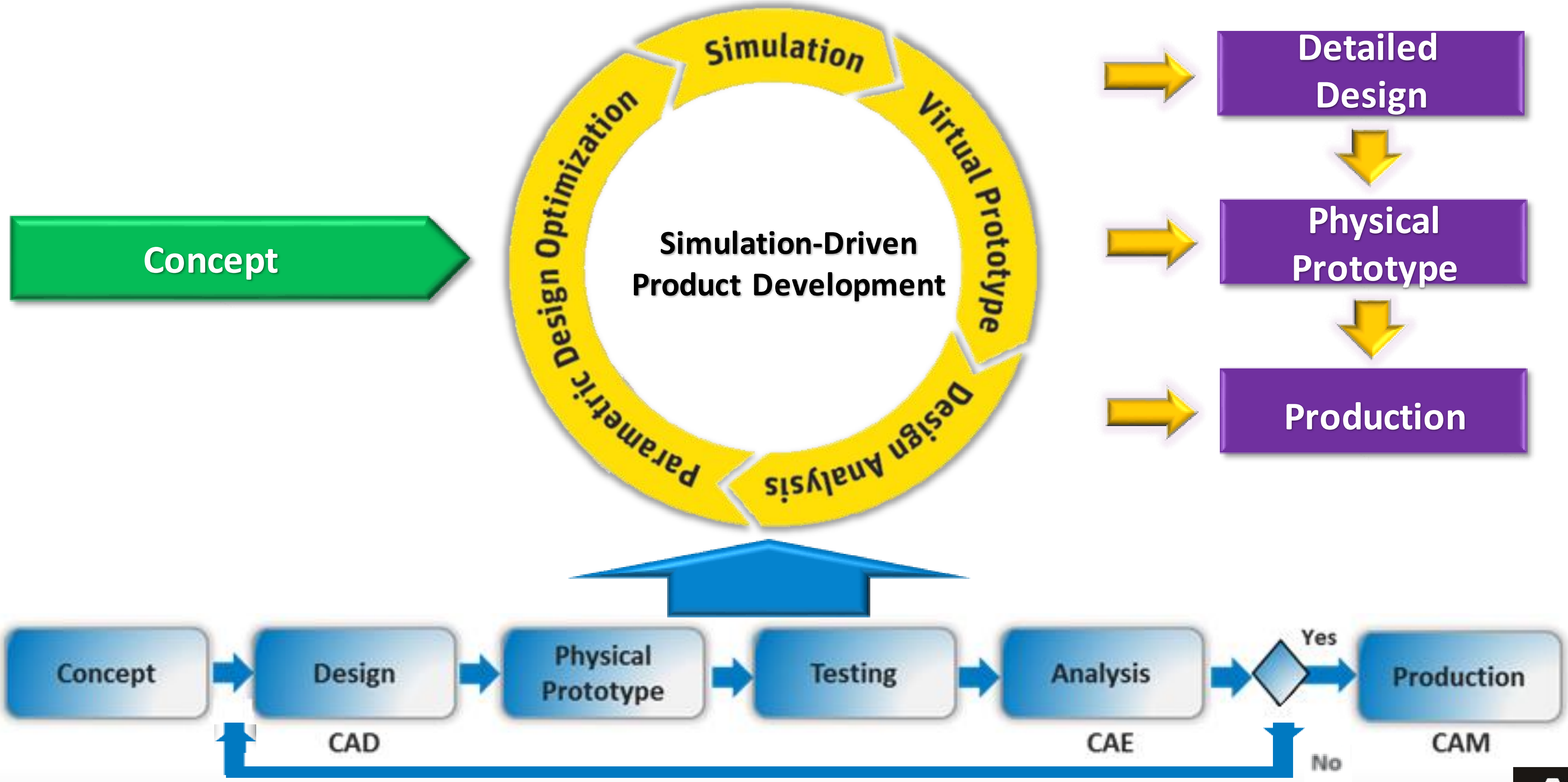
Systems:
From Data Sharing



To Multi-Domain System Analysis

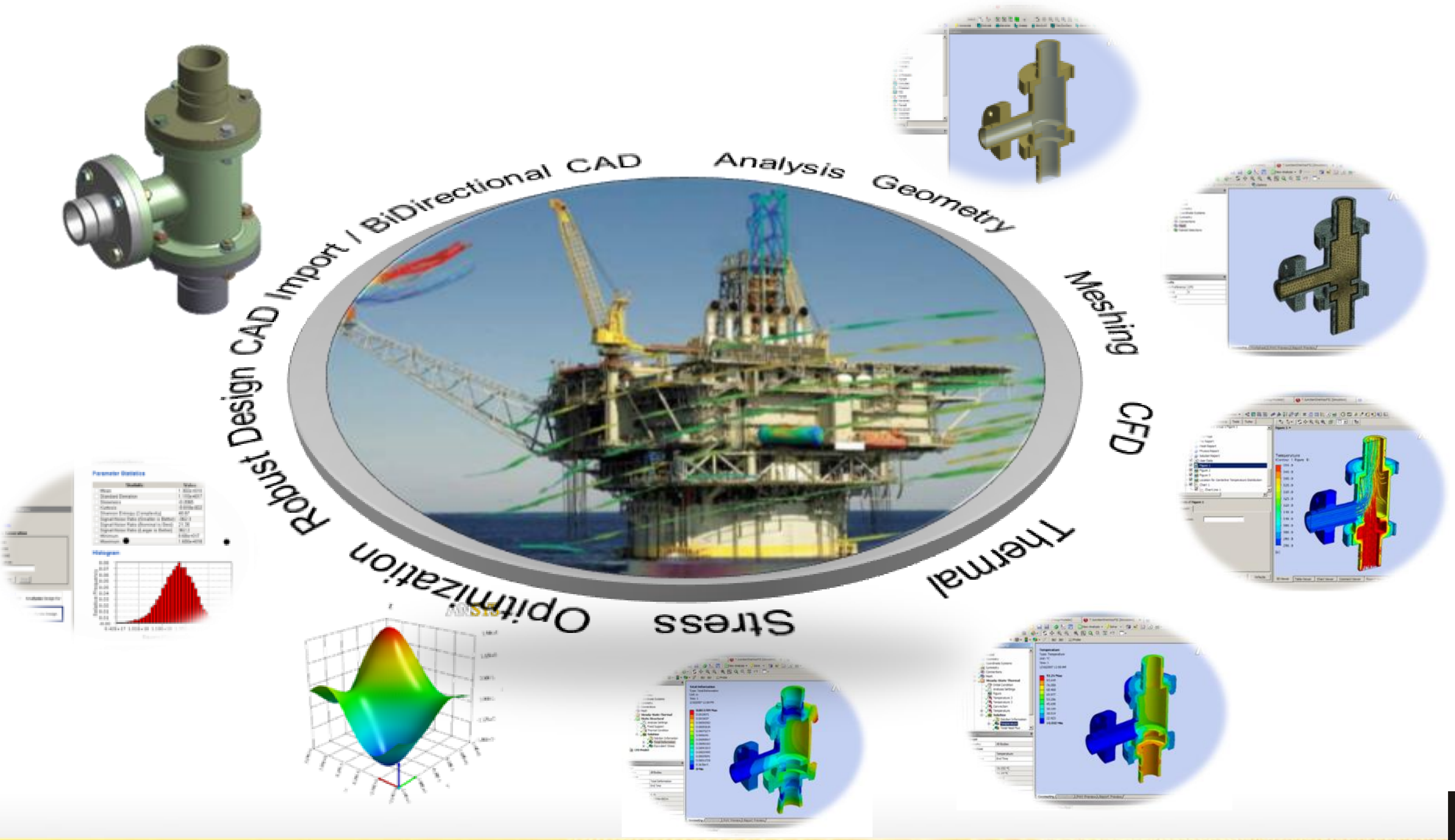


Our Vision: Simulation Driven Product Development



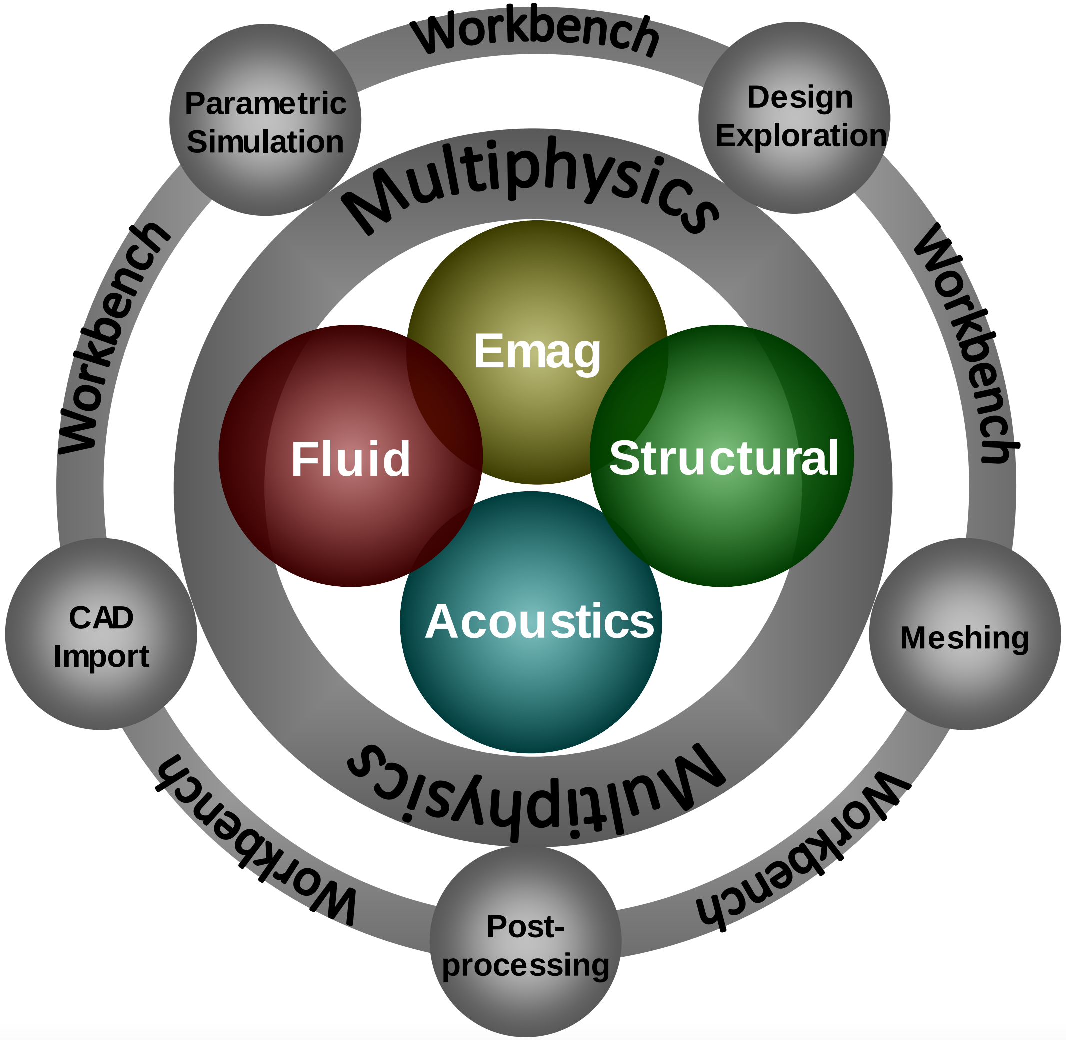
Streamlined Workflow Strategy

Workbench End-To-End Solutions In a Unified Environment



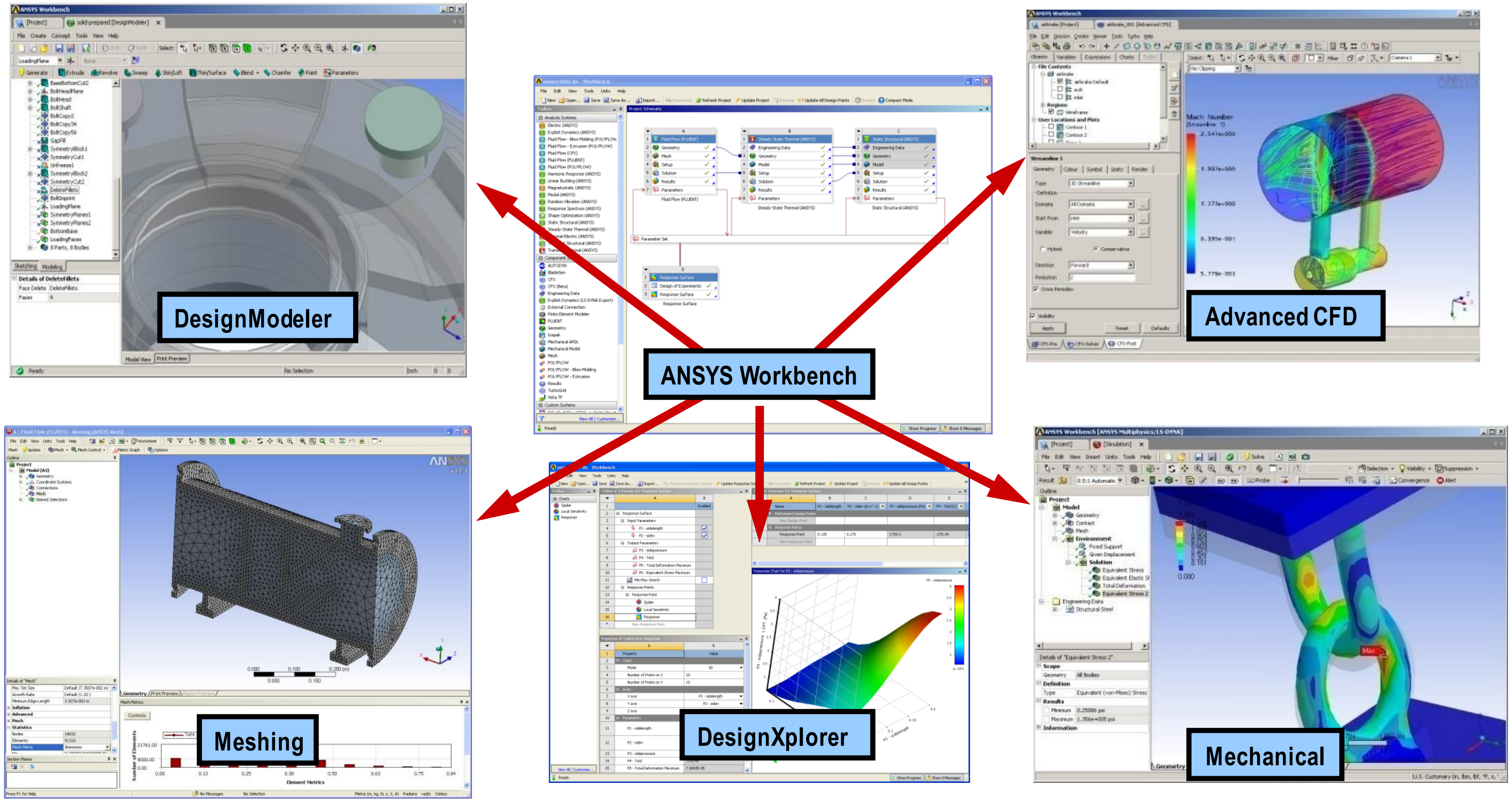
ANSYS, Technologies

- **ANSYS design, develops, markets and globally supports a comprehensive range of engineering simulation software**
- **Proven software technologies for**
  - **Fluid Dynamics (FLUENT, CFX) for CFD**
  - **Structural Mechanics**
  - **Acoustics**
  - **Electromagnetics**
  - **Multiphysics**
- **Specialized tools, including**
  - **ANSYS Icepak (thermal/flow for electronics)**
  - **ANSYS nCode DesignLife (for fatigue)**



ANSYS Workbench

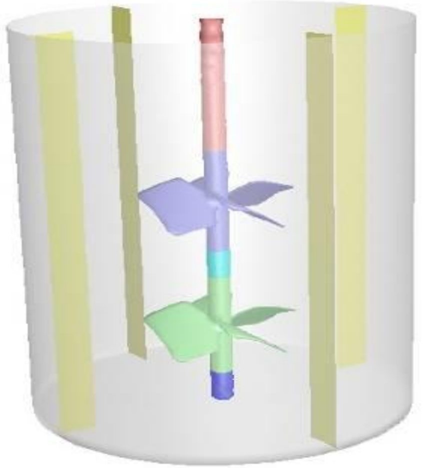
A common environment integrating ANSYS tools for multi-disciplinary CAE simulation

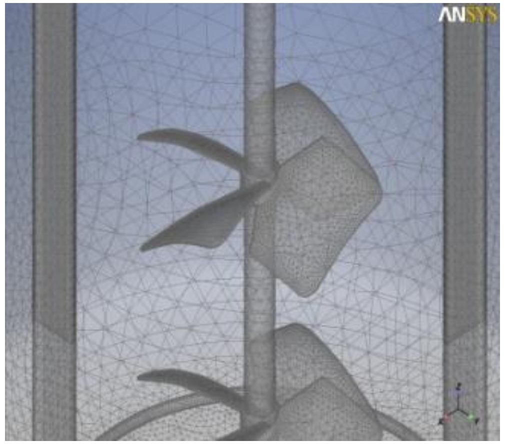


What is CFD?

- **Flow simulation, or Computational Fluid Dynamics (CFD), is the science of predicting fluid flow, heat transfer, mass transfer, chemical reactions, and related phenomena by solving the <u>mathematical equations (normally PDE's)</u>**

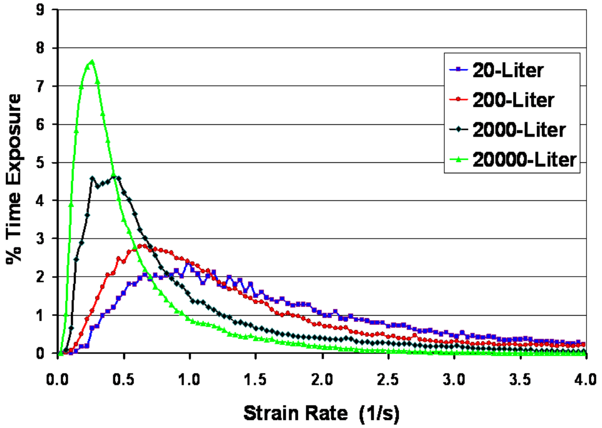
Geometry and Meshing

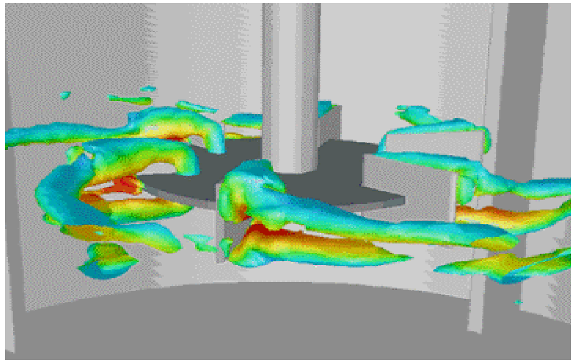




- **Three Step Process**
  1. **Geometry and Mesh**
  2. **Set-up and Solution**
  3. **Results analysis**

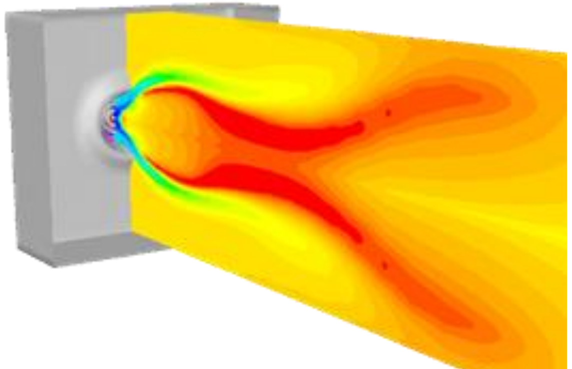
Results Analysis



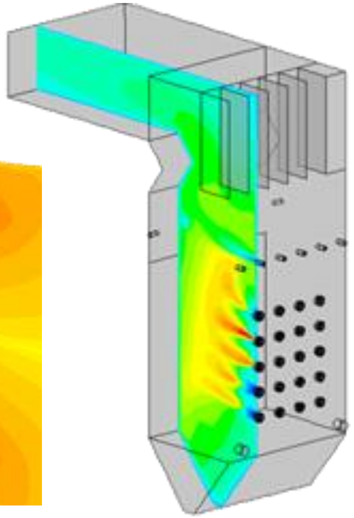


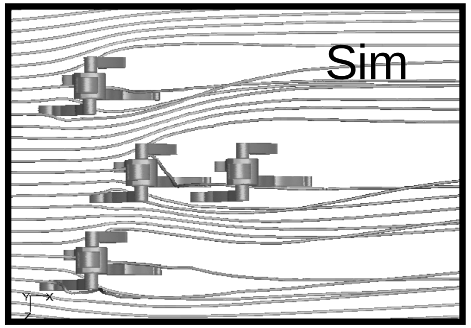
Computational Fluid Dynamics (CFD)

- **Fluid mechanics that uses numerical methods and algorithms**
- **Solve, analyze problems that involve fluid flows**
  - ✓ Flow characteristics
  - ✓ Heat and mass transfer
  - ✓ Chemical reactions, etc.
- **Fundamental basis**
  - ✓ Solves Navier-Stokes Equations, numerically
  - ✓ To conserve mass, momentum, energy, species
  - ✓ ANSYS CFD solvers based on Finite Volume Method

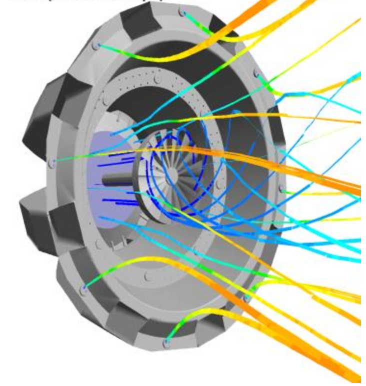


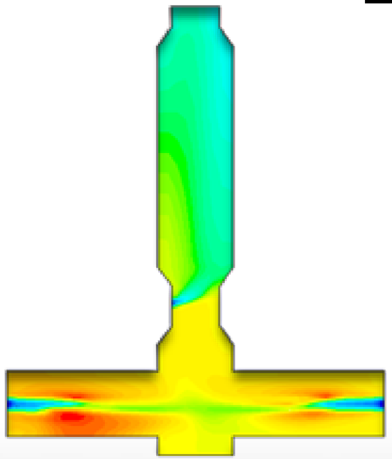
Courtesy of Mitsui Babcock Energy Ltd.



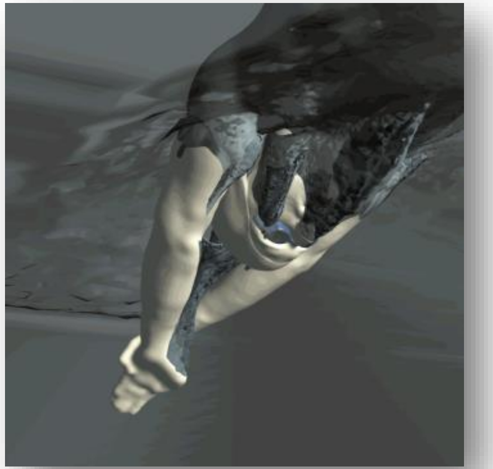


Courtesy of John Zink Company





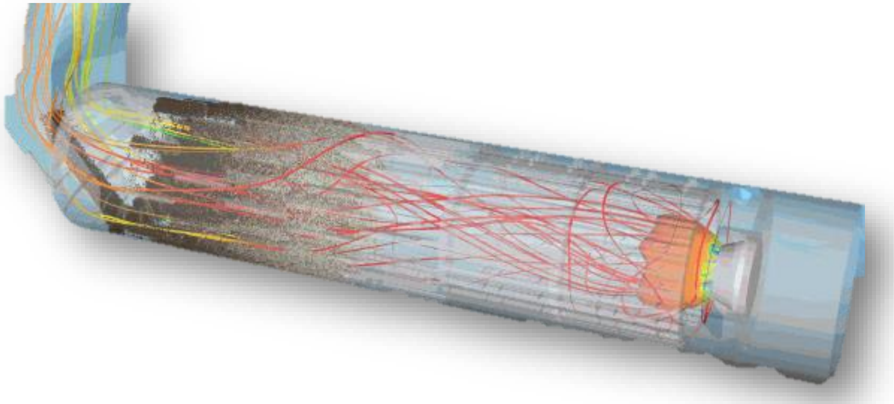
ANSYS Fluent



Courtesy Speedo

Widest array of modeling capabilities

Accurate capabilities to simulate a wide range of phenomena: aerodynamics, combustions, hydrodynamics, mixtures of liquids/solids/gas, particles dispersions



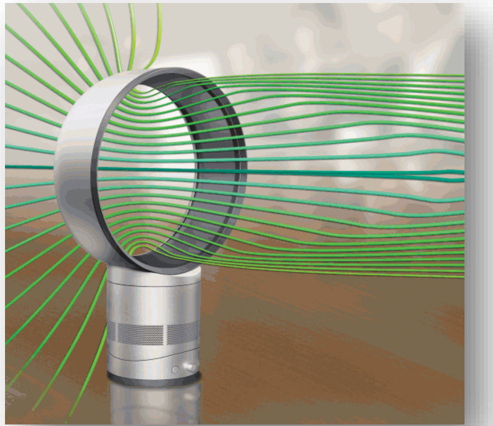
Courtesy Astec, Inc.

Customizable numerical models

Customizable to extend the capabilities to your specific CFD needs, and include your "secret ingredients" like material properties, simulation models, etc.

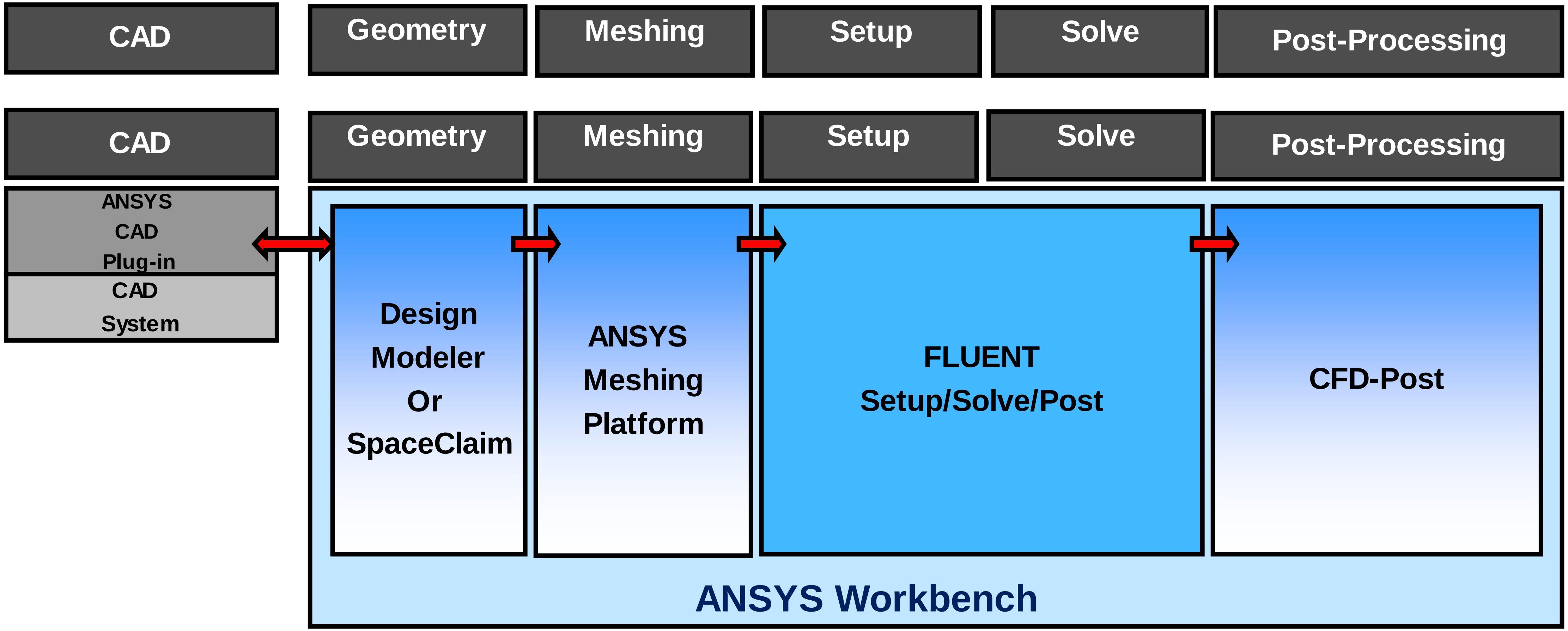
Best solver speed and HPC scalability

A fast solver: industry-leading multi-processor solver technologies ensure that you get the fastest time to solution



Courtesy Dyson Ltd.

ANSYS FLUENT Workflow

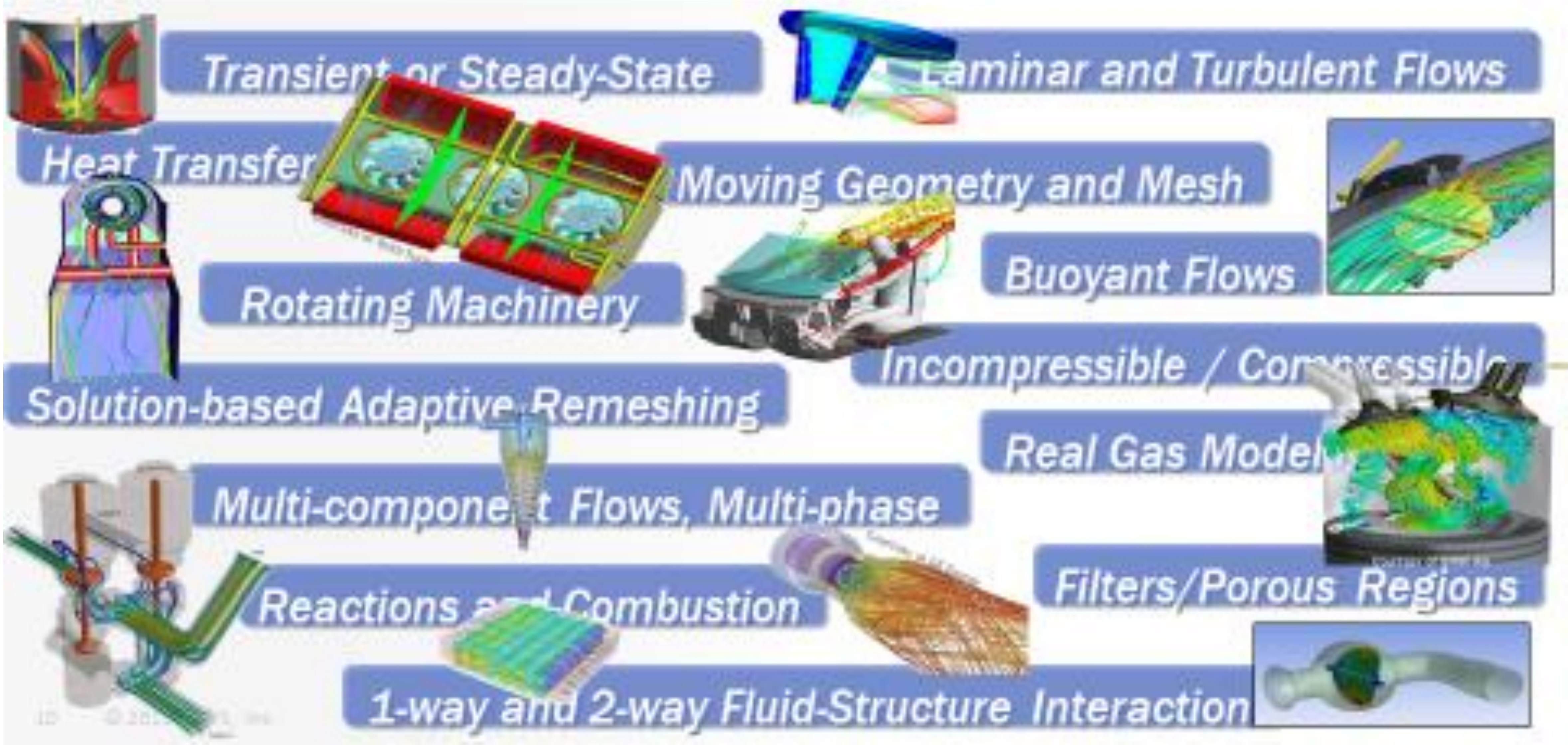


Consolidated Tools
for CAD, Geometry,
Meshing &
Post-Processing

Integration in ANSYS Workbench

- Flexible Workflows
- Connect to other Simulation tools for Multi-Physics Analysis
- Parameterization for Optimization

Modeling Flow Physics in FLUENT



CFD Methodology

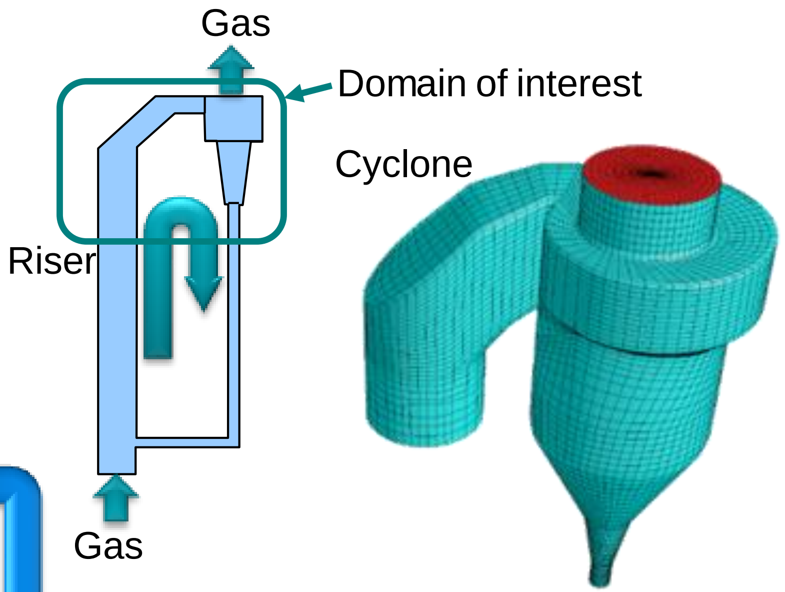
Problem Identification
- Define goals
- Identify domain

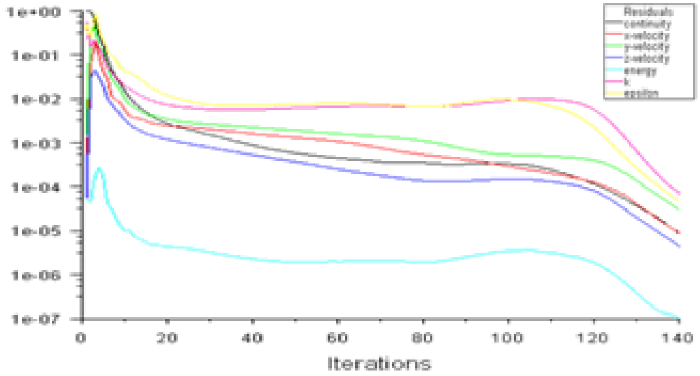
Pre-Processing
- Geometry
- Mesh
- Physics
- Solver Settings

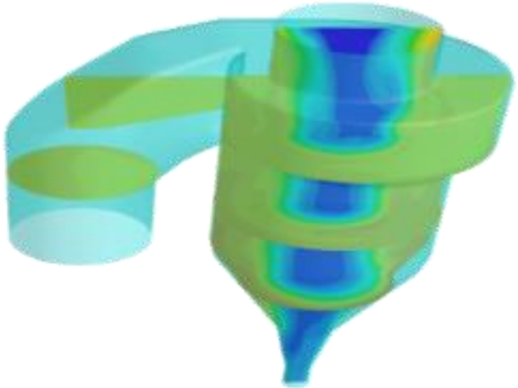
Solve
- Compute solution

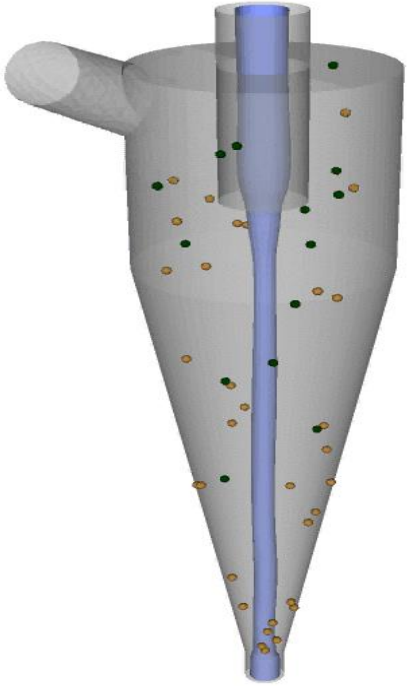
Post Processing
- Examine results

Update Model









Solids volume fraction contours (5 micron particles)

Courtesy: Fuller Company

Motivation for Modeling

- Reacting Flow Devices are very complex
  - Complex geometry, complex BCs, complex physics (turbulence, multi-phase, chemistry, radiation,…), complex systems, …
- Tool to gain insight and understanding
  - Predictions of flow field and mixing characteristics
  - Temperature field
  - Species concentrations
  - Particulates and pollutants
- Reduce expensive experiments
- Eventually design!

Reacting Flow Applications

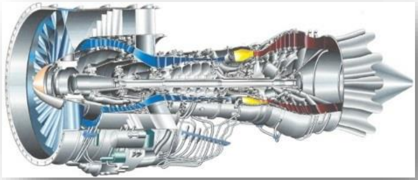
ANSYS CFD contains models which are applicable to a wide range of homogeneous and heterogeneous reacting flows

- ✓ Furnaces
- ✓ Boilers
- ✓ Process heaters
- ✓ Gas turbines
- ✓ Rocket engines
- ✓ IC engine
- ✓ CVD, catalytic reactions

Importance

- ✓ More Efficient (Energy Efficiency)
- ✓ Cleaner (Pollutant Regulations)
- ✓ Safer (Safety Regulations)

Gas Turbine Combustors



Climate change & Energy sustainability

Propulsion & Engines

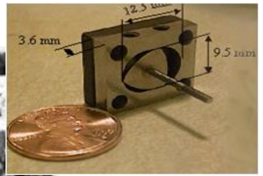
Biomedicine & Biochemistry

Fired Heaters

Environment & Emissions control

Gas Flares

Micros & Nanos



Fire & Fire protection

IC Engines

Burners

Boilers

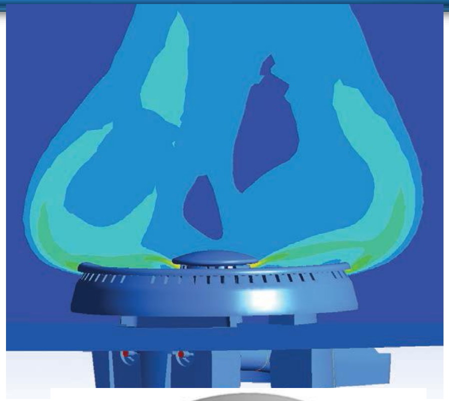
Whirlpool Reduced Burner Model Prep Time by 90 percent with ANSYS SpaceClaim

Designing a Better Burner

- Whirlpool Brazil relies heavily on simulation to design gas burners for freestanding ranges, built-in ovens and cooktops.
- Engineers required a tool to prepare models for simulation so that they could quickly explore a range of designs to come up with the best burner that would meet all criteria.

ANSYS in Action

- Whirlpool chose ANSYS SpaceClaim Direct Modeler, which enables easy geometry cleanup and generation of closed volumes required for CFD.
- Engineers then used ANSYS Fluent to perform combustion simulation using the EDC combustion and SST turbulence models.

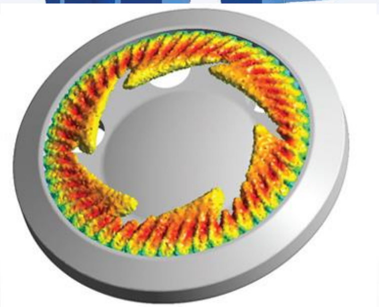


Key Results

- Using ANSYS SpaceClaim Direct Modeler, the model was ready for meshing and simulation in only four hours.
- Engineers increased primary air entrainment from 36 percent to 52 percent. This generated a stable flame with nearly complete combustion, high levels of efficiency and low levels of carbon monoxide.

Reduced time to analysis by 90%

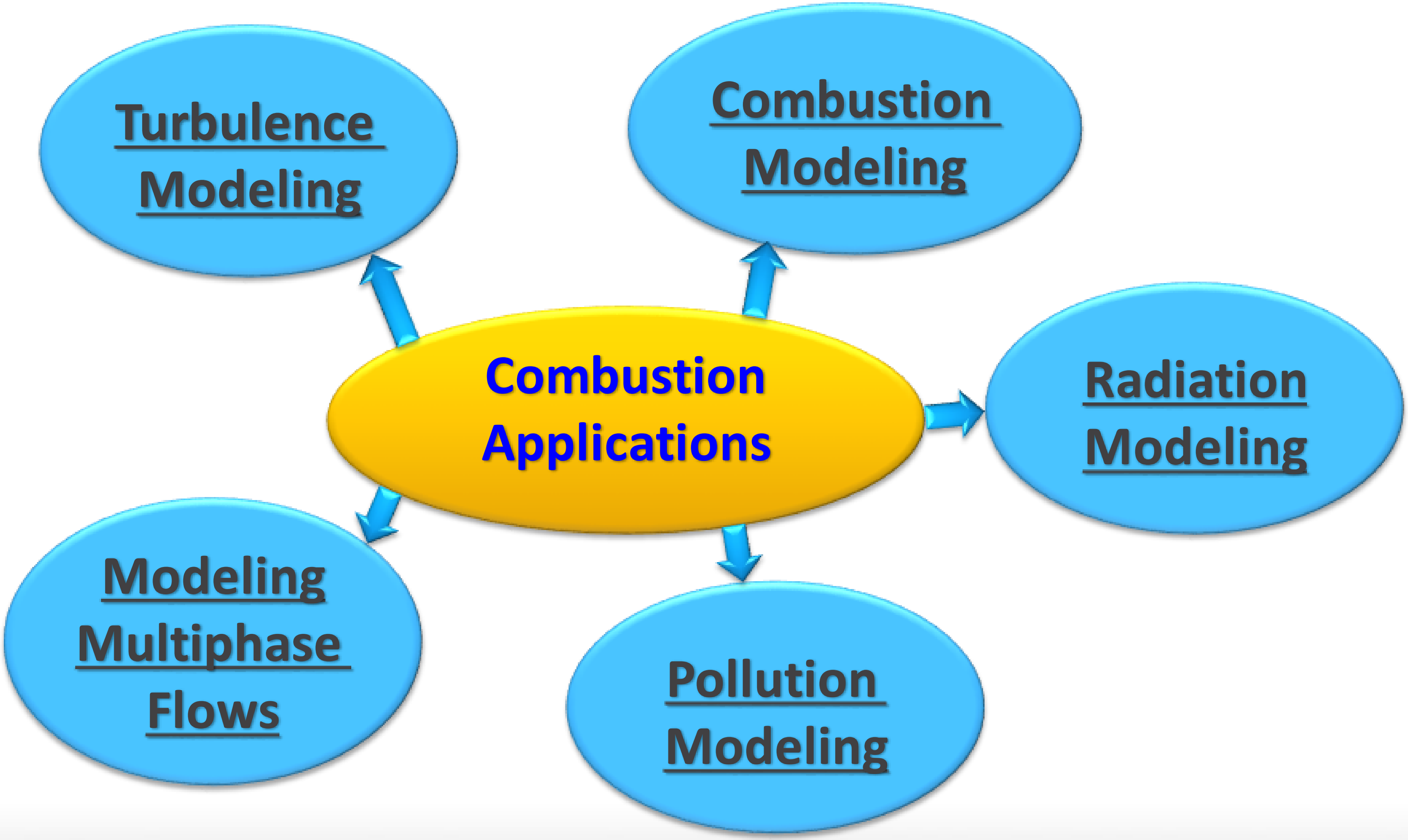
Reduced design time by 35%



"This application demonstrates the time- and cost-savings that can be achieved by enabling simulation engineers to quickly and easily prepare design geometry for simulation, as well as how an efficient design can be determined using simulation."

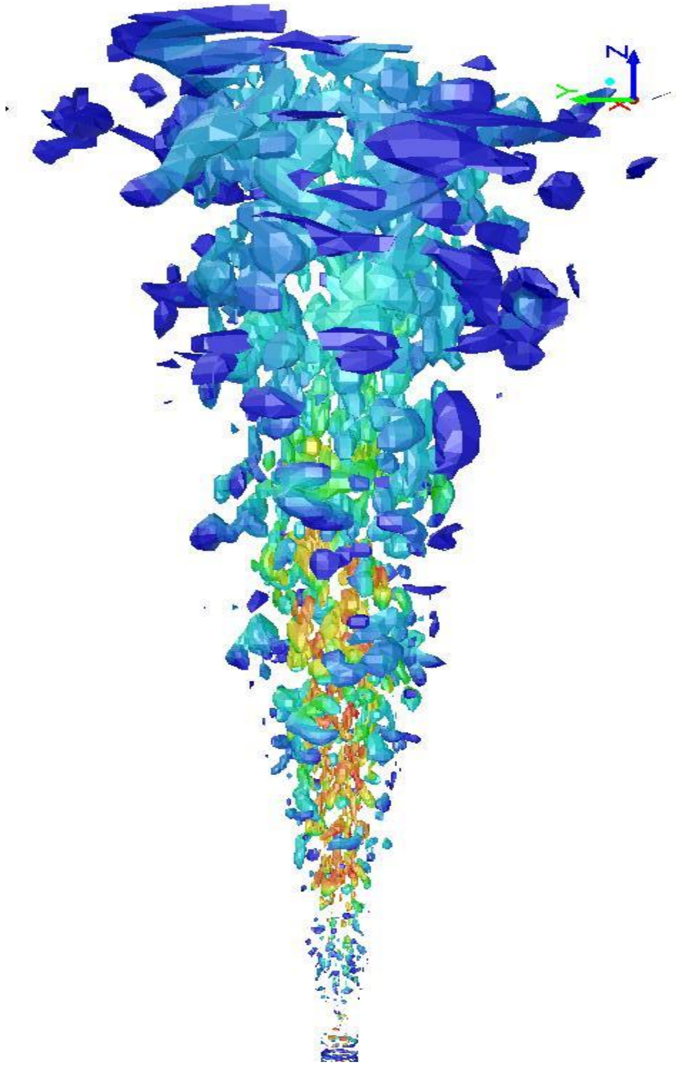
Pablo Filgueira Rodeiro
Senior Manager — Simulation-Based Design
Whirlpool Corporation

CFD Models involved in Reacting Flows

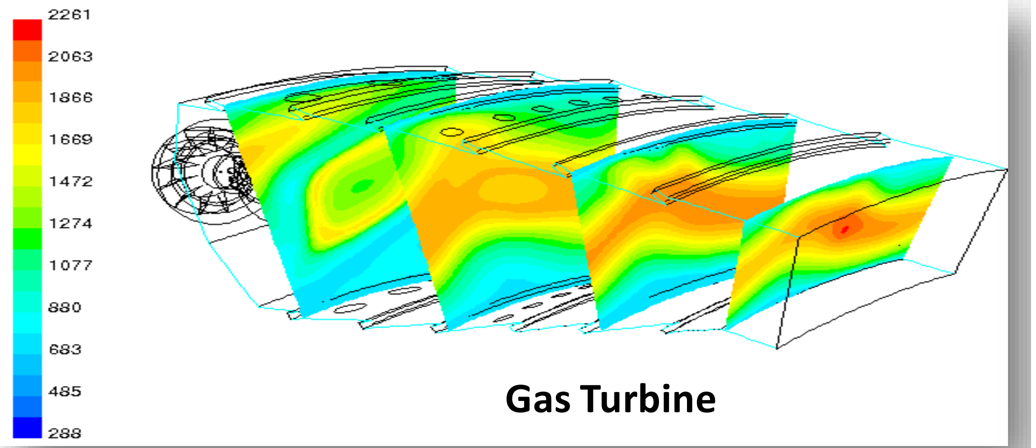


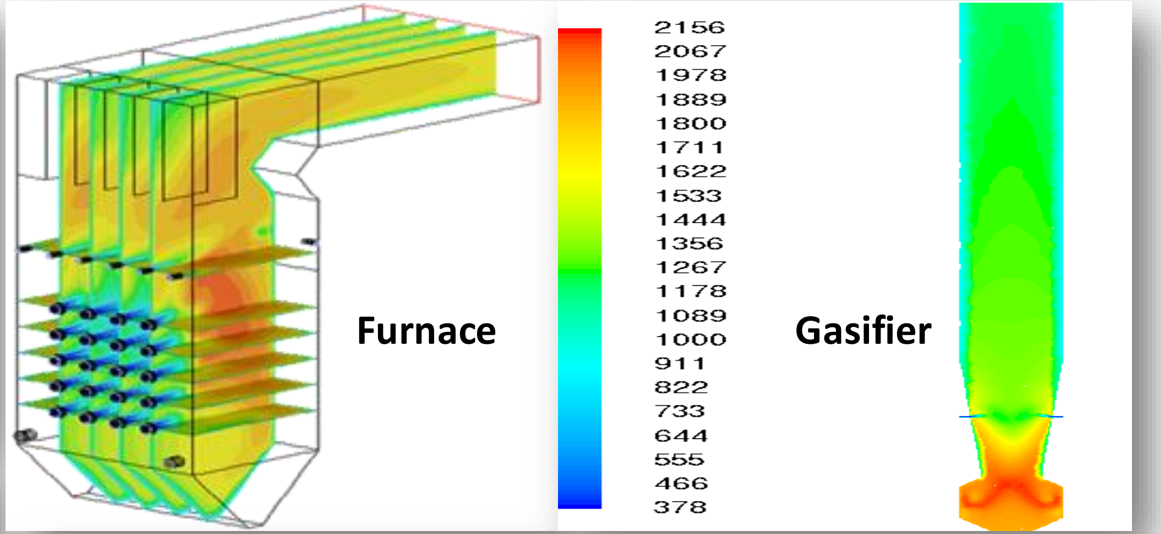
Role of Turbulence in Reacting System

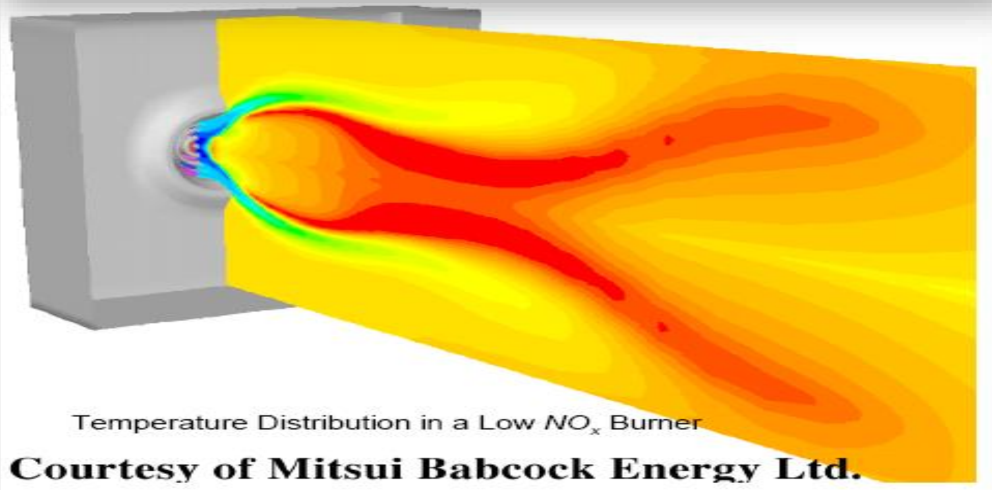
- **Flows encountered in most of the Practical Reacting Systems are turbulent**
- **Reactions and Turbulence affect each other**
  - **Turbulence-chemistry interaction**
- **Turbulence is modified by flames**
  - **Through flow acceleration, modified kinematic viscosity**
- **Modified turbulence alters the flame structure**
  - **Enhanced mixing and chemical reactions (through temp fluctuations)**
- **Mixing time scale (τ_F) relative to chemical time scale (τ_{chem})**
  - **An important parameter to decide whether the reaction is mixing limited or chemically limited**
  - **Mixing time scale in turbulent flows** $= \frac{k}{\epsilon}$
  - **Damkohler Number (*Da*)** $= \frac{\tau_F}{\tau_{Chem}}$
  - **If *Da* > 1 → Fast chemistry and *Da* $\leq$ 1 → Finite rate chemistry**

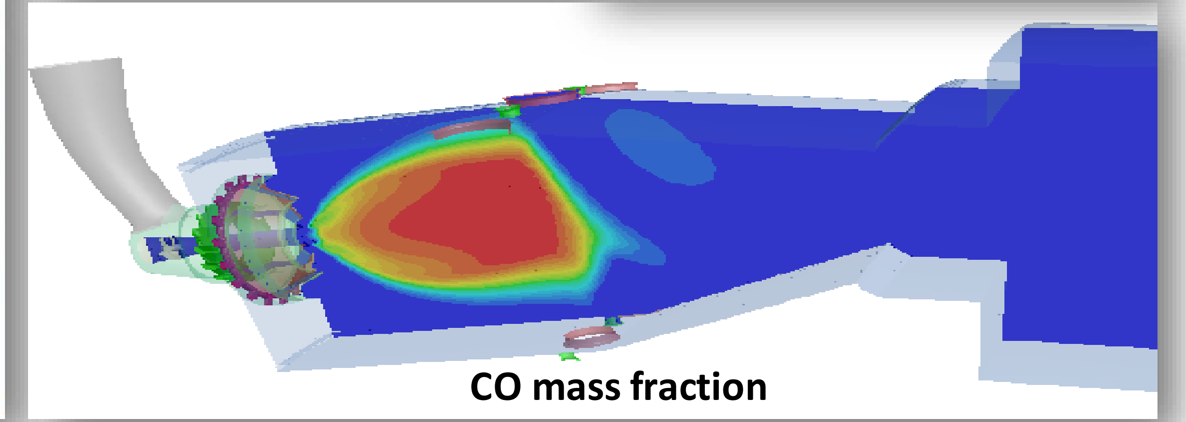


Modeling Examples: Fast Chemistry

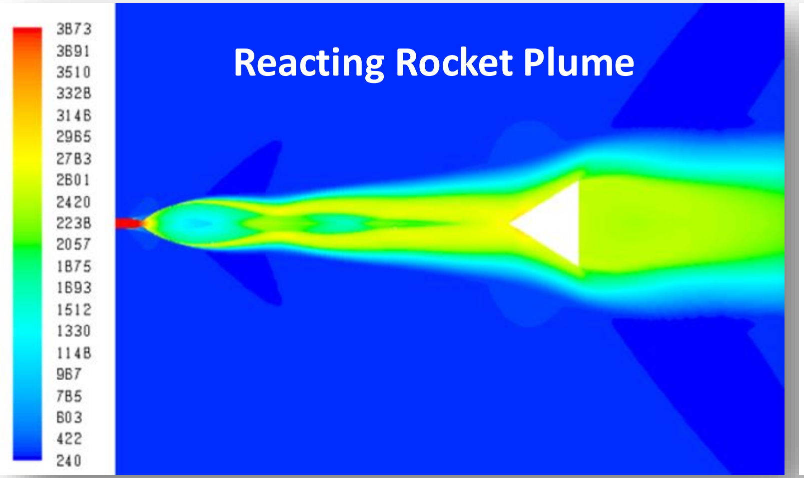


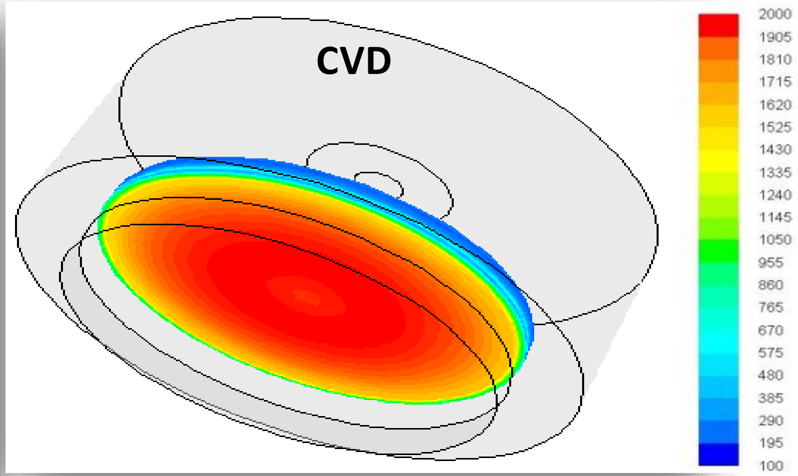


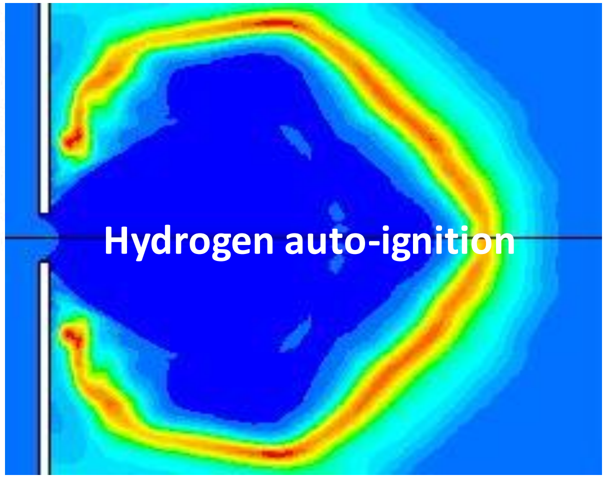


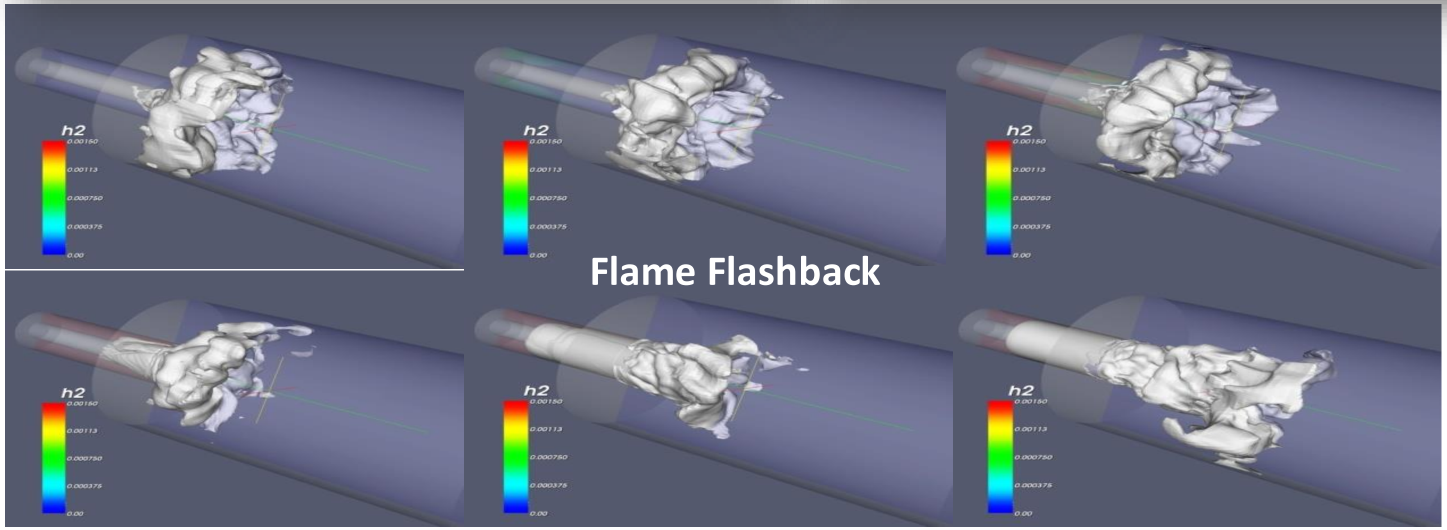


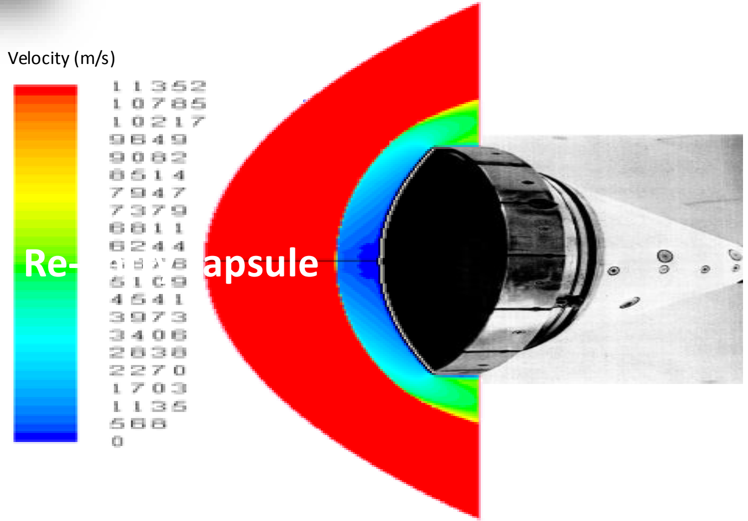
Modeling Examples: Slow Chemistry











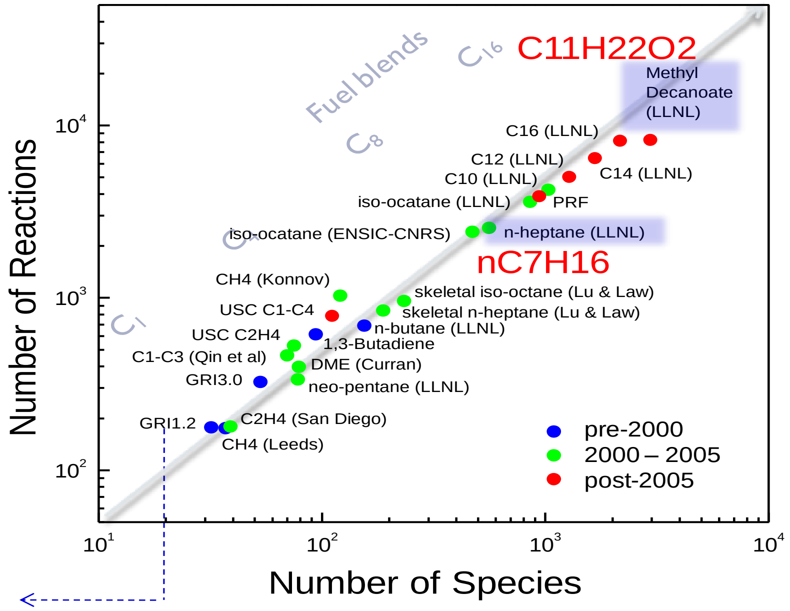
Challenges in Modeling Turbulent Reacting Flows

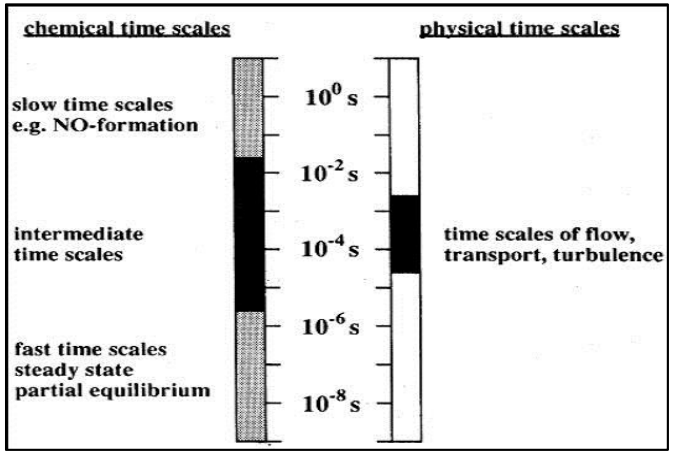
Turbulence

- Most industrial flows are turbulent.
- DNS of non-reacting and reacting turbulent flows is not possible because of the wide range of time and length scales.

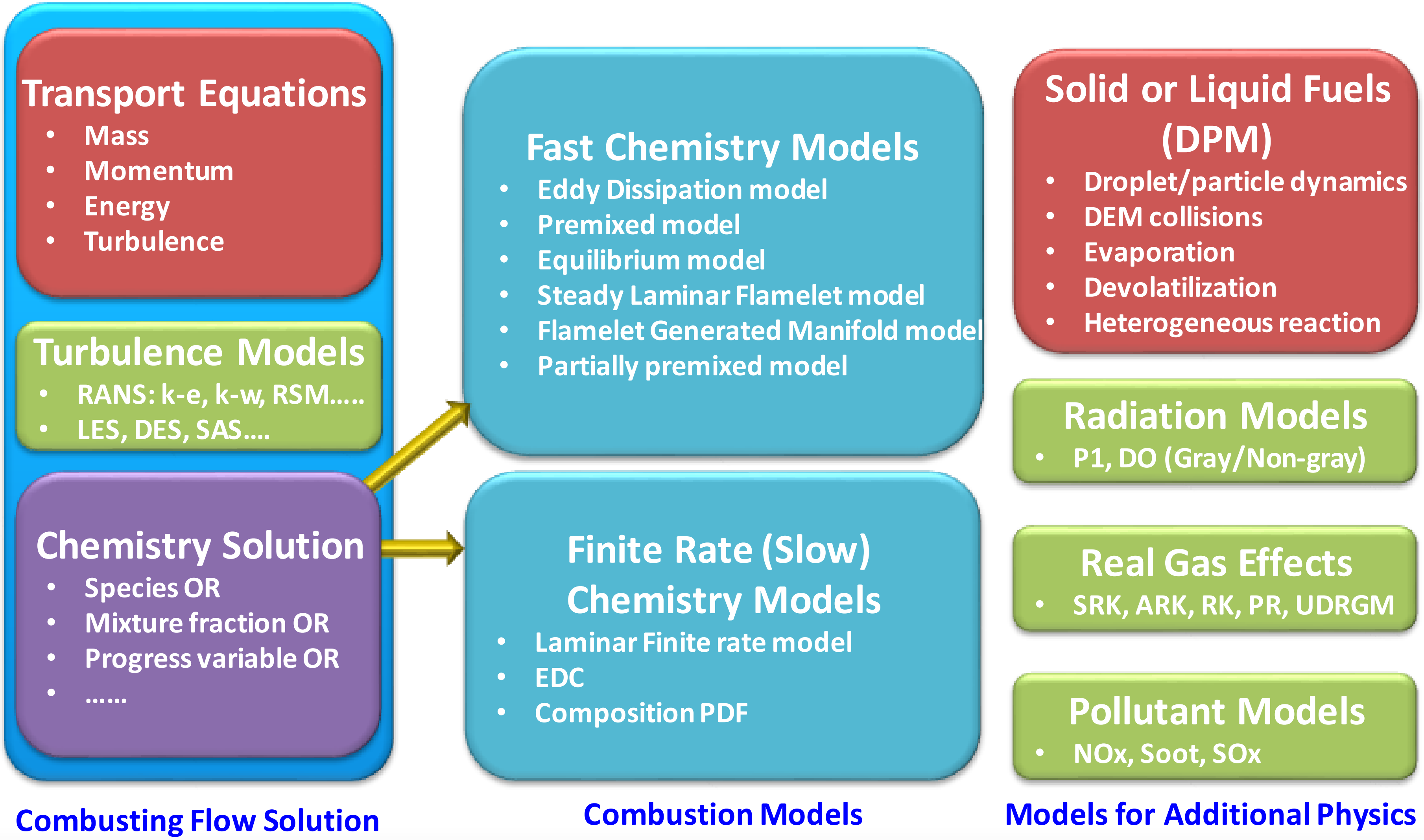
Chemistry

- *Realistic chemical mechanisms cannot be described* by a single reaction equation.
  - Tens of species, hundreds of reactions
  - Known in detail for only a limited number of fuels
- Stiff kinetics (wide range of reacting time scales)
- Turbulence-Chemistry Interaction
- The sensitivity of reaction rates to local changes is complicated by enhanced mixing of turbulent flows.





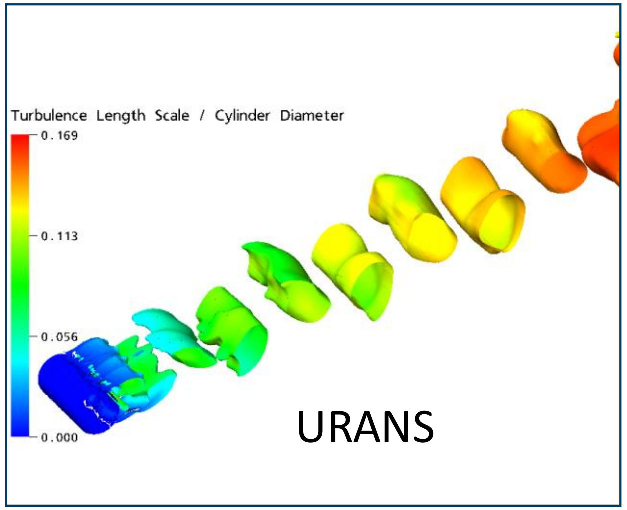
Overview of Combustion Modeling

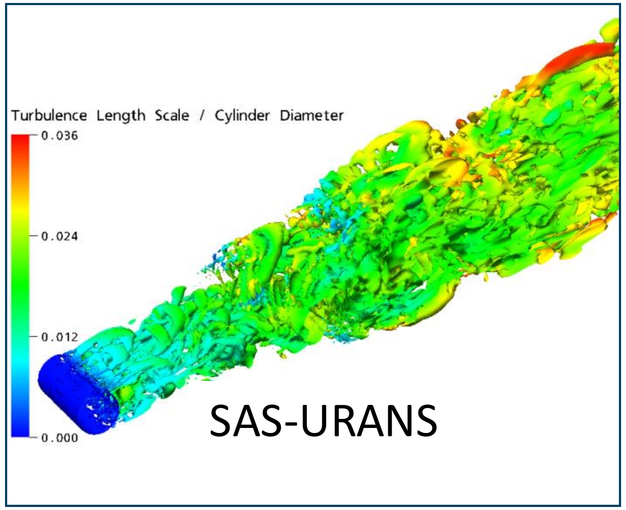


Turbulence Models

- RANS (K-epsilon, k-omega, SST, RSM..)
- URANS
  - URANS gives unphysical single mode unsteady behavior
- LES (Large Eddy Simulation)
  - High resolution requirements in boundary layers
- DES (Detached Eddy Simulation)
  - First industrial-strength model for high-Re with LES-content
  - Increased complexity (grid sensitivity) due to explicit mix of two modelling concepts
- ELES (Embedded LES)
  - Interface between RANS-LES: coarse mesh for the RANS and fine mesh for LES
- SAS (Scale-Adaptive Simulation)
  - Provides 'LES' mode in unsteady regions
  - Avoid explicit mesh dependency
  - Resolved length scale determined from solution
  - Scale-adaptation based on von Karman length scale
  - RANS/LES switch based on local L/LvK ratio

$$L_{vK} = \kappa \left| \frac{\partial U / \partial y}{\partial^2 U / \partial y^2} \right|$$





Types of Flames

Diffusion (or Non-Premixed) flames

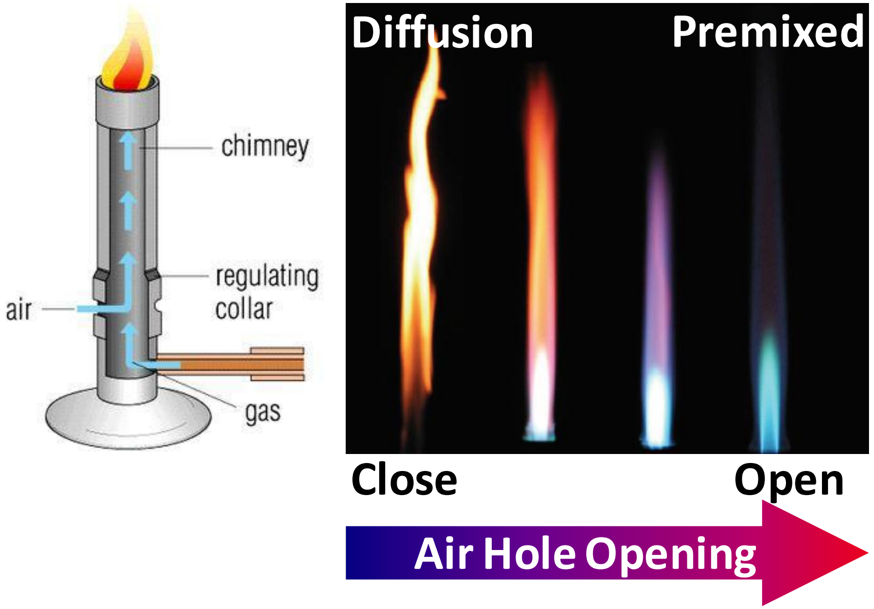
- Separate streams for fuel and oxidizer
- Convection or diffusion of reactants from either side into a flame sheet

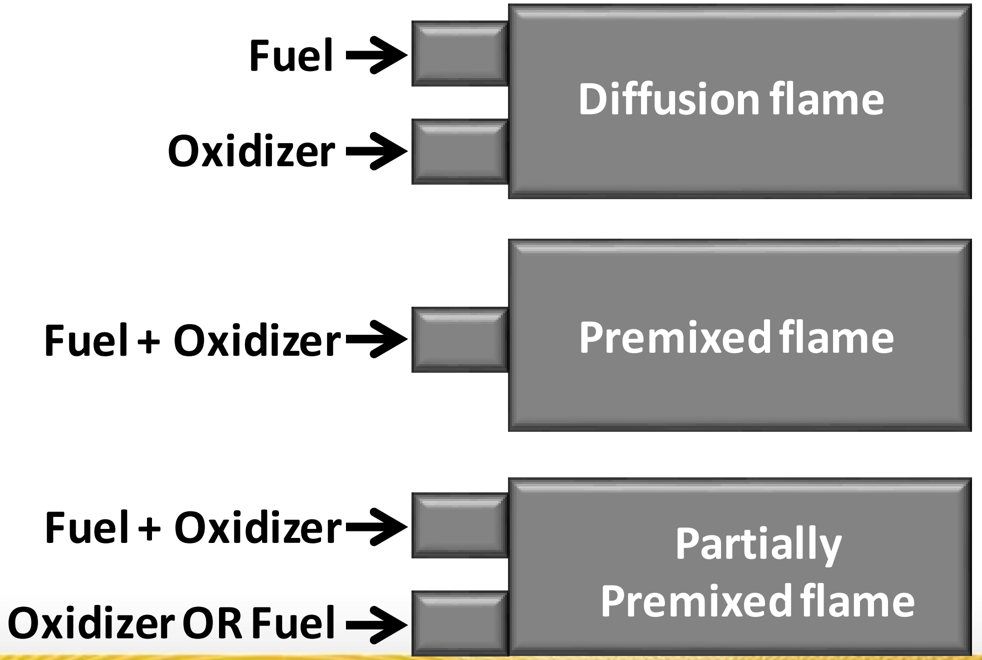
Premixed flames

- Fuel and oxidizer are already mixed at the molecular level prior to ignition
- Diffusion heat and radicals from the products to the reactants
- Rate of propagation (flame speed) depends on the internal flame structure

Partially Premixed flames

- Reacting systems with both non-premixed and premixed fuel/oxidizer streams





  June 2, 2016

Approaches for Modeling Reacting Flows

Damköhler Number (Da) = $\frac{\tau_F}{\tau_{Chem}}$

- Simplify the chemistry
  - Considers global chemical reaction mechanism
    - Eddy Dissipation model (or Finite Rate/Eddy Dissipation)

- Decouple chemistry from flow (Fast Chemistry models – *Da* >> 1)
  - Use progress variable (C) approach
    - Premixed model
  - Use mixture fraction (Z) approach
    - Non-Premixed model
  - Use progress variable and mixture fraction approach
    - Partially Premixed model
  - Incorporate finite rate chemistry effects with laminar flamelets based models

- Model detailed chemistry (Finite Rate Chemistry models – *Da* ~ 1)
  - CPU intensive (large number of transport equations + stiff kinetics)
  - Use of Stiff Chemistry Solver will allow larger time steps to be used
  - Chemistry Acceleration tools can help to speed up the calculation
  - This includes :
    - Laminar Finite Rate model
    - Eddy Dissipation Concept model
    - Composition PDF Transport model

Overview of ANSYS Fluent Reacting Flows Models

Flow Configuration

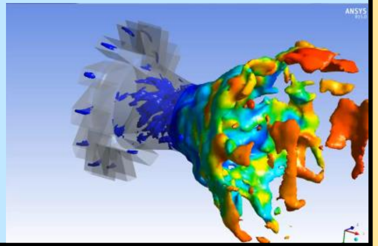
Chemistry

	Premixed Combustion	Non-Premixed Combustion	Partially Premixed Combustion
Fast Chemistry	Finite Rate/Eddy Dissipation Model (Species Transport)		
	Premixed Combustion Model Reaction Progress Variable	Non-Premixed Equilibrium Model Mixture Fraction	Partially Premixed Model Reaction Progress Variable + Mixture Fraction
		Laminar Diffusion Flamelet Model (Steady/Unsteady)	
	Flamelet Generated Manifold Model		
Finite Rate Chemistry	Laminar Finite Rate Model		
	Eddy-Dissipation Concept (EDC) Model		
	Composition PDF Transport Model (Eulerian/Lagrangian)		

ANSYS Reacting Flow Solution(s)

ANSYS CFD

- Flow simulation (Turbulent flows, steady/unsteady)
- Solid or liquid fuels (droplet, coal particles, etc.)
- Full range of combustion capabilities (premixed, partially premixed, non-premixed)
- Pollutant modeling
- Radiation modeling
- Real Gas modeling



CHEMKIN-CFD/API

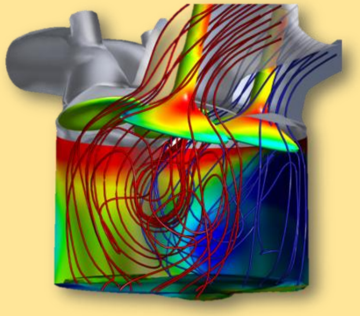
- Advanced chemistry computation for use in CFD

CHEMKIN-PRO

- Advanced chemistry for 0-D, 1-D reactor and flames (flame speeds, flamelets)

FORTÉ CFD

- IC Engine 3-D Simulation

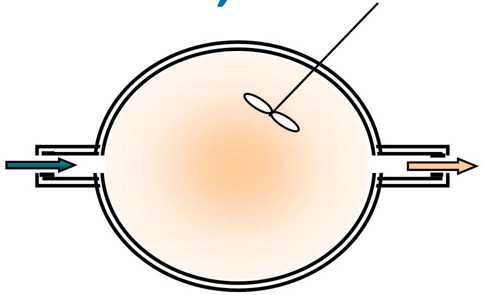


Gas turbines combustion, furnaces, coal combustion, reformers, boilers, materials, chemical vapor deposition, chemical processing

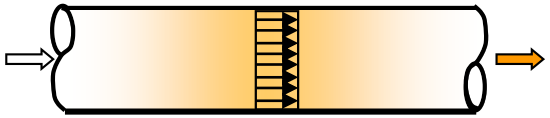
IC Engines

CHEMKIN-PRO® focuses on Chemistry using Engineering Approximations of the Flow

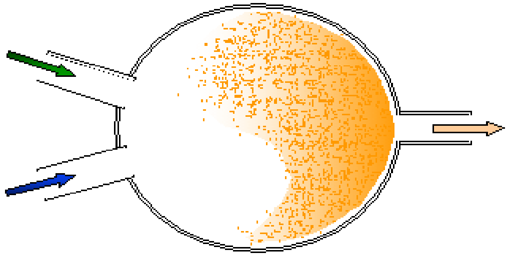
0-D, 1-D and 2-D approximations of industrial flow conditions



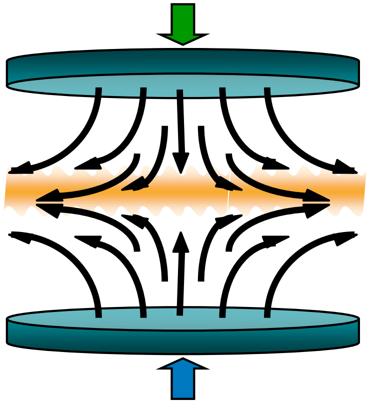
Perfectly Stirred Reactor (PSR)



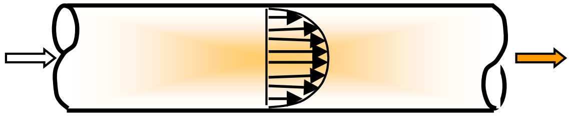
Plug-flow Reactor (PFR)



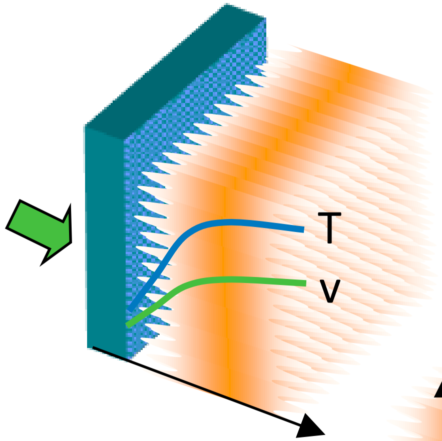
Partially Stirred Reactor



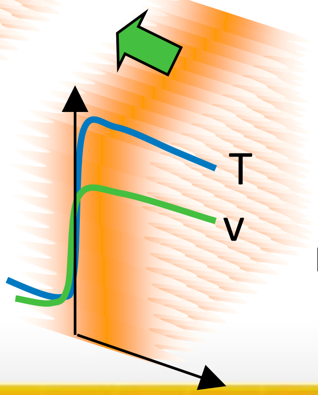
Opposed-flow Diffusion Flame



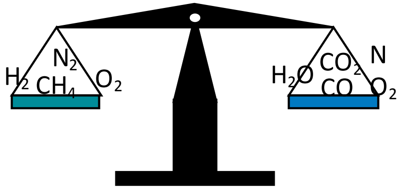
Shear-layer Channel-flow Reactor



Pre-mixed Flame



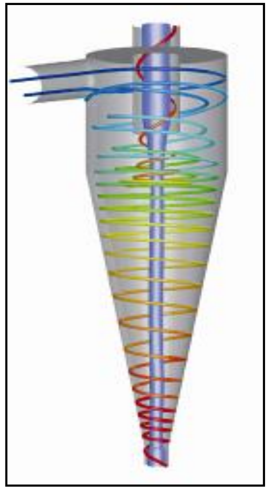
Flame-speed Calculation



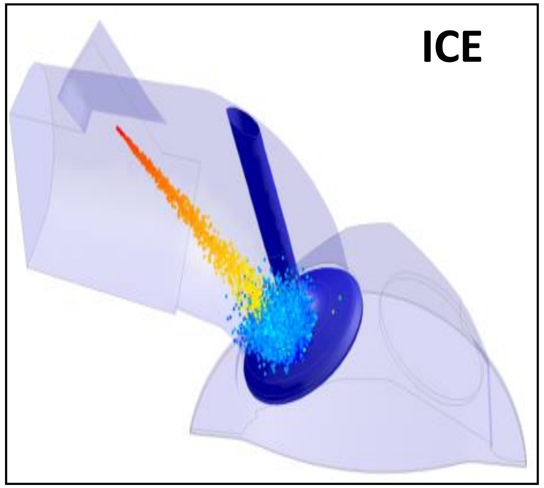
Equilibrium Calculator

DPM & Spray Injection

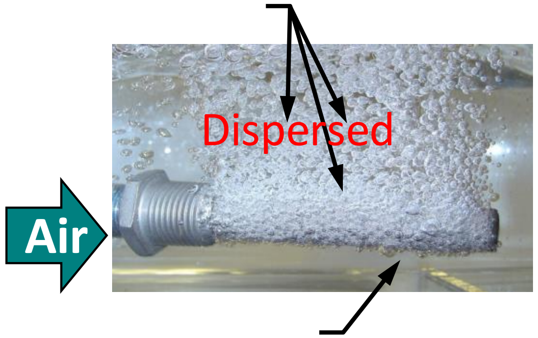
Spray injection in a highly turbulent environment



Cyclones

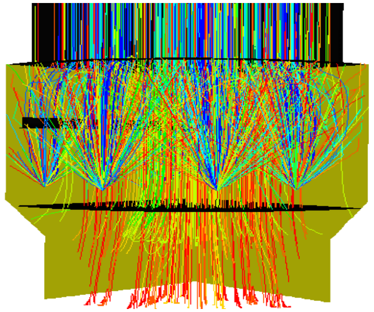


Dispersed Phase

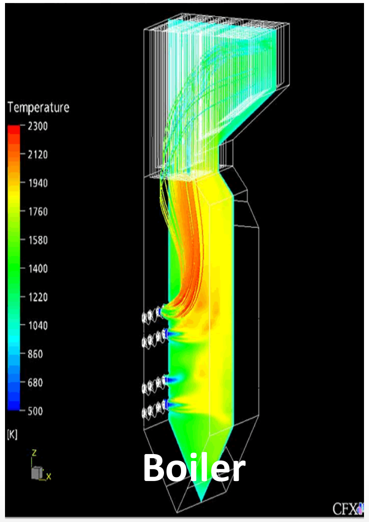


Continuous Phase

Scrubber



Courtesy of Lurgi



- **Assumptions :**
  - A discrete phase < 10%
  - Negligible particle/particle interactions

- **Example applications:**
  - Cyclone Separator
  - Pulverized coal/oil fired boilers
  - Internal combustion engine
  - Scrubbers, spray powders.
  - Gas turbine engines

Liquid Evaporation and Burning

Applications

– IC engines; Gas turbines; Oil fired boilers, scrubbers; etc.

Combined action of fluid dynamics and surface tension causes liquid break up

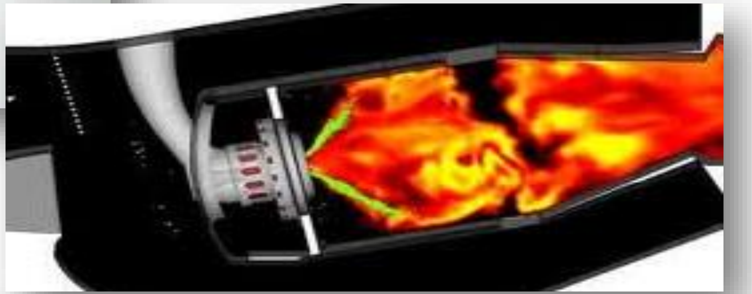
– Unstable liquid sheet → ligaments → droplets

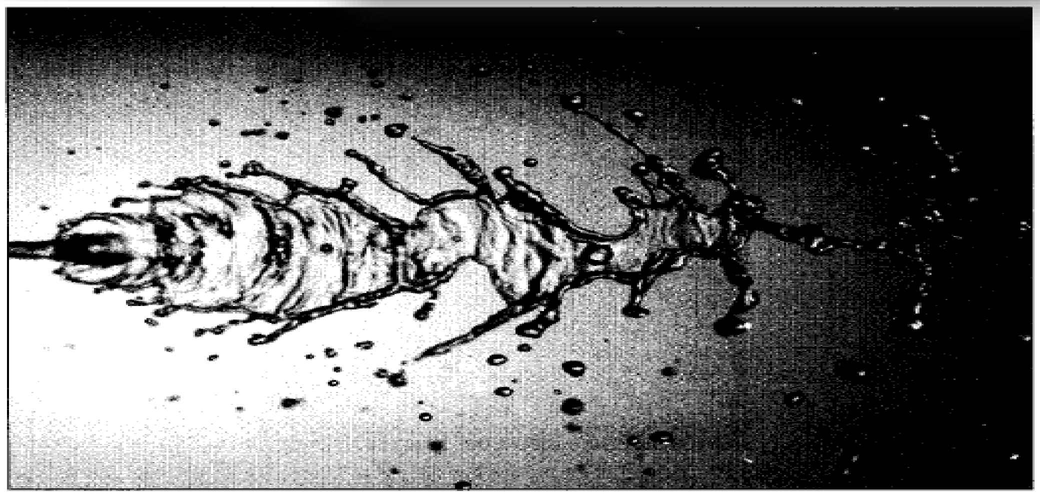
Vaporization

– Droplet evaporation and boiling

Mixing and Reactions in Gas Phase

Gas turbine combustor





Modeling Pollutant Formation

- Pollutants with usually very low concentrations compared to major components participating in combustion
  - Does not affect much to the flow distribution and heat transfer
- Three approaches: Fully coupled, decoupled chemistry and post-processing

✓ Fully coupled

- ❖ Solution of pollutant equations together with those of major species
- ❖ Computationally more expensive

✓ Decoupled chemistry

- ❖ Solution with sub-mechanism for pollutants in post-processing step
- ❖ Species and temperature field from any of the combustion models
- ❖ Computational efforts in between fully coupled and post-processing

✓ Post-processing

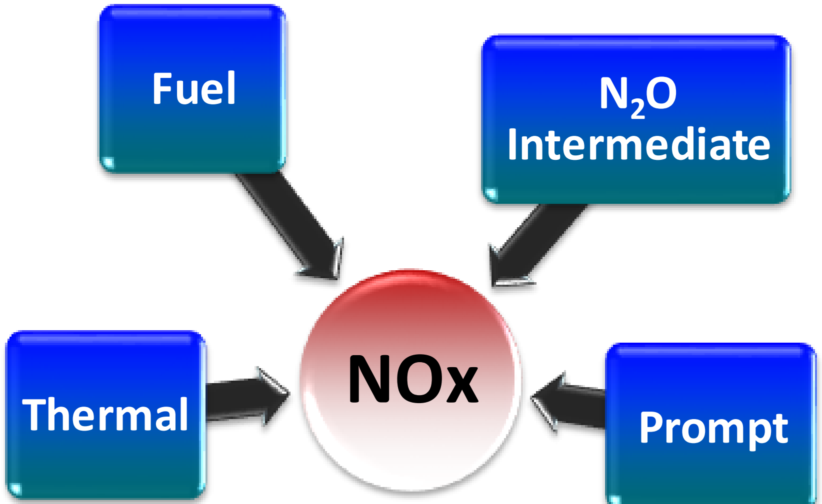
- ❖ Solution of pollutant with frozen velocity, turbulence and species composition field
- ❖ Accuracy is governed by the combustion solution
- ❖ Computationally economical
- ❖ ANSYS CFD has NOx, SOx and Soot formation models

Post-processing Pollutant Models

- **NOx**
  - Mainly consists of Nitric oxide (NO)
  - Nitrogen peroxide (NO_2) and Nitrous oxide (N_2O) to the smaller extent
  - Thermal, Prompt, Fuel and N_2O intermediate mechanisms are available
- **Soot**
  - Formed in fuel rich zones with strong temperature gradients
  - Complex nucleation, surface growth, coalescence, aggregation phenomenon can be included
  - One-step Khan & Greeves model, Two-step Tesner model, Moss-Brookes model and Moss-Brookes-Hall model are available
- **SOx**
  - Consists of SO_2, SO, SO_3
  - Eight-step reduced mechanism is used

NOx Modeling

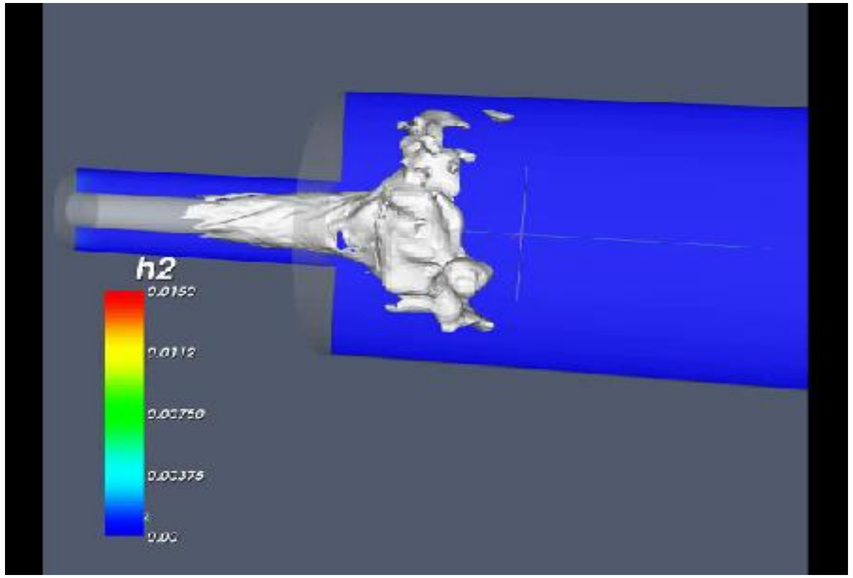
- Transport equations for
  - NO, HCN, NH_3 and N_2O
- Thermal NOx using extended Zeldovich mechanism
- Fuel NOx sources for gaseous, liquid, and coal fuels are considered separately
- NOx contribution from N_2O intermediate using formulation of Melte and Pratt
- Prompt NOx using global kinetic parameters suggested by DeSoete
- For turbulent flows, turbulent-chemistry interaction using joint PDF in terms of
  - Normalized temperature
  - Normalized species mass fraction
  - The combination of both
  - Or mixture fraction



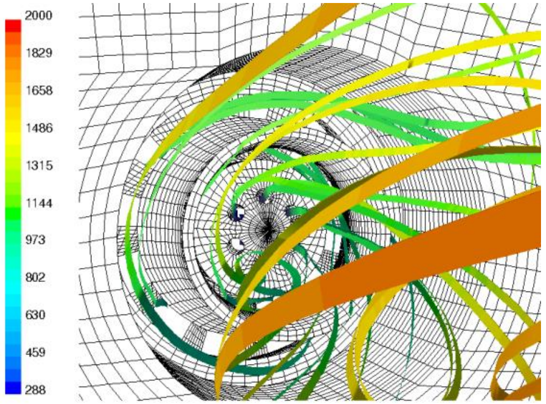
Combustion Systems: Burners/Combustors

Challenges

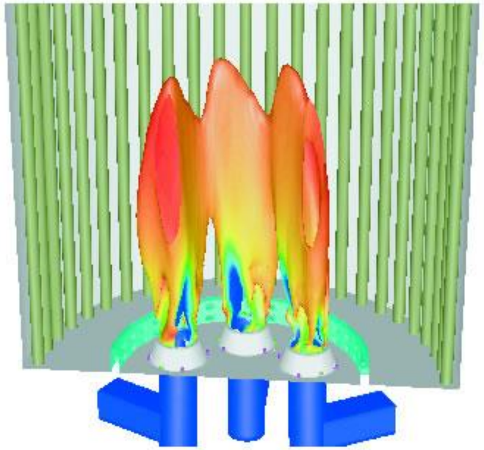
- Burner performance
- Back mixing and burner design
- Pollution and NOx reduction
- Fatigue and creep from thermal stresses
- Flame shape, instability and interaction



Courtesy of NETL (USA)



Pathlines colored by temperature gas Turbine Combustor (NOVA Chemicals)



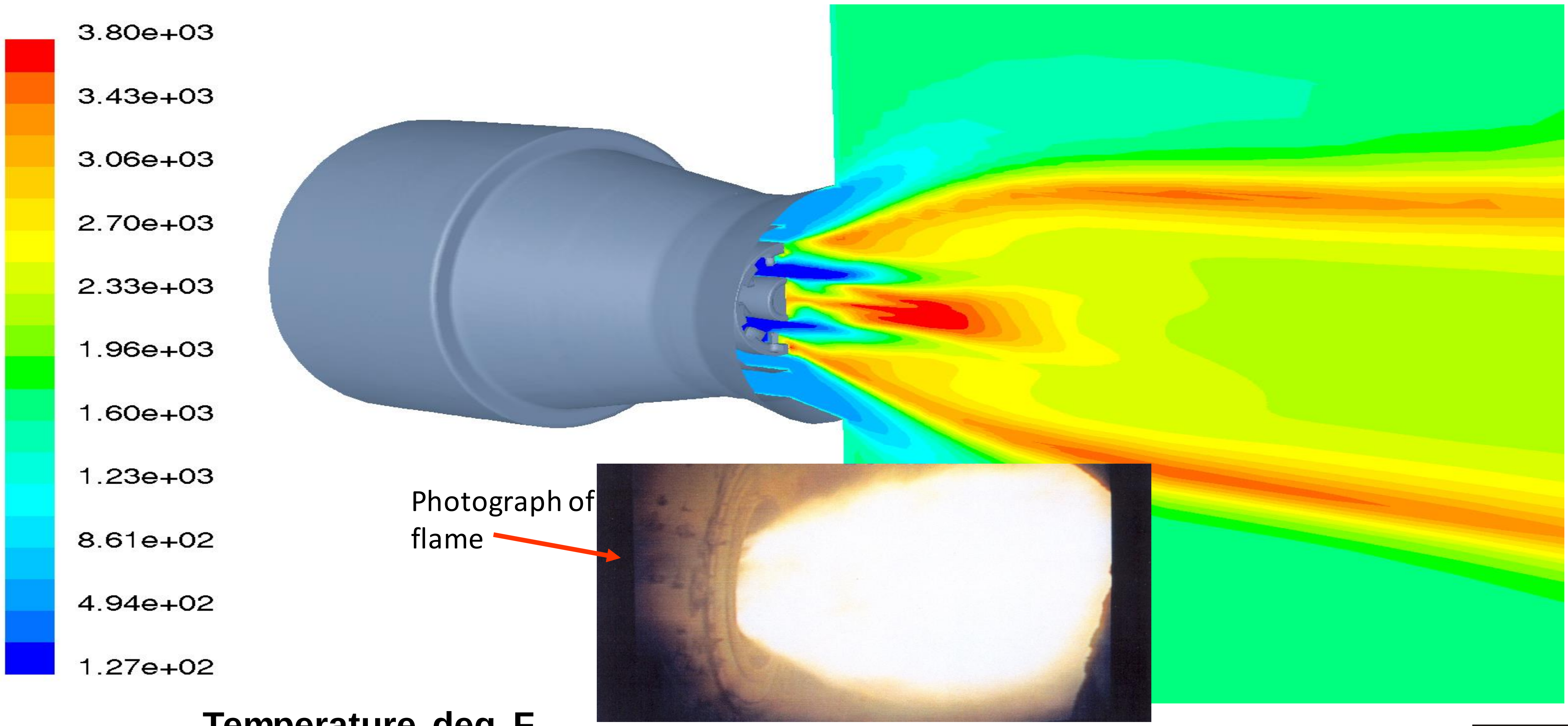
Contours of Flame temperature in a 3 burner design (John Zink)

CFD Advantages

- Burner design and performance for various fuel
- Help in developing low and ultra-low NOx burners
- Predicting temperature, NOx, with varying fuel, load, swirl
- Predicting thermal loads and stresses for different designs
- Burner spacing, orientation and the resulting thermal performance of the system

Low-NOx Burner Simulation

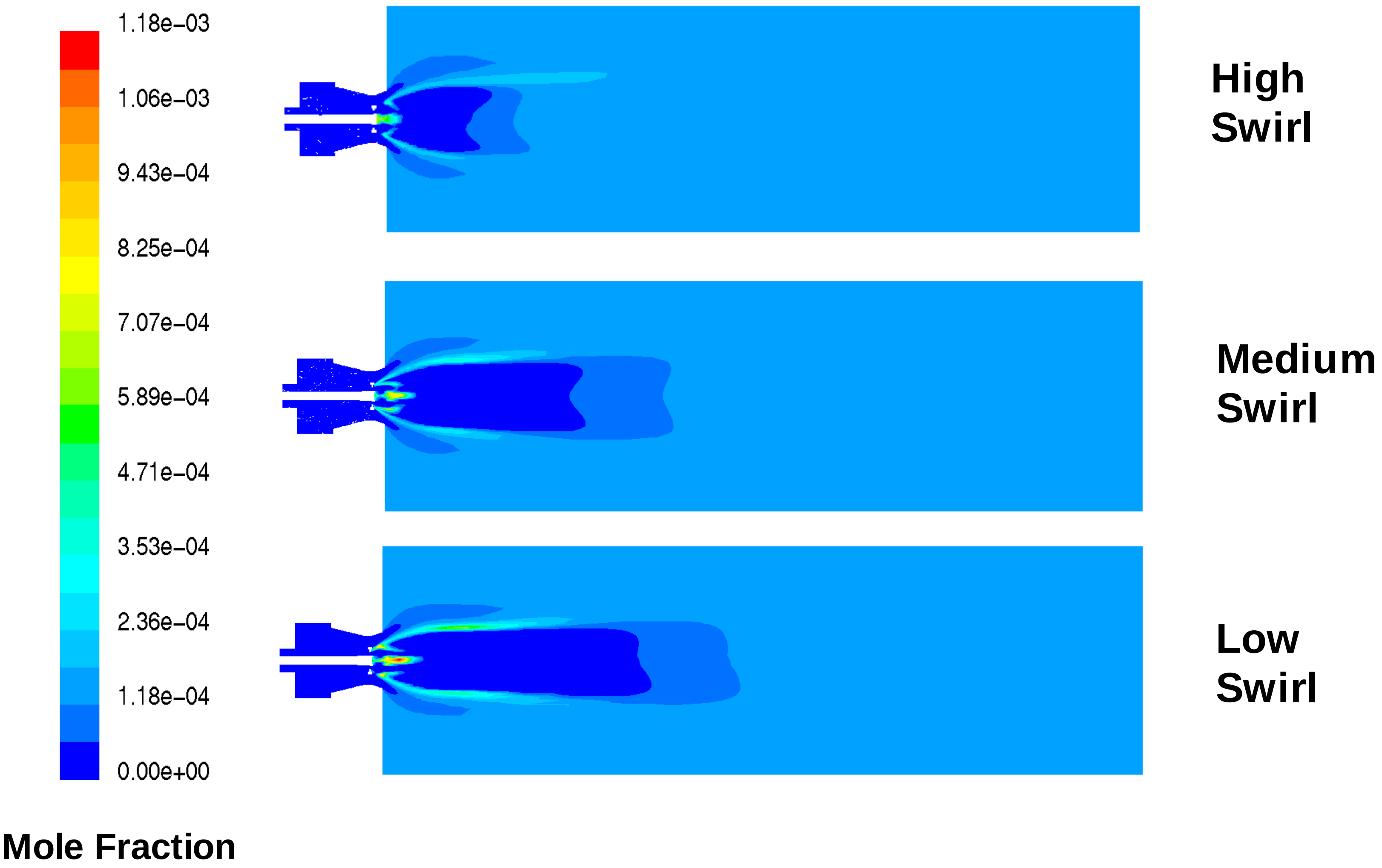
CFD simulation captured the flame shape and spreading as observed in experiment



Temperature, deg. F

Courtesy Of: GE Energy and Environmental Research Corporation

NOx Concentration Profile(s)



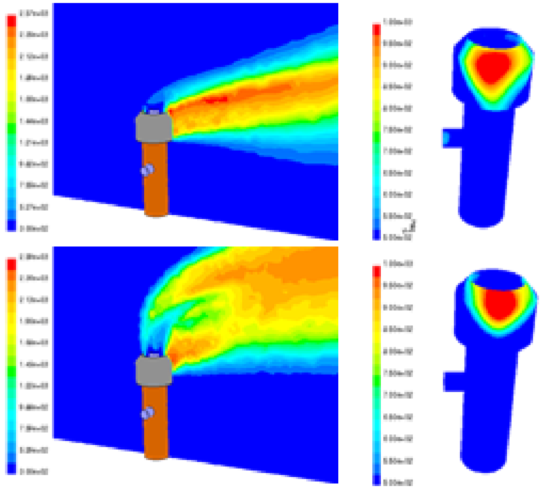
NOx concentration decreases with increasing swirl as observed in experiments.

Courtesy Of: GE Energy and Environmental Research Corporation

Combustion Systems: Flares

Challenges

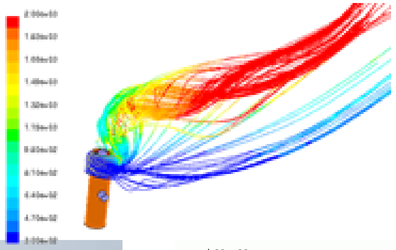
- Control flame shape and flare performance for different fuel and wind velocity
- Avoid back mixing and flame blow out
- Design flare support system and placement
- Reduce maintenance cost

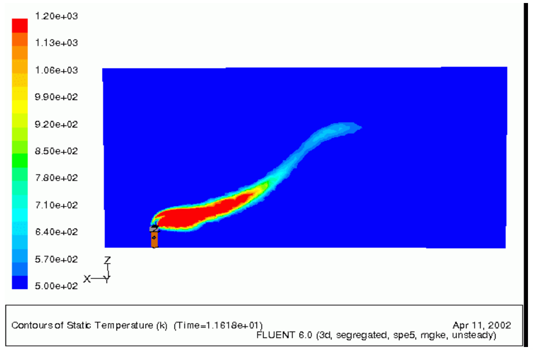


Fuel to Wind ratio 1:2

Fuel to Wind ratio 2:1

Flame shape and shroud surface temperature for two different fuel and wind ratios



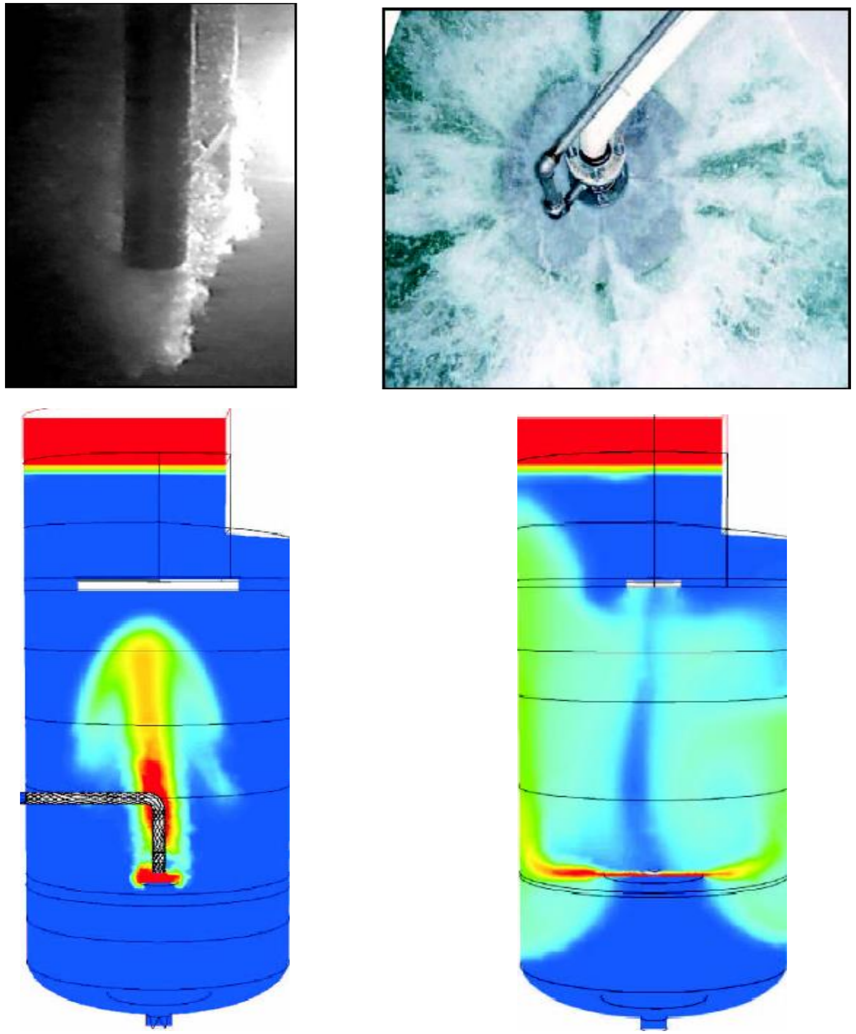


Flare flow pathlines, colored by temperature

CFD Advantages

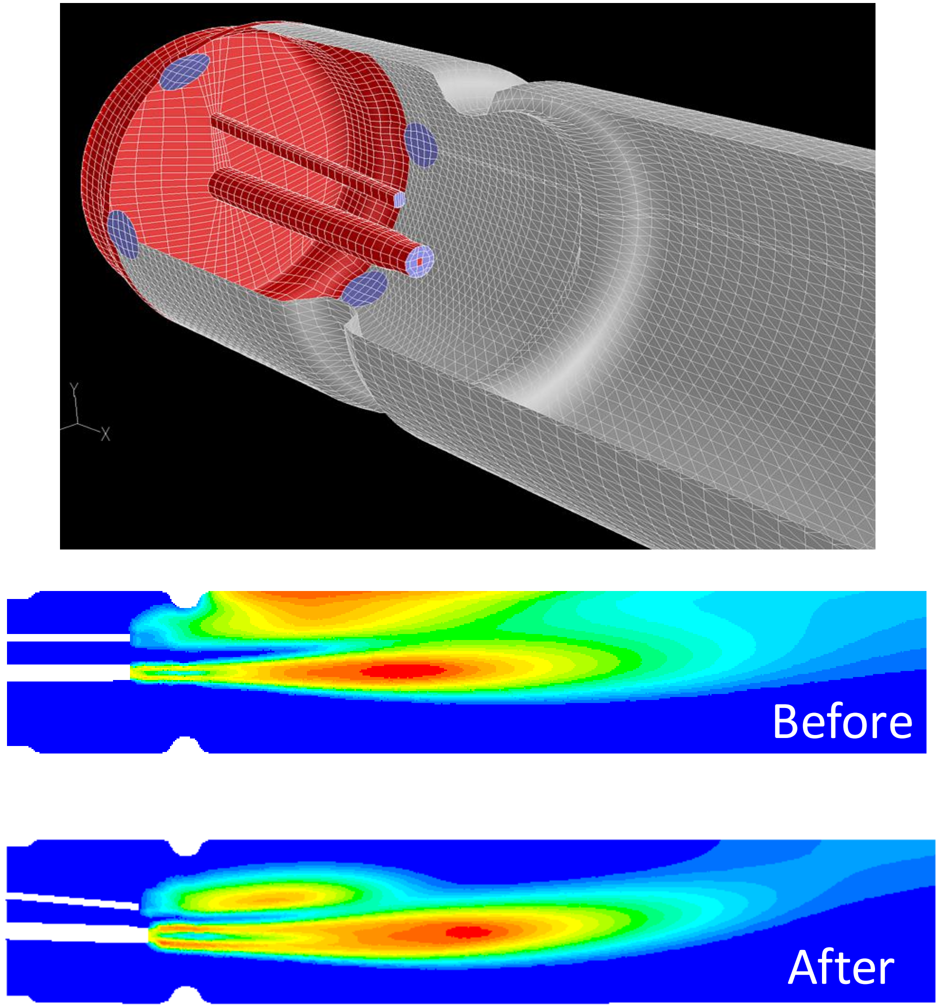
- Optimize flare design, shape and burner internals
- Compare performance of different arrangements and best placement
- Perform radiation and heat transfer studies from the flame
- Learn about thermal and structural stresses

Troubleshooting and Optimization



Gas Distributor Optimization

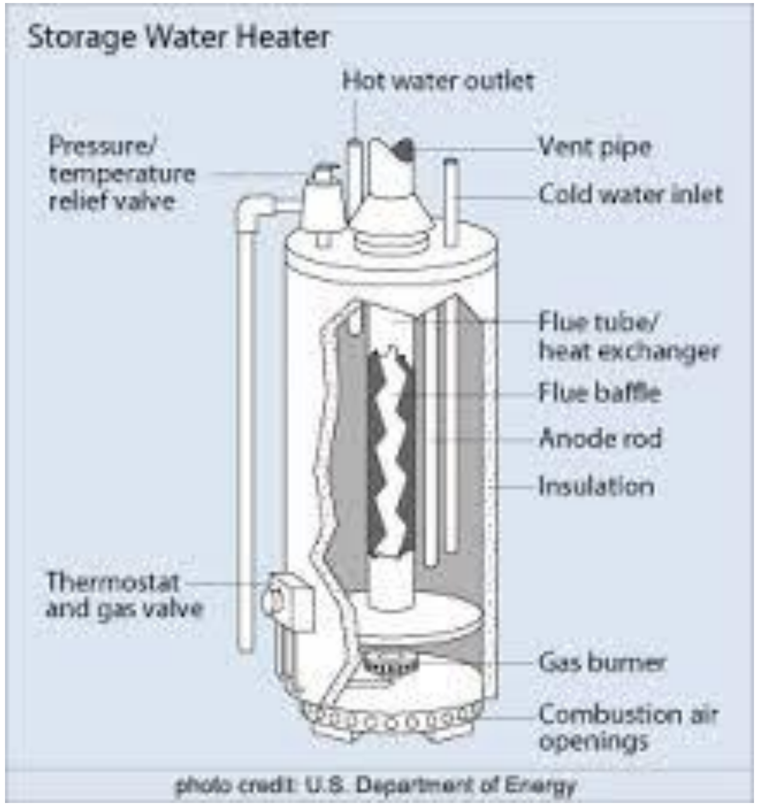
Courtesy of NATCO group Inc.



Troubleshooting a kiln burner

Courtesy of Coen Company

Water Heater Design



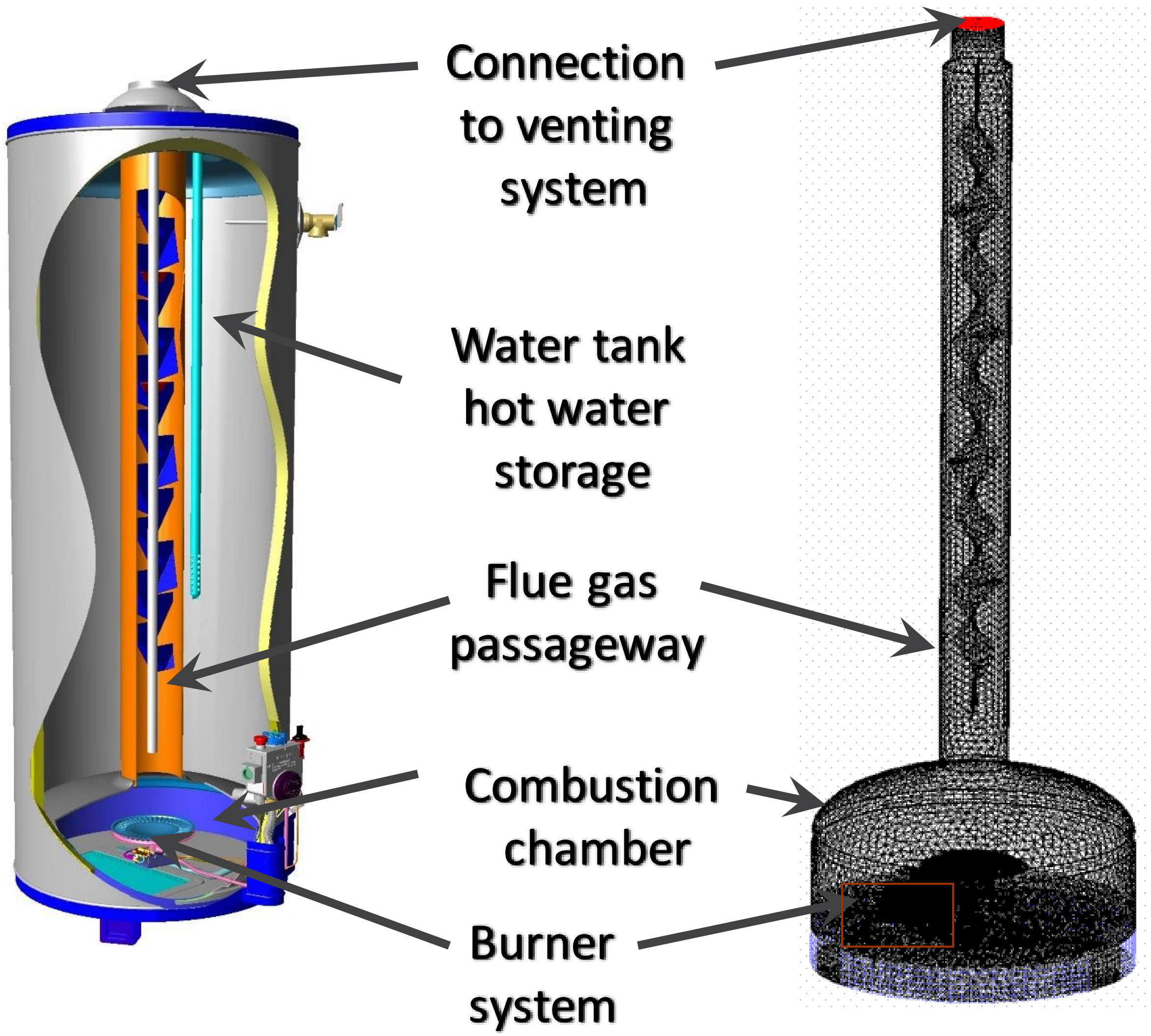
Emission
Flame stability
Heat transfer
Wall/solid temperature

Increased safety

Higher service efficiency

Lower CO and NO_x emissions

Water Heater Design



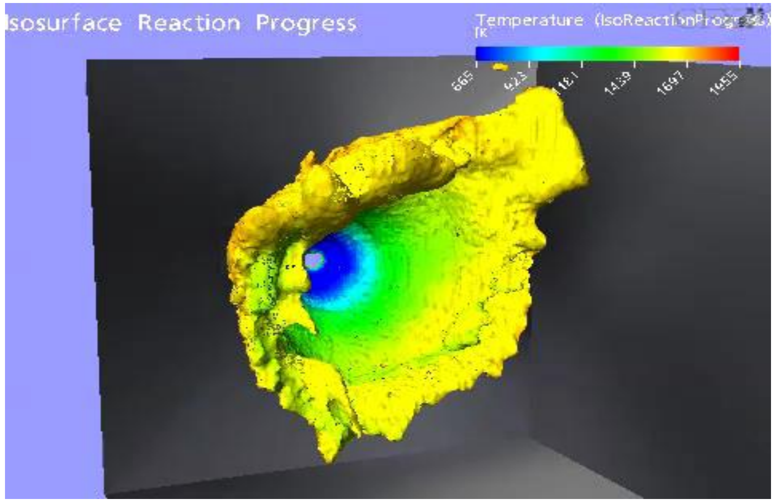
CFD will help …

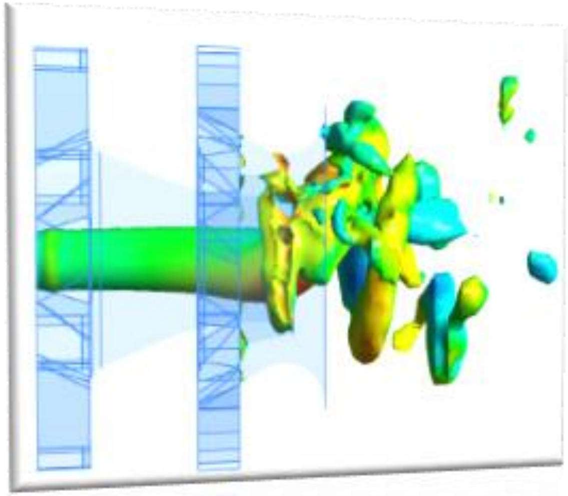
- Optimization of the burner operation
- Identify optimal location of temperature sensor
- Determine possible hot spots on the combustion chamber wall and flue gas passageway that might lead to premature failure
- Emission

Benefits of Scale Resolving Models

Next generation Combustion Simulations requires to capture unsteady Phenomena

- **Models like LES proved to be more accurate**
- **Prediction of Combustion Dynamics**
- **Prediction of Flame instabilities which can lead to catastrophic phenomena like Blow-Off or Flashback**



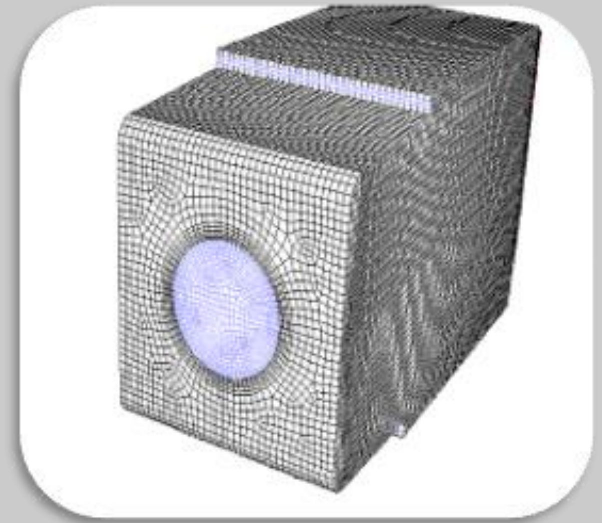


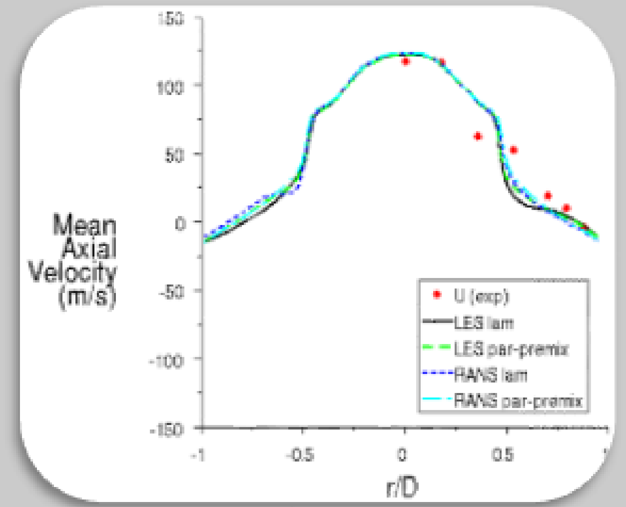
State of the Art Scale Resolving Models in ANSYS CFD

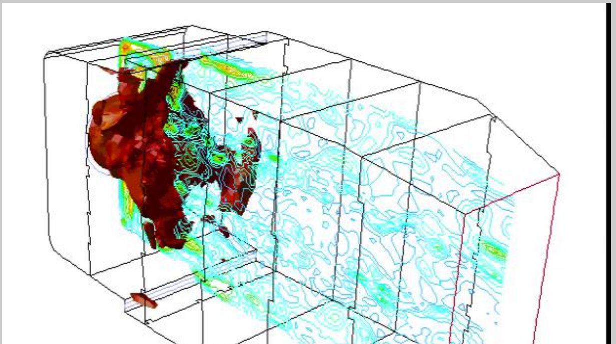
- Scale Adaptive Simulation
- Detached-Eddy Simulation
- Delayed Detached-Eddy Simulation
- Embedded Large-Eddy Simulation
- Large-Eddy Simulation

Scale Resolving Methods for Combustion Simulations
LES Example

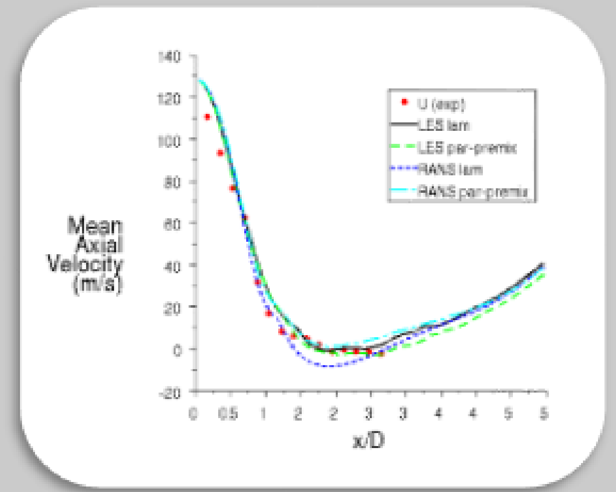
- **Challenge**
  - Simulating Combustion Processes in the GE LM6000 Gas Turbine Combustion Chamber
  - Predict the Flame location and velocity fields
- **Solution**
  - High Quality Mesh
  - State of the Art Turbulence Models (LES)
  - State of the Art Combustion Models (Premixed Model)
- **Results**
  - Accurate Prediction of the Combustion Processes
  - Accurate Prediction of Velocity Fields







Contour lines of vorticity magnitude on the combustor center-plane and contours of temperature on the flame surface (c=0.4)



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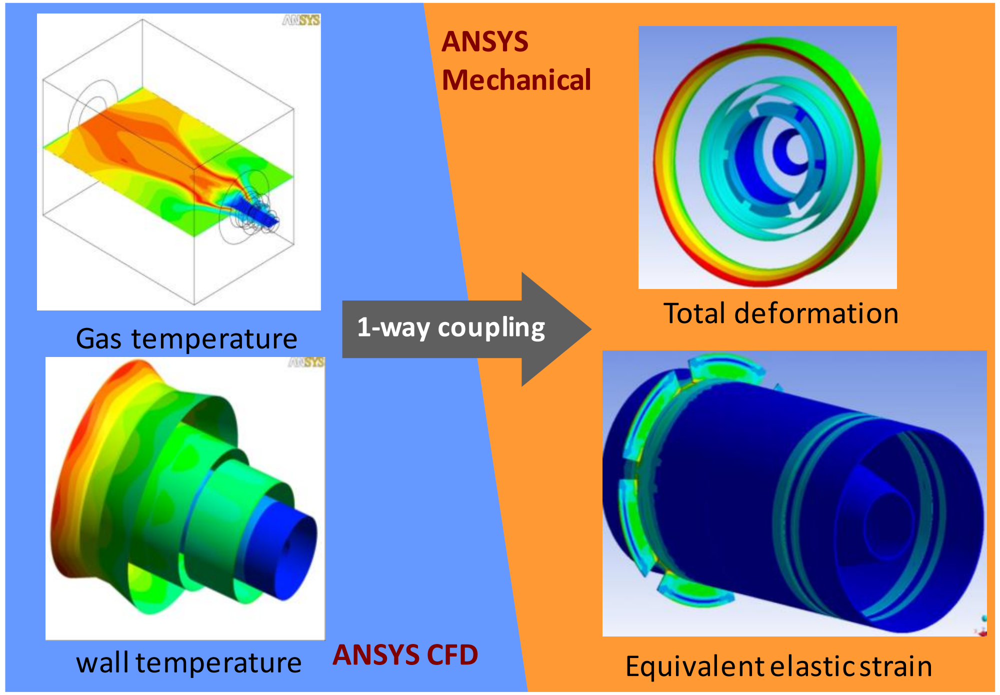
Full Power of ANSYS
Coupling FEA / CFD & Optimization

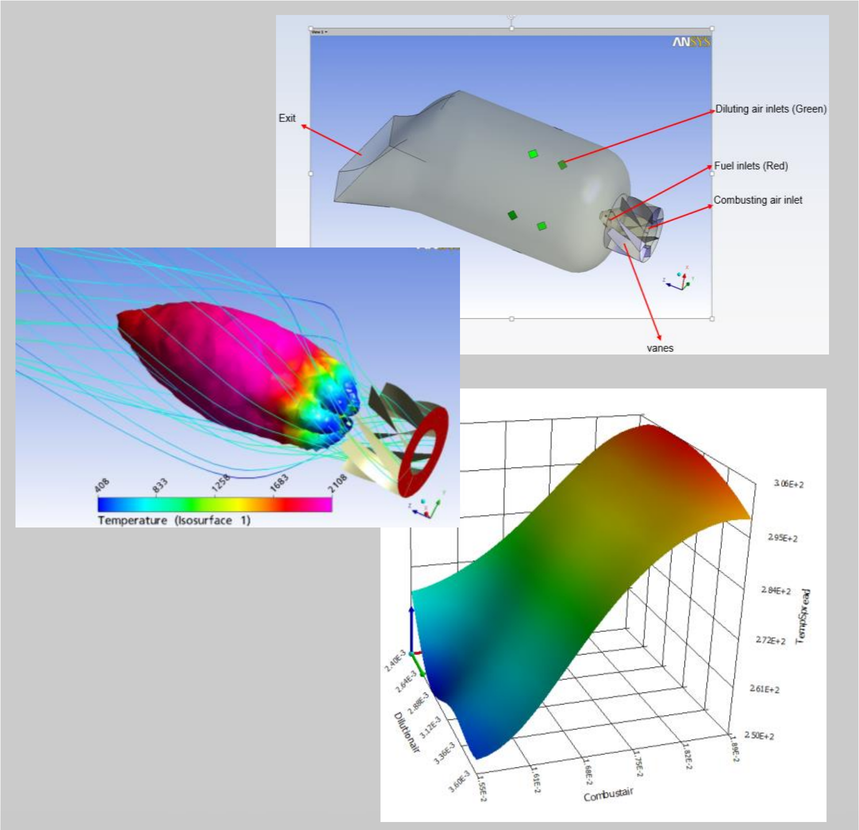


ANSYS Workbench – Fluid Structure Interaction (FSI)

- Couples CFD and Structural Simulations
- Transfer Pressure Loads, Temperature Loads, CHT data, etc.
- 1- and 2-way FSI

Design Optimization – Examples:

- Optimize a geometry
- Optimize operating conditions



Summary

- **ANSYS provides Powerful Combustion & Multiphysics Capabilities**
- **A large variety of models in ANSYS CFD including:**
  - ✓ Combustion
  - ✓ Turbulence
  - ✓ Radiation
  - ✓ Liquid Sprays
  - ✓ Pollutants
- **ANSYS Workbench integration can be used for Coupled Mechanical-Thermal-Combustion Analysis & Parametric Design Optimization**
- **For Advanced Combustion Analysis one can consider using Scale Resolving Simulations based Models**