Our Mission

TRDDC was founded in 1981…

"to apply existing knowledge for the benefit of our industry and our people"

- J.R.D. Tata

Motivation

Software and process engineering R&D is directed towards:

- adding quality to the process
- adding value to the product

The goal is to replace informal methods by a precise, predictable process with measurable quality

Process Engineering Research

Pradip

CFD, FEA
Population Balance
Statistical Methods

Surface Colloid Chemistry
Particle Science
Separation Science

Mineral Processing
Ceramics, Cements
Paints & Pigments

Reaction Engineering
Solid/Gas Reaction
Thermodynamics

Process Engineering
@
TRDDC

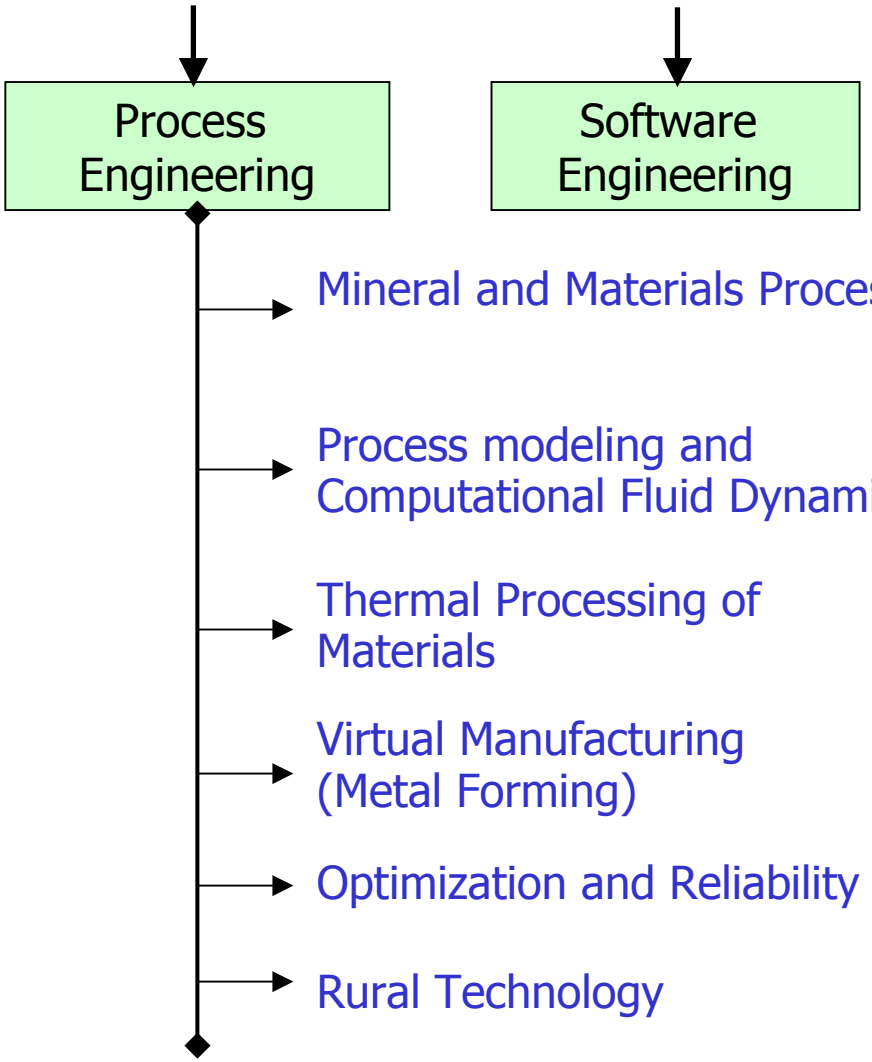
Iron and Steel Making
Casting
Welding

Solidification
Deformation processing
Thermal processing

Optimization & Control
Statistical Methods
Software Engineering

Metal forming
Heat Treatment
Furnaces

About TRDDC



Modeling & Simulation

Manufacturing Processes

Mathematical Modeling & Simulation

Computational Fluid Dynamics
Finite Element Analysis
Optimization & Control

Materials Processing

Casting & Solidification
Deformation processing
Thermal processing

Data Based Modeling

Reliability Prediction
Statistical Methods
Forecasting

Computational Fluid Dynamics (CFD)

- Materials Processing
  - Continuous Casting
  - Electron Beam and Laser Welding
  - Single Crystal Production (Czochralski & Bridgman)
- Turbomachinery
  - Compressors
  - Axial Fans (Placements of blades)
- Combustion
  - Boilers (Prevention of hotspots)

Design of a Centrifugal Compressor

Challenge:

2% increase in overall efficiency

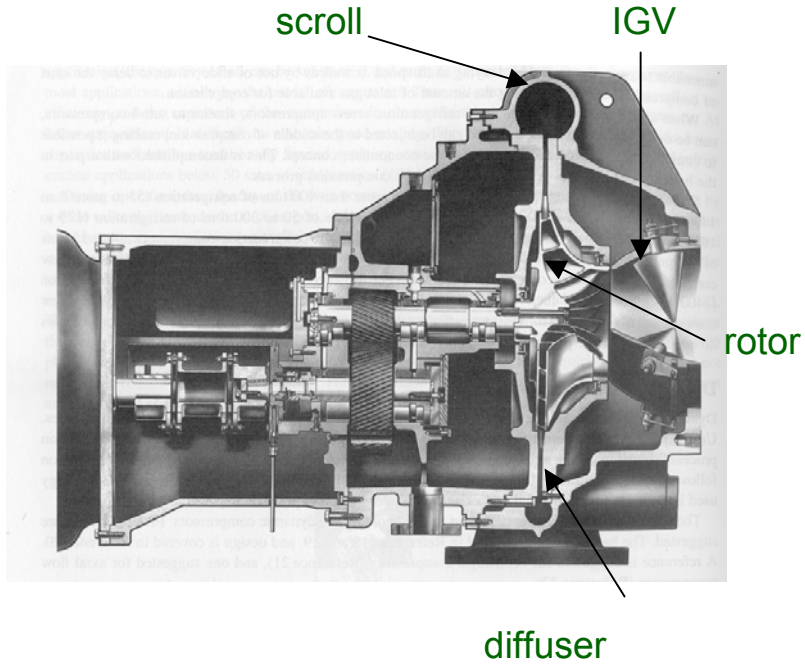
ASHRAE 90.1 Standard

Technology:

CFD in compressible Flow

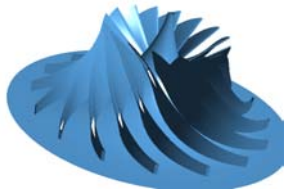
Constraints:

Size and Speed

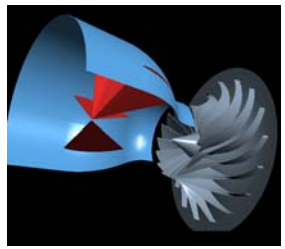


Compressor Design Solution

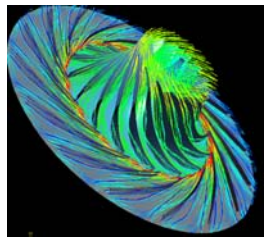
Preliminary Design



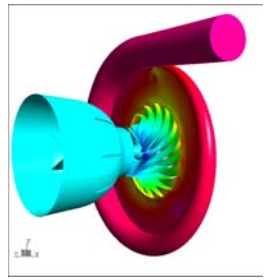
Rotor



Rotor with IGV



Flow in Rotor and Diffuser



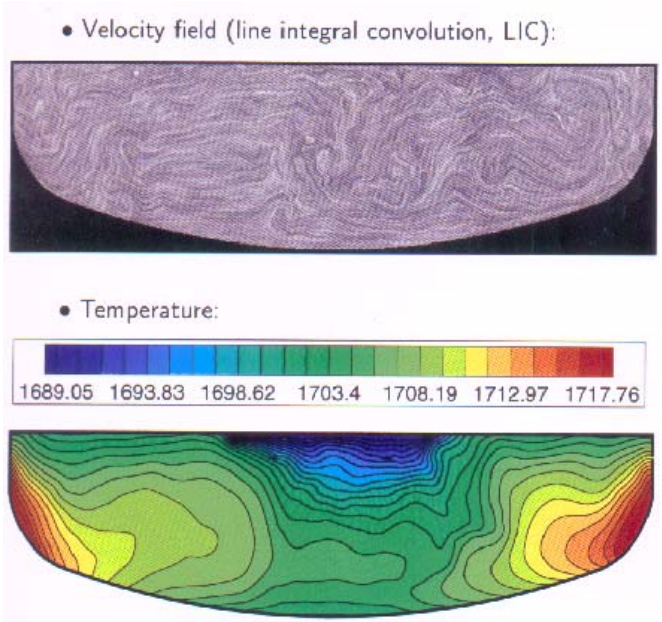
Complete Compressor

Structural Integrity

Enhancement of Overall Efficiency : 4.5 %
Design delivery : 6 months

Optimisation of Single Crystal Production (Czochralski Process)

- Manufacturing of Pure Silicon Crystal
- Control of fluid-mechanical instabilities
- **D**irect **N**umerical **S**imulation of turbulence

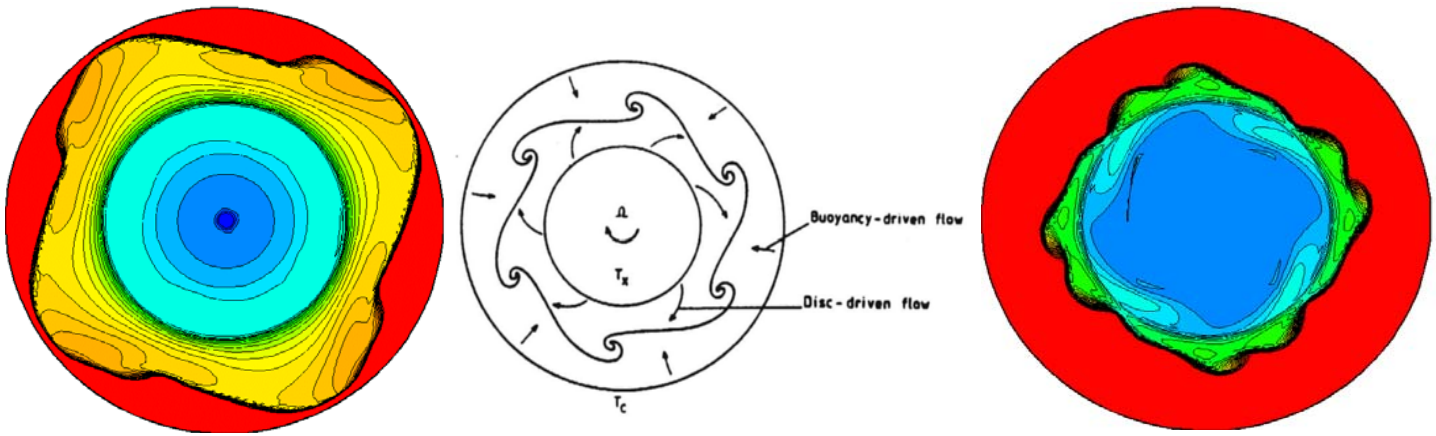


Mean $\Delta T(t)$: 4.12 K (P) and 3.8 K(M)

Collaboration :Institute of Fluid Mechanics Germany.

Optimisation of Single Crystal Production
(Czochralski Process)

- "Direct Numerical Simulation" in materials processing
  - 4 Processors in NEC SX-4
- Prediction & control of surface waves [**$Gr/Re^2 < 235$**]

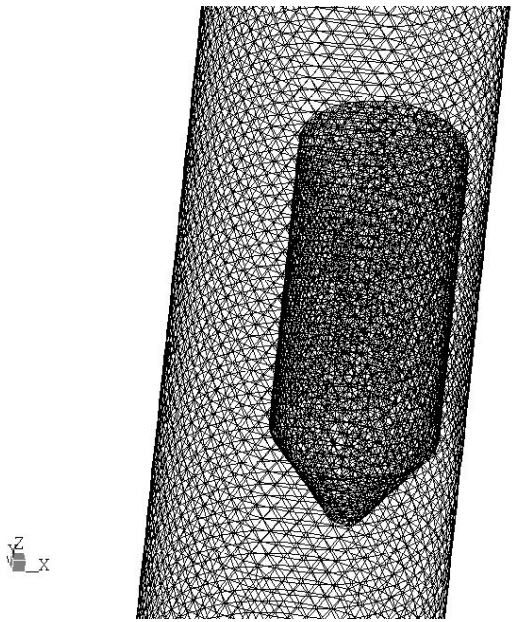


Collaboration : Institute of Fluid Mechanics, Germany.

B. Basu, et al, J Crystal Growth, 2000

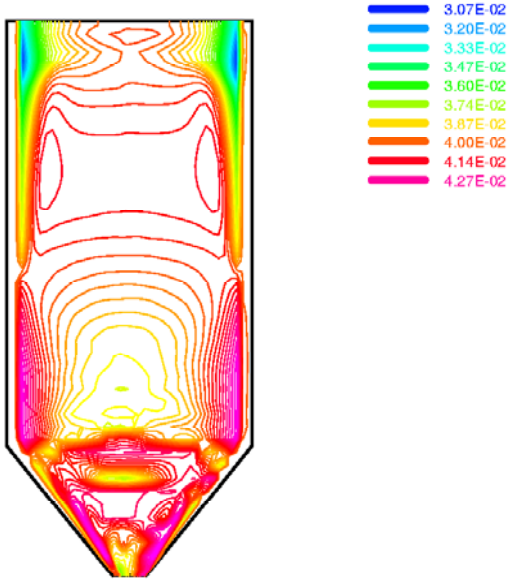
Optimization of Bridgman Crystal Growth Cd-Zn-Te (CZT)

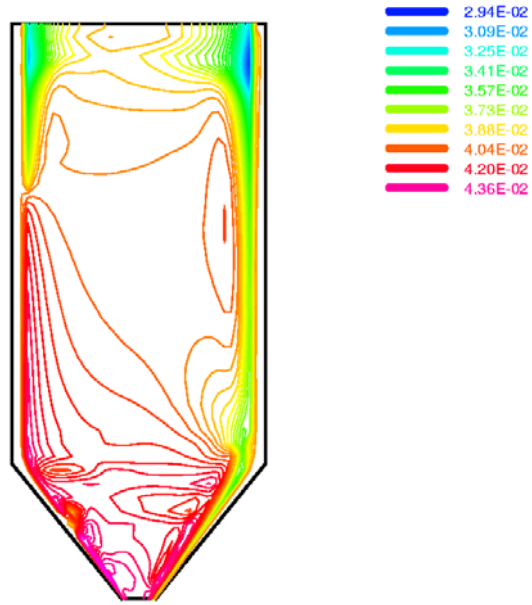
- CFD based modeling to explain the phenomena (asymmetric crystal growth leading to high yield) and to optimize the process parameter for a scaled-up furnace



Optimization of Bridgman Crystal Growth of CZT

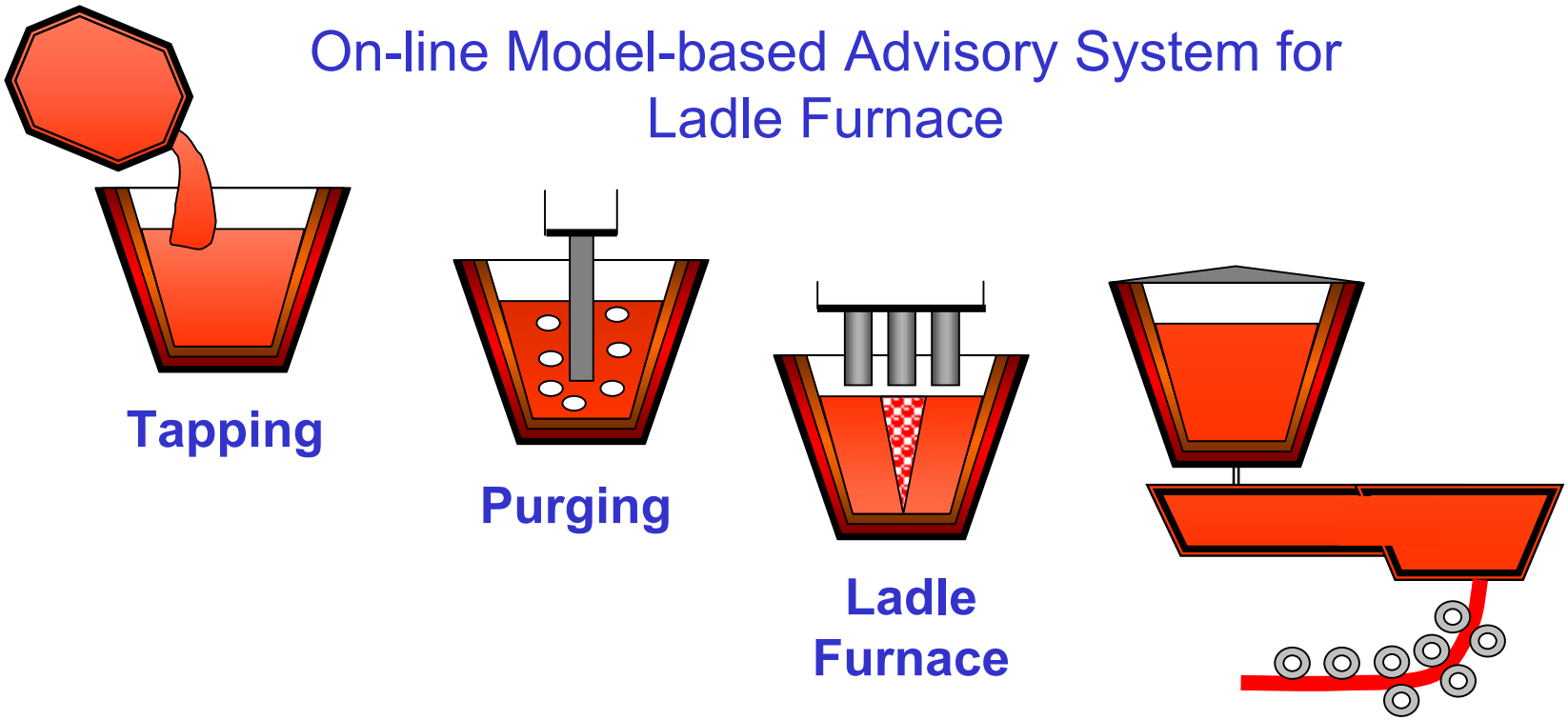
- Asymmetric Crystal Growth leading to improved quality and yield





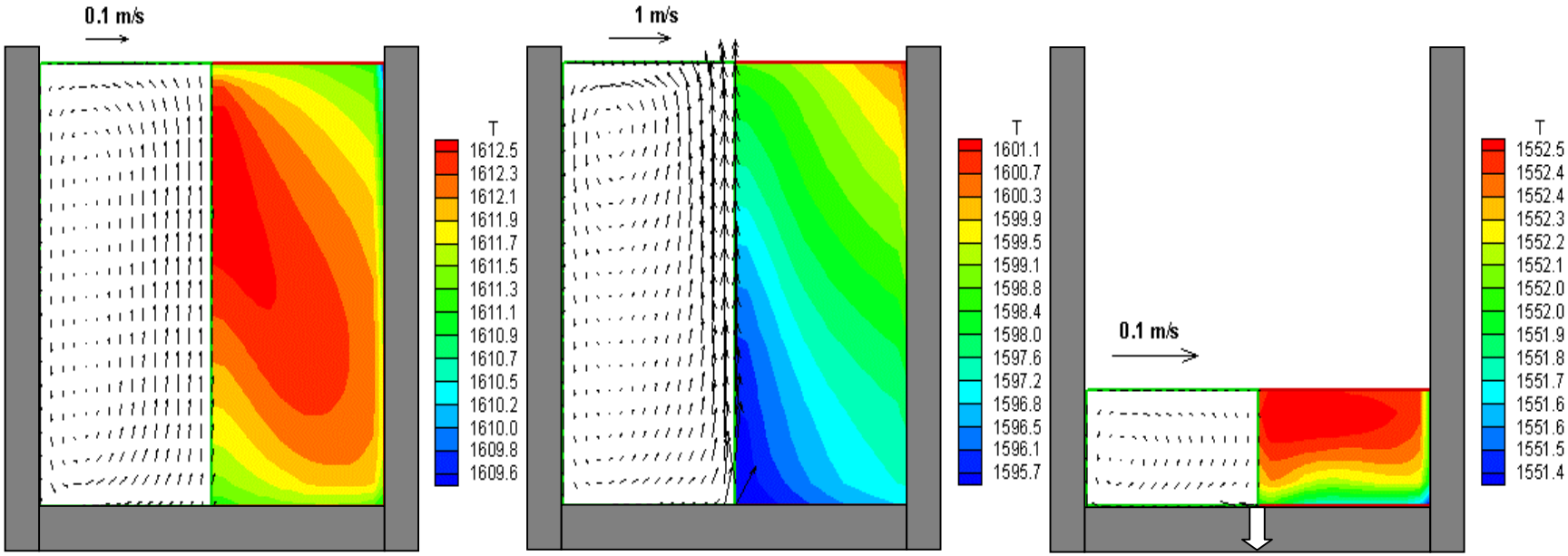
LFOR

On-line Model-based Advisory System for Ladle Furnace



High Speed Casting With Consistent Quality

Ladle Furnace Modeling

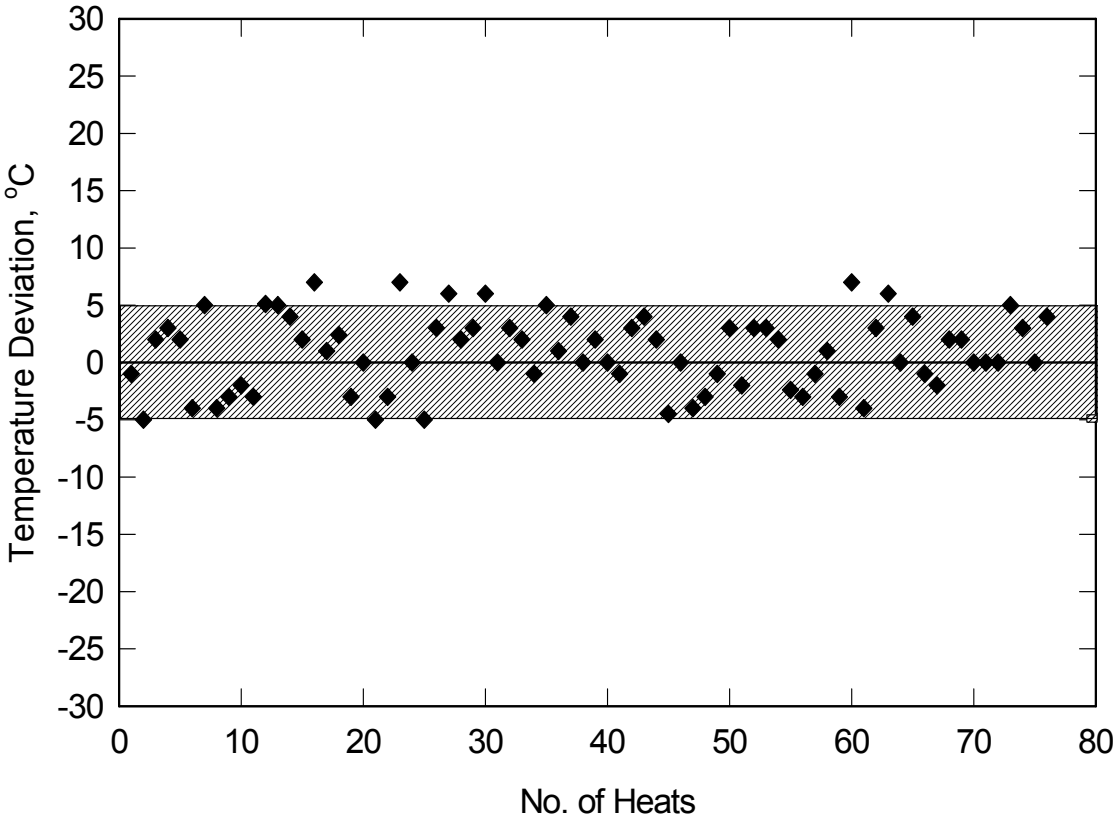


Holding
(0.1 m/sec)

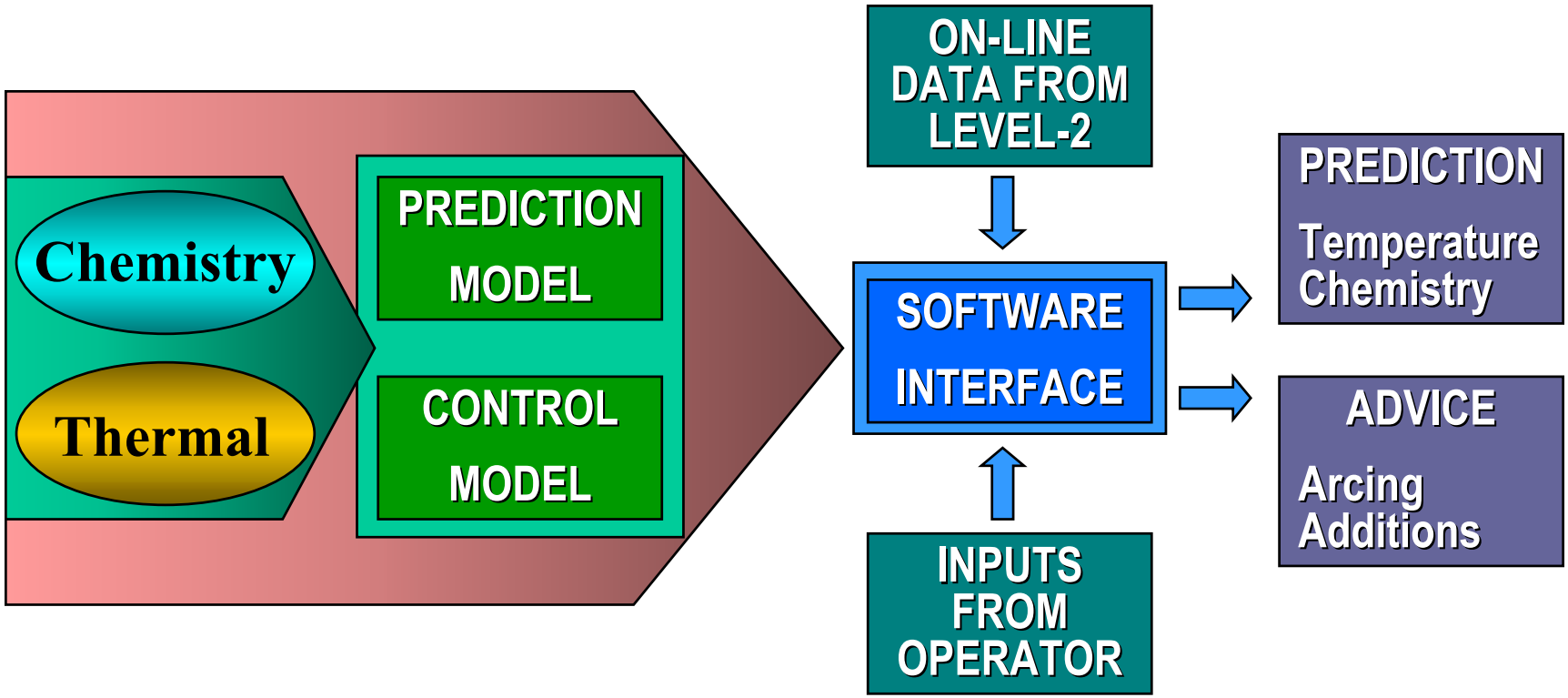
Purging
(1 m/sec)

Teeming in Tundish
(0.1 m/sec)

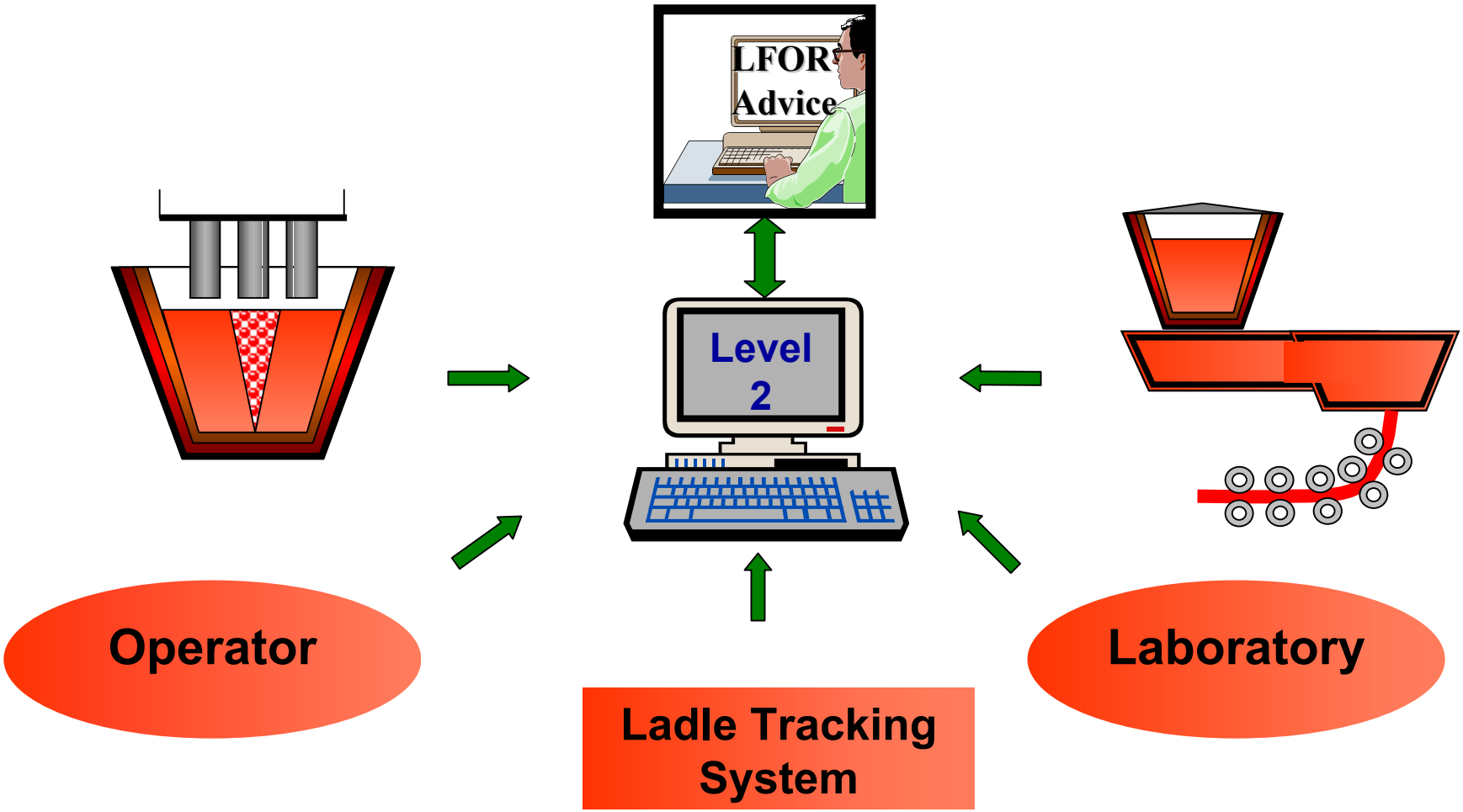
Ladle Furnace Modeling



Ladle Furnace Modeling



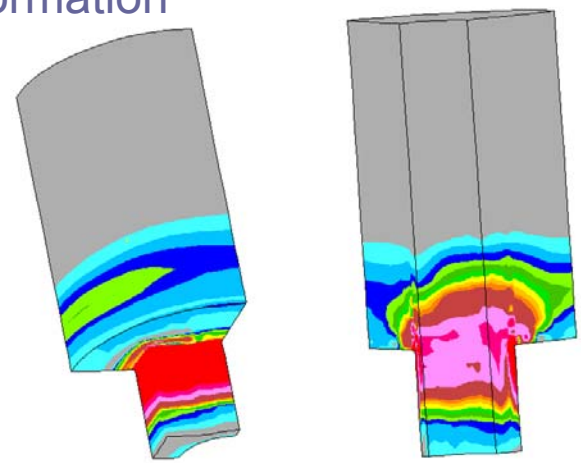
LFOR: Plant Implementation



Deformation Processing

- Research on simulation tools for metal forming
  - In house developed nonlinear *Finite Element* models
  - In a powerful *Arbitrary Lagrangian Eulerian* framework
  - Efficient solid type formulations for hot & cold deformation

- Applied to
  - Large deformation of solids and structures
  - Extrusion & drawing
  - Forging



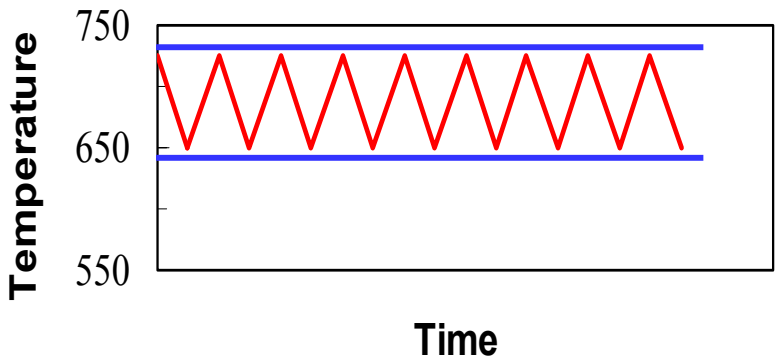
Extrusion of Aluminum

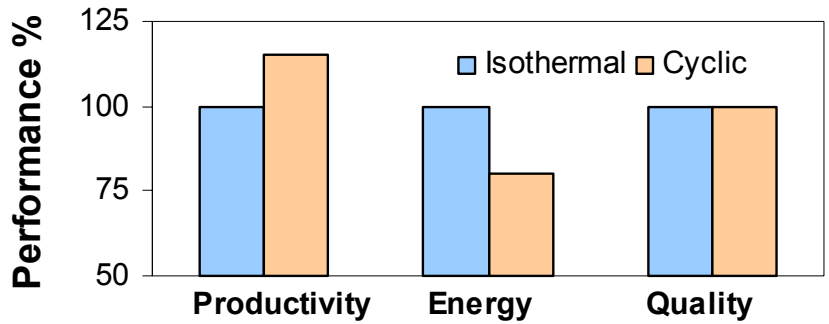
- Some key achievements
  - Prediction of *dead metal zone* & flow in the die for aluminum extrusion
  - *Cost effective* simulator for design of preform for cold ring rolling

Thermal Processing of Materials

- Modeling & optimization of thermal processing
  - Cost model, integrated process models for microstructural modeling
  - Successfully optimized several industrial scale operations

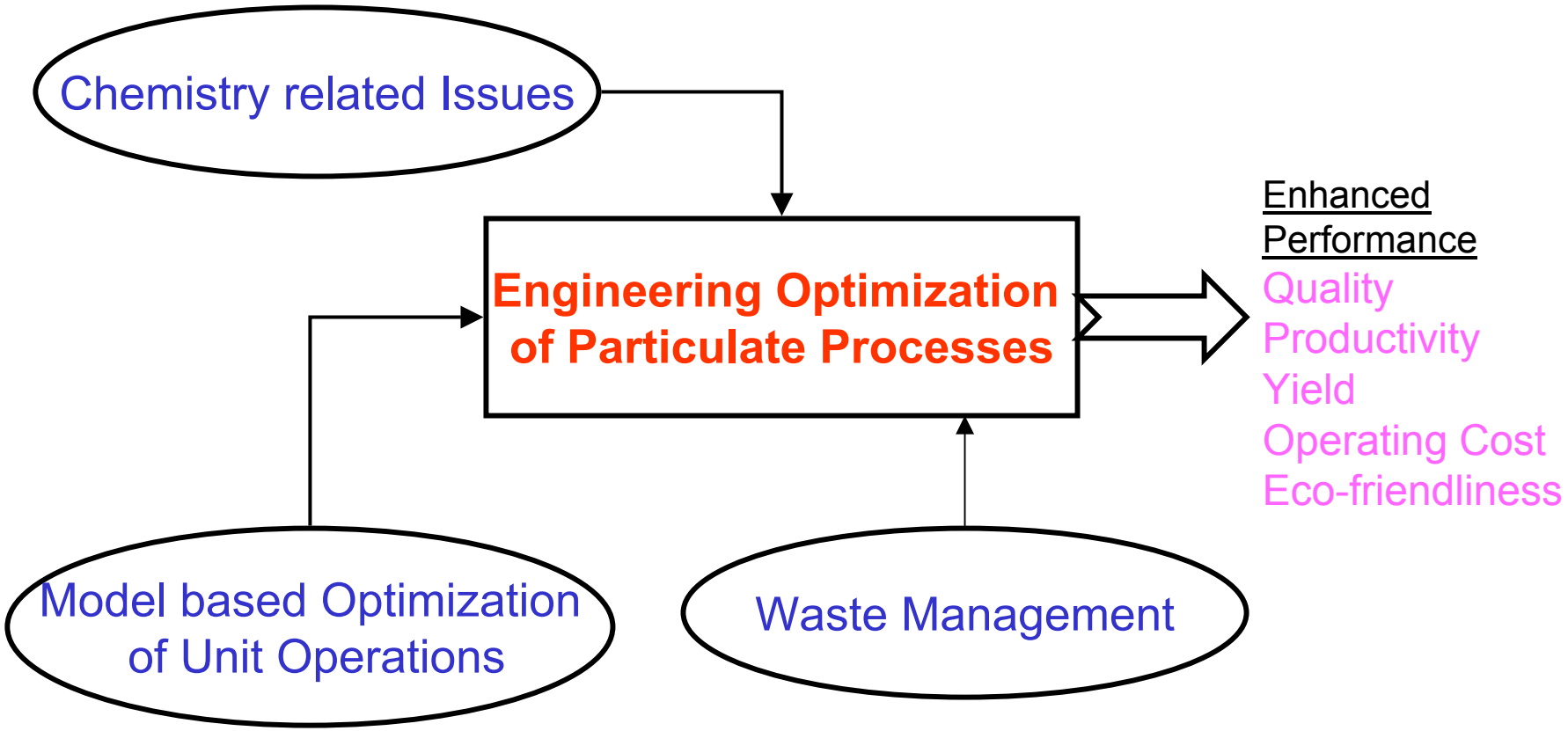
- Efficient non-isothermal processing of materials
  - Kinetics of non-isothermal processing faster than isothermal processing
  - Experimentally shown in several transformations and material system





Ref: Sahay *et al.* Acta Materialia (2003), HTP 2003, Physica B (2004)

Mineral and Materials Processing



Particle Science & Technology

Interfacial Chemistry and Reagents Design

- Rational design of additives/surfactants
  - *Molecular Modeling/MD Simulation*
  - *Molecular recognition phenomena at interfaces*
- Rheology of multi-component particulate fluids
  - *Colloidal processing of advanced ceramics*
  - *Pressure filtration*
  - *Semi-dry disposal of mine tailings*

Engineering Optimization of Particulate Processing Operations (Minerals & Materials)

- Comminution circuits
- Flotation separation circuits
- Gravity separation units (spirals)
- Pelletization and agglomeration units
- Iron ore sintering
- Solid state sintering (sintering cycle optimization)
- Flocculation – Dispersion in suspensions
- Dewatering of particulate slurries
- Silicon Carbide Production by Acheson Process

Model based optimization of unit operations

⇒

Enhanced Performance
Quality, Productivity, Yield, Operating Cost, Eco-Friendliness

- Lignin Separation from black liquor (pulp & paper mills)
- Sulfur recovery from waste sludges
- Cement from industrial & mining wastes (alinite & sulfo-aluminate)
- Recovery of Copper Oxide from etchant wastes
- Recovery of values from fine talilings
- Rice husk ash based water filter (Removal of turbidity, pathogens, fluoride, heavy metals, arsenic)

Waste Management

Nanoscience and Technology

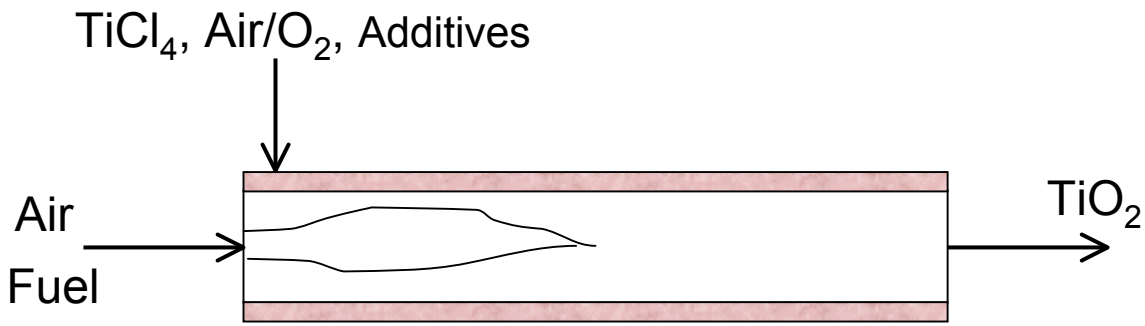
- Rational Design of Performance Chemicals
  - Molecular Modeling Tools
  - Adsorption/Self-assembly of Molecules at Interfaces
  - Industrial Additives and Specialty Chemicals
    - Flotation
    - Dewatering
    - Dispersion & Flocculation
- Synthesis of Nanoparticles
  - Population Balance Modeling
  - Particle Size Distribution is the most important property
  - Modeling of Aerosol Flame Reactors
  - Titania, Silica and Carbon Black

Application-oriented, Industrially Relevant & Scientifically Challenging

Modeling of Titania Nanoparticle Synthesis
(Aerosol Flame Reactor)

Process Variables

- Flame Temperature Profile
- Residence Time
- Reactant flow rate & Concentration
- Reactor Pressure
- Additives



Length ~ 3 m

residence time ~ 50 msec

Temperature > 1000 °C

Process is characterized by high temperatures and low residence times

Modeling Issues

- Particle Size Distribution
  - PSD depends on gas/flame dynamics
- Gas/Flame Dynamics
  - Gas/Flame temperature profiles
  - gas velocity profiles
  - gas concentration profiles

Population Balance

Computational Fluid Dynamics

Necessary to integrate particle growth kinetics with gas/flame dynamics in order to predict effects of process inputs on product characteristics

Prediction of Size Distribution of the synthesized Titania Nanoparticles

Titania particle size distributions

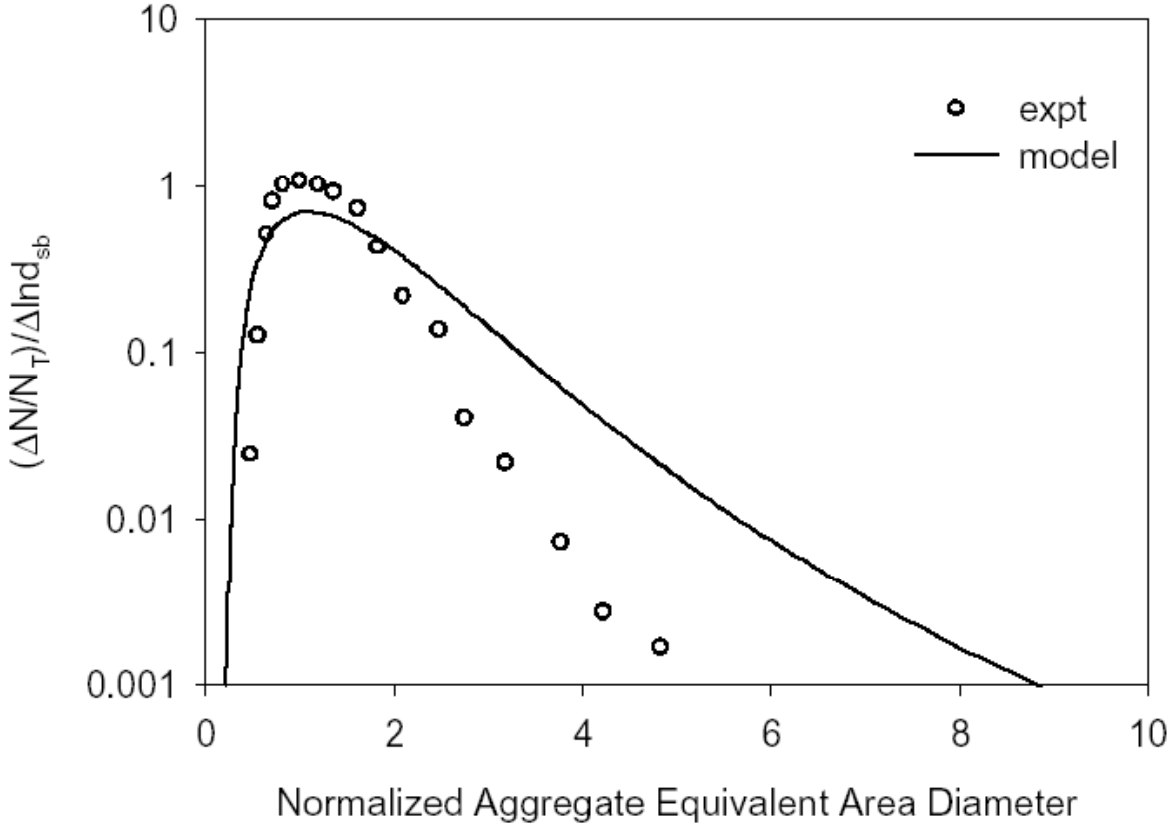
Comparison of predictions with experimental data from an aerosol flame reactor

Pressure: 1 atm

Temperature: 1400 K

Residence Time: 1.6 sec

$[TiCl_4]$: 9.34×10^{-6} mol/lit



Expt. Data from Akhtar et al., *A. I. Ch. E. Journal*, **37**, 1561-1570 (1991)

Summary

- Multidisciplinary expertise in modeling-simulation and control
- Industrial problem solving skills
- In house programs on selected areas of relevance to industry
- Experience of taking R&D to industry
- Creation of intellectual assets
- Partnership with academia and industry

Thank you for your kind attention