Computational Fluid Dynamics for Natural Circulation- NEEDS and V&V

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Presented at
IAEA Course on Natural Circulation in Water-Cooled Nuclear Power Plants,
International Centre for Theoretical Physics (ISP), Trieste, Italy
25th to 29th June 2007

Contents

1. Introduction

- NEED FOR CFD
  - DESIGN: – Evolutionary Process
  - Design – Analyze - Predict Performance – Modify Design
  - CFD Can Help in Optimization

  - NEW PRODUCT DEVELOPMENT: CFD is a very good tool for Analysis
  - Generates Complete Flow Field Information
  - 1D, Empirical, Lumped Loss Modeling cannot be Extended to Unknown Territory - CFD has Better Chance for Success, since Modeling is done at Microscale Level

Experimentation – Extremely Difficult & Expensive

- Measurement Techniques, Sensors, Instrumentation not yet Developed
- Measurement Volume Inaccessible, Small for Intrusive/Non-intrusive measurement
- Intermittent/Unsteady, Multicomponent, Multiphase Flow
- Hostile Environment: High Temperature, Contaminants (Dirt), radioactive

CFD Appears to be a Logical Scheme to Complement Experimentation

CFD Applications in Nuclear Field during the Last Few years:

Pressurized thermal shock
Flow in tee junctions
Containment flow in LOCA
Sump screen debris
Flow storage
Boron mixing
Natural Circulation
Reactor cavity Cooling System
Gas cooled reactors, etc.
…………………………
CFD Tsunami hits nuclear industry!!!!

2. Conservation Equations

- (Single-phase) conservation equations
- Ensemble averaged equations & Reynolds
- Filtered equations & Subgrid model

Conservation Equations
Single-Phase

- Mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \mathbf{u} \right) = 0$$

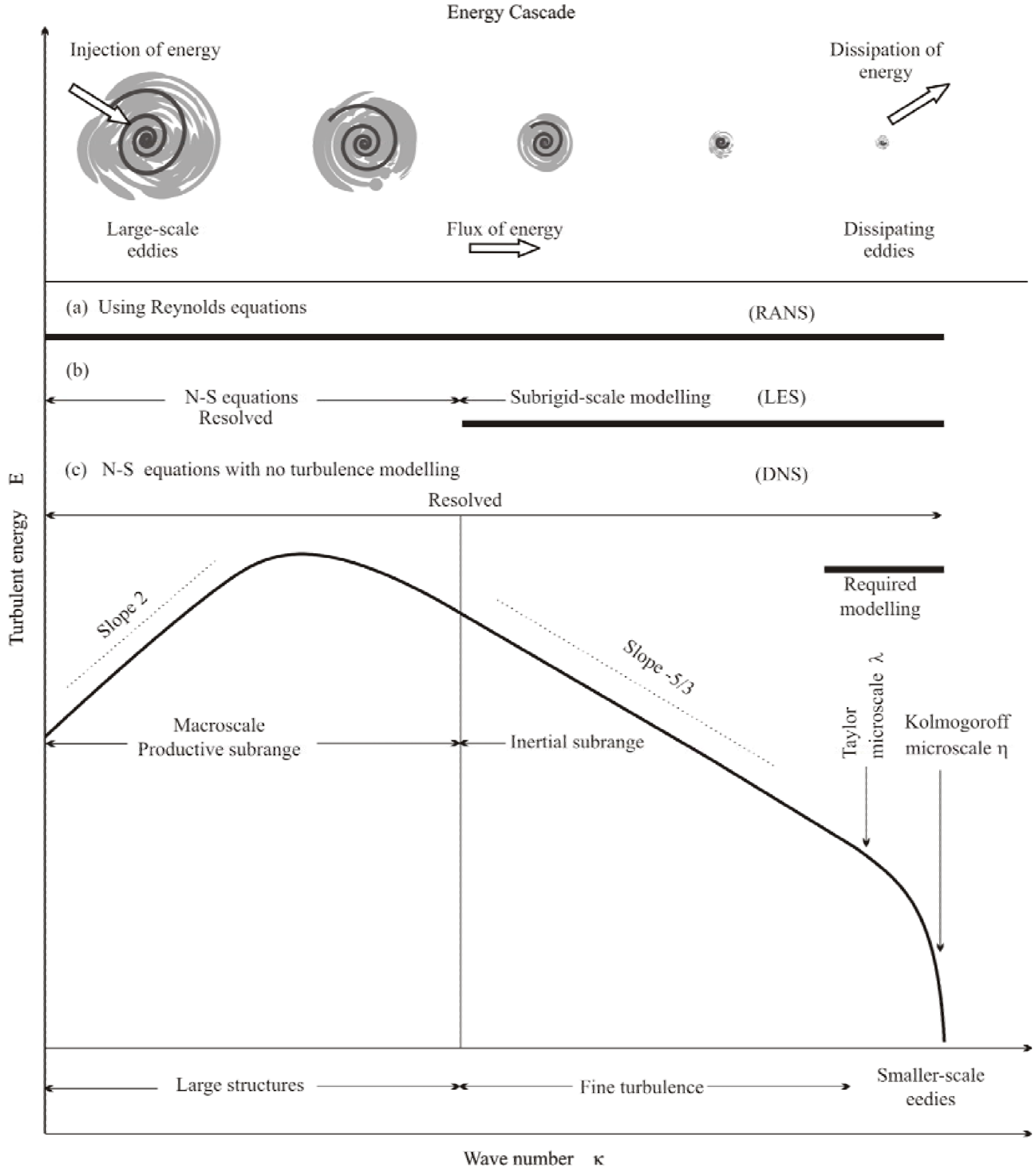
- Momentum:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{f}$$

- Energy:

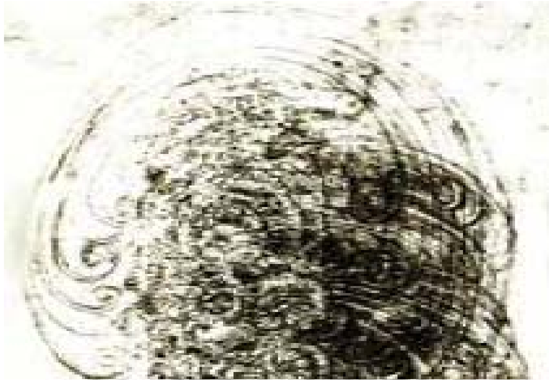
$$\rho \frac{\partial}{\partial t}\left(e + \tfrac{1}{2} u^2 \right) + \rho \mathbf{u} \cdot \nabla \left(e + \tfrac{1}{2} u^2 \right)$$
$$= -\nabla \cdot \left(p \mathbf{u} \right) + \nabla \cdot \left(\boldsymbol{\tau} \cdot \mathbf{u} \right) - \nabla \cdot \mathbf{q} + \rho \, \mathbf{f} \cdot \mathbf{u} + \dot{q}$$

$$\boldsymbol{\tau} = \lambda \left(\nabla \cdot \mathbf{u} \right) \boldsymbol{\delta} + \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \qquad \mathbf{q} = -\kappa \nabla T$$



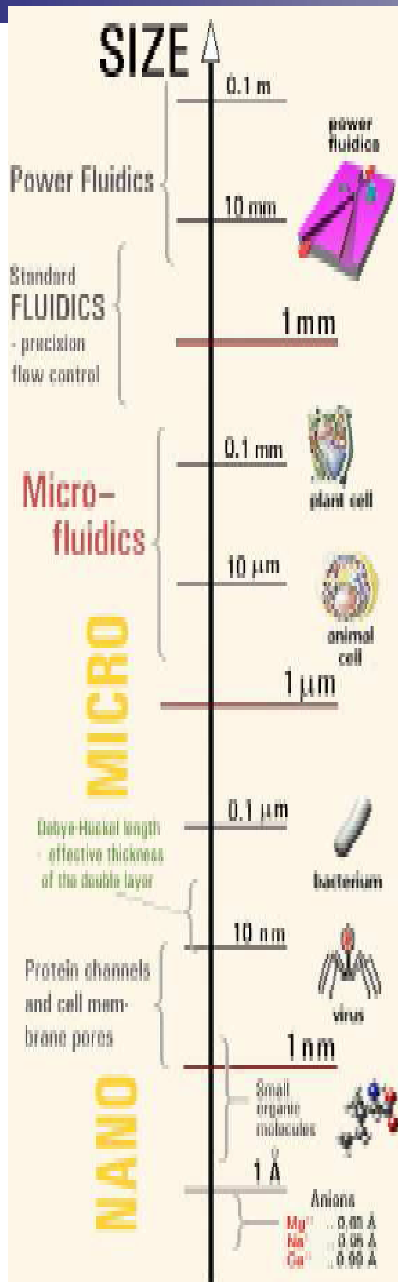
Turbulence Model Concepts

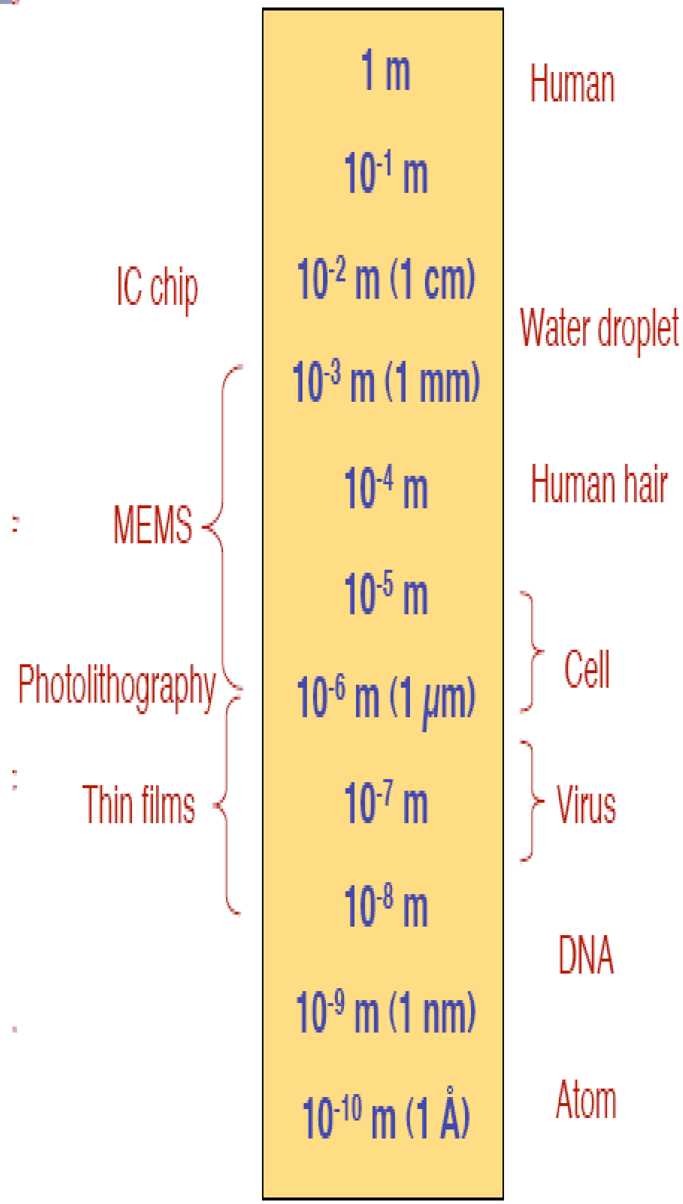
Leonardo da Vinci (1452-1519), his drawing and statement of coherent vortices around piers (The Royal Library, Windsor Castle)



Sketch of Leonardo da Vinci

Turbulence Has a Wide Range of Scales





Putting Size in Perspective

(1) Direct Numerical Simulation (DNS)

- It is possible to directly solve the Navier-Stokes equations for laminar flow cases and for turbulent flows when all the relevant length scales can be contained on the grid. This solution approach of resolving all the scales is known as Direct Numerical Simulation (DNS). Because all the length and time scales have to be resolved. DNS is computationally expensive. In general, the range of length scales appropriate for flows of practical importance is larger than even today's massive supercomputers can model.

Limitations of DNS

- Too many nodes is required.
  - Turbulence have the broad range of scale.
  - To describe the smallest scale of turbulence, practically impossibly due to many numbers of meshing of $Re^{9/4}$ are required.
  - Representative Reynolds number
    - Model airplane (L=1 m,U=1 m/s): $Re \sim 7 \cdot 10^4 \rightarrow 8 \cdot 10^{10}$ mesh pts
    - Cars (U=3 m/s): $Re \sim 6 \cdot 10^5 \rightarrow 10^{13}$ mesh pts
    - Airplanes (U=30 m/s): $Re \sim 2 \cdot 10^7 \rightarrow 2 \cdot 10^{16}$ mesh pts
    - Atmospheric flows: $Re \sim 10^{20} \rightarrow 10^{45}$ mesh pts

(2) RANS

- The Reynolds averaged Navier equations (RANS) are obtained by ensemble average of the conservation equations which introduces new apparent stresses known as Reynolds stress.
- Various models are developed to provide different levels of closure.

(3) Large Eddy Simulation (LES)

- Large Eddy Simulation is a compromise between RANS and DNS methods.
- LES uses a spatial filtering technique where scales of turbulence above the grid size are resolved.
- Scales of turbulence below the grid size are modeled as dissipation (these scales are generally more universal).
- These are known as subgrid scale models.

Large Eddy Simulation

- Convolution filter used to separate instantaneous flow variables into resolved (large) and unresolved (subgrid) scales:

$$\bar{f}\left(x,t\right)=\int\bar{G}\left(x,x'\right)f\left(x',t\right)dx'$$

Continuity

$$\frac{\partial\bar{u}_i}{\partial x_i}=0$$

Momentum

$$\frac{\partial\bar{u}_i}{\partial t}+\frac{\partial\bar{u}_i\bar{u}_j}{\partial x_j}=-\frac{1}{\rho}\frac{\partial\bar{p}}{\partial x_i}+\nu\frac{\partial^2\bar{u}_i}{\partial x_j\partial x_j}-\frac{\partial\tau_{ij}}{\partial x_j}$$

Subgrid Scale Modeling

- The goal of SGS modeling is to express the unresolved components in terms of the known values.
- The Smagorinsky model

$$\tau_{ij} - \frac{1}{3}\delta_{ij}\tau_{kk} = -2\nu_T \bar{S}_{ij} \qquad \left|\bar{S}\right| = \left(2\bar{S}_{ij}\bar{S}_{ij}\right)^{1/2}$$

$$\nu_T = \left(C_S \Delta\right)^2 \left|\bar{S}\right| \qquad \bar{S}_{ij} = \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)$$

Subgrid Scale Modeling

- Although the Smagorinsky model is the most widely used subgrid model, it has several drawbacks:
  - Incorrect behavior near walls (damping necessary)
  - Poor representation of Reynolds stresses (compared to DNS data)
  - Does not allow SGS energy backscatter
  - Model coefficient is flow dependent

Dynamic Subgrid Scale Model

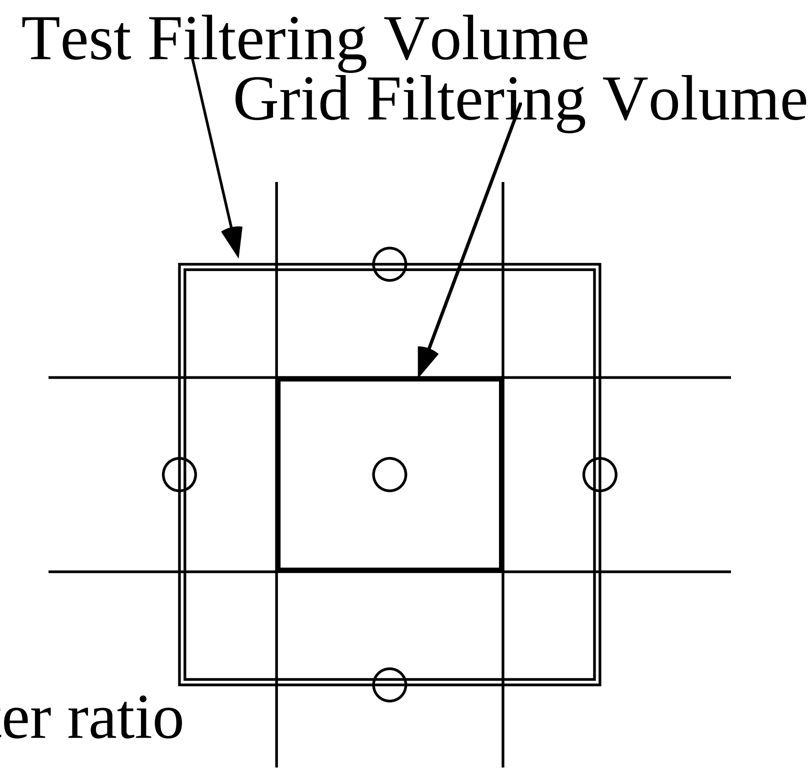
- A dynamic procedure is used to evaluate the model coefficient.

$$L_{ij} = \widehat{\bar{u}_i \bar{u}_j} - \hat{\bar{u}}_i \hat{\bar{u}}_j = T_{ij} - \hat{\tau}_{ij}$$

$$C = -\frac{1}{2}\frac{L_{ij} M_{ij}}{M_{ij} M_{ij}}$$

$$M_{ij} = \hat{\bar{\Delta}}^2 \left|\hat{\bar{S}}\right| \hat{\bar{S}}_{ij} - \bar{\Delta}^2 \widehat{\left|\bar{S}\right| \bar{S}_{ij}}$$

Only input parameter: grid to filter ratio



Dynamic Subgrid Scale Model

- This model overcomes the deficiencies of the Smagorinsky model but may observe numerical instabilities.
- Spatial and temporal low-pass filters damp out high frequency oscillations.

$$\hat{\bar{f}}\left(x\right)=\int \hat{\bar{G}}\left(x,x'\right)\bar{f}\left(x'\right)dx'$$

$$C^{n+1}_{filtered}=\left(1-\varepsilon\right)C^{n}+\varepsilon C^{n+1}$$

- Total viscosity cutoff.

Wall Modeling

- Resolving wall layer may use up to 50% of resources.
- Wall models relate the wall shear stress to the velocity at the first grid point.
- Logarithmic law is generally used in turbulent flows.
- In LES wall shear stresses are distinguished in each direction.

Subgrid-scale modeling

In addition to:

- Smagorinsky model
- Dynamic model

Several new subgrid models are being developed.

(4) Detached Eddy Simulation (DES)

- In wall bounded flows, the computational cost of a LES becomes quickly unaffordable as the Reynolds number increases.
- In DES the domain is ideally divided into **two sub-domains:**

  a RANS region, where a suitable RANS model is solved, typically near the boundary layer AND **a LES region** where, the LES equations are solved.
- This is practically done by a switch in the turbulent viscosity dependent on the grid itself and the distance from the wall.
- Typically in the LES region the RANS model itself is used as a SGS model.

3. Methodology and Solution Techniques

- **Common Procedures**
  1. The **geometry** (physical bounds) of the problem is defined.
  2. The volume occupied by the fluid is divided into **discrete cells (mesh)**. The mesh may be uniform or non-uniform, structured or unstructured mesh.
  3. The **physical modeling** is defined; i.e. the conservation equations
  4. **Boundary conditions** are defined. This involves specifying the fluid behavior and properties at the boundaries. For transient problems, the initial conditions are also defined.
  5. The equations are **solved iteratively.**
  6. **Analysis** and **visualization** of results

Boundary Conditions

- **Periodic boundary conditions**
  - which can be used in directions of statistical homogeneity of the flow. The size of the domain must be chosen so that fluctuations can not spuriously interact with themselves through periodic boundaries.
- **Outflow boundary conditions**
  - which must be designed to prevent spurious reflextions on the boundary.
- **Wall boundary conditions**
  - In case the no-slip condition associated to the wall is not relevant, because scales of motion in the very near wall region are not captured. As a consequence, a specific subgrid model for the inner layer, referred as a wall model, must be defined, which should provide the simulation with adequate conditions on the variables and/or the fluxes.
- **Inflow conditions**,
  - the main problem arises when the incoming flow is turbulent, because all the resolved scales of motion should be prescribed at the inlet. This requires a priori a deterministic description of the turbulent flow on the inlet plane. A few existing methods for the inflow velocity field are employed such as, the random method in which the incoming velocity is split to stationary and fluctuating part. The stationary part is assumed to be known from experiments, RANS simulations or theory, while the fluctuating part is defined as a random function.

3.1 Discretization Methods

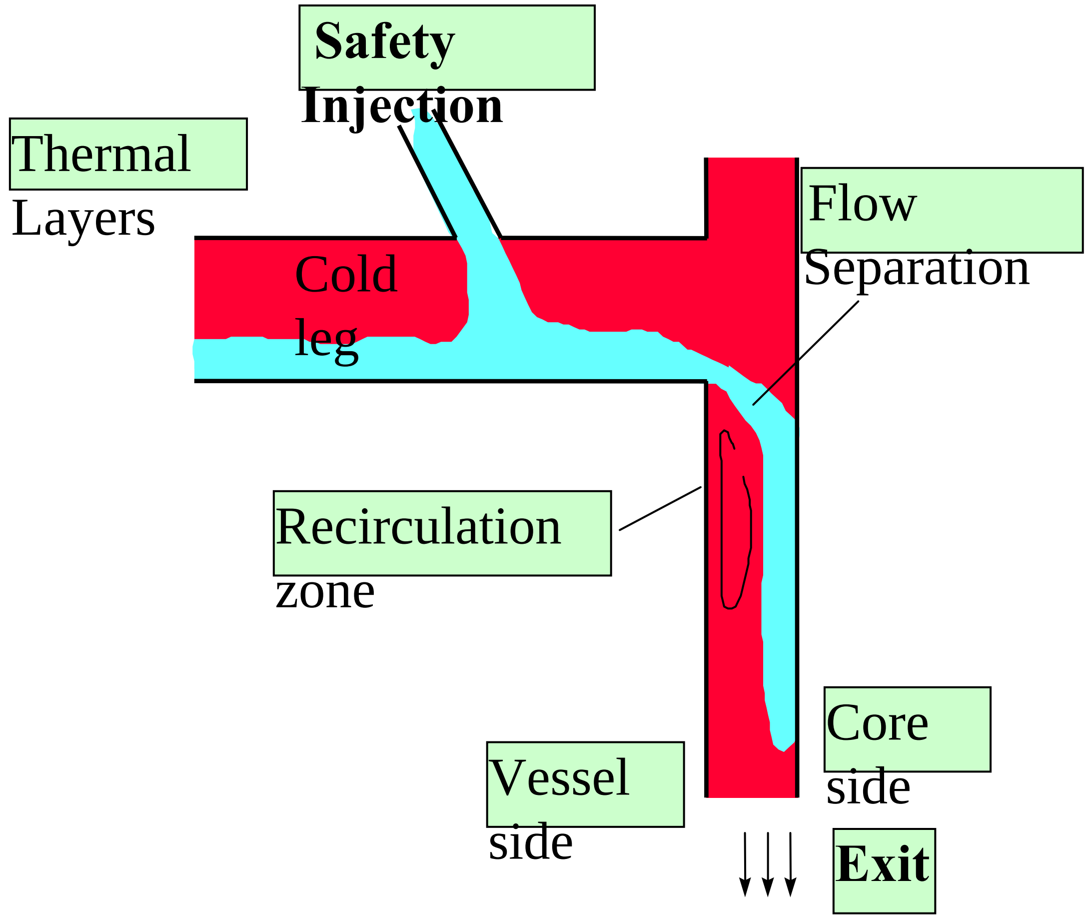
- Finite difference method
- Finite volume method
- Finite element method
- Boundary element method
- Spectral method

3.2 Solution Techniques

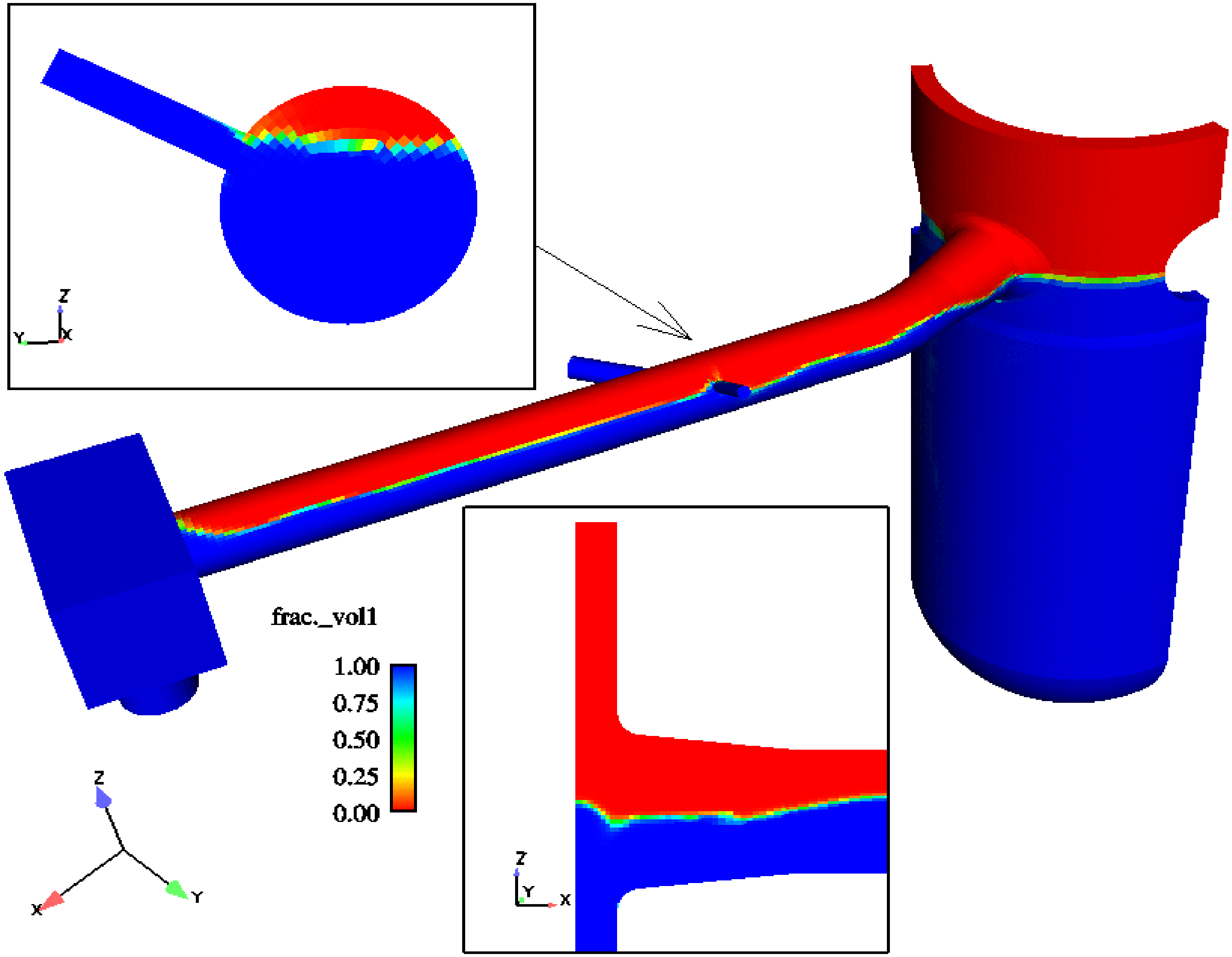
CFD in Natural Circulation and Nuclear Applications

Examples:

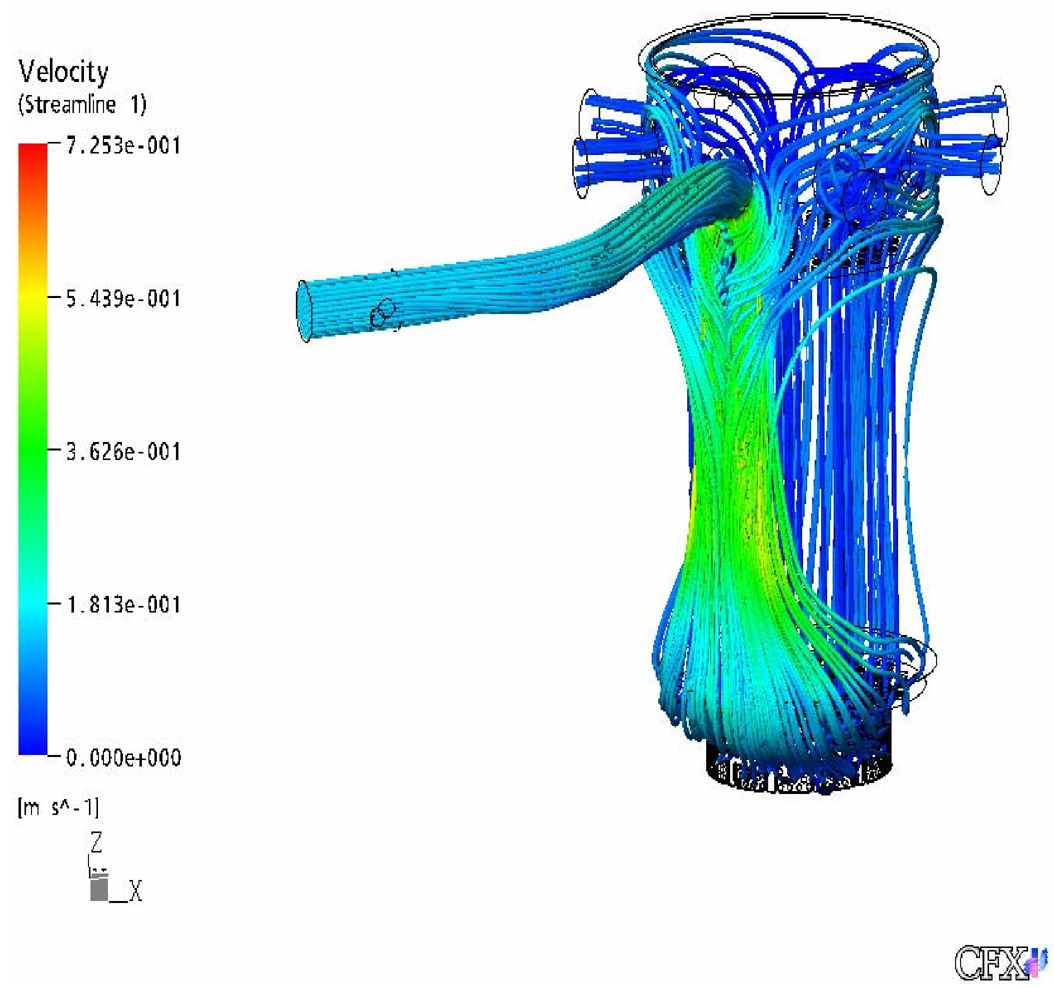
- Mixing (PTS and Boron Dilution)
- Flow in Tee Junctions



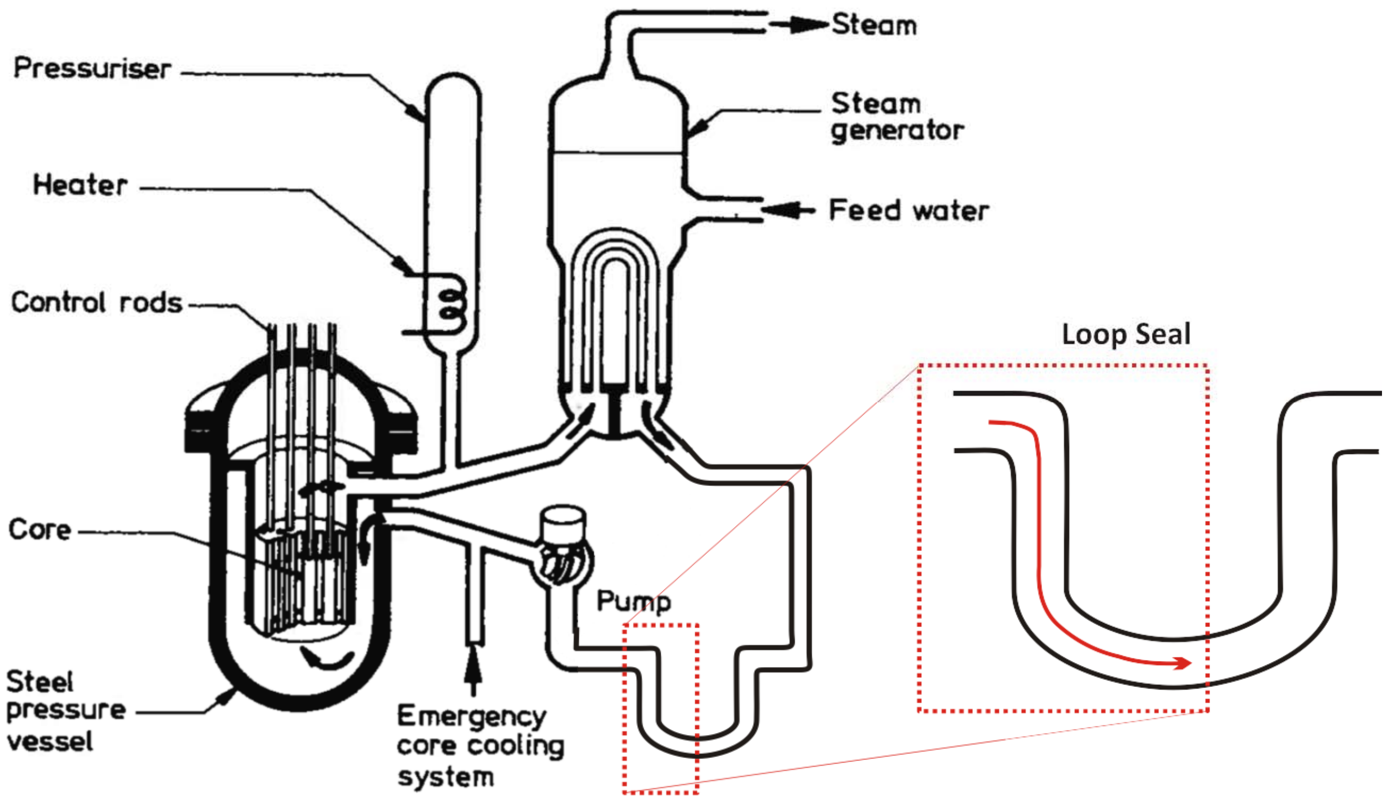
Mixing in cold leg of PWR



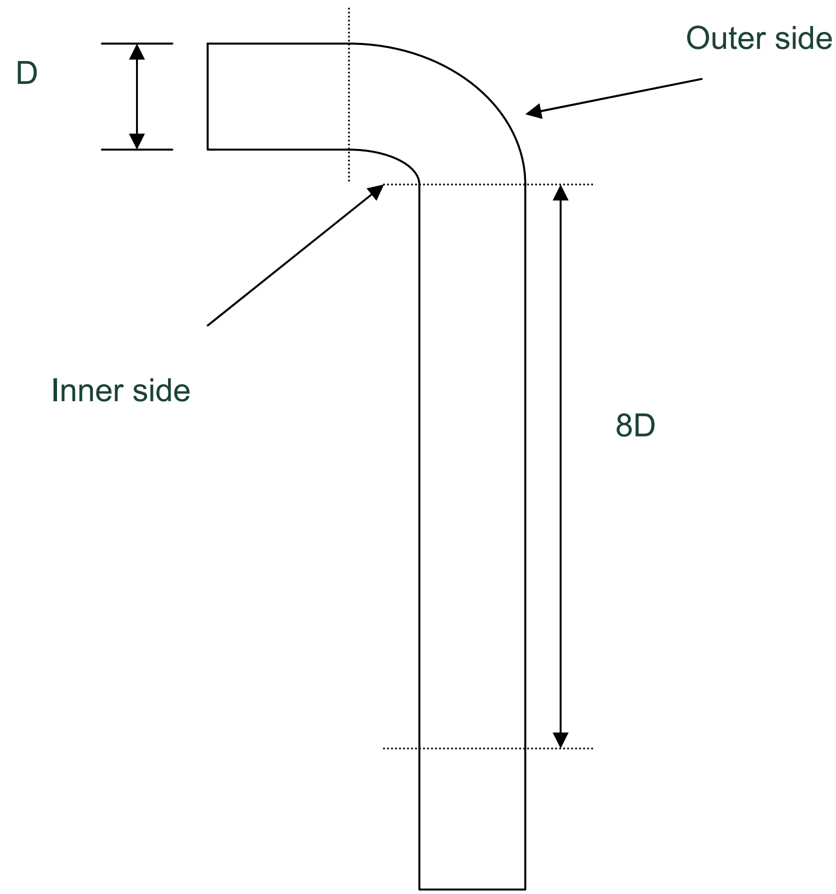
Temperature distributions in the cold leg and downcomer from CFD calculations (Hohne et al, 2005)



Pathlines of mixing after the buoyancy suppression at time=23 S (Hohne et al, 2005)

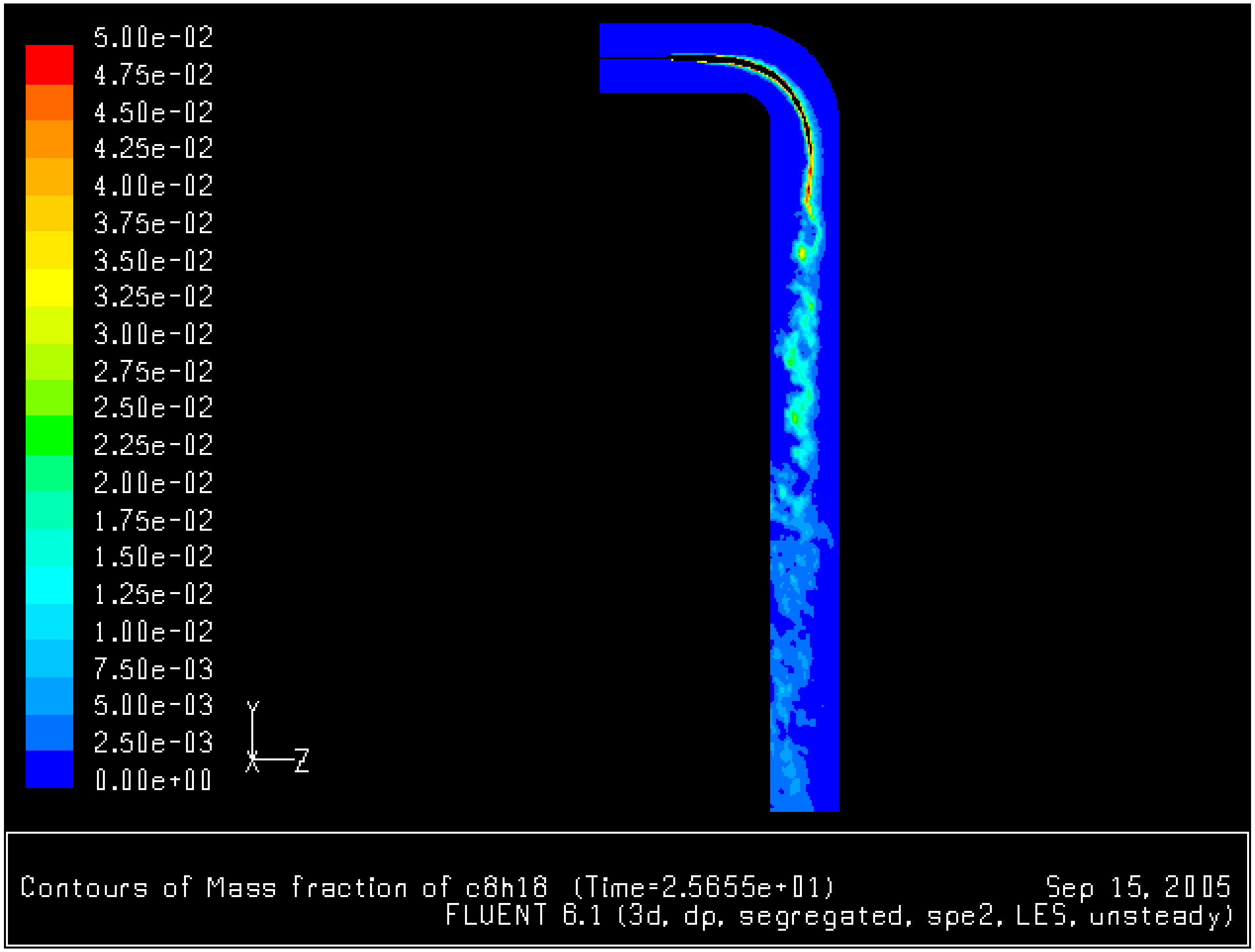


Schematic of PWR with loop seal

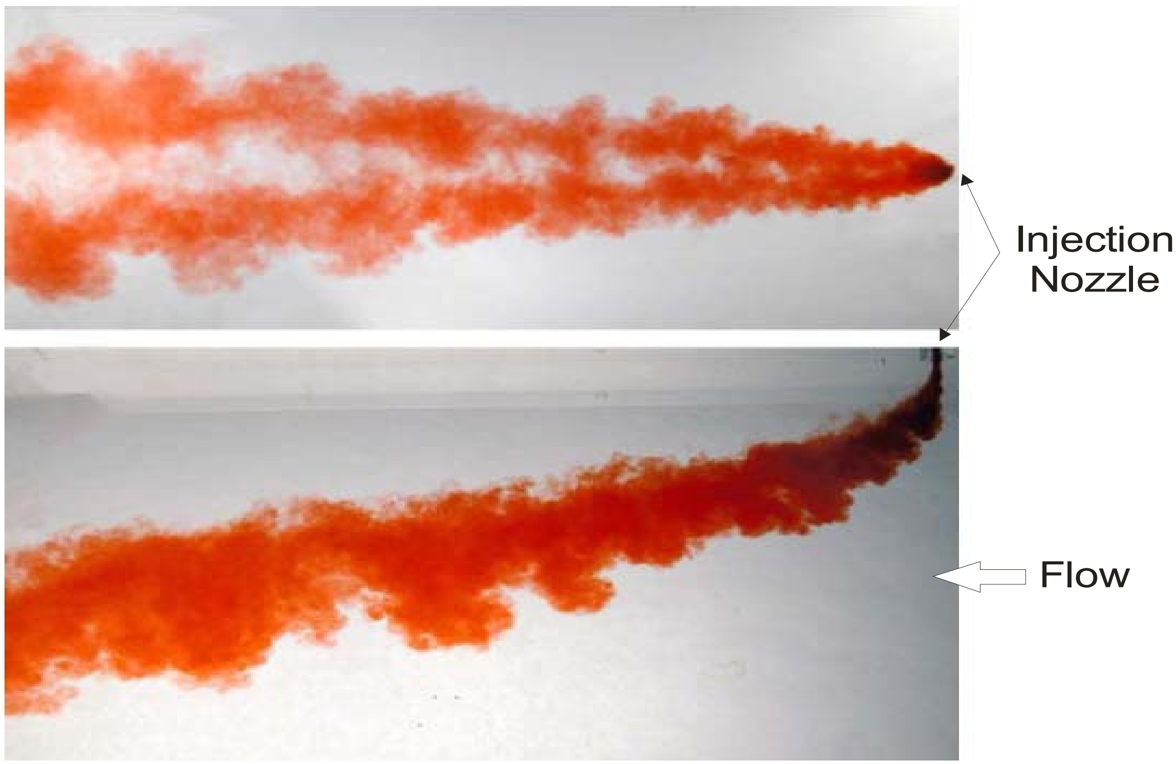


Simulated elbow

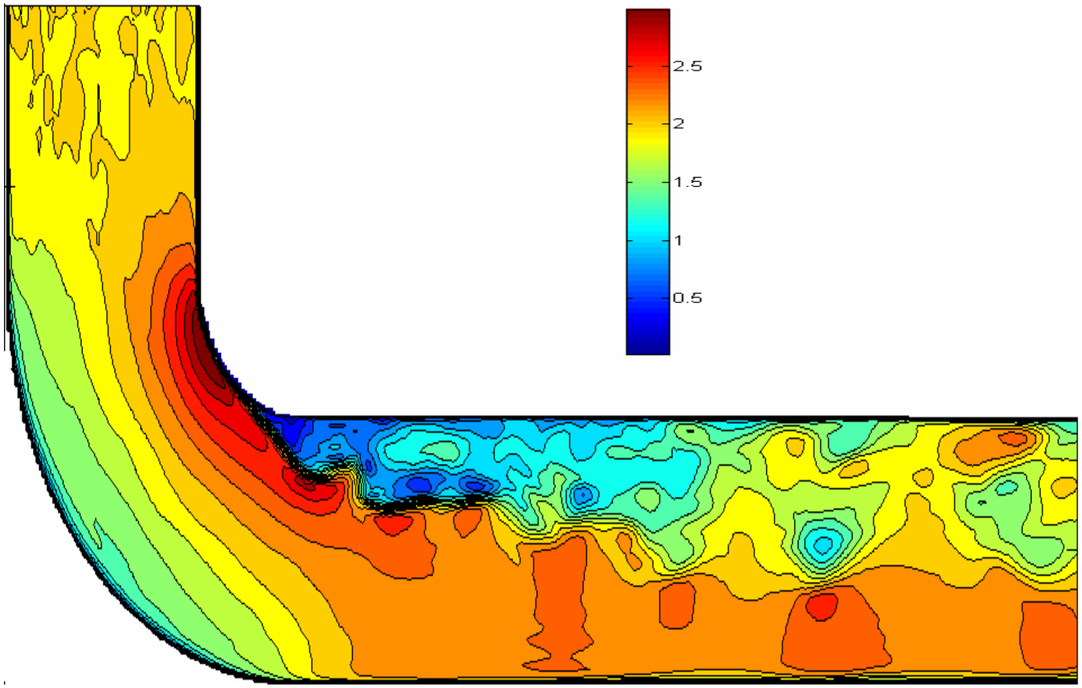
Mixing (PTS and Boron Dilution)



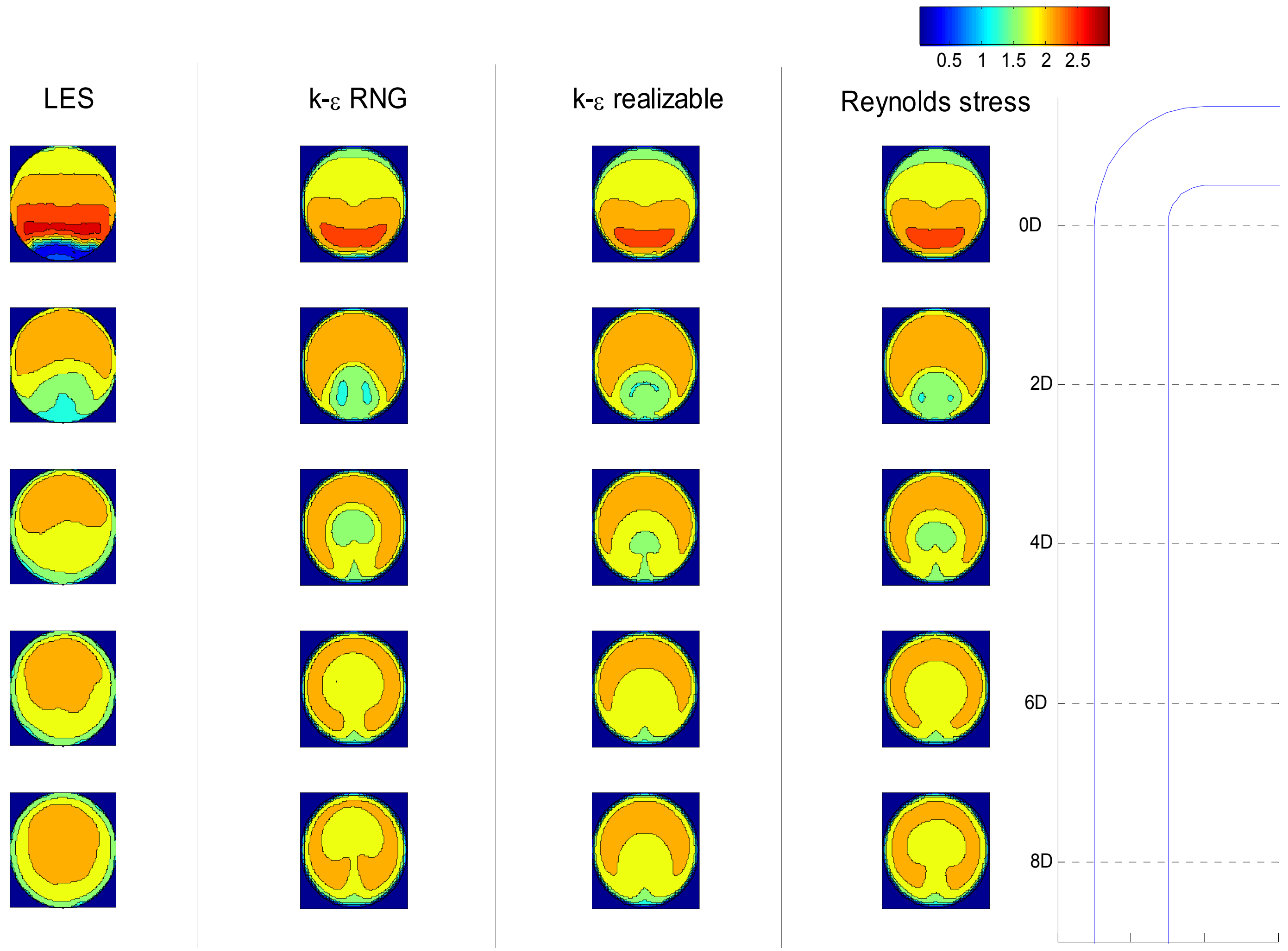
LES Concentration contour dynamic



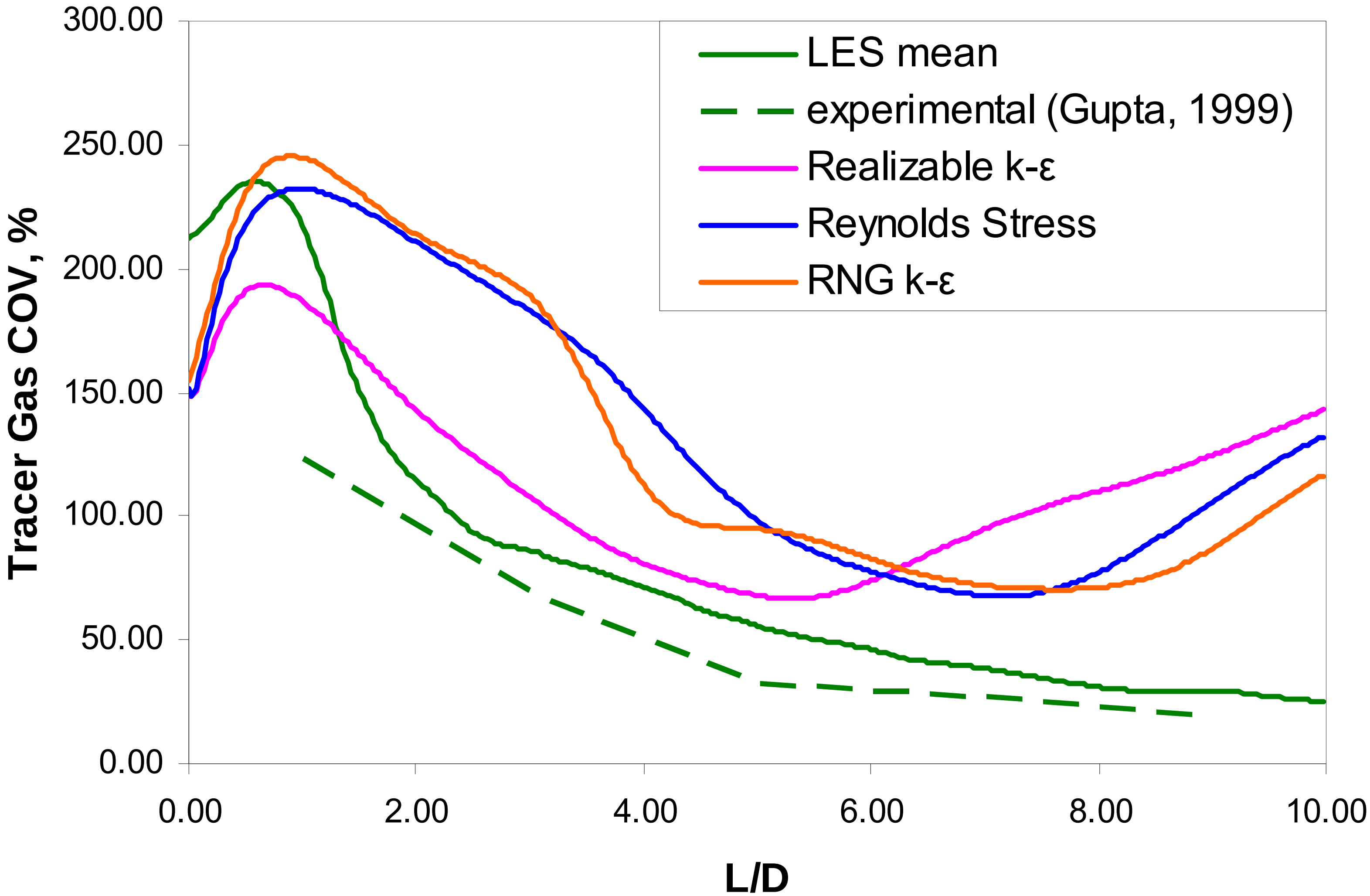
Visualization of the penetration properties of a steady turbulent jet in a uniform crossflow. The upper image shows the top view where as the lower image shows the side view



Contours of instantaneous velocity magnitude through mid symmetry plane of the elbow

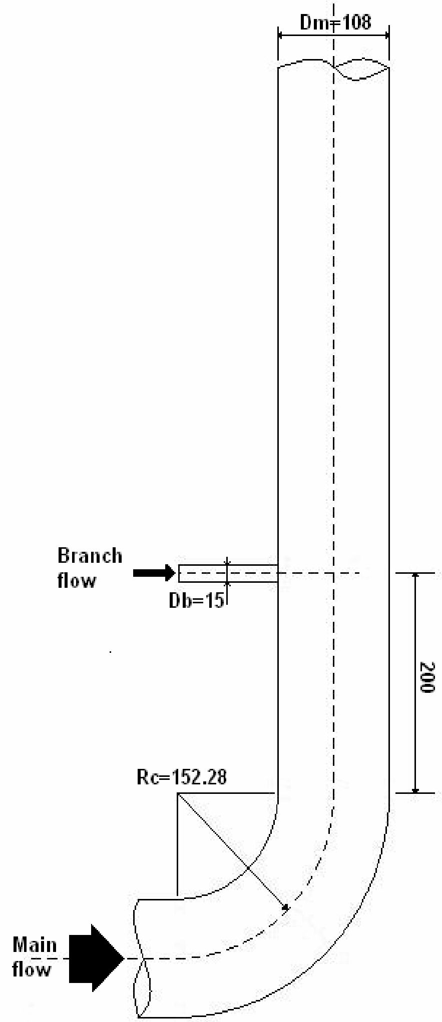


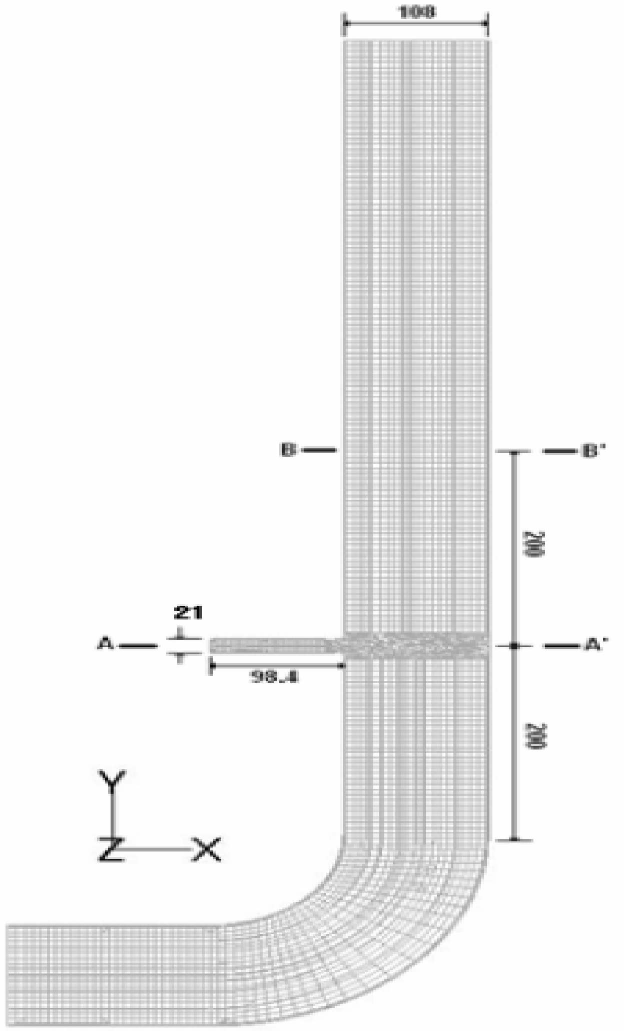
Comparison of the mean velocity profiles through the pipe cross sections at various axial elevations using several turbulence models.



Concentration *COVs* are plotted against the downstream distance from the exit plane of the elbow

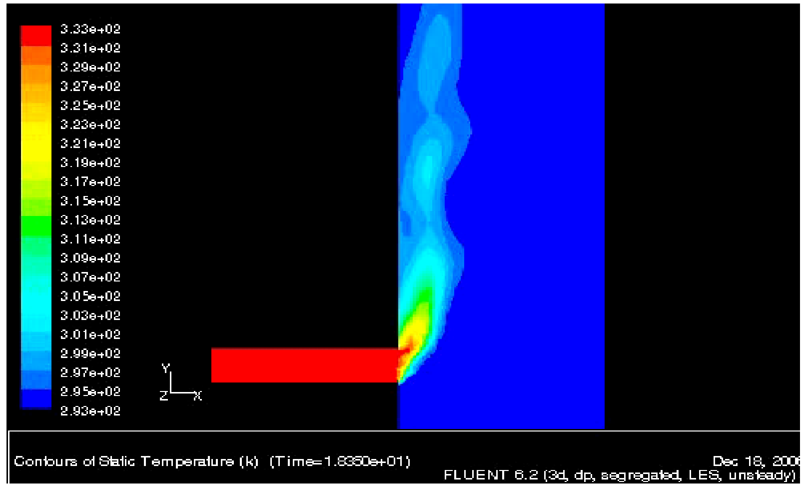
Flow in Tee Junction



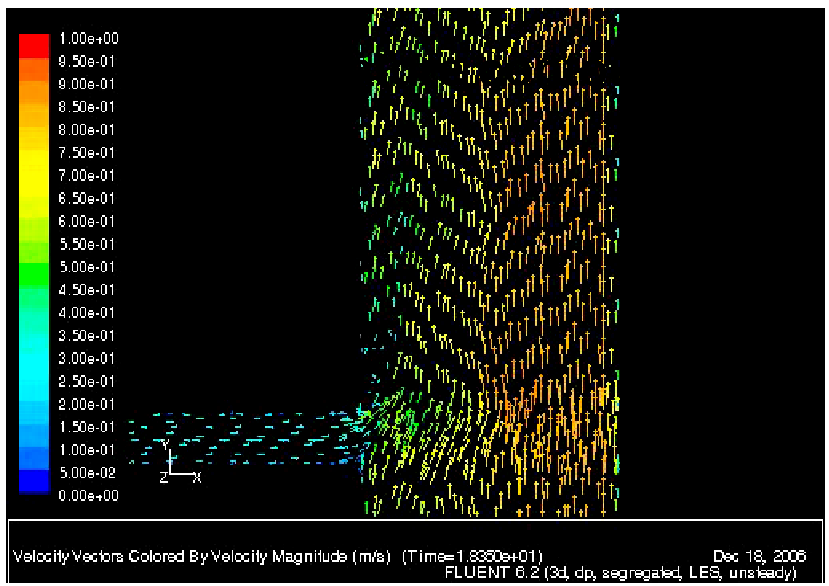


Tee-junction and CFD three-dimensional nodalization scheme

Temperature contour



Velocity Vector



Case A:

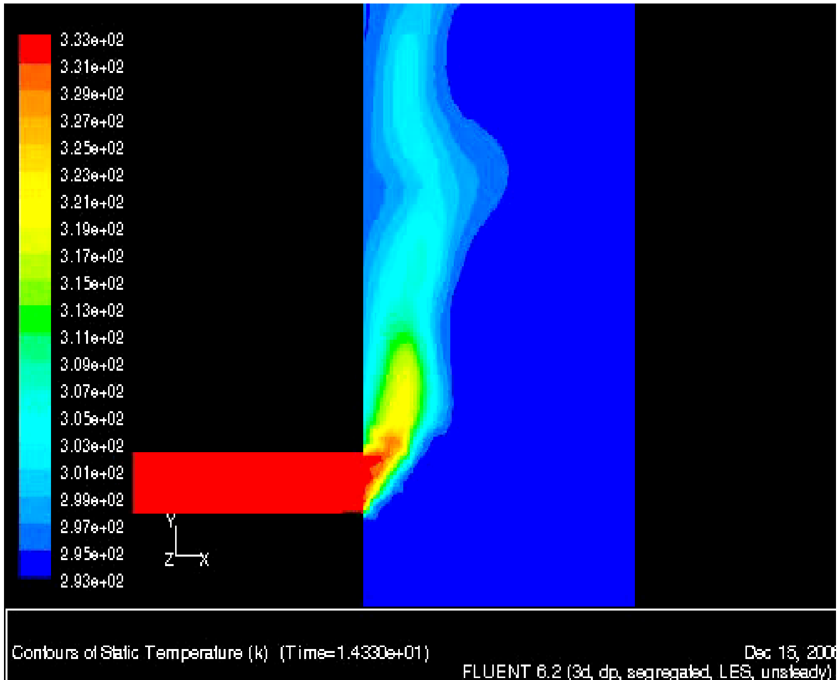
U_{main}= 0.72 m/s

&

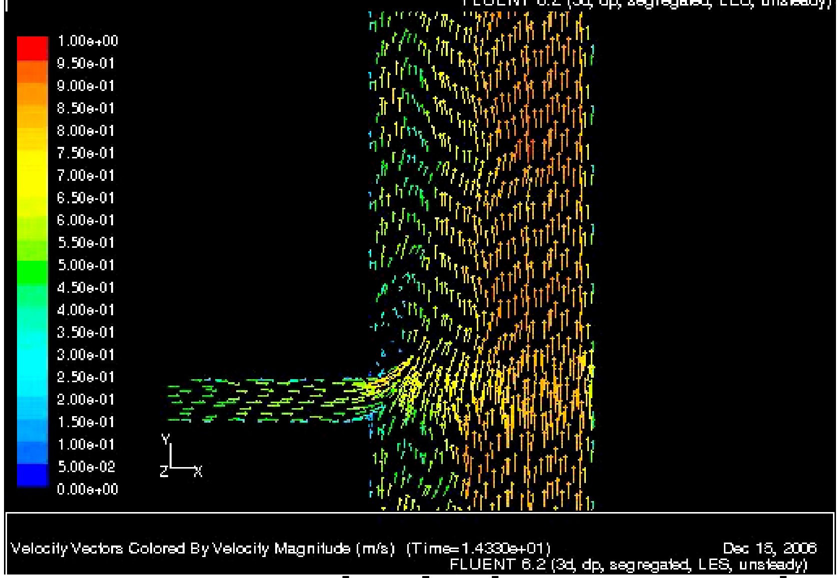
U_{branch}= 0.24 m/s

Temperature and velocity contours in a Tee-junction for various flow rates of the branch section.

Temperature contour



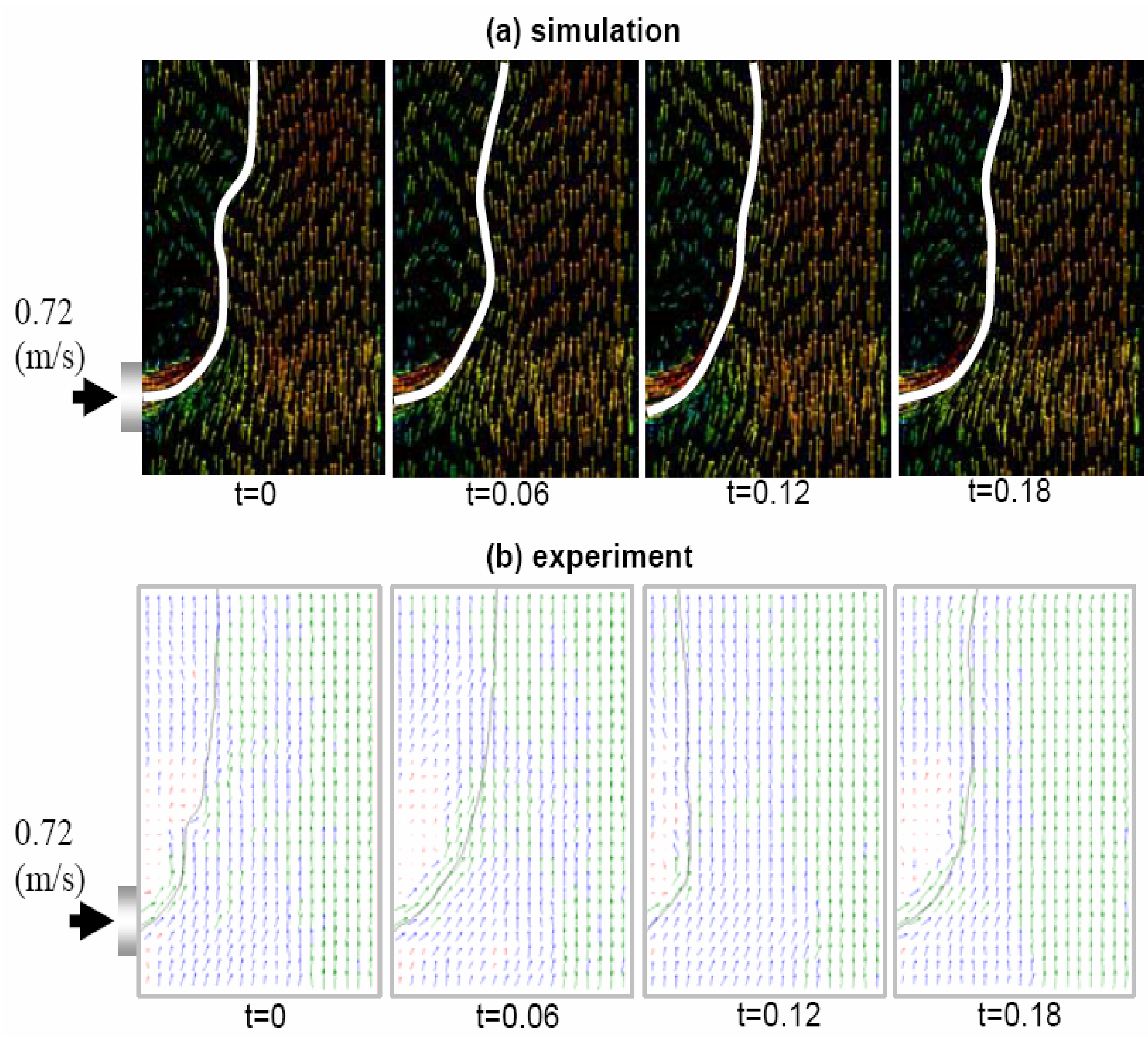
Velocity Vector



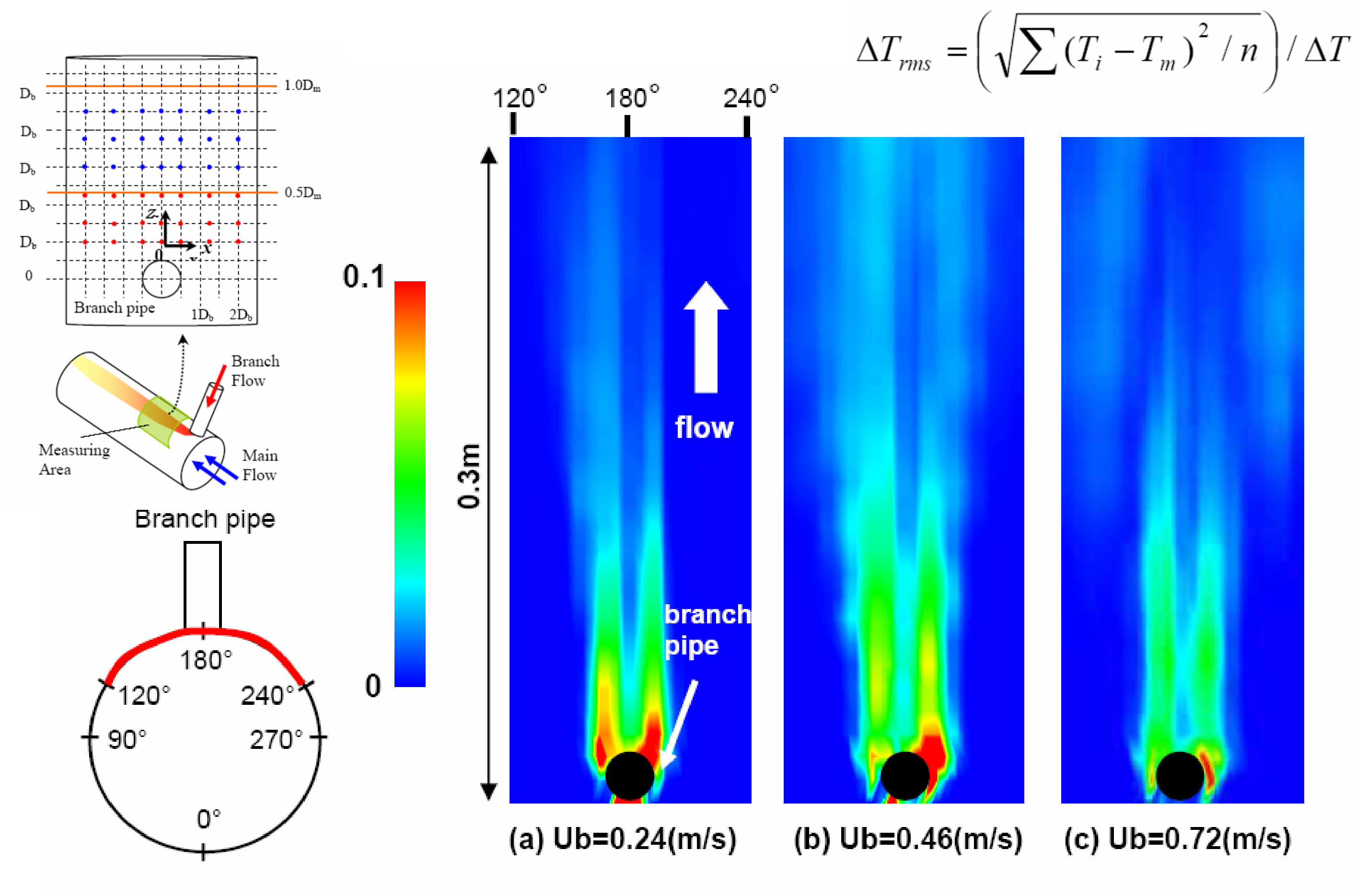
Case A:
Umain= 0.72 m/s

&
Ubranch= 0.46 m/s

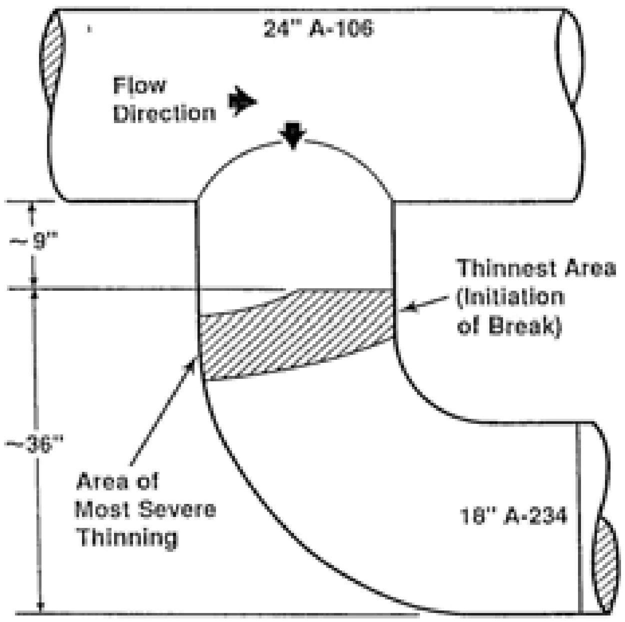
Temperature and velocity contours in a Tee-junction

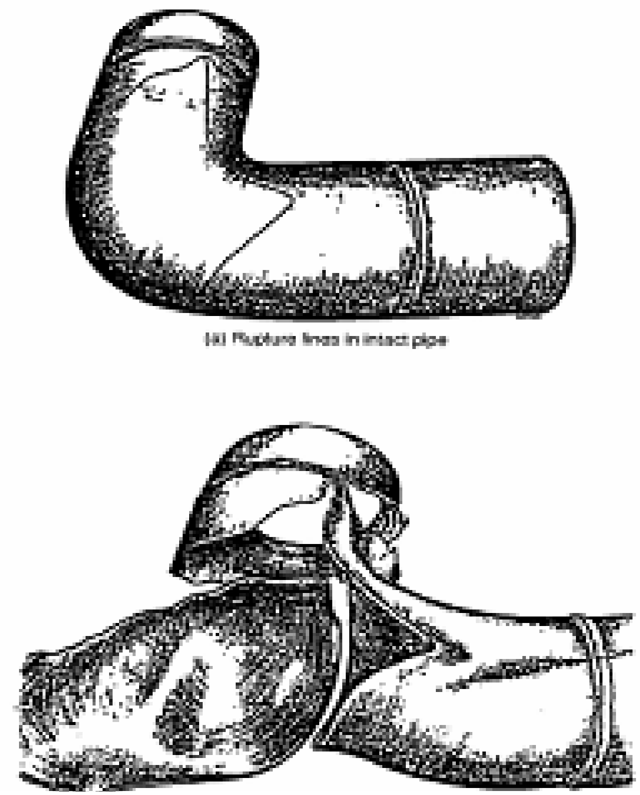


Comparison of the CFD velocity profile prediction with the experimental data for case C. The simulation is the top figure (a), and the experiment is the bottom one (b).



Fluctuation temperature intensities predictions





Schematic result of Surry unit 2 wall thinning

Subcooled and Bubbly Flows Challenges

Complexity of multidimensional multiphase thermal hydraulic processes in nuclear components

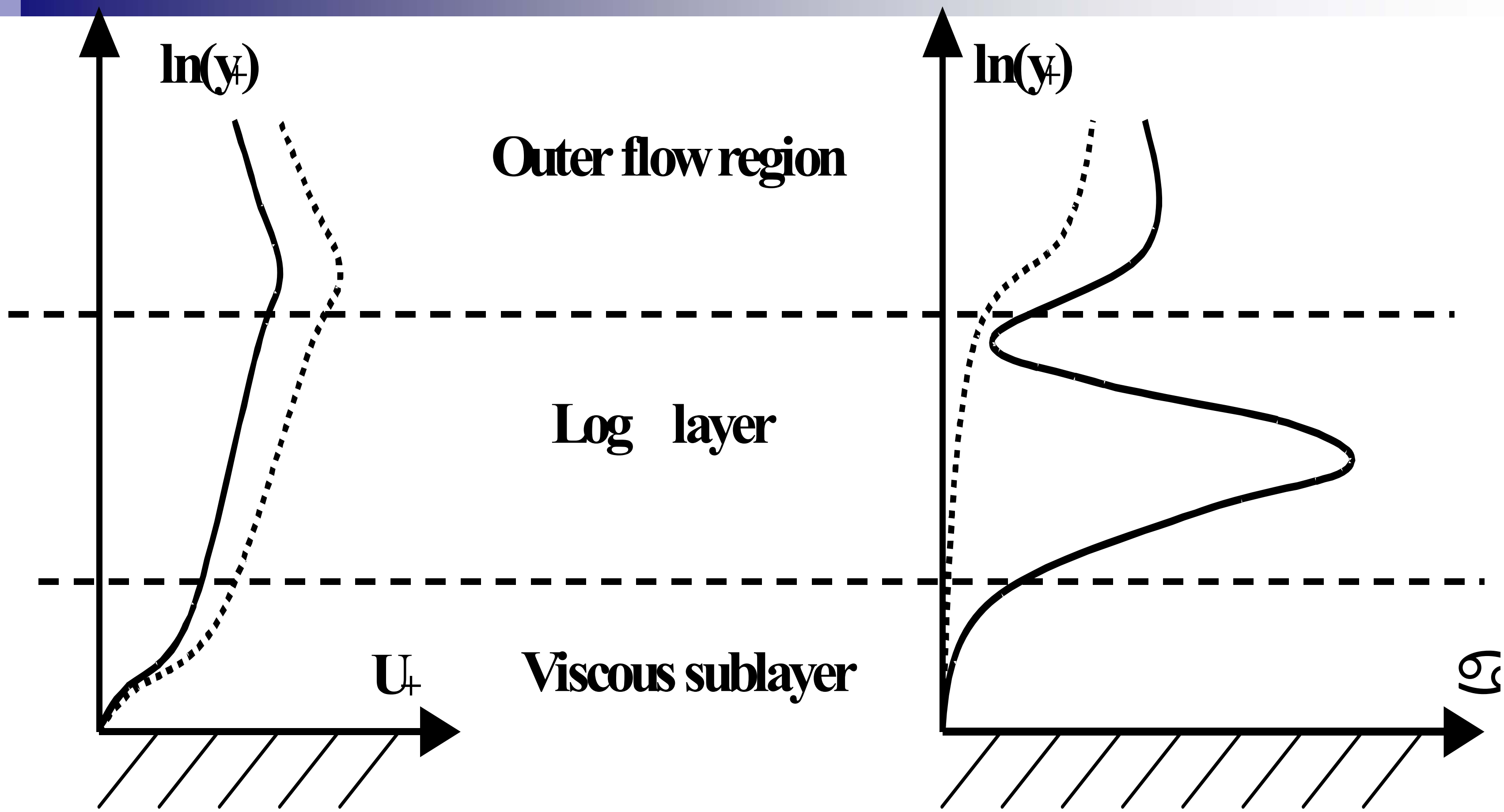
Mass Conservation (field-j, phase-k)

$$\frac{\partial\left(\alpha_{jk}\rho_{k}\right)}{\partial t}+\nabla\bullet\left(\alpha_{jk}\rho_{k}\underline{\bar{v}}_{jk}\right)=\Gamma_{jk}+m'''_{jk}$$

Momentum Conservation (field-j, phase-k)

$$\frac{\partial\left(\alpha_{jk}\rho_{k}\underline{\bar{v}}_{jk}\right)}{\partial t}+\nabla\bullet\left(\alpha_{jk}\rho_{k}\underline{\bar{v}}_{jk}\underline{\bar{v}}_{jk}\right)+\nabla\left(\alpha_{jk}p_{jk}\right)$$

$$-\nabla\bullet\left(\alpha_{jk}\left[\underline{\underline{\bar{\tau}}}_{jk}+\underline{\underline{\tau}}^{T}_{jk}\right]\right)-\alpha_{jk}\rho_{k}\underline{g}-\underline{M}_{jk}-\underline{M}^{w}_{jk}=\Gamma_{jk}\underline{v}_{i}+m'''_{jk}\underline{v}_{jk}$$



Two-phase turbulent boundary layer structure: solid line denotes upward flow, dotted line denotes downward flow.

However, all CFD codes use Single-Phase Flow Wall Function

5. Verification and Validation

- **Verification** is the process of determining that a computational model accurately represents the underlying mathematical model and its solution.

- **Validation** is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended use of the model.

- CFD is Cheaper & Quicker than Experimentation
- Complete Flow Field Information
- Good Optimization Tool
  - Data Preparation & Set up – Complex & Time Intensive
  - Results – Credibility?

CFD is a Better & <u>good Choice</u> in Many Instances
Feasible / Cost Effective &
Efficient <u>if Computed Correctly</u>

CFD CHALLENGES

- Infinite Degrees of Freedom
- Grid Generation is still a Challenge
    - Complex Geometry
        - Non Stationary, Unsteady Volumes
- B. C. - Relies on Experiments
- Modeling & Solution – Complex Geometry, 3   Dimensionality, Non-stationary, Unsteady Volumes, Wide Range of Flow scales, Multi Component, Multiphase

CHALLENGES

- CFD is Still an Immature Science

  Codes Based Mainly on Laboratory Flows

  Multiple Strain Fields, Multiple & Wide Range of Scales

  Neither Universal Turbulence Model is Available Nor Probable – DNS cannot Solve the Problem
- Validation Limited to Gross Features & Expensive
- Cannot be Used as a Black Box

SOME THOUGHTS for CONSIDERATION

- Efficiency, Cost & Reliability Improvements are Demanding the Use of CFD
- CFD is not a Magic Wand
- Validation, Caution & Critical Judgment are Important for application and Use of CFD
- Tune CFD Development to Industrial Needs – Need Concerted Effort by the CFD Community

CONCLUSIONS

CFD is a Better & Optimal Choice in Many Instances
Feasible / Cost Effective &
Efficient if Computed Correctly

Verification and Validation are the key to better predictions (accurate algorithms + Physics + Experiments)

Best Practice Guidelines are necessary for selecting a modeling approach, a nodalization, to control the numerical errors …