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An Overview of Modeling and Simulation Activities in the Laboratory for Thermal-Hydraulics (LTH)

B. Niceno

Laboratory of Thermal-Hydraulic, Nuclear Energy and Safety, PSI

Laboratory of Nuclear Energy Systems, Institute of Energy Technology, ETH Zurich

Structure of the Presentation

- **Introduction – Modeling and Simulation Group (MSG) embedding**
  - Scope and Strategy of **LTH**
  - Scope and Strategy of **MSG**
- **Technical contents – divided by the spatial scales**
  - **System** scale
  - **Integrated Components** scale
  - **Component** scale
  - **Component** scale, Generation IV
  - **Micro** scale
  - **Nano** scale
- **Concluding remarks**

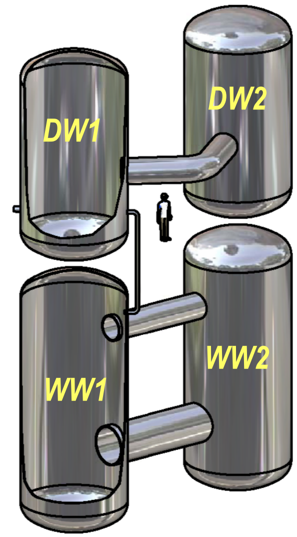
Scope and Strategy of LTH

- **LTH, led by Prof. H.-M. Prasser, is divided in three groups:**
  - Experimental group, Leader: D. Paladino;
  - **Modeling and Simulation group, Leader: B. Niceno**;
  - Severe Accident Group, Leader: T. Lind.
- **Fundamental research on cross-cutting TH issues from Gen II to IV**
  - **Fields**: **reactor**, **plant** and, **containment** Thermal-Hydraulics (TH), **severe** accidents.
  - **Tools**: unique (**home-grown**) experimental and analytical capabilities.
- **LTH strives for excellence in fluid dynamic instrumentation.**
- **Embraces collaboration with other institutes and universities.**
- **Supports and integrates education.**

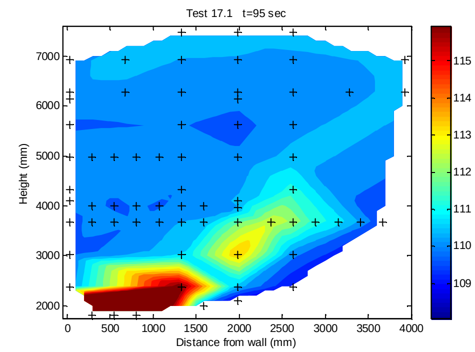
Experimental Group

❖ PANDA experimental facility

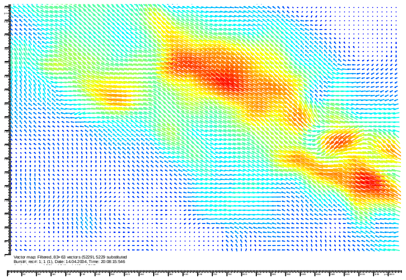
- **Unique** large-scale experimental model of a **LWR**, combined with extensive instrumental capabilities.
- **Large** scale. Compared to **SBWR**:
  - **Height**: 1:1 (25 m);
  - **Volume**: 1:25;
  - **Power**: 1:25.
- **Dense network** of (combined) gas composition and temperature measurements.
- **Enhanced quality** of PIV, novel velocity, temperature and concentration sensors.



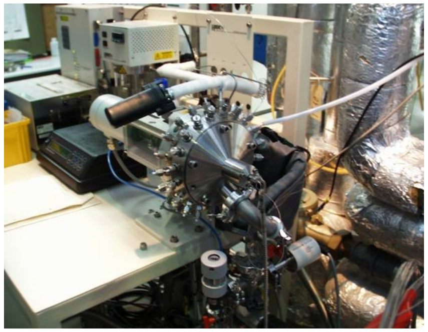
PANDA scale



Thermocouple distribution



PIV measurement



Dense measurement network

Severe Accident Group

❖ **ARTIST:**

Aerosol ReTention In STeam generator

❖ **PWR steam generator tube rupture:**

- **Frequent** occurrence in design basis (**DB**);
- **Low frequency** in severe accident (**SA**);
- Potential for significant **release of radioactivity** due to **by-pass** of the containment in DB and SA.
- ARTIST provides data for **radioactive aerosol retention** in SG secondary side:
  - Aerosol retention in **dry secondary** side;
  - Aerosol retention in **flooded secondary** side;
  - **Droplet retention** under DBA conditions.

Scope and Strategy of MSG

- **Unlike Experimental and Severe Accident groups, MSG does not have its flagship (big) facilities, and will never have any.**
- **Instead on size, we focus on computer power and thematic diversity, and that means:**
  - We work on **multiple scales;**
  - We work on issues relevant for **four generations** of Nuclear Power Plants (NPP);
  - We collaborate on **twelve** national and international **projects;**
  - We are strongly devoted to **collaboration** (within LTH, NES, PSI, ETHZ and beyond);
  - We use **nine different codes** for simulation, **third party** and **in-house;**
  - We are devoted to **education** (giving lectures at ETHZ, host master students).

Many Generations

❖ NPP generations covered by MSG

Generation I

Early Prototype Reactors

- Shippingport
- Dresden
- Fermi 1

Generation II

Commercial Power Reactors

- PWR and BWR (LWR)
- CANDU
- All Swiss NPPs

Generation III

Advanced Light Water Reactors

- AP1000 Westinghouse
- ABWR GE
- EPR AREVA

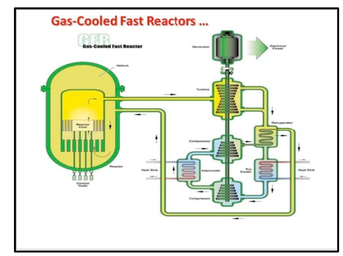
Generation III+

Evolutions from Generation III offering improved passive safety and economics

- APR1000 Westinghouse
- ESBWR
- KERENA (AREVA)

Generation IV

Future Theoretical Nuclear Reactors



- Highly economical, safe
- Minimal waste and risk of proliferation

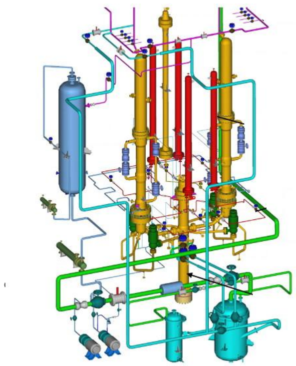
1950 1960 1970 1980 1990 2000 2010 2020 2030

Multiple Scales

❖ Spatial scales covered by MSG

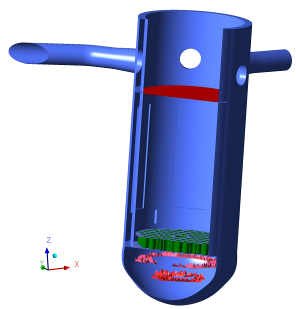
System

Dynamic response of entire systems



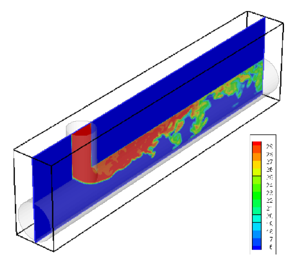
Integrated

Three-dimensional effects on systems



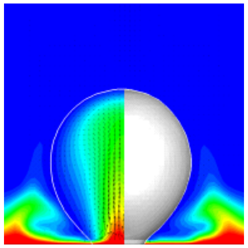
Component

Insight into multiphase and turbulent effects on components



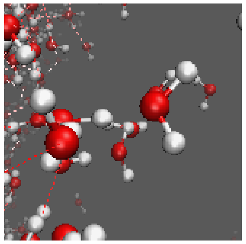
Micro

Basic study of phase change, turbulence and interface dynamics



Nano

Basic study of inter-phase phenomena



System Codes
(RELAP5)

Computational Fluid Dynamics (CFD)
(FLUENT, OpenFOAM, PSI-Boil, …)

Molecular Dynamic (MD) simulations
GROMACS
LAMMPS

Containment Code
(GOTHIC)

Direct Numerical Simulation (DNS)
(PSI-Boil)

Involvement in Many Projects

- **SETH and SETH 2 (Int., Gen 3)**
  - **Gas distribution** inside the **containment**; system and containment.
- **ERCOSAM (Int., Gen 2-3)**
  - **Containment** thermal-hydraulics of current and future LWRs; containment.
- **PLiM II – PLiM IV (Nat., Gen 2, with LNM)**
  - Thermal mixing leading to **fatigue**; component scale.
- **NURESIM, NURISP and NURESAFE (Int., Gen 2)**
  - **Loss Of Coolant Accident (LOCA)**; component scale.
  - **Pressurized Thermal Shock (PTS)**; integral part and component scale.
  - **Departure from Nucleate Boiling (DNB)**; micro-scale.

Involvement in Many Projects

- **SiC for fuel cladding (Nat., Gen 2-4, with LNM)**
  - Replacement of **Zr** alloys by **SiC** for **cladding**; component scale.
- **PINE-II (Int., Gen 4, with LNM)**
  - **Innovative fuel** designs; component scale.
- **Applied projects with utilities:**
  - **Spent fuel basin** analysis for Kernkraftwerk (KK) Beznau;
  - **PTS** for KK Goesgen;
  - **H_2 distribution** in containments for KK Goesgen;
- **Applied non-nuclear project**
  - **Stirred** chemical reactor **vessel** simulations for ThyssenKrupp Uhde.

swissnuclear
Nuclear Energy Section of swisselectric

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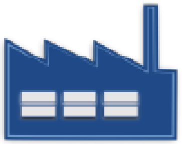
Involvement in Many Projects



- **MOTHER (Int., Gen 2)**
  - Thermal mixing leading to **fatigue**; component scale.
- **THINS (Int., Gen 4):**
  - Mixing of **gases** at very high density ratios; component scale;
  - Modeling of **supercritical** fluids; component scales.
- **MSMA (Nat., Gen 2-3)**
  - Basic study of **boiling phenomena**, micro and nano scales.
- **PASSPORT (Nat., Gen 2-3, with LRS)**
  - Development and validation of a **novel computational methodology** for the performance assessment of LWR safety systems.

Modeling and Simulation Group

Organigram

Leader

Dr. B. Niceno

Alumni

Dr. B. Smith

Scientists

Dr. M. Andreani

Dr. A. Badillo

Dr. M. Sharabi

Dr. Y. Sato

Post Doc PhD

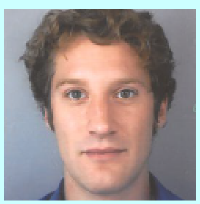
Dr. D. Papini

H. Badreddine

C. Braga

M. Draksler

Master Students



B. Krohn

A. Saxena

S. Lal

The Technical Content – Divided by Spatial Scales

❖ System Scale

- **ATLAS** Facility

❖ Integrated Component Scale

- Containment analysis in **PANDA**

❖ Component Scale

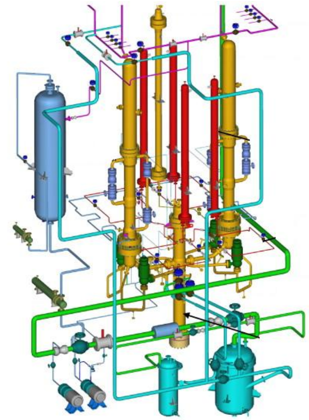
- Mixing in **T-junctions**

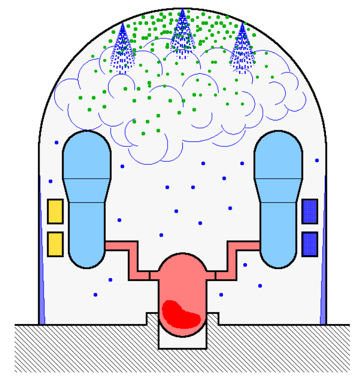
❖ Micro Scale

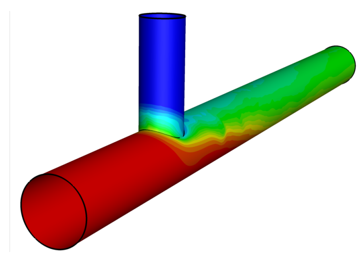
- Modeling of **boiling**

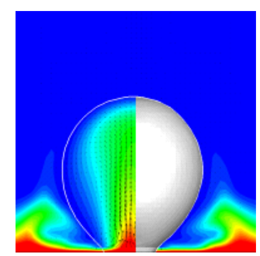
❖ Nano Scale

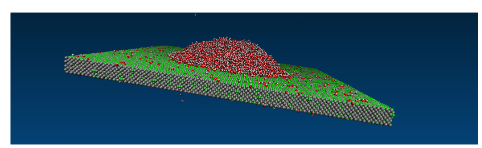
- **Molecular Dynamic (MD)** simulations









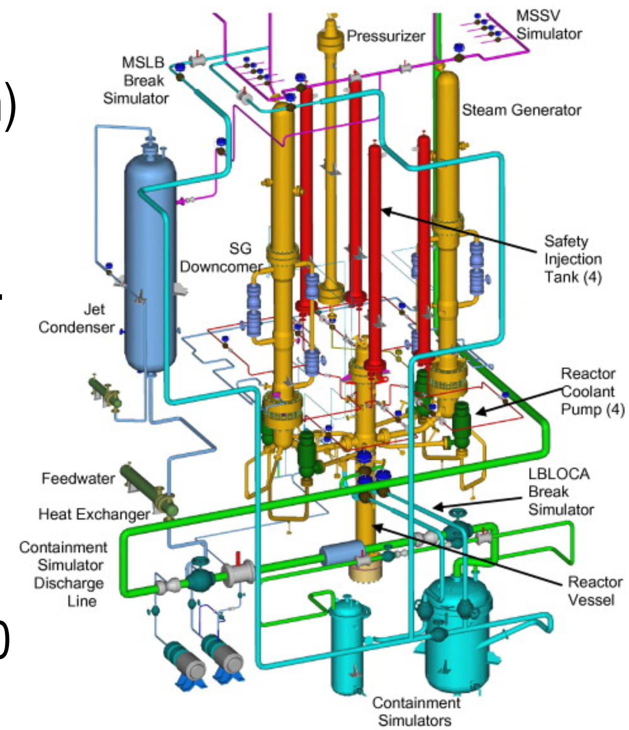


Line-Break in the ATLAS Facility

Sharabi

❖ Summary of the exercise:

- **International Standard Problem 50 (ISP-50)** exercise is sponsored by **NEA/CSNI** and focuses on the 50% (6 inch) of the cross section **Direct Vessel Injection (DVI)** line break scenario offering relevant **integral effect test** data.
- The ISP-50 helps to better **understand** the behavior of nuclear reactor **systems with the DVI**.
- Offers data for **validation** of **system codes**.
- A total of **19 organizations** are participating in the ISP-50
- MSG is taking part in this activity for the transient calculations using the **RELAP5** code.



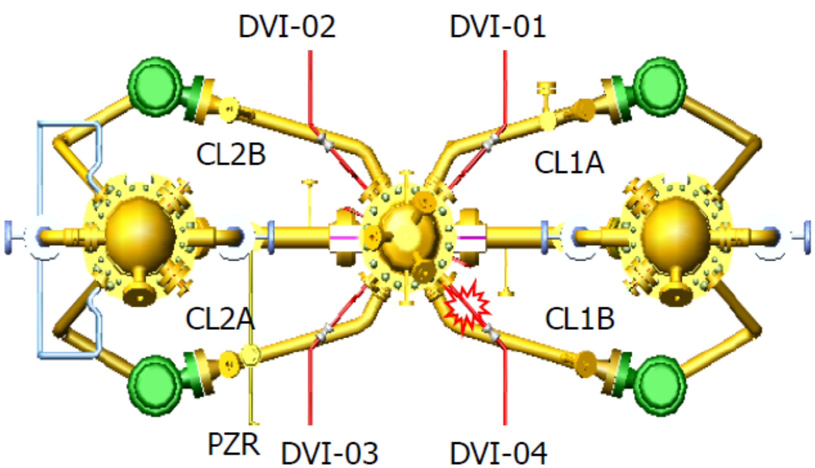
ATLAS facility

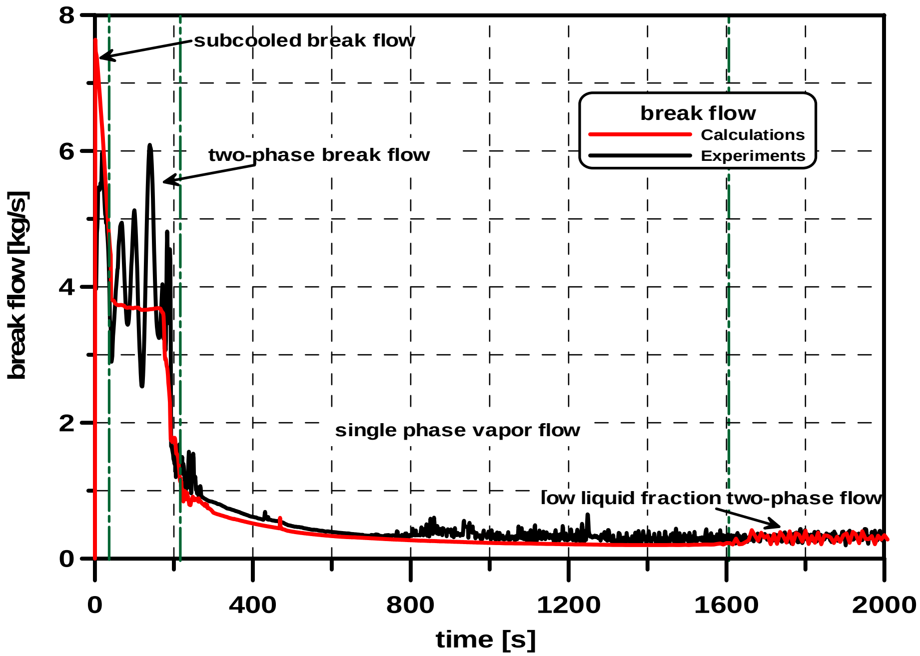
Line-Break in the ATLAS Facility

Main outcomes

- The time trend of the break **mass flow rate** is **well** reproduced.
- **Underestimation** of the break flow in the **two-phase** discharge flow regime.

RCP loop configuration in ATLAS with DVI break

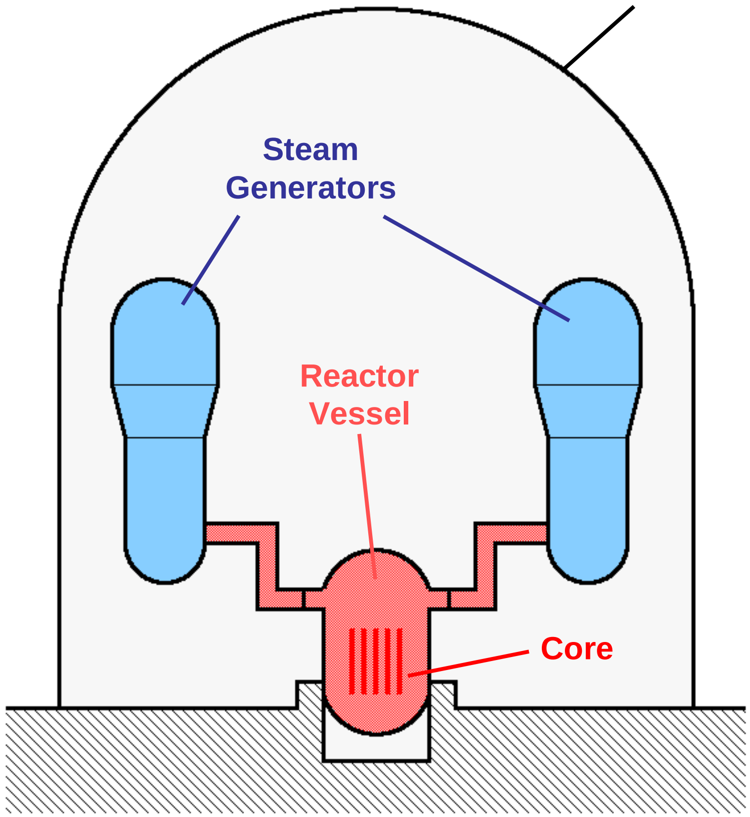




Time trend of the break mass flow rate

Build-Up / Break-Up of Stratification in Containment

- Importance

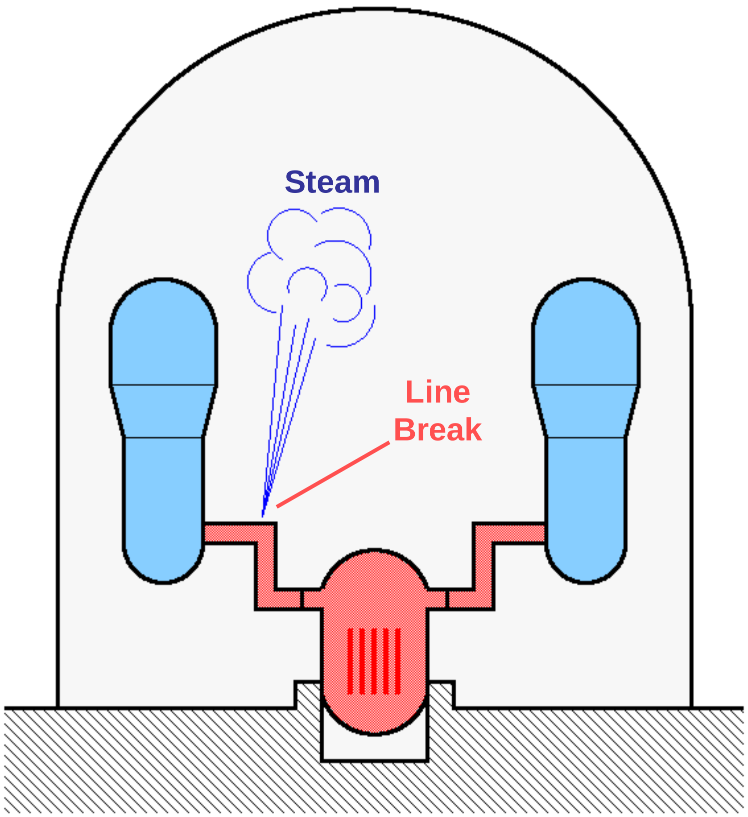


PWR during normal operation

Build-Up / Break-Up of Stratification in Containment

❖ Importance

- In case of a **line break**, leg releases **steam** …

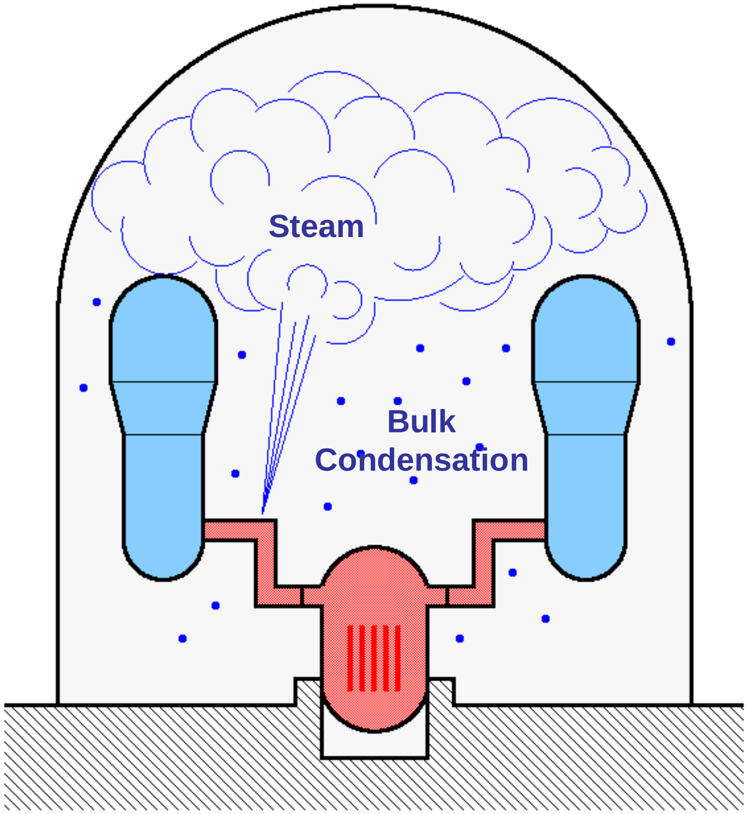


Hot leg breaks, releasing steam

Build-Up / Break-Up of Stratification in Containment

Importance

- In case of a line break, leg releases steam …
- … leading to an **increase** of **pressure**.

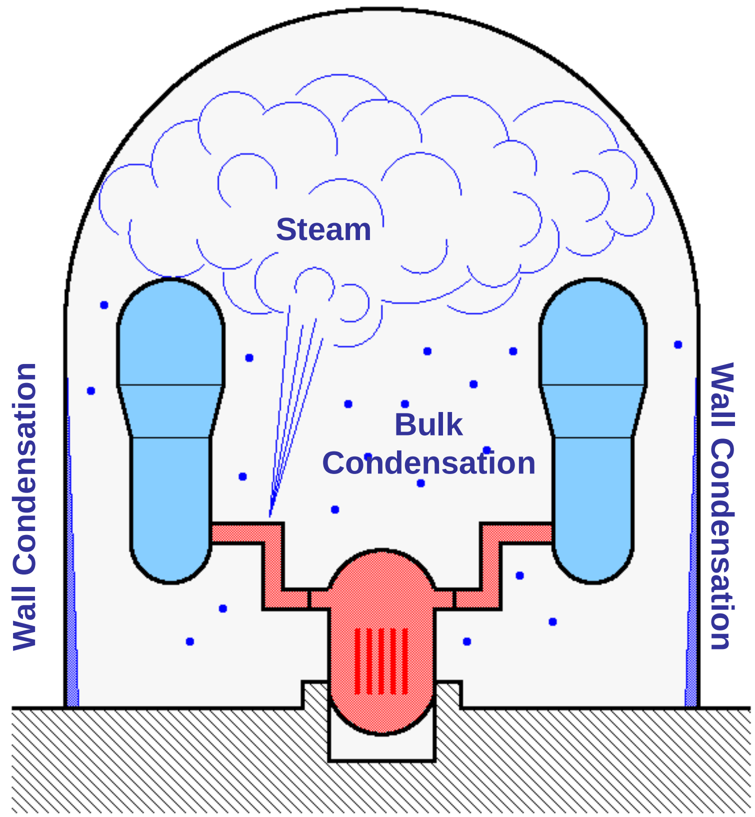


Released steam builds the pressure in the containment up.

Build-Up / Break-Up of Stratification in Containment

Importance

- In case of a line break, leg releases steam …
- … leading to an increase of pressure.
- Steam **condenses** on the walls to some extent.

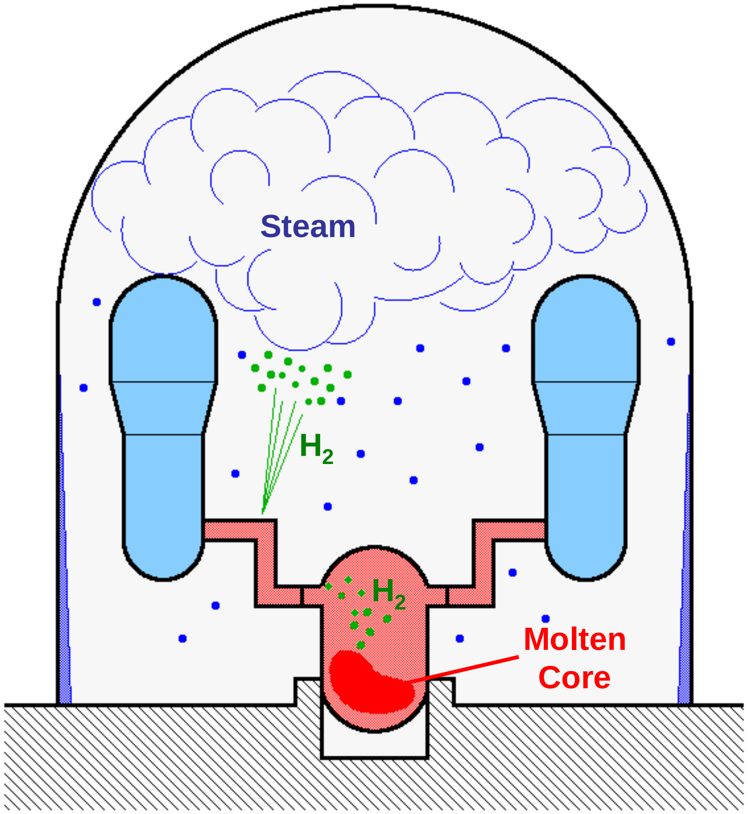


Released steam builds the pressure in the containment up.

Build-Up / Break-Up of Stratification in Containment

Importance

- In case of a line break, leg releases steam …
- … leading to an increase of pressure.
- Steam condenses on the walls to some extent.
- The **core** might **melt down** later, releasing H_2 …

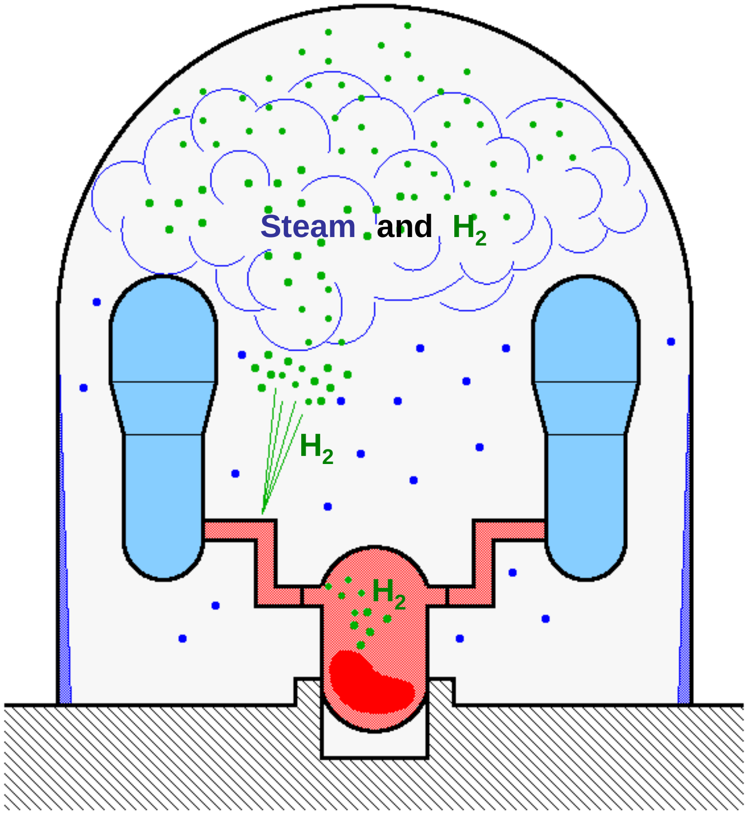


Core releases H_2 (and other non-condensables)

Build-Up / Break-Up of Stratification in Containment

Importance

- In case of a line break, leg releases steam …
- … leading to an increase of pressure.
- Steam condenses on the walls to some extent.
- The core might melt down later, releasing H_2 …
- H_2 **mixes** with steam, but because it is lighter

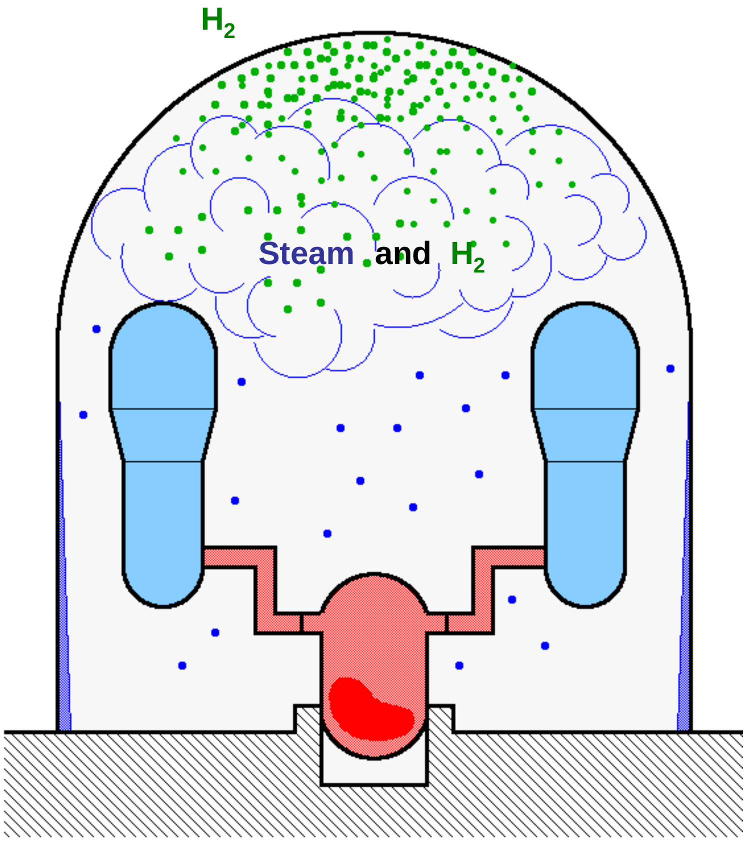


Core releases H_2
(and other non-condensables)

Build-Up / Break-Up of Stratification in Containment

Importance

- In case of a line break, leg releases steam …
- … leading to an increase of pressure.
- Steam condenses on the walls to some extent.
- The core might melt down later, releasing H_2 …
- H_2 mixes with steam, but because it is lighter …
- … its concentration **rises on top** …

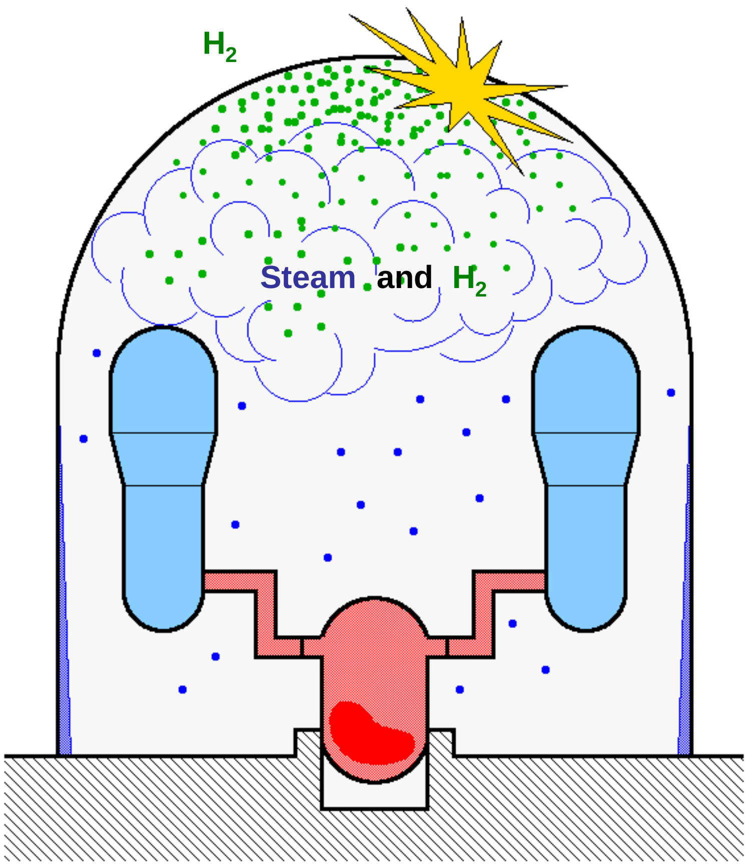


A stratified layer of H_2 forms on top of the containment

Build-Up / Break-Up of Stratification in Containment

Importance

- In case of a line break, leg releases steam …
- … leading to an increase of pressure.
- Steam condenses on the walls to some extent.
- The core might melt down later, releasing H_2 …
- H_2 mixes with steam, but because it is lighter
- … its concentration rises on top …
- … which may lead to **deflagration**.

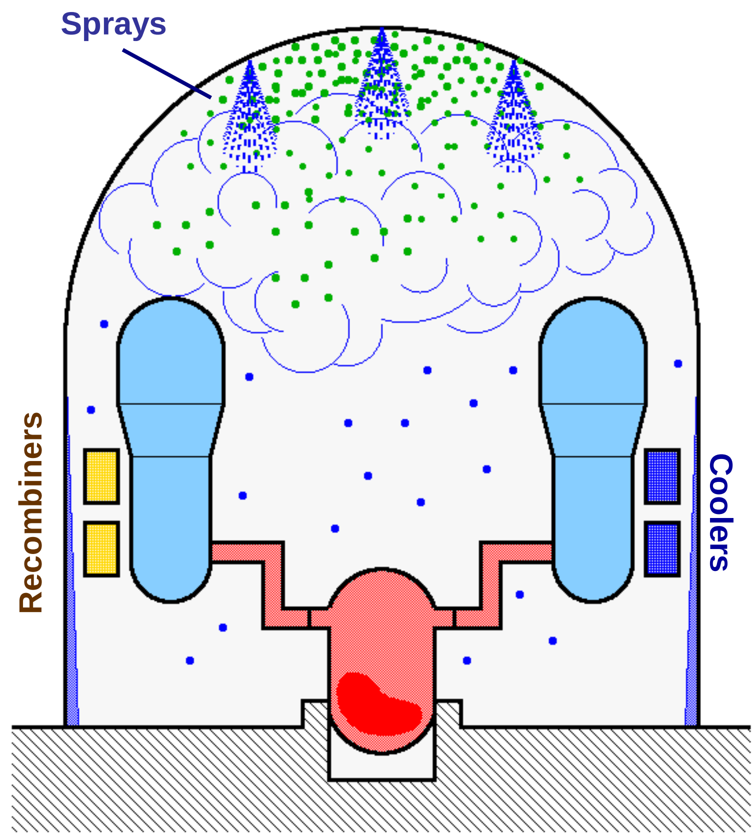


High concentrarion of H_2 may lead to deflagration

Build-Up / Break-Up of Stratification in Containment

Importance

- In case of a line break, leg releases steam …
- … leading to an increase of pressure.
- Steam condenses on the walls to some extent.
- The core might melt down later, releasing H_2 …
- H_2 mixes with steam, but because it is lighter
- … its concentration rises on top …
- … which may lead to deflagration.
- We perform containment **analysis** to study **measures** to avoid high concentration build-up of H_2.



Various measures to avoid break-up the stratified layers of H_2

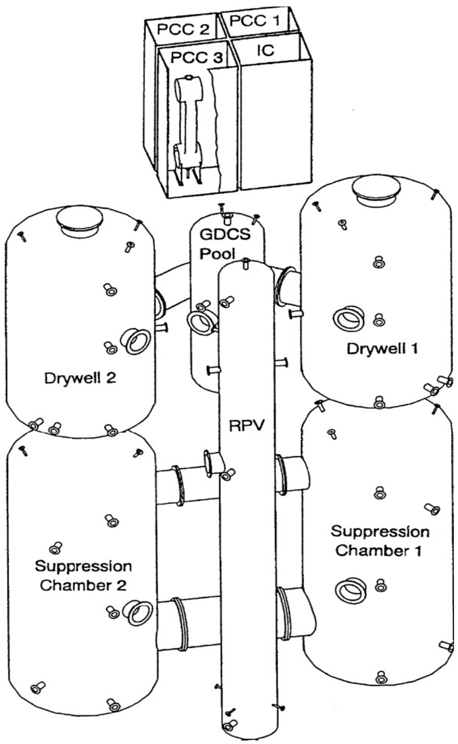
Containment Analysis with GOTHIC


Papini


Andreani

- **The complex scenario during an accident, goes in two phases, which can be studied separately**
  - Stratification **build-up** (**SETH** project)
  - Stratification **break-up** (**SETH 2** project)

- **Stratification break-up by a vertical jet**
  - Typical **model** used for analysis of SETH-2 tests:
    - **3D** and **2D** coarse representation of both vessels
    - cells in Vessel 1: ~ **0.1** to **0.2 m** each side
    - cells in Vessel 2: larger cells
    - ~ 600 cells for the interconnecting pipe
    - k-ε turbulence model



PANDA vessels used in present experiment

Integrated Component Analysis

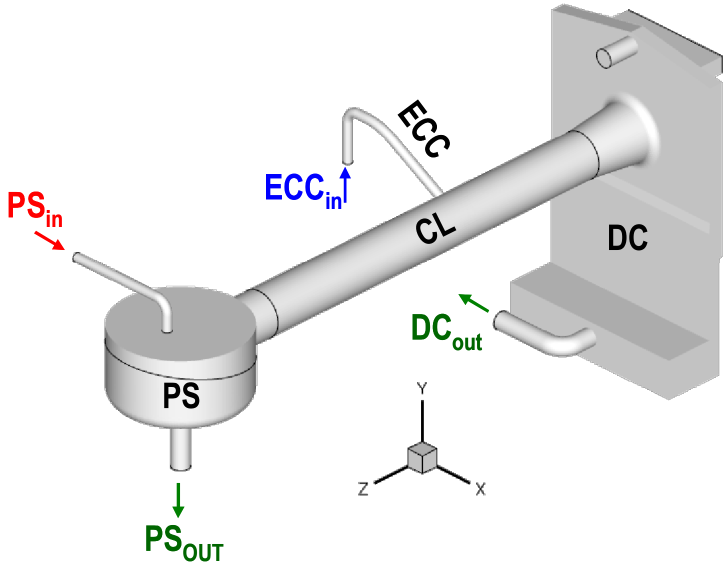
Pressurized Thermal Shock

Niceno

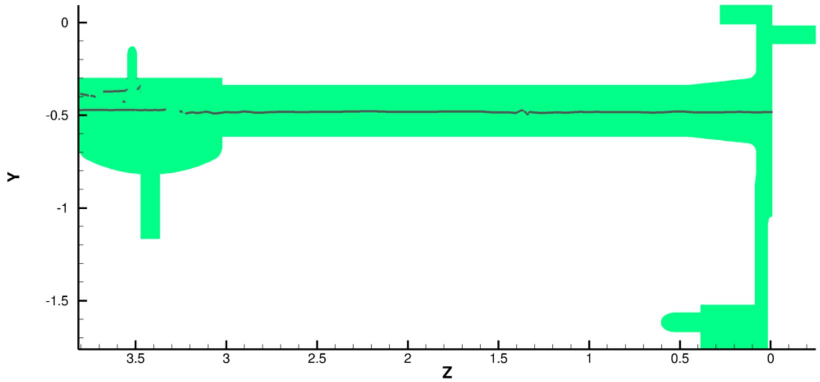
Saxena

❖ TOPFLOW-PTS

- Models thermal mixing in a reactor's cold leg after injection of emergency coolant.



Sketch of the TOPLFLOW-PTS facility



Simulated evolution of temperature in the cold leg, in TOPLFLOW-PTS facility

Mixing in T-junctions


Niceno


Sharabi


Smith

Relevance:

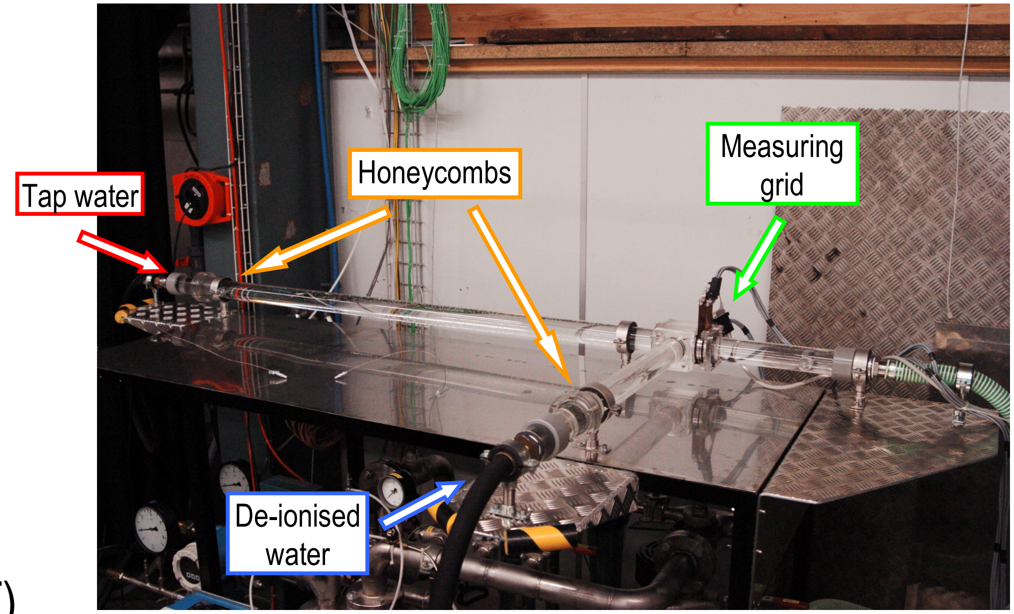
- Mixing of streams at **different temperatures** can lead to temperature **fluctuations**, which may lead to thermal **fatigue**.

Experimental approach:

- Use **analogy** of temperature and scalar transport, analyze streams with different **conductivities**.

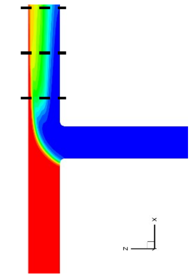
Numerical approach:

- Check state-of-the art turbulence modeling strategy (**LES** in FLUENT)



Experimental Setup For Mixing in T-junctions

Mixing in T-junctions

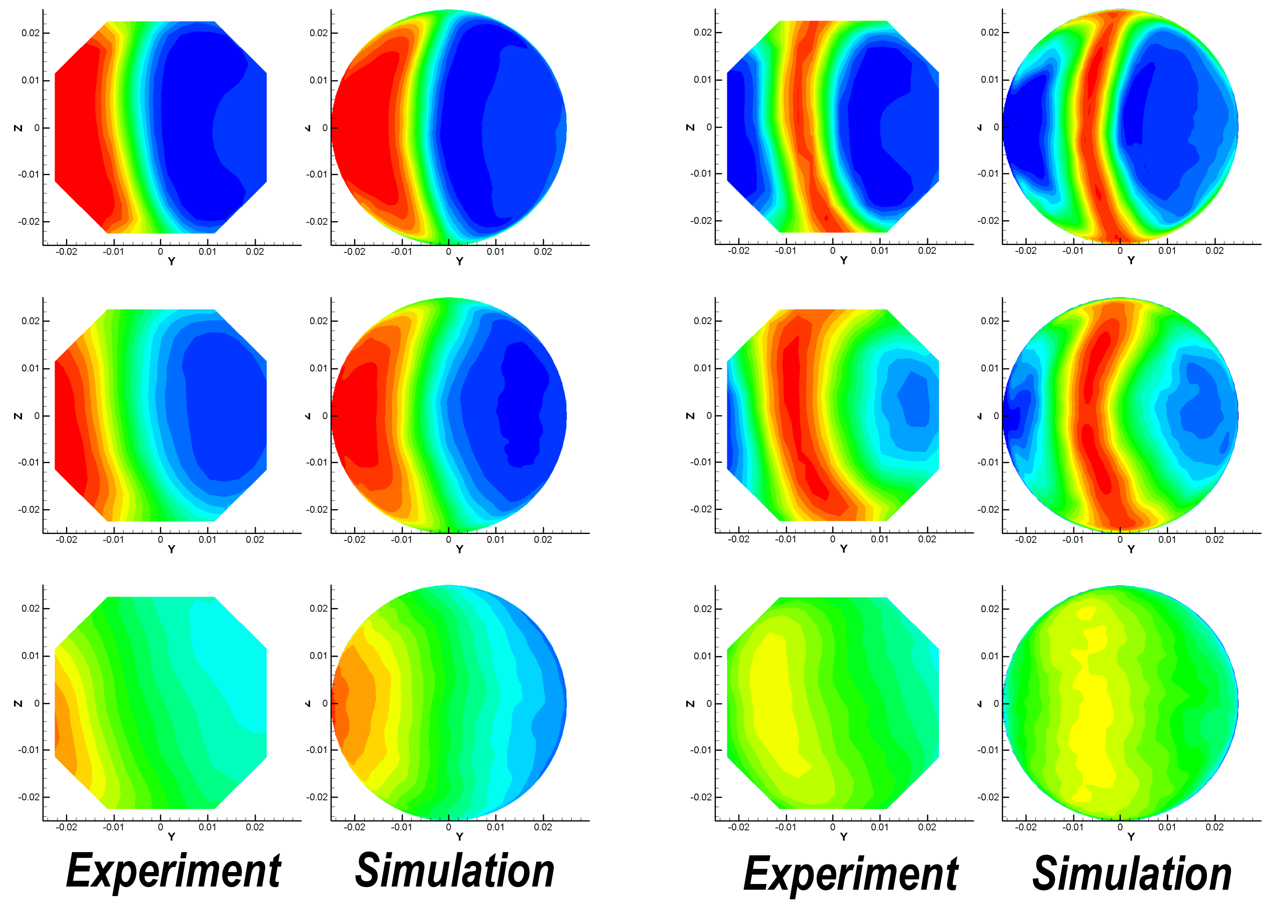


❖ Distributions of conductivity and its fluctuations in planes:

x/D = 1.0

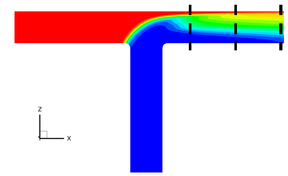
x/D = 2.2

x/D = 4.6

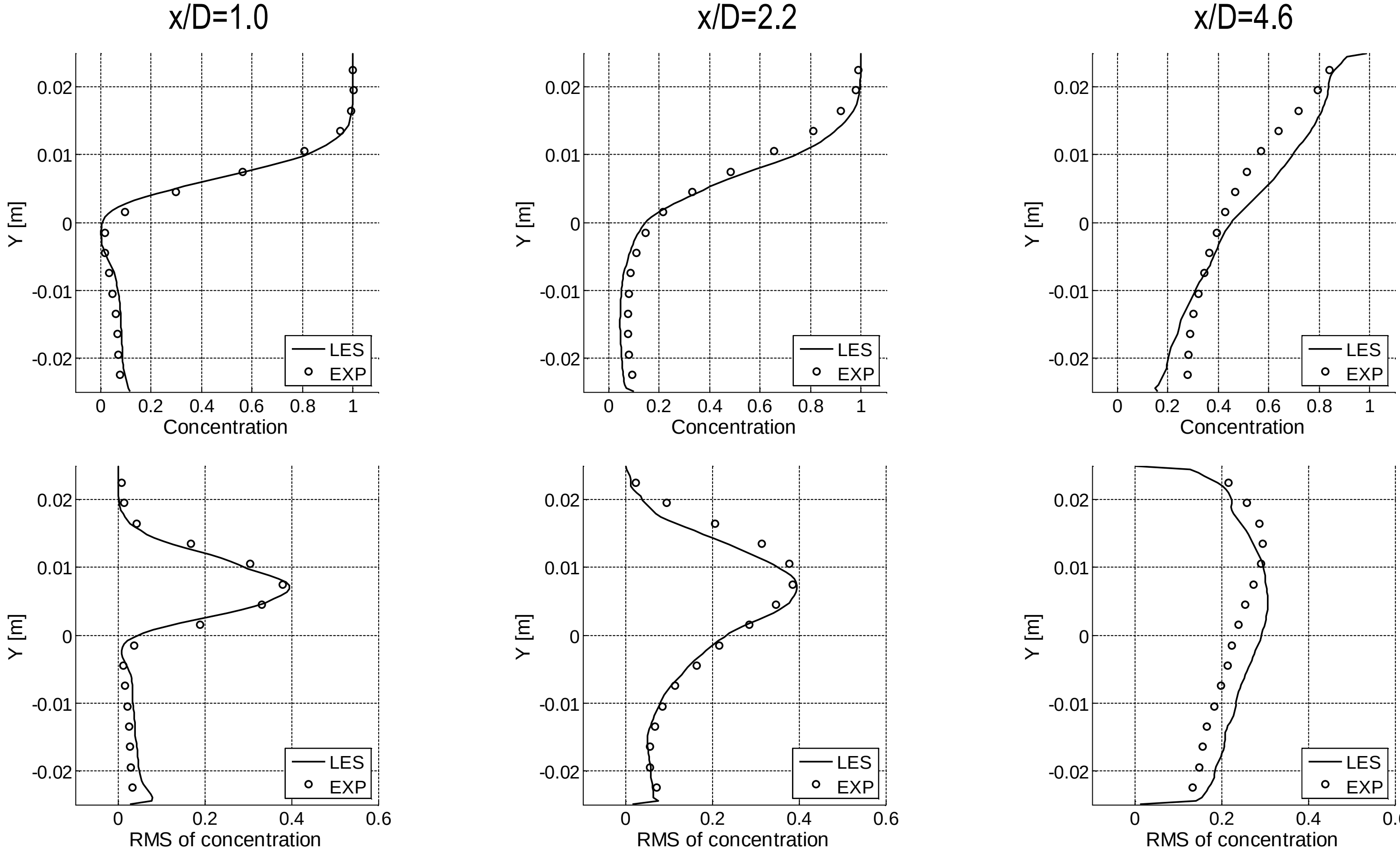


Component Scale

Mixing in T-junctions



- **Distributions of conductivity and its fluctuations in horizontal lines:**

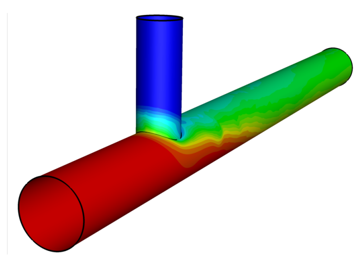


Real T-junction Cases

❖ Coupling with ABAQUS

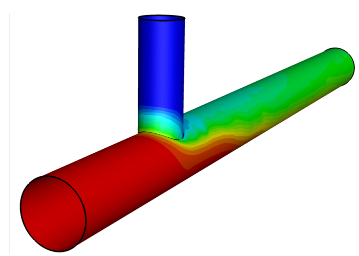
- During the **FLUENT CFD** simulation, transient temperatures in the solid and pressures at the fluid-solid interface are exported to **ABAQUS** format at a frequency of 40 Hz, using subroutines developed earlier within the **PLiM** projects.
- A **database** with transient results from 65 s – 85 s is transferred to **LNM**

FLUENT →



Temperature at 65 s

…



Temperature at 85 s

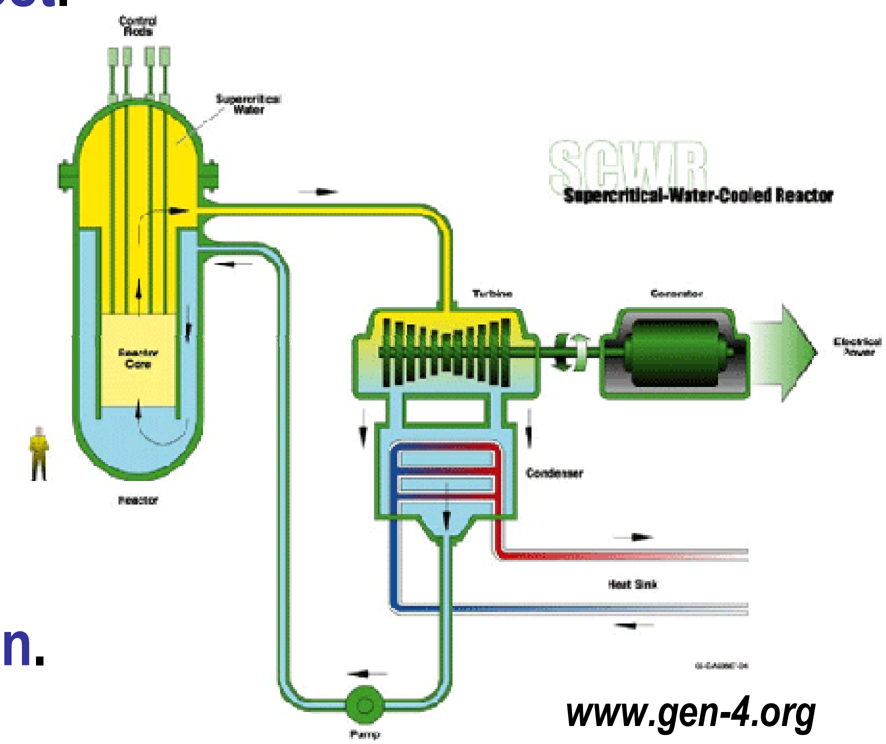
→ **ABAQUS**

SC-Water-cooled Reactor (SCWR)


Niceno

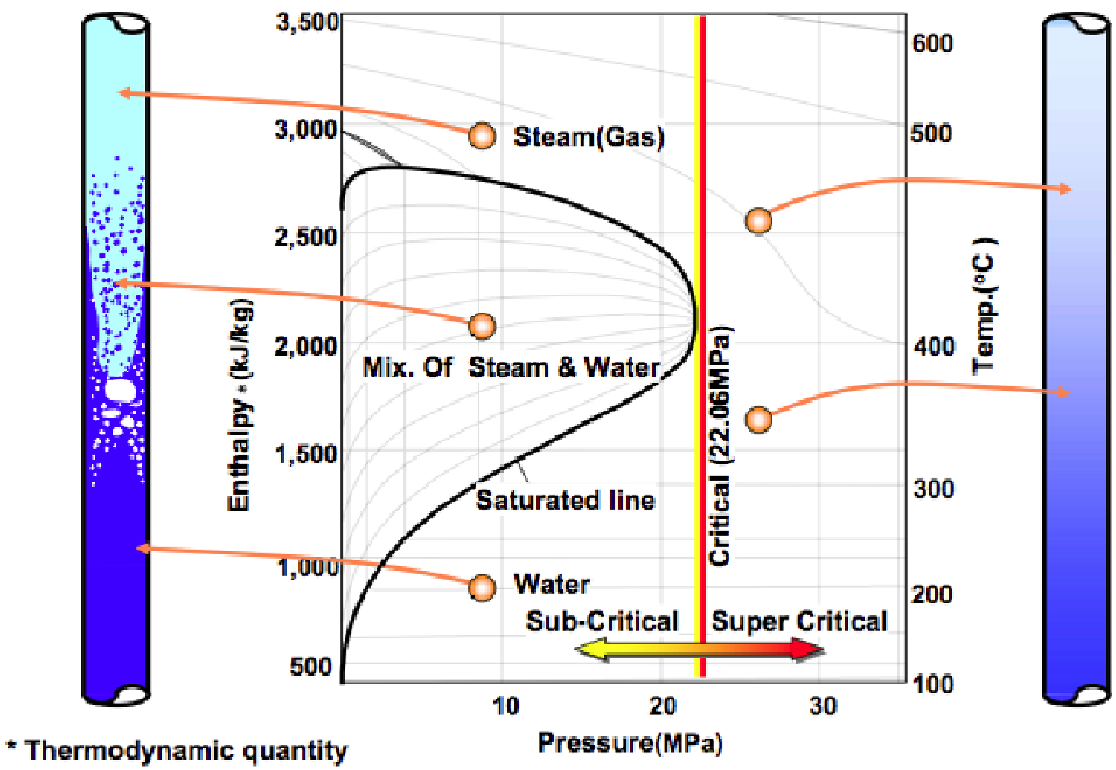

Sharabi

- One of the **Gen-IV** reactor concepts.
- Generates electricity at **lower cost**.
- High **conversion ratio.**
- Elimination of **dryout.**
- Realization of the core in the **fast neutron** spectrum.
- Potential for **waste transmutation**.



www.gen-4.org

SC Water: State of Matter



Diagram's courtesy of Vijay Jain, Dalhousie University

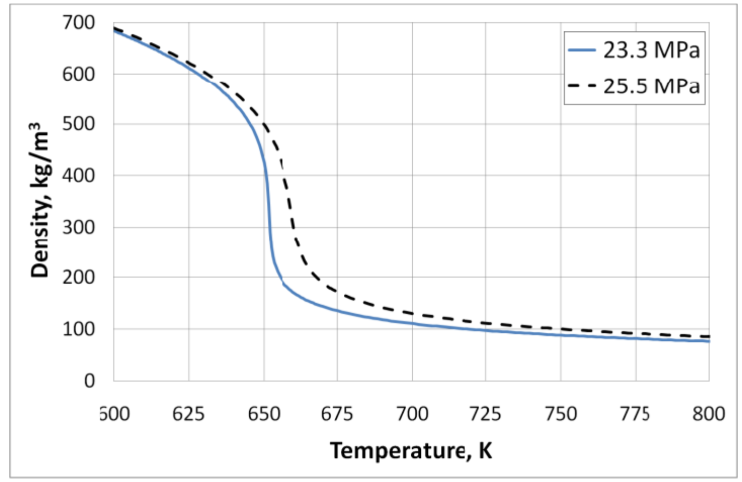
- **Continuous change from liquid-like to gas-like state.**
- **No liquid-gas boundary, no surface tension.**
- **It shares *characteristic* of liquid *and* of gas**
  - It is **disolving** like liquid, but has good **diffusivity** like gas

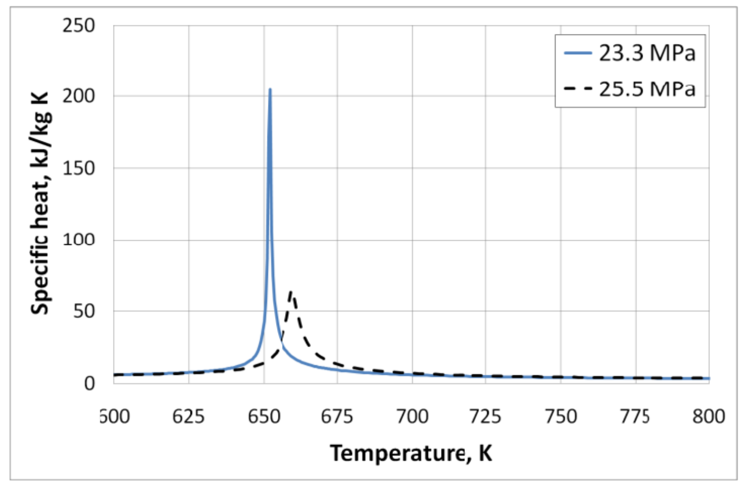
Heat Transfer at Super-Critical Pressures

SC Fluid Properties

- Thermo-physical properties vary strongly in the vicinity of pseudo-critical temperature.

- Different heat transfer regimes
  - **Normal** – convective heat transfer to subcritical fluids.
  - **Improved** – leading to reduction of wall temperature.
  - **Deteriorated** – leading to rise of wall temperature.



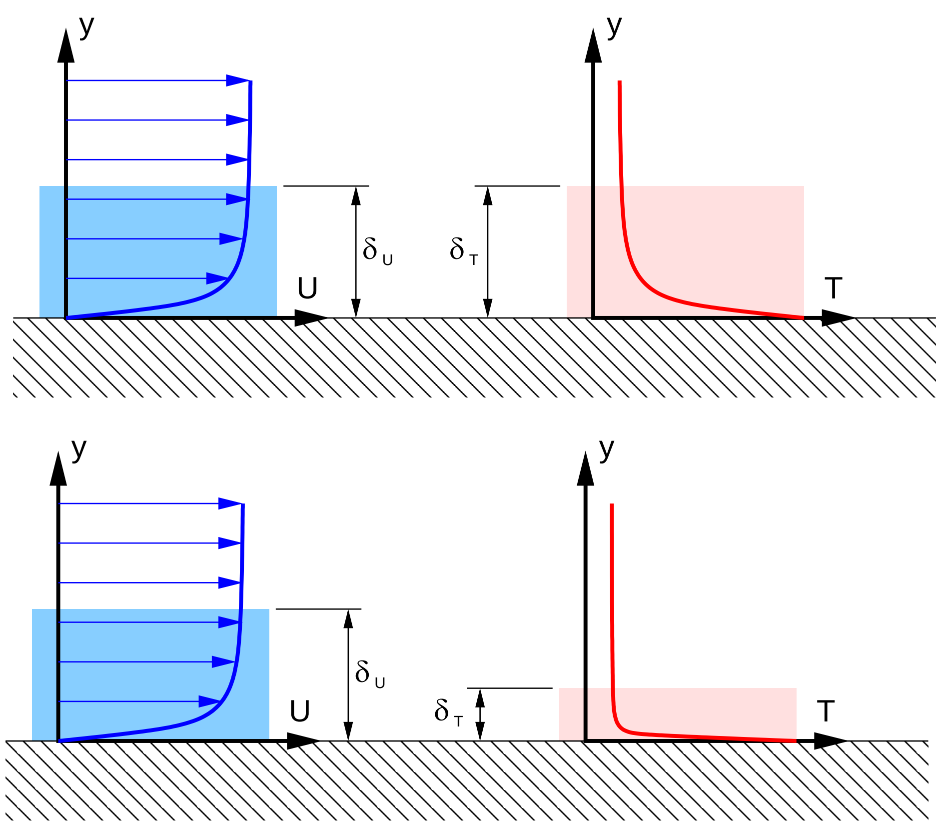


SC-water density and heat capacity variation with temperature

Modeling Issues Rising From Reynolds Analogy

$$Pr = \nu / \alpha$$

$$\alpha_{eff} = \mu_{eff} / Pr_t$$



Prandtl close to unity

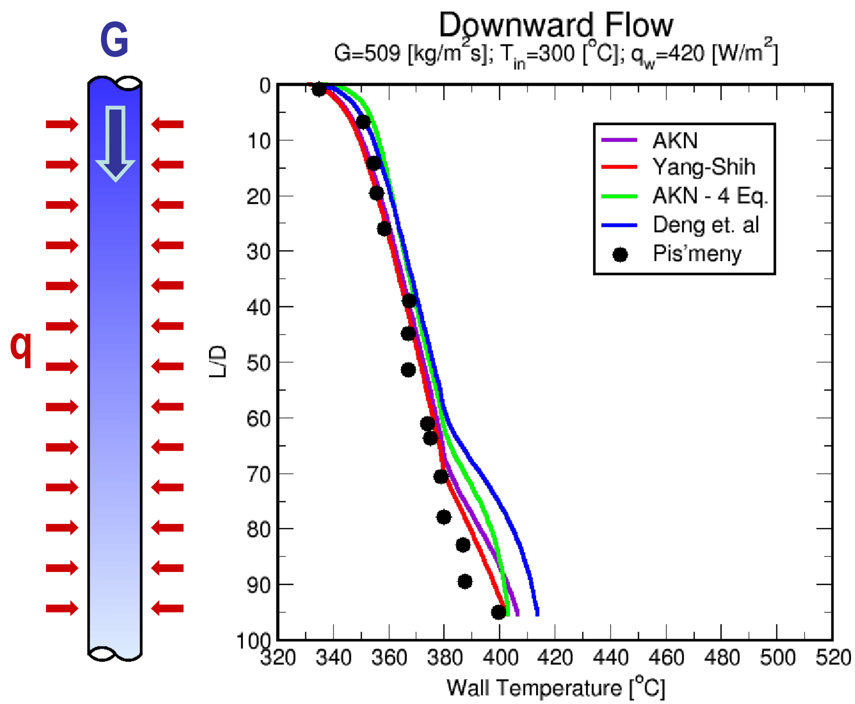
- In most **gasses**
- Reynolds analogy **holds**
- Wall functions ...
- ... or $\Delta + < 1$

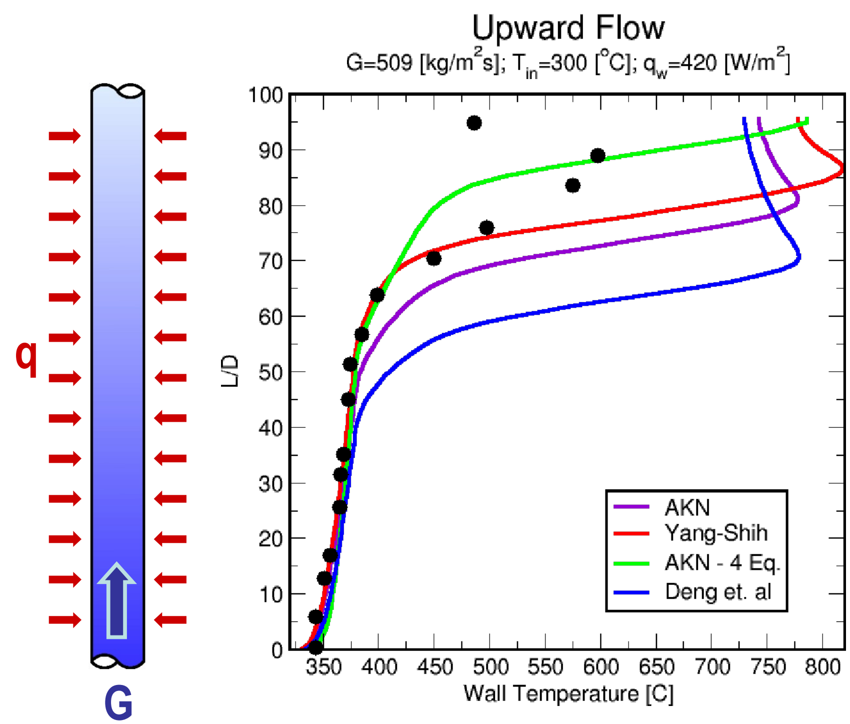
Prandtl greater than unity

- **Supercritical** fluids
- Reynolds analogy **invalid**
- Wall functions **mustn't** be used
- ... or $\Delta + << 1$

Turbulence Modeling by RANS

- It would be **economic** to apply **RANS**, but it **doesn't** predict the **heat transfer deterioration** in SC water very well ☹



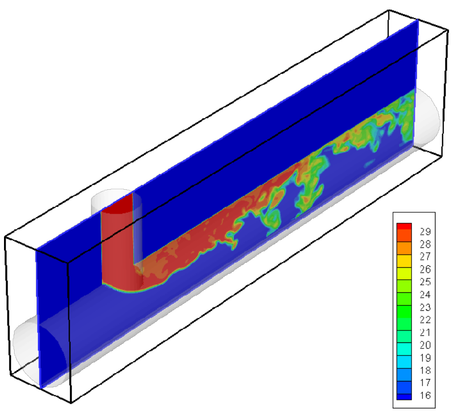


Heat Transfer at Super-Critical Pressures

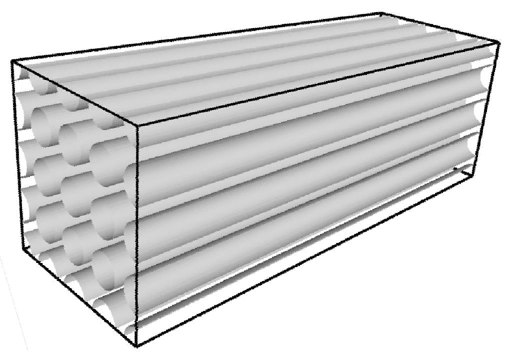
For LES, we use PSI-BOIL, a home-grown tool

Niceno

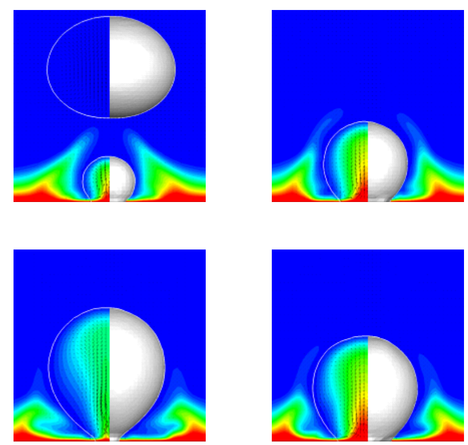
- **Features**
  - **Cartesian** grid, finite volume method with **staggered** arrangement
  - **CIP-CSL2** method for surface tracking (third order accuracy)
  - **Algebraic Multi-Grid** (AMG) solution procedure; scales with problem size,
  - **Immersed Boundary Method** (**IBM**) to handle complex geometries).



T-junction simulation



Flows in rod-bundles

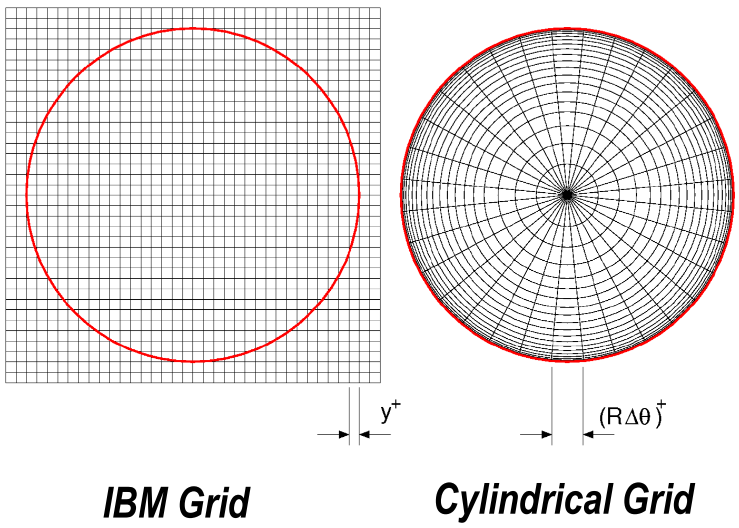


Boiling simulation

Heat Transfer at Super-Critical Pressures

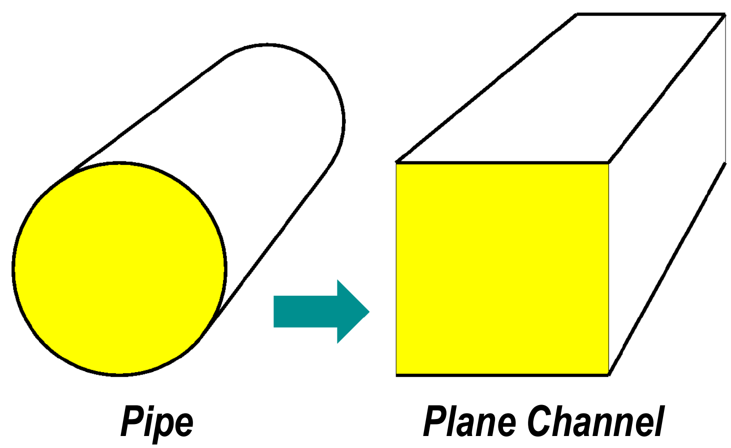
Concerns

- Small enough y^+ could difficult to achieve with IBM
- With cylindrical coordinates, problem could be reaching fine enough $(R\Delta\theta)+$



Solution

- Focus on plane channel with same hydraulic diameter



Computational domain

- **Streamwise (x): L = 1 [m]**
- **Normal (y): H = 3.14 [mm]**
- **Spanwise (z): W = 2 [mm]**

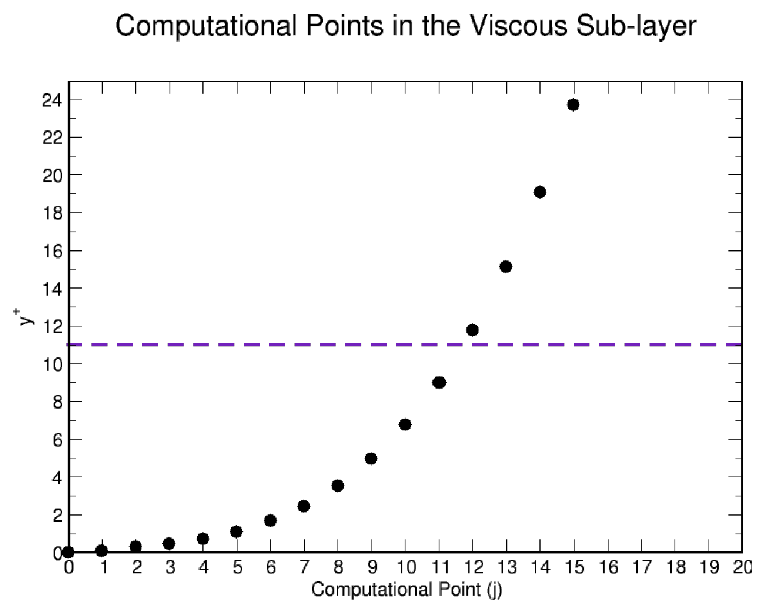
Elongated domain, stiff equations

Hard for pressure solution.

We could solve only with **AMG** solver, using **CG-IC with fill-in**.

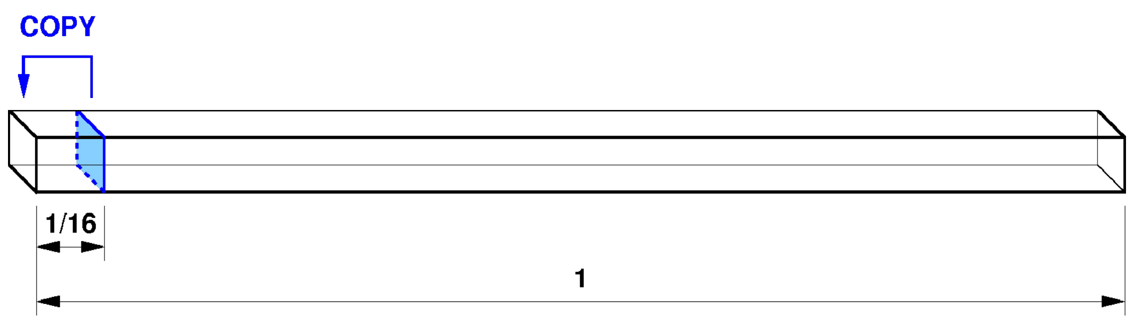
Computational grid

- **Resolution: 4096 × 48 × 64**
- **In wall units:**
  - $y^+ = \mathbf{0.09}$
  - $\Delta x^+ = \mathbf{70}$
  - $\Delta z^+ = \mathbf{9}$



Inlet conditions

- Obtained by copying one planar realization of the velocity field from inside of the back to the inlet of the computational domain.



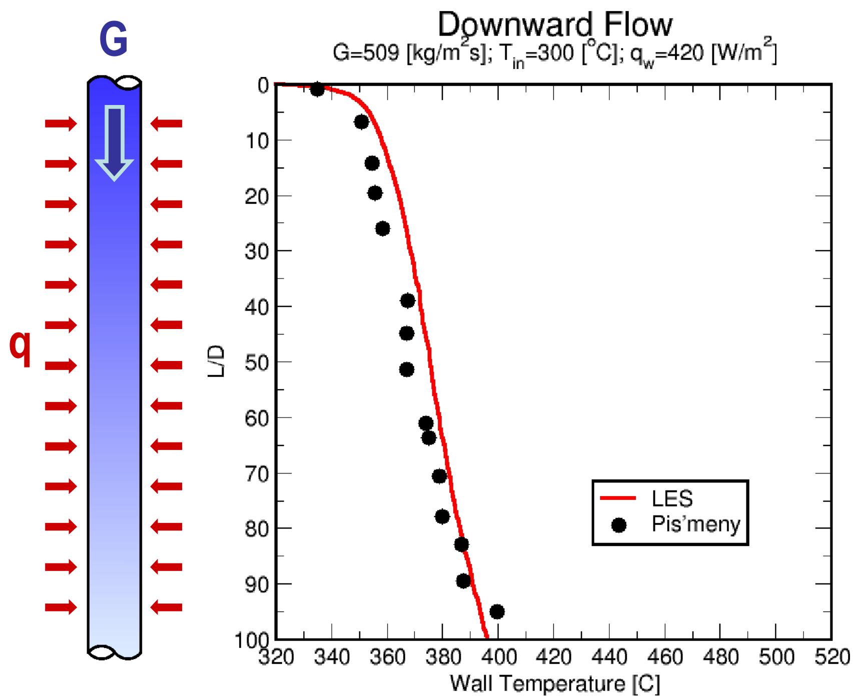
Statistics

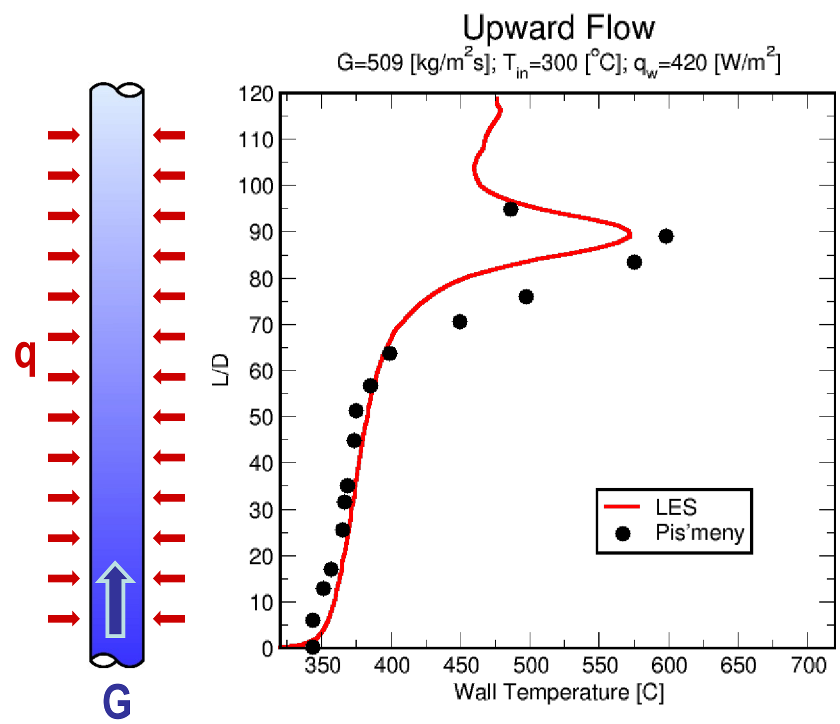
- Flow development: 130 000 time steps = 2.6 [s] = 90 [LETOT]
- Gathering statistics: 80 000 time steps = 1.6 [s] = 55 [LETOT]
- Total: 210 000 time steps = 4.2 [s] = 145 [LETOT]

Wall Temperatures

Results

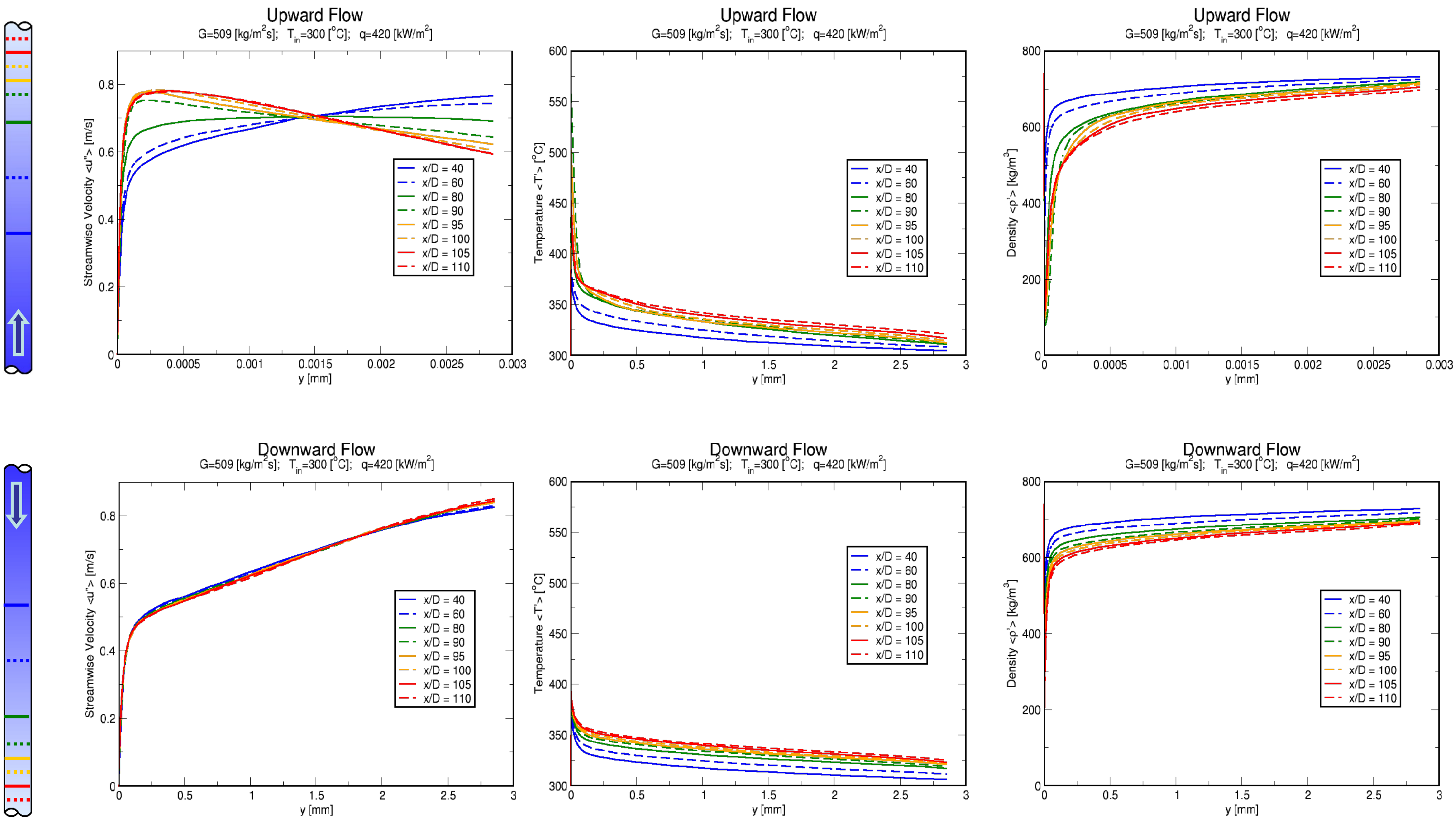
- **Wall temperatures predicted well with LES**





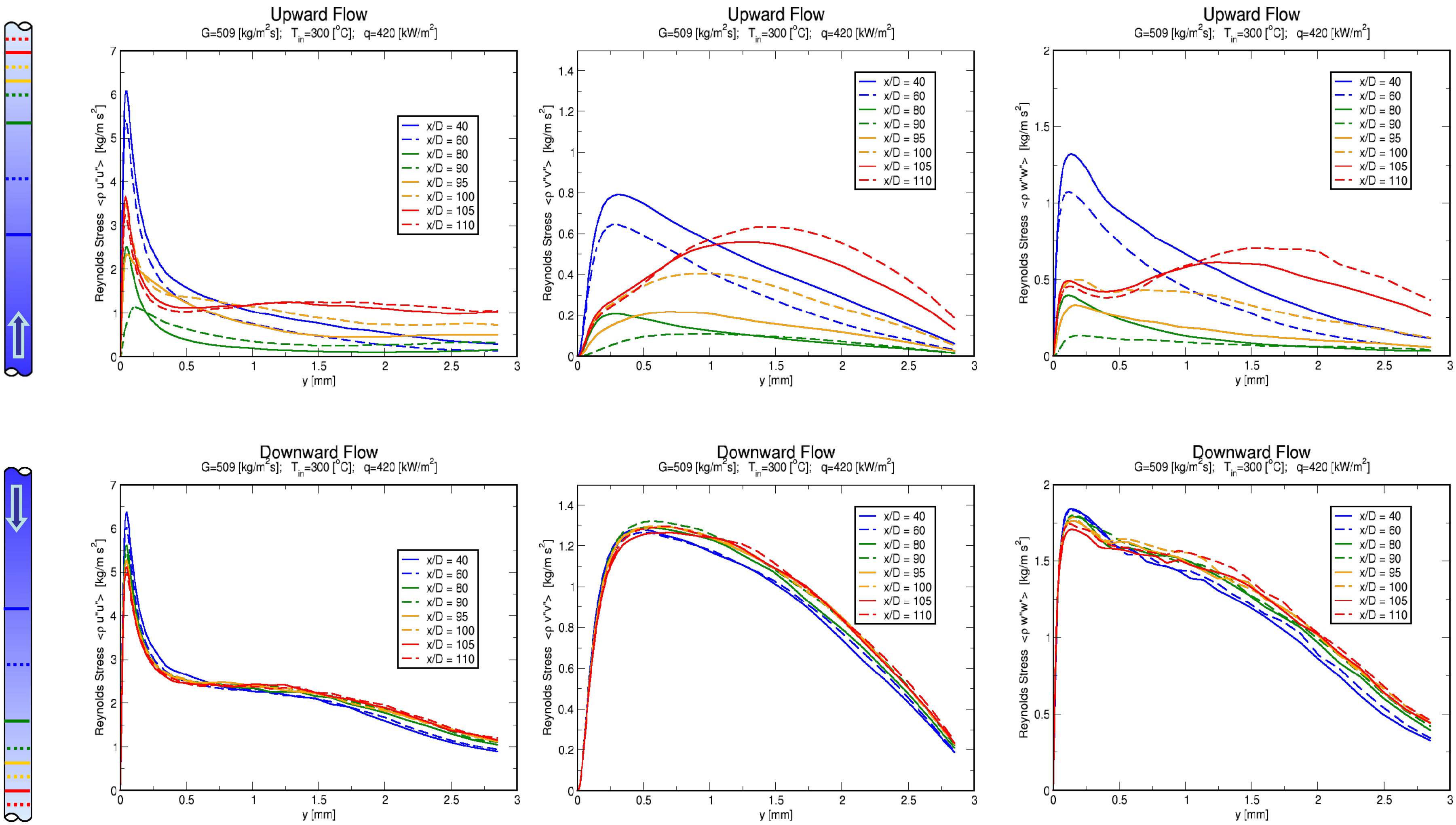
- **Relief: heat transfer deterioration effect present in the channel ☺**

Mean Values



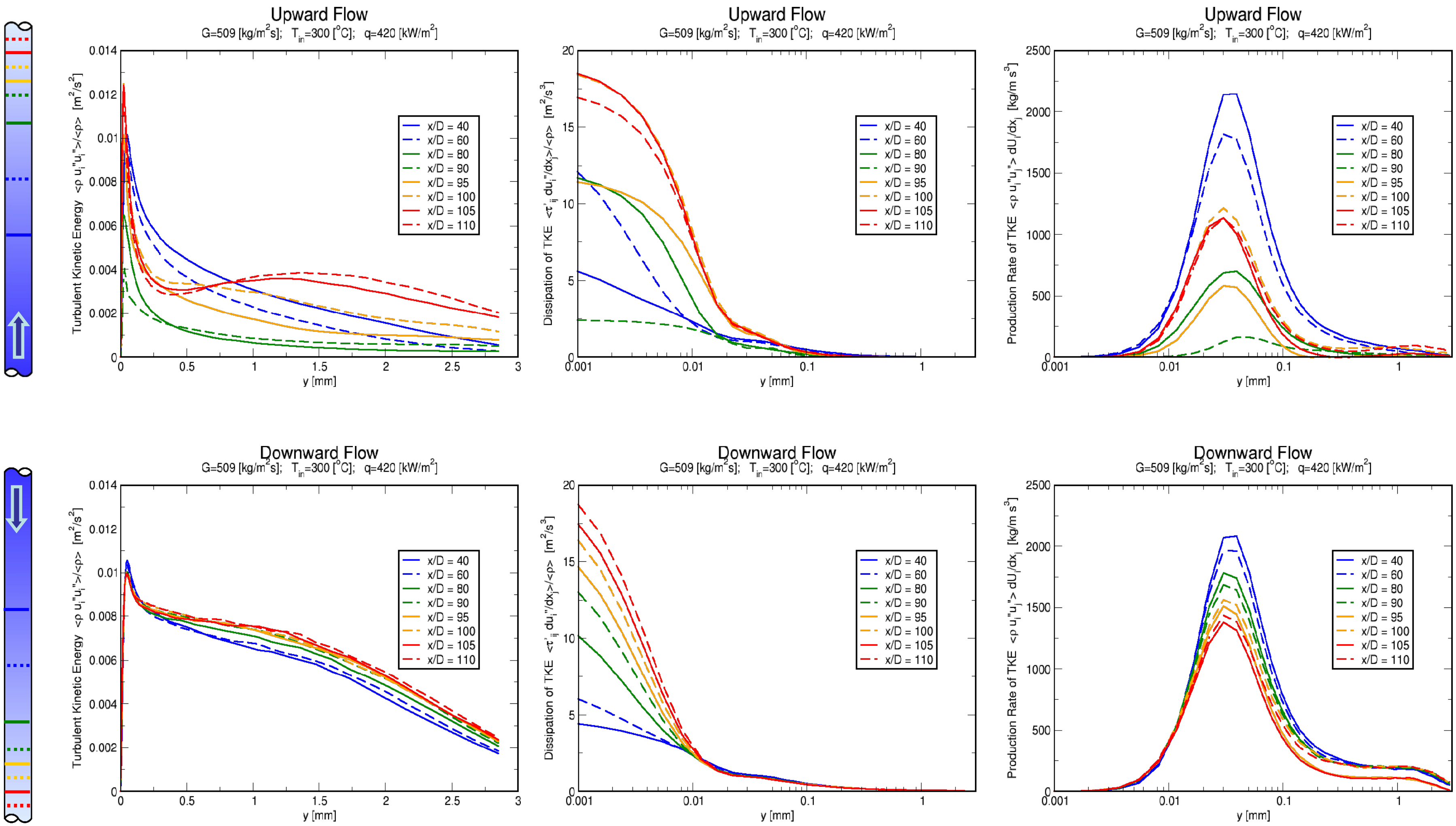
Streamwise velocity <u'> ***Temperature <T'>*** ***Density <ρ'>***

Reynolds Stresses



Streamwise <ρ'u''u''> ***Normal <ρ'v''v''>*** ***Spanwise <ρ'w''w''>***

Kinetic Energy, Dissipation, Production



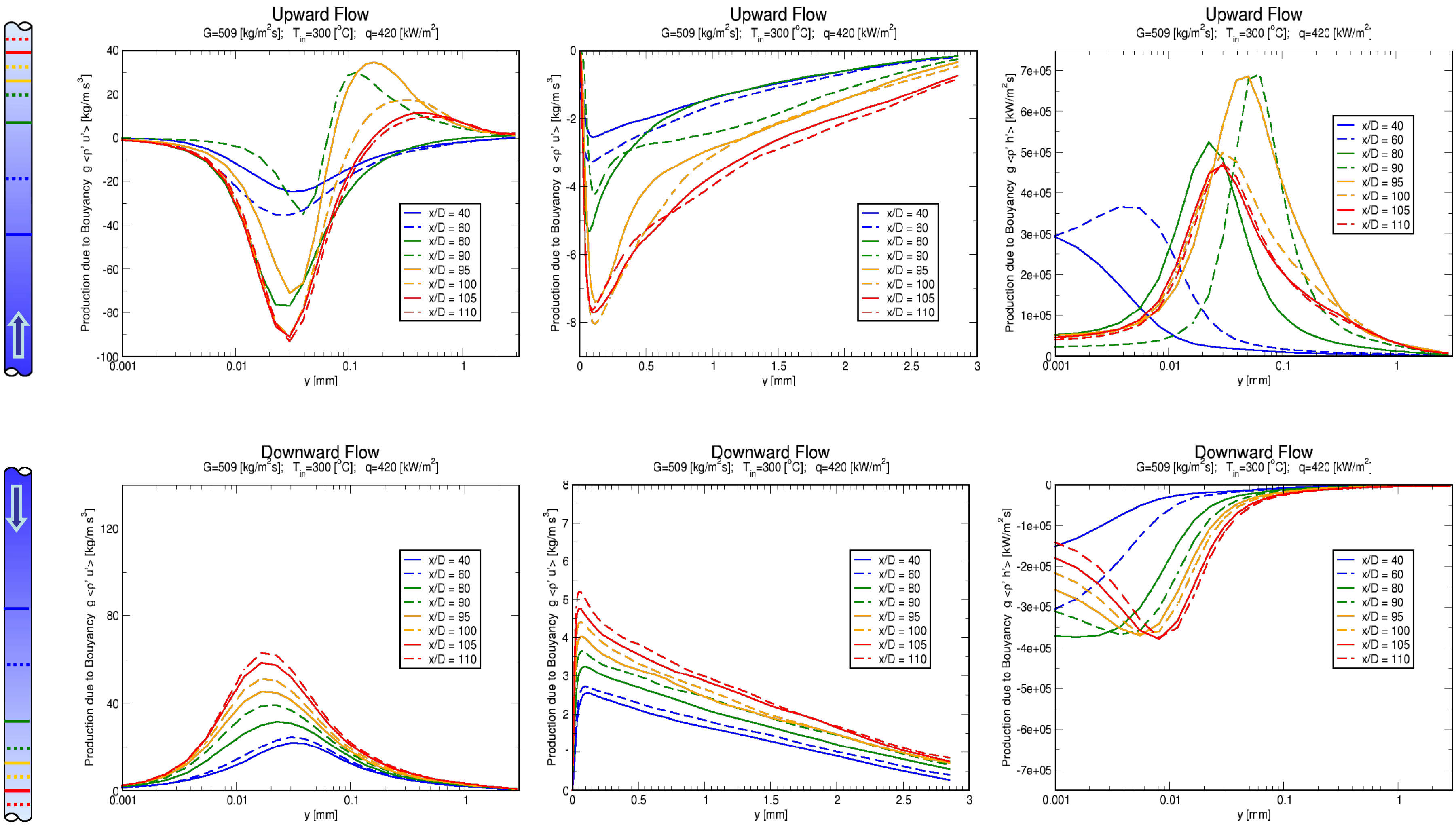
k $<\rho' u_i'' u_i''> <\rho>^{-1}$

ε $<\tau_{ij}' du_i''/dx_j> <\rho>^{-1}$

P_k $<\rho' u_i'' u_j''> dU_i/dx_j$

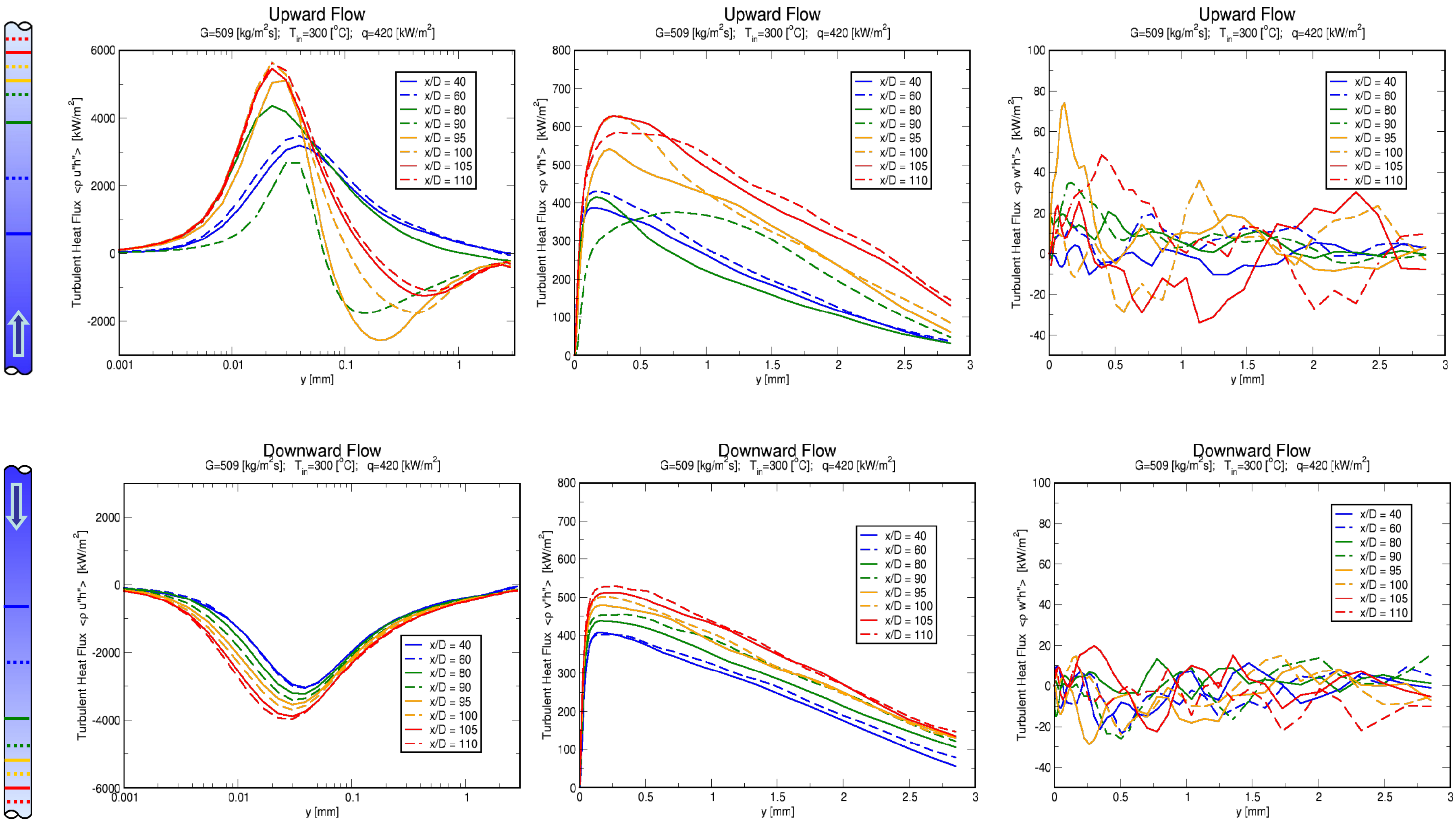
PAUL SCHERRER INSTITUT

Production due to Buoyancy



$g<\rho' u'>$ $g<\rho' v'>$ $g<\rho' h'>$

Turbulent Heat Fluxes



g <ρ'u''h''> **g <ρ'v''h''>** **g <ρ'w''h''>**

Boiling Simulations


Sato

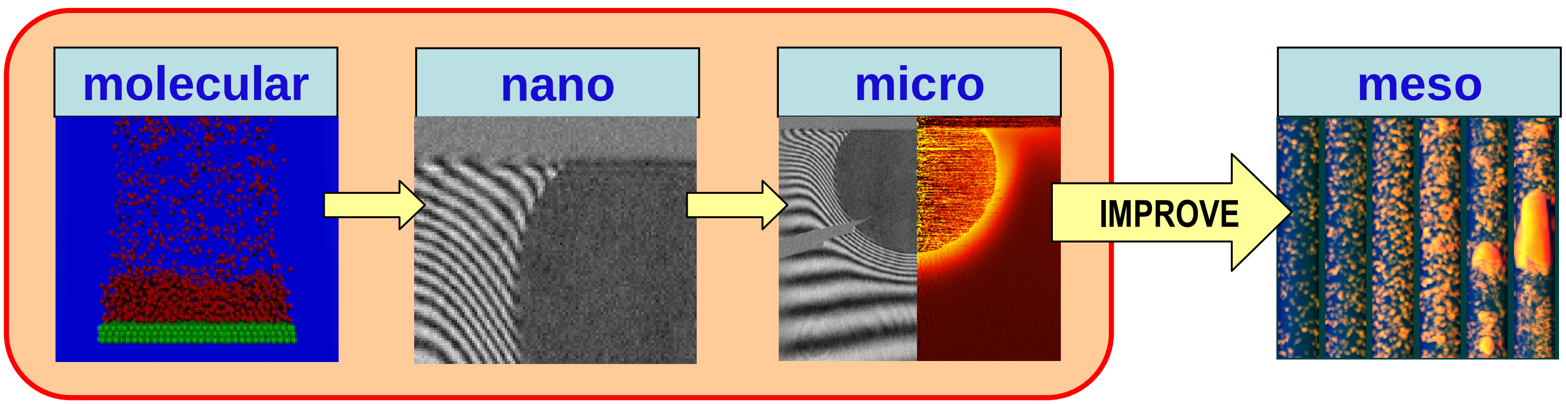

Badillo


Niceno


Andreani

❖ Multi-Scale Modeling Analysis

- Sponsored by **Swissnuclear** (prize **Project of the Year** awarded for **2008**)
- Goal: development of **physically based boiling closure laws** for CFD …
- derived from improved **understanding** of the physics of boiling from **experiments** and numerical **simulations** at different **scales**.



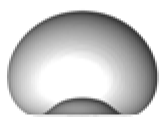
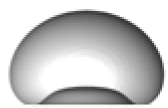
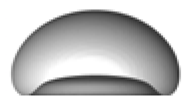
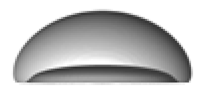
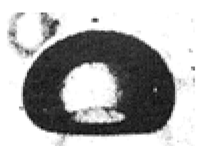
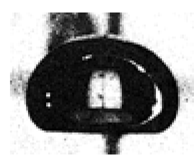
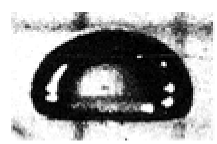
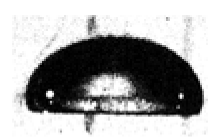
- An integral part: new **DNS** tool with interface tracking **PSI-BOIL**.

Boiling – Interface Tracking

Sato

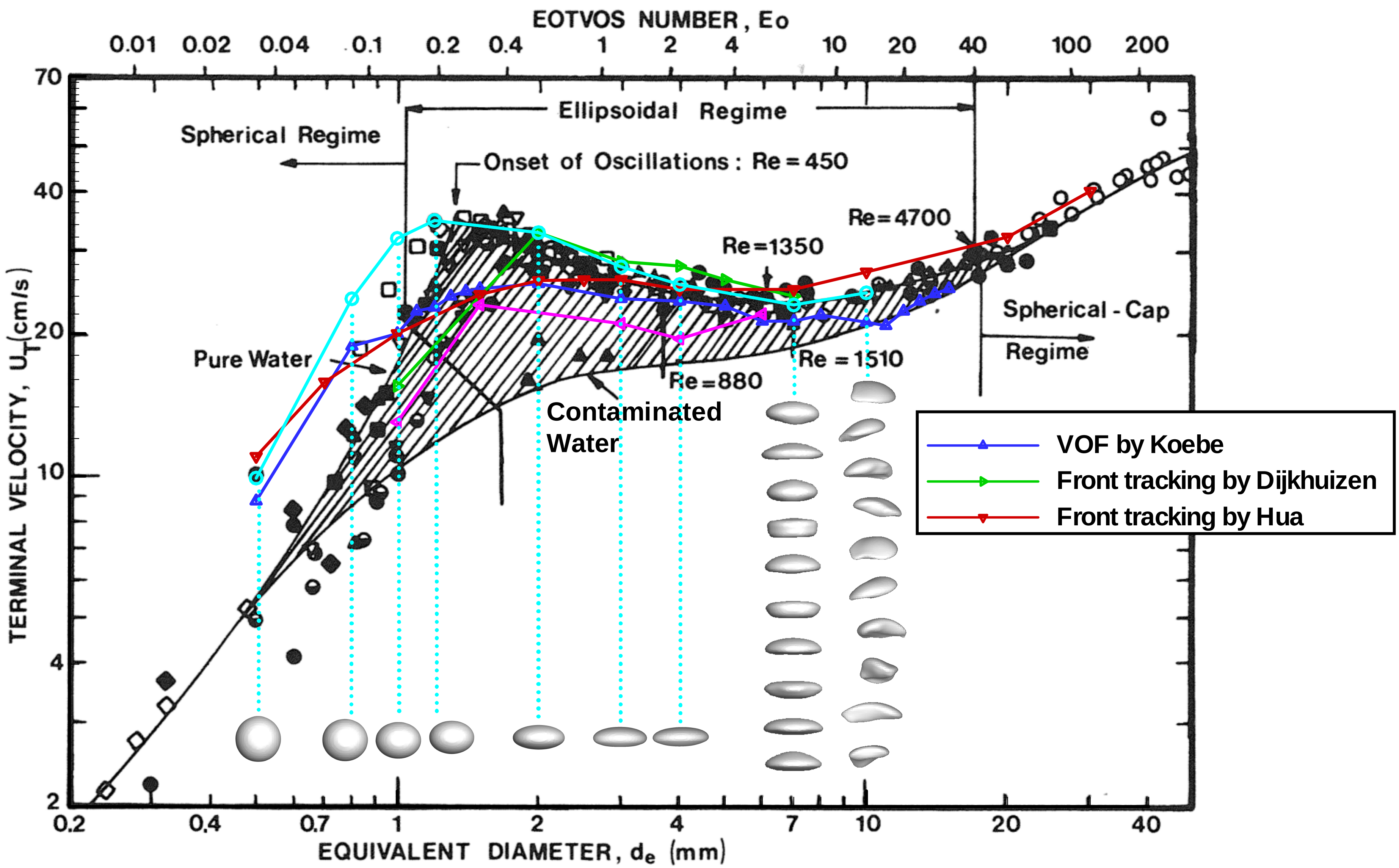
❖ CIP-CSL2 method with local sharpening scheme

- Highly **accurate** scheme for convection term using **gradient** of variable.
- Exactly **conservative** method.

Case		(a)	(b)	(c)	(d)
Condition	E	116	116	116	116
	M	848	266	41.1	5.51
Computed					
	Re	2.85	4.31	7.80	13.7
Experiment					
	Re	2.47	3.57	7.16	13.3

Validation *(single air bubble in oil)*

Micro Scale



EOTVOS NUMBER, Eo
0.01 0.02 0.04 0.1 0.2 0.4 1 2 4 10 20 40 100 200
70
40
20
10
4
2
TERMINAL VELOCITY, U_T (cm/s)
Spherical Regime
Ellipsoidal Regime
Onset of Oscillations: Re = 450
Re = 4700
Re = 1350
Pure Water
Re = 1510
Re = 880
Contaminated Water
Spherical - Cap Regime
VOF by Koebe
Front tracking by Dijkhuizen
Front tracking by Hua
0.2 0.4 0.7 1 2 4 7 10 20 40
EQUIVALENT DIAMETER, d_e (mm)

Micro Scale

Boiling – Results

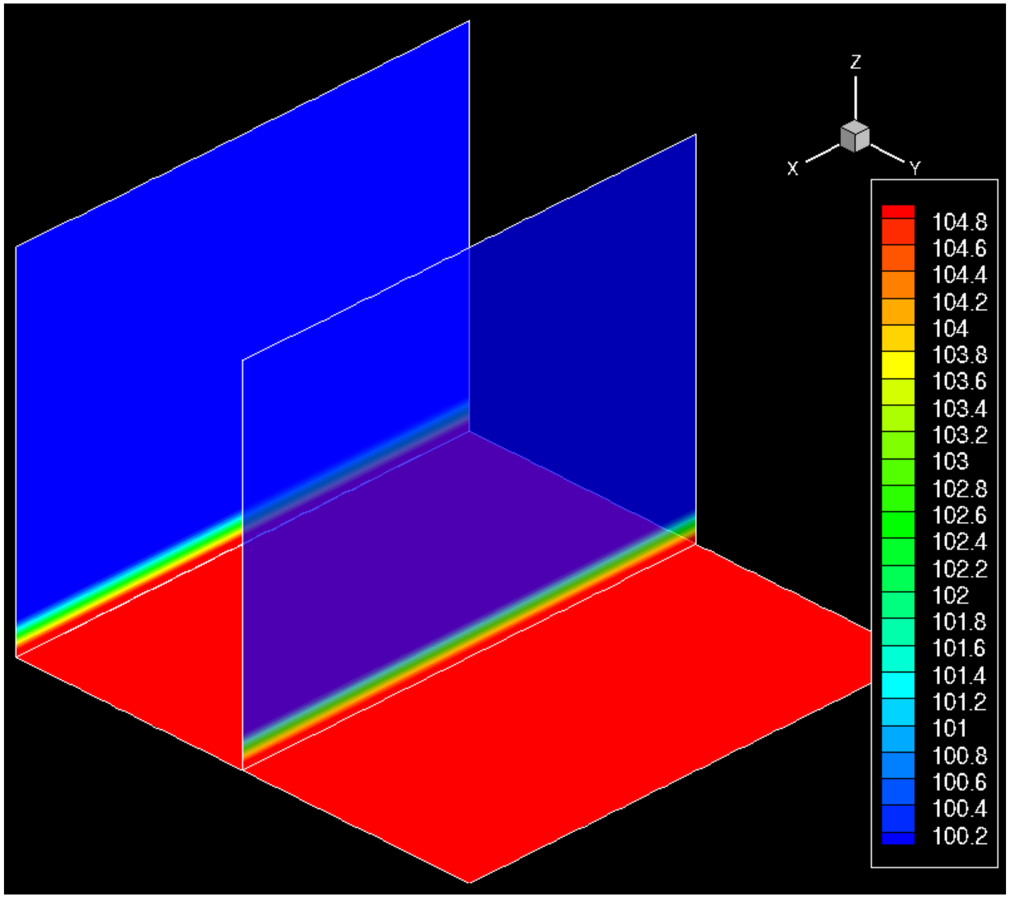

Sato


Lal

❖ Saturated pool boiling.

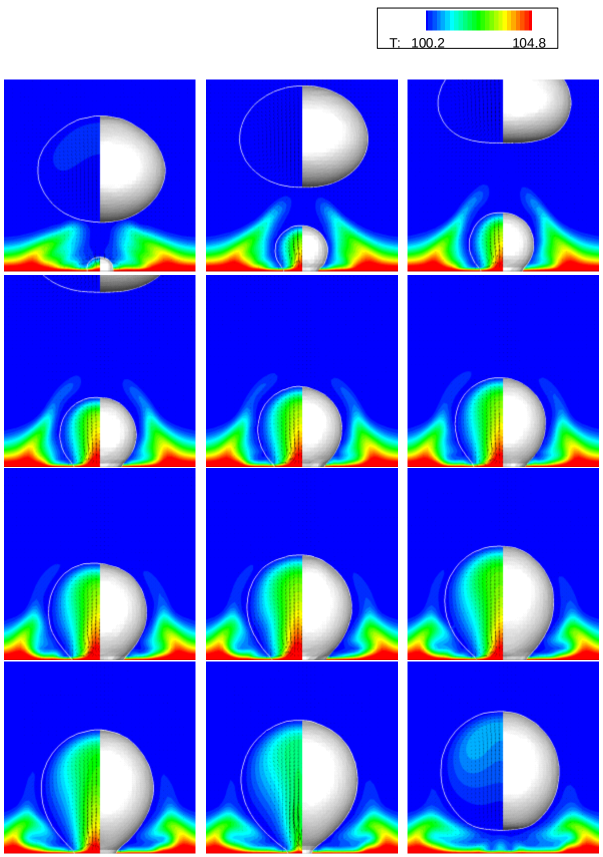
- **Boundary Condition**
  - Bottom wall: Temp. = 106.2 °C
  - Contact angle = 38°
- **Initial Condition**
  - Bubble shape: hemisphere
  - Bubble diameter = 0.25mm
- **Computational parameters:**

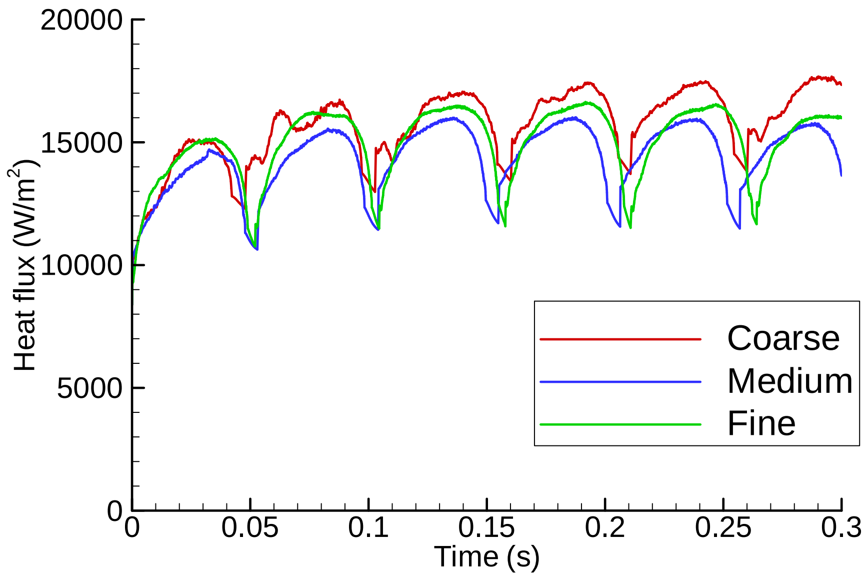
Grid	h [μm]	No. Cell
Coarse	125	150 000
Medium	83	350 000
Fine	63	1 200 000



Boiling – Results

- Bubble departure diameter and frequency





		Experiment	Simulation
Diameter	[mm]	2.1 ~ 2.4	2.4
Period	[sec]	0.035 ~ 0.043	0.05

No experimental uncertainty is given.

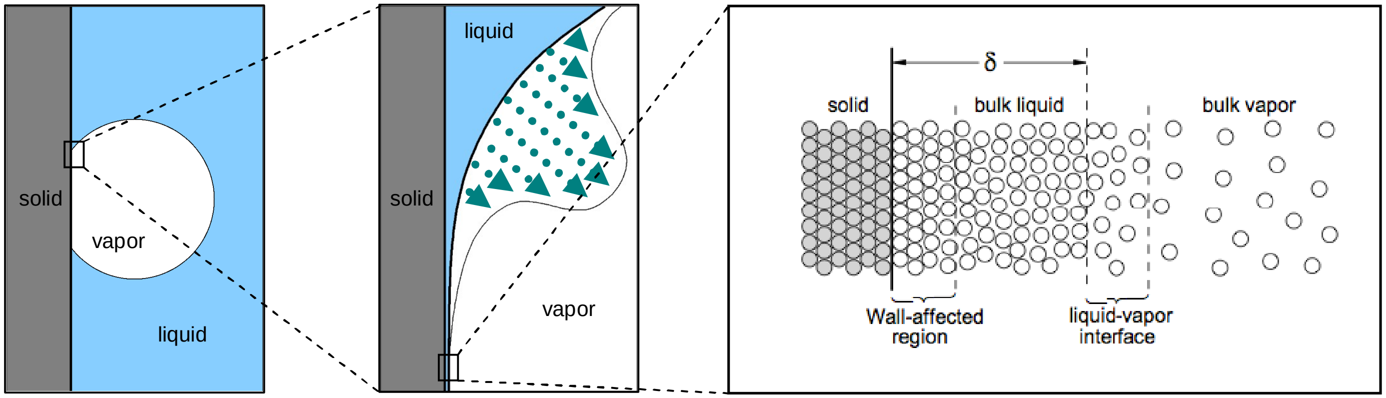
Below a Vapor Bubble


Krohn


Badillo

Motivation

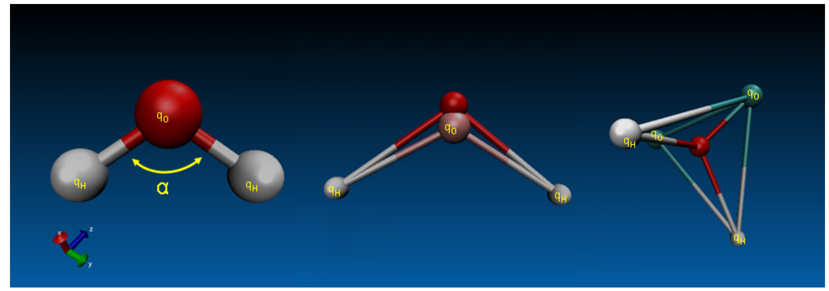
- At micro-scale, **triple-line** is one computational cell
- But in reality, it is a very **dynamic region**, where many important phenomena take place, such as most intensive mass transfer, variable surface tension, etc.



- In order to build better **model** for micro-scale, we conduct analysis of the triple line at nano-scales, i.e. we perform MD simulations.

Below a Vapor Bubble

❖ Theory of MD



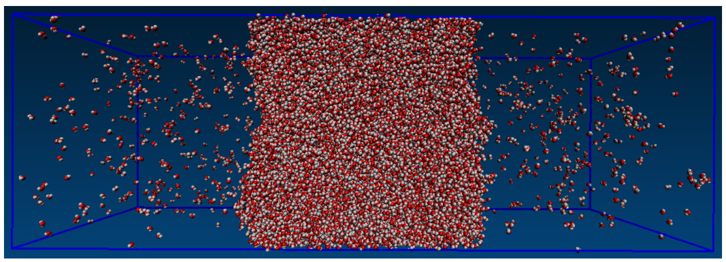
Molecule models used in this study

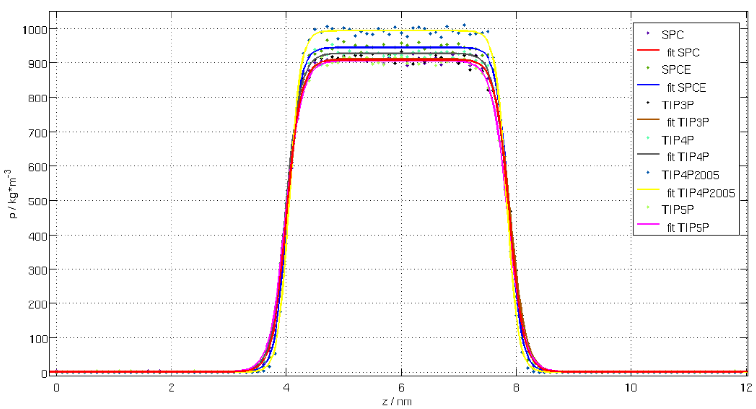
- Hamiltonian $\mathcal{H} = f(\vec{r}^N, \vec{P}^N) = \mathcal{K}(\vec{P}) + \mathcal{U}(\vec{r})$
- Newtonian $\dfrac{\partial^2 x_i}{\partial t^2} = \dfrac{F_{x,i}}{m_i}$
- Taylor series $r(t+dt) = r(t) + v(t)\delta t + \frac{1}{2}a(t)\delta t^2 + \ldots$
- Van der Vaals and Coulomb: $U(r_{ij}) = U_{short}(r_{ij}) + U_{Coulomb}(r_{ij}) = \sum_{i\in 1}\sum_{j\in 2} U_{short}(r_{ij}) + \sum_{i\in 1}\sum_{j\in 2}\dfrac{q_i q_j}{r_{ij}}$
- Leonard-Jones potential: $U^{LJ}(r_{ij}) = \left(\dfrac{A}{r_{ij}}\right)^{12} - \left(\dfrac{B}{r_{ij}}\right)^{6}$

Below a vapor bubble

❖ Validation

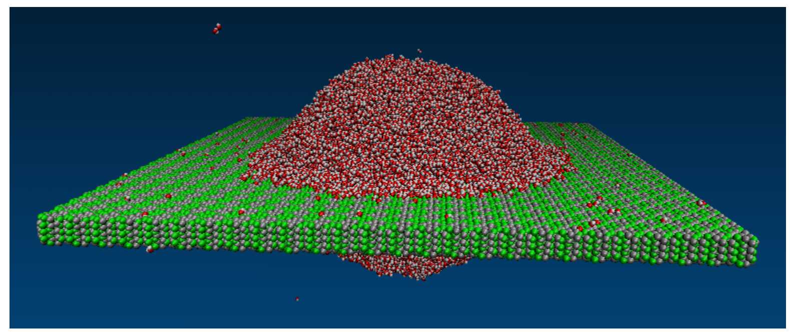
- Liquid-vapor equlibrium





❖ Results

- Droplet sitting on a solid



- With further increase in resolution (number of molecules) we may deduce the existence of the micro-region and contact angle.

Concluding Remarks

- **MSG works on a number of topics, ranging in spatial scale (system to nano) and scope (Gen II – Gen IV reactors).**
- **Associated with that, the number of project in which we are involved is also relatively big.**
- **In order to cover this wide range of topics and projects, the group has evolved. (Since 2007: from 3 to 13 members.)**
- **Recruitment was facilitated by:**
  - Involvement in **education** (lectures at ETHZ);
  - Dedication to **networking**, through international **projects** we are involved in.