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# Thermal–hydraulics and CFD for Molten Salt Reactors

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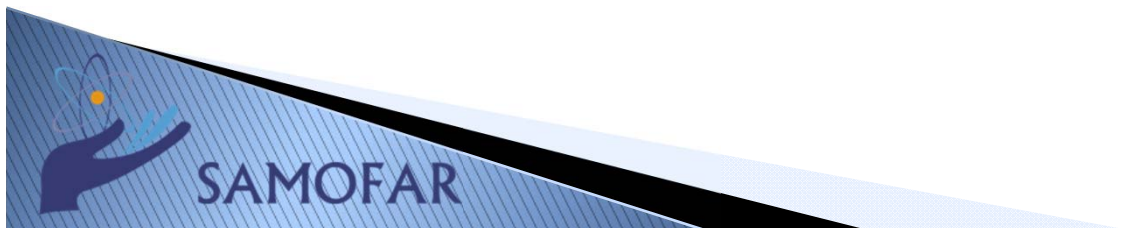


SAMOFAR



# Overview

- ▶ Why Thermal-Hydraulics (T&H) design is needed?
- ▶ Simplified flow governing equations
- ▶ Computational Fluids Dynamics (CFD)
- ▶ Current research efforts on molten salt T&H modeling



# References

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- ▶ *Computational Fluid Dynamics – The basics with applications*, Anderson, McGraw–Hill (1995).
- ▶ *Turbulent flows*. Pope, S. B. (2001).
- ▶ Best practice guidelines for the use of CFD in nuclear reactor safety applications, NEA/CSNI/R(2007)5.
- ▶ *Near-wall behavior of RANS turbulence models and implications for wall functions*, Kalitzin, Medic, Iaccarino and Durbin, Journal of Computational Physics, 204 (2005) 265–291.
- ▶ *Solidification: –Revised & Expanded*. Dantzig, J. A., & Rappaz, M. (2016). EPFL press.



# WHY THERMAL HYDRAULICS DESIGN IS NEEDED?

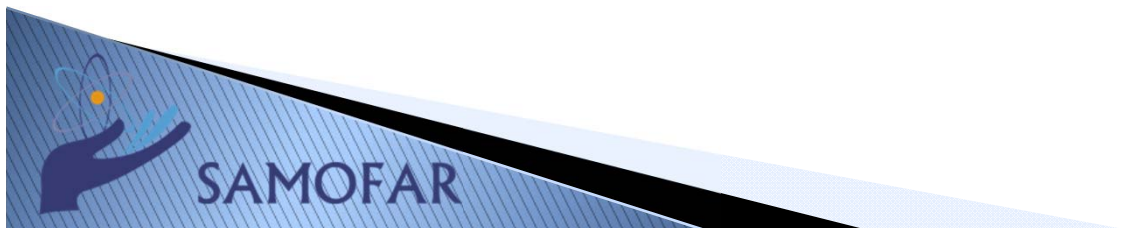
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- Design and safety criteria
- MSFR T&H design

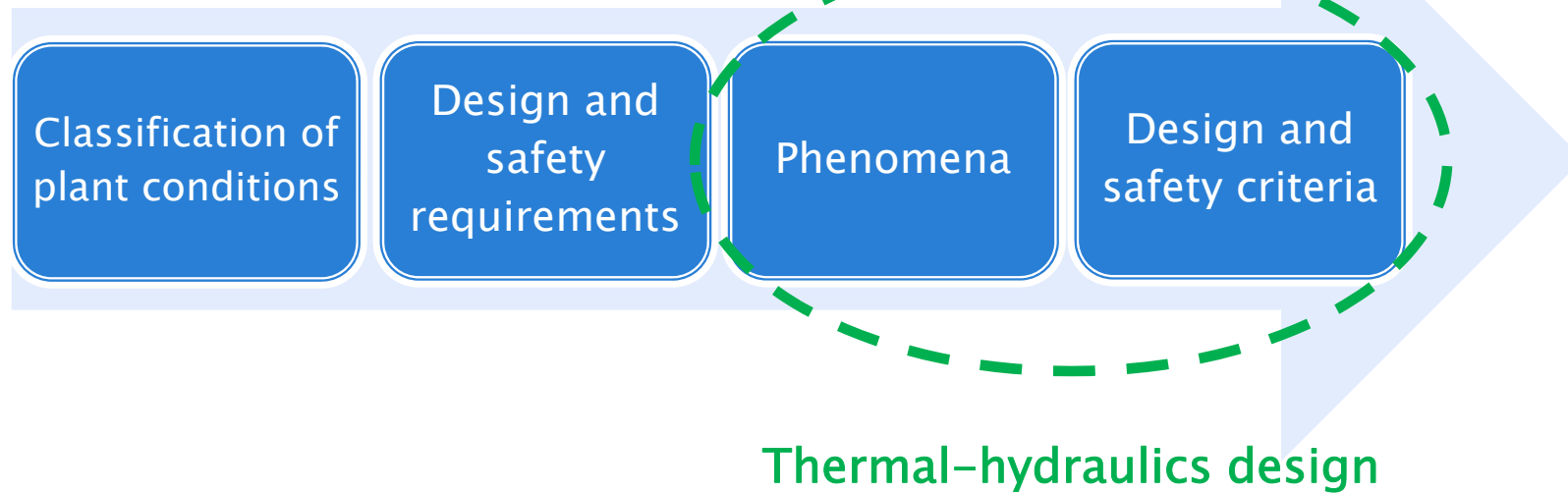


# Why performing T&H studies?

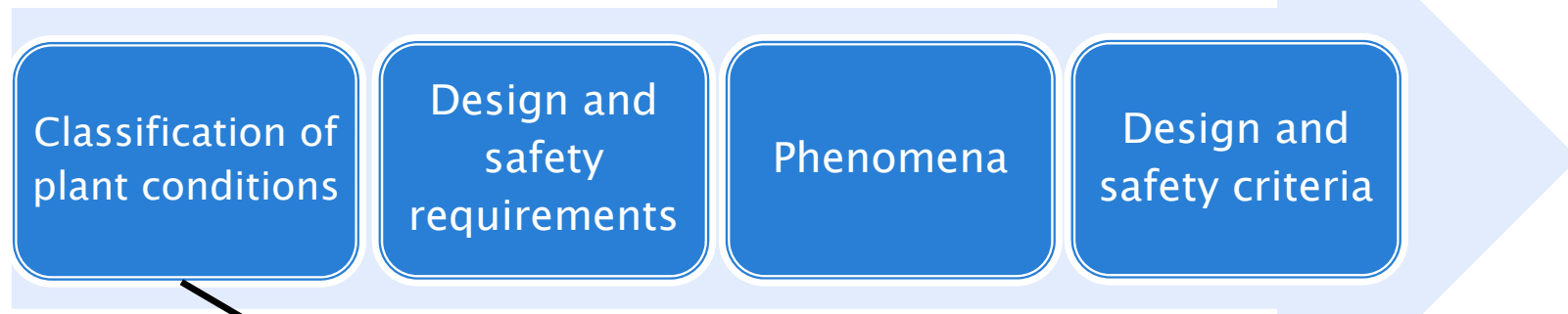
- ▶ To verify that the reactor design and safety criteria are met !
- ▶ And also to optimize the electricity generation cost...



# Nuclear design/safety criteria verification process



# Plant conditions



## Example of classification of plant conditions for a PWR (ANS 51.1)

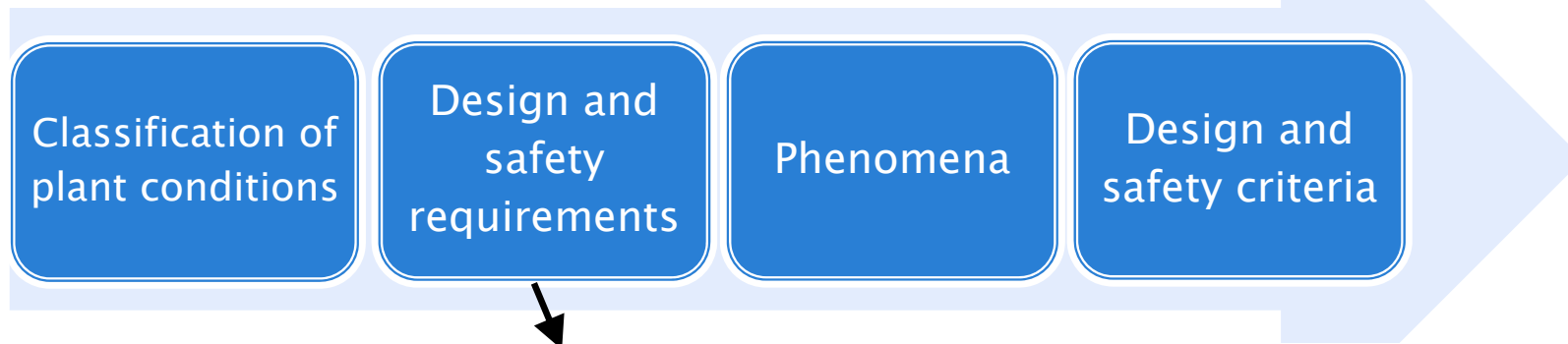
Condition I: Normal operation and operational transients

Condition II: Faults of moderate frequency

Condition III: Infrequent faults

Condition IV: Limiting faults

# Design and safety requirements



## Example of Design and safety requirements for a PWR

Condition I: Barriers integrity is kept

Condition II: The reactor shall rapidly come back to normal operation.  
Barriers integrity is kept

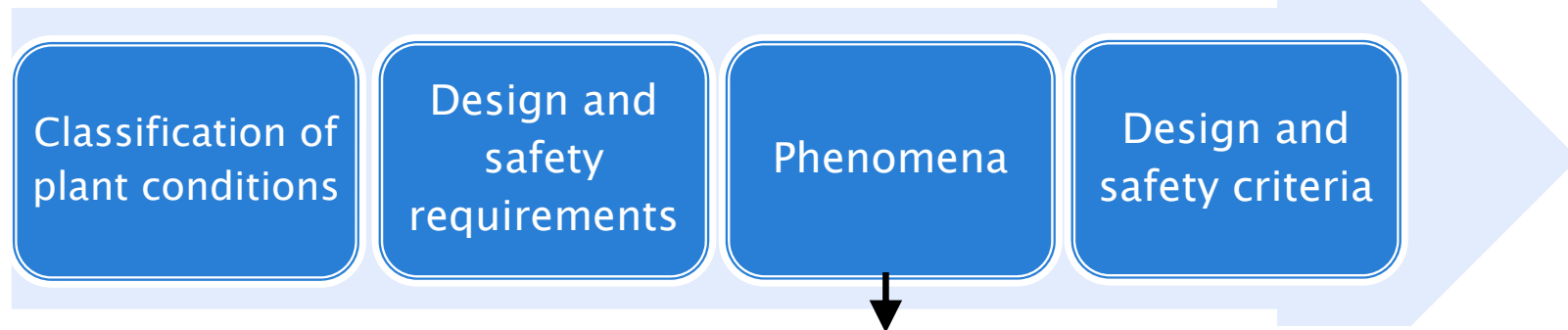
Condition III: Immediate come back to normal operation is no longer required. A limited volume of fuel salt that may leak could be allowed

Condition IV: The reactor shall come to a safe state and the fuel salt maintained sub-critical and cooled in a specific containment. Integrity of all barriers is not guaranteed





# Phenomena

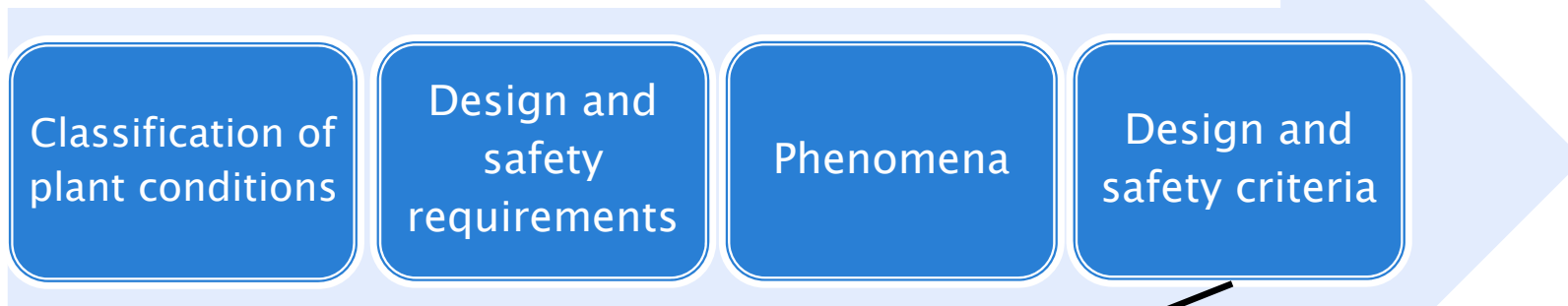


## Example of phenomena for a PWR fuel assembly

Departure from Nucleate Boiling (DNB): the formation of a steam layer over the cladding rapidly deteriorates the heat transfer coefficient and causes an excessive increase of the cladding temperatures

Fuel pellet melting: fuel pellet melting is considered as a cladding failure mechanism

# Design and safety criteria



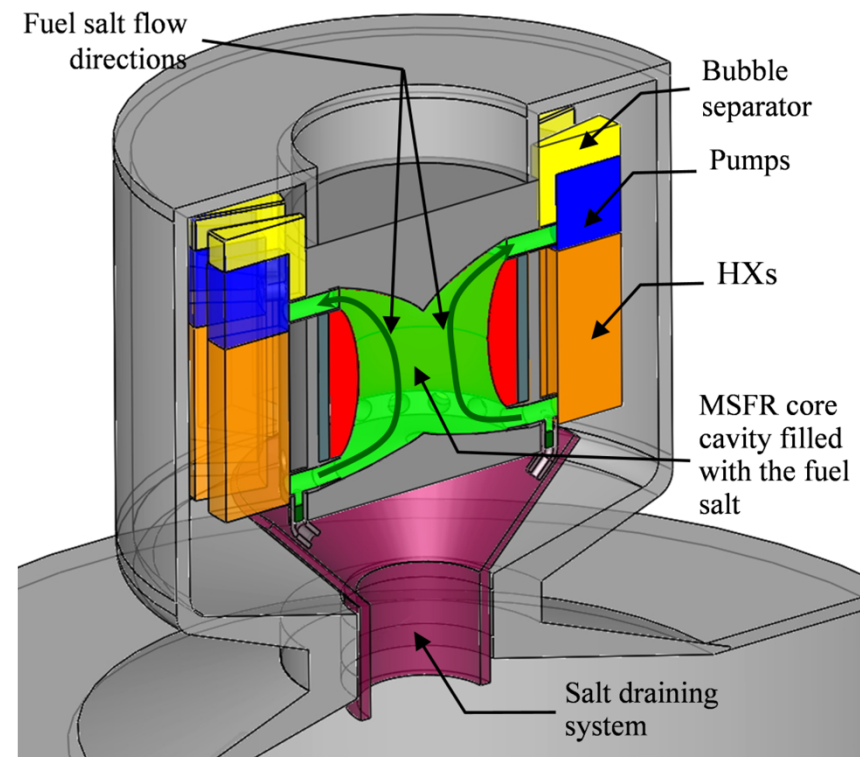
## Example of Design and Safety criteria for a PWR fuel assembly

Departure from Nucleate Boling (DNB): probability of at least 95% with a confidence of 95% that DNB does not occur in the limiting fuel rods

Fuel pellet melting: probability of at least 95% with a confidence of 95% that the fuel rod linear power does not exceed the value corresponding to the melting temperature of the fuel centerline

# The MSFR concept

- ▶ Main differences with respect to LWR designs
  - Liquid fueled reactor using a molten salt as fuel matrix and coolant (LiF)
  - Based on a Thorium fuel cycle ( $^{232}\text{Th}$  /  $^{233}\text{U}$ )
  - No solid moderator in the core -> fast neutron spectrum reactor
  - No core internal structures
  - Online refueling and reprocessing
- ▶ Three reactor loops
  - Fuel salt loop
  - Intermediate loop
  - Thermal conversion loop
- ▶ Fuel loop operating conditions
  - High temperatures ( $\sim 750^\circ\text{C}$ )
  - Low pressures ( $\sim 1$  bar)
  - Fuel salt recirculation time  $\sim 4$  s



# MSFR features impacting the reactor design and safety

## ▶ Liquid fuel

- Molten salt acts as nuclear fuel and coolant
- A significant part of the fissile inventory is outside the core
- Components of the fuel circuit exposed to high temperatures/neutron flux

## ▶ No control rods in the core

- Reactivity is controlled by the heat removal in the HXs and fuel salt feedback coefficients, continuous fissile loading and geometry of fuel salt mass
- Not need to control neutron flux shape (no DNB, uniform fuel irradiation, etc.)

## ▶ Fuel salt draining

- Cold shutdown can be obtained by draining the molten salt from the fuel circuit
- Changing the fuel geometry allows for adequate shutdown and cooling margins
- Fuel draining can be done passively or by operator action



# Key specific MSFR phenomena

- ▶ Circulation of delayed neutron precursors (e.g. effective delayed neutron fraction depends on the flow field)
- ▶ Large core cavity with significant 3D and turbulence effects
- ▶ Flow distribution impacts the reactor feedback coefficients and the core wall temperature distribution
- ▶ Complex heat transfer: conduction, convection and radiative
- ▶ Phase change: possibility of undesirable fuel salt solidification in the fuel loop with complex solid phase morphology (and properties)
- ▶ Volumetric heat source



# Comparison of T&H design and safety criteria for different designs

	Pressurized Water Reactors (PWRs)	Sodium-Cooled Fast Reactor (SFRs)	Molten Salt Fast Reactor (MSFR)
T&H criteria	<ul style="list-style-type: none"> <li>✓ MDNBR</li> <li>✓ Linear rod power</li> <li>✓ Clad oxidation thickness</li> </ul>	<ul style="list-style-type: none"> <li>✓ Maximal cladding temperature</li> <li>✓ Linear rod power</li> <li>✓ Sodium boiling</li> <li>✓ Maximal coolant velocity</li> </ul>	<ul style="list-style-type: none"> <li>✓ Maximal salt temperature</li> <li>✓ Maximal temperature, temperature gradient and thermal fatigue on the core walls, pipes and HX plates</li> <li>✓ Minimum salt temperature</li> <li>✓ Maximal coolant velocity</li> </ul>
Codes models	Subchannel or porous medium	Subchannel or porous medium	Only CFD codes





# Particularities of MSFR T&H modeling

- ▶ Requires Numerical resolution of the Navier-stokes equation for turbulent flow
  - Classical approaches such a porous media or sub-channel models are in general not well suited
- ▶ Coupled neutronics and T&H numerical simulations are needed
  - The CFD model is usually coupled to a neutronics model of the reactor which provides the power distribution. The neutronics model could be based on for example a neutron diffusion code or a Monte Carlo code
- ▶ Both steady and transient calculations are necessary for normal and transient conditions
- ▶ CFD models have to integrate all the specific salt phenomena



# SIMPLIFIED FLOW GOVERNING EQUATIONS

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- Navier–Stokes Equations
- Turbulence RANS Equations





# Conservation of mass

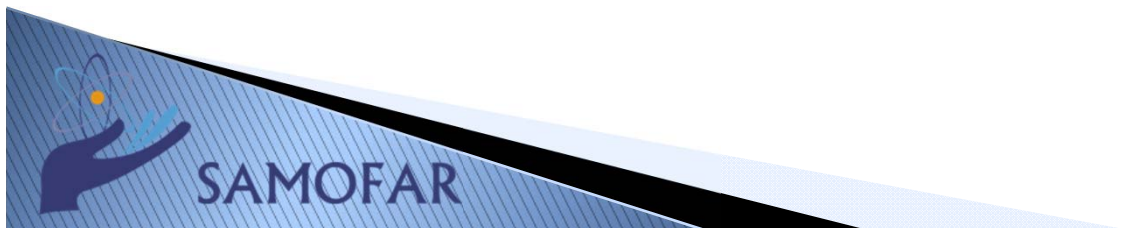
- ▶ Setting aside nuclear reactions and relativistic effects mass is neither created nor destroyed in a fluid. Thus individuals mass elements may be tracked within a flow field
- ▶ In addition, assuming no phase change, then it can be considered that the mass of a specific collection of neighboring fluid particles is constant
- ▶ The continuity equation is a scalar equation reflecting the conservation of mass for a moving fluid. It has the following form:

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

in index  
notation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0$$

where  $\rho$  and  $\vec{u}$  are the fluid density and flow velocity, respectively.

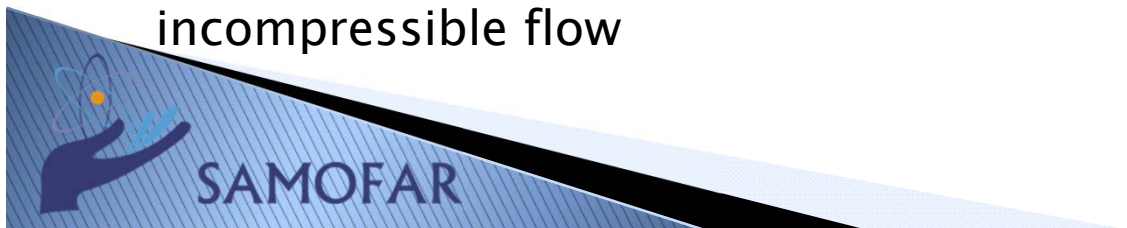


# Conservation of mass

- ▶ For an incompressible flow where density of the fluid particles does not change (i.e. the material derivate of the density is zero)

$$\frac{D\rho}{Dt} = \frac{\partial\rho}{\partial t} + \vec{u} \cdot \nabla(\rho) = 0 \quad \text{thus} \quad \boxed{\nabla \cdot \vec{u} = 0}$$

- ▶ Therefore the divergence of the velocity field of incompressible flows is zero
- ▶ Constant density flows are a subset of incompressible flows
- ▶ A fluid is usually called incompressible if its density does not change with pressure.
- ▶ Liquids are almost incompressible. The general form of the continuity is required when the material derivative of the density is not zero because of changes in the pressure, temperature or molecular composition of fluid particles
- ▶ In most of our applications, molten salt can be often considered as incompressible flow



# Conservation of momentum

- ▶ The momentum equation is a vector equation that represents the application of Newton's 2<sup>nd</sup> law of motion to a fluid element
- ▶ It relates the fluid-particle acceleration to the net body ( $\rho \vec{G}$ ) and surface force ( $\nabla \cdot \vec{\tau}$ ) on the particle (also called Cauchy's equation)

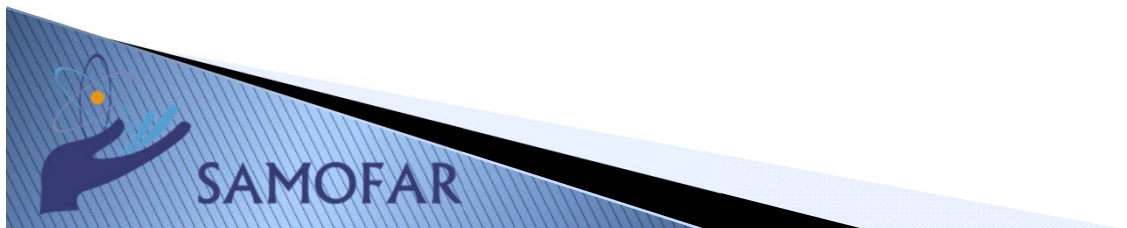
$$\rho \frac{D\vec{u}}{Dt} = \rho \vec{G} + \nabla \cdot (\vec{\tau})$$

in index  
notation

$$\rho \frac{Du_i}{Dt} = \rho g_i + \frac{\partial}{\partial x_i} (\tau_{ij})$$

where  $\vec{G}$  is a body force (i.e. gravitation) and  $\vec{\tau}$  is the fluid stress tensor

- ▶ This equation does not provide a complete description of fluid dynamics, even combined with the continuity equation because the number of dependent field variables is greater than the number of equations



# Stress tensor

- ▶ The state of stress at a point can be specified by a nine component tensor  $\vec{\tau} = \tau_{ij}$ . Its two free indices specify two directions; the first (i) indicates the orientation of the surface on which the stress is applied while the second (j) indicates the component of the force per unit area on that surface.
- ▶ The stress tensor can be written as a the matrix as follows:

$$\tau = \begin{bmatrix} \tau_{11} & \tau_{12} & \tau_{13} \\ \tau_{21} & \tau_{22} & \tau_{23} \\ \tau_{31} & \tau_{32} & \tau_{33} \end{bmatrix}$$

- ▶ It can be shown that the stress tensor is symmetric ( $\vec{\tau} = \vec{\tau}^T$ ) based on the conservation of the angular momentum. Therefore the stress tensor has only six independent components
- ▶ The net force  $d\vec{F}$  on a surface area element  $d\vec{A} = \vec{n} dA$  is thus:

$$d\vec{F} = \vec{n} \cdot \vec{\tau} dA = \vec{\tau} \cdot \vec{n} dA$$



# Newtonian fluid constitutive equation

- ▶ The relationship between the stress and the deformation rate in a continuum is called a constitutive equation
- ▶ A fluid that follows the simplest possible linear constitutive equation is known as a Newtonian fluids
- ▶ The stress tensor can approximately be written as follows:

$$\tau_{ij} = -p \delta_{ij} + \sigma_{ij}$$

where  $p$  is the thermodynamic pressure (fluid static pressure) and  $\sigma_{ij}$  is the deviatoric stress tensor (or fluid dynamic stress) due to viscosity (with both diagonal and off-diagonal components). For a incompressible flow it can be shown that  $p = \bar{p} = -\frac{1}{3}\tau_{ii}$



# Newtonian fluid constitutive equation

- ▶ Considering that the fluid is isotropic, a linear relationship between the stress tensor and the flow strain rate tensor can be obtained

$$\tau_{ij} = -p \delta_{ij} + 2\mu \left( S_{ij} - \frac{1}{3} S_{mm} \delta_{ij} \right) + \mu_v S_{mm} \delta_{ij}$$

where

$$S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad \text{is the strain rate tensor}$$

$$\mu_v = \lambda + \frac{2}{3} \mu \quad \text{is the coefficient of bulk viscosity (set to 0 under Stokes assumption). The coefficients } \mu \text{ and } \lambda \text{ are scalars that depend on the local thermodynamics state}$$



# Navier–Stokes momentum equation

- ▶ The momentum conservation equation for a Newtonian fluid (Navier–Stokes momentum equation) is obtained by substituting the constitutive equation for the stress tensor into the Cauchy's equation to obtain:

$$\rho \frac{Du_j}{Dt} = -\frac{\partial p}{\partial x_j} + \rho g_i + \frac{\partial}{\partial x_i} \left[ \mu \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) + \left( \mu_v - \frac{2}{3} \mu \right) \frac{\partial u_m}{\partial x_m} \delta_{ij} \right]$$

The viscosities  $\mu$  and  $\mu_v$  can depend on the thermodynamics state and indeed  $\mu$  display a rather strong dependency for most fluids

- ▶ When temperature differences are small within the flow this reduces to

$$\rho \frac{Du_j}{Dt} = -\frac{\partial p}{\partial x_j} + \rho g_i + \mu \frac{\partial^2 u_j}{\partial x_i^2} + \left( \mu_v + \frac{1}{3} \mu \right) \frac{\partial}{\partial x_j} \frac{\partial u_m}{\partial x_m}$$

- ▶ If in addition the flow is incompressible ( $\frac{D\rho}{Dt} = 0$  and thus  $\nabla \cdot \vec{u} = 0$ ):

$$\rho \frac{Du_j}{Dt} = -\frac{\partial p}{\partial x_j} + \rho g_i + \mu \frac{\partial^2 u_j}{\partial x_i^2} \quad \text{in index notation}$$

$$\rho \frac{D\vec{u}}{Dt} = -\nabla p + \rho \vec{G} + \mu \nabla^2 \vec{u}$$





# Energy conservation equation

- ▶ The energy equation is a scalar equation that represents the application of the 1<sup>st</sup> law of thermodynamics to a flow
- ▶ Assuming that:
  - Heat transfer is caused by thermal conduction and there is no phase change
  - The irreversible conversion of mechanical energy to thermal energy through the action of viscosity (viscous work) for a Newtonian fluid
- ▶ Then the energy conservation equation can be written as follows:

$$\rho \frac{De}{Dt} = -p \frac{\partial u_m}{\partial x_m} + \underbrace{2\mu \left( s_{ij} - \frac{1}{3} \frac{\partial u_m}{\partial x_m} \delta_{ij} \right)^2 + \mu_v \left( \frac{\partial u_m}{\partial x_m} \right)^2}_{= \rho \varepsilon} + \frac{\partial}{\partial x_m} \left( k \frac{\partial T}{\partial x_i} \right)$$

where

$e$  is the fluid internal energy per unit mass

$k$  is the fluid thermal conductivity (depends on thermodynamics conditions)

In index notation

$$\rho \frac{De}{Dt} = -p \nabla \cdot \vec{u} + \rho \varepsilon + k \nabla^2 T$$



# Boussinesq approximation

- ▶ This approximation assumes that density changes in the fluid can be neglected except where  $\rho$  is multiplied by  $g$  (i.e.  $\rho$  is constant in continuity and momentum equations, except for the gravity term). Other fluid properties ( $\mu$ ,  $k$ ,  $C_p$ ) are usually treated as being constants
- ▶ Valid if pressure–compressibility effects are small and density changes are caused by temperature variations alone and these variations are small
- ▶ Assuming that  $\Delta\rho = -\beta \rho_o \Delta T$  (where  $\beta$  is the thermal expansion coefficient) then the flow momentum equation can be simplified to:

$$\frac{D\vec{u}}{Dt} = -\frac{1}{\rho_o} \nabla p' + \frac{\rho'}{\rho_o} \vec{G} + \frac{\mu}{\rho_o} \nabla^2 \vec{u}$$

where  $p' = p - p_s$ ,  $p_s$  is the hydrostatic pressure and  $\rho' = \Delta\rho$ .

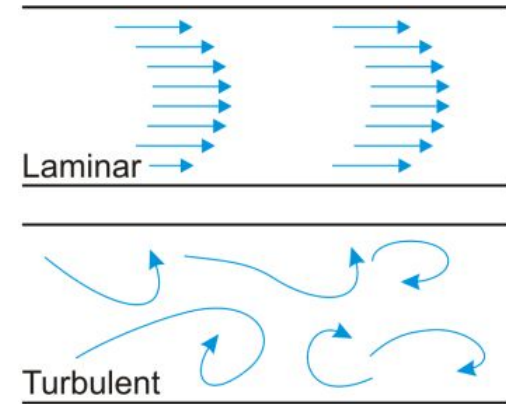
- ▶ In addition the energy equation takes the form:

$$\frac{DT}{Dt} = \left( \frac{k}{\rho C_p} \right) \nabla^2 T$$

since the heating term due to viscous dissipation of energy is negligible under the restrictions underlying the Boussinesq approximation

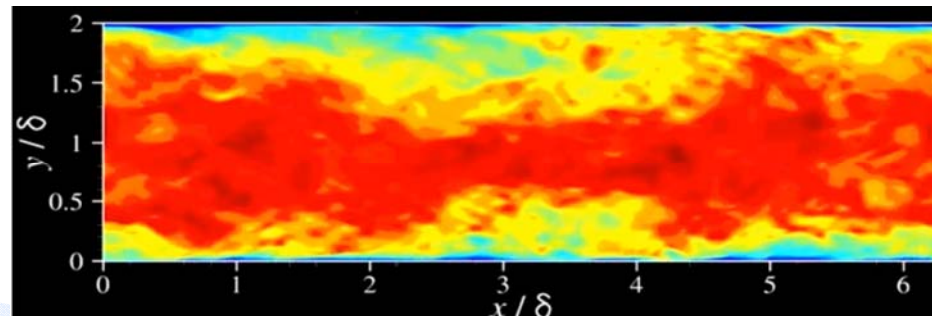
# Turbulent versus laminar flows

- ▶ Navier–Stoke (NS) equations are highly non-linear with only a few very simple analytical solutions
- ▶ In addition, very different regimes of flows may exist in an hydraulics component:
  - a) Laminar flow
  - b) Turbulent flow
  - c) Transitional flow
- ▶ The resolution strategy of the NS equations will strongly depend on the type of flow being studied
- ▶ Nearly all macroscopic flows encountered in engineering practice are turbulent:
  - Flows with Reynolds numbers larger than 5000 are typically (but not necessarily) turbulent, while those at low Reynolds numbers usually remain laminar
  - The flow regime in most of the MSFR components is then turbulent
- ▶ A turbulent fluid velocity field conserves mass, momentum and energy while a purely random time-dependent vector field need not
- ▶ Useful predictions are possible using deterministic or statistical analysis



# Turbulence generic characteristics

- ▶ What is turbulence? : turbulence can be defined as a dissipative flow state characterized by non–linear fluctuating three–dimensional vorticity field
- ▶ Some basic features of turbulence are:
  - Fluctuations : observed in the dependent–field quantities (velocity, pressure, temp., etc.)
  - Nonlinearity: once a critical value (e.g.  $Re$ ) is exceeded small perturbations can grow until reaching a new equilibrium which can also become unstable
  - Vorticity: characterized by fluctuating vorticity. Identifiable in a turbulent flow, particularly those that spin, are called eddies. Eddy sizes decrease with  $Re$ .
  - Dissipation: Persistent turbulence requires supply of energy. Energy is transferred from larges vortex to the smaller, until the smallest eddies transform the energy in heat by the action of viscosity
  - Diffusivity: characterize by high rate of mixing and diffusion of species, momentum and heat compared to equivalent laminar flows



# Statistic for turbulent flow

- Flow variables can be described by using the theory of stochastic processes and random variables (but turbulence is not entirely random)
- The Reynolds decomposition separates a dependent-field variables into its first moment and its fluctuation. The estimation of the first moment can be done in different ways

- ☐ **Non stationary flow** (or flow unsteady in the mean):  
defined as the ensemble average of  $u$

$$\overline{u(x, t)} = \langle u(x, t) \rangle \equiv \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N u(x, t; n)$$

where  $u(x, t; n)$  is nth the realization in the ensemble.

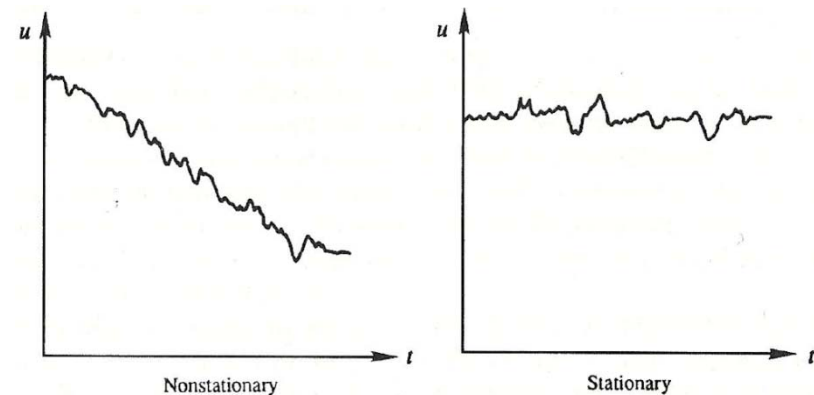
- ☐ **Stationary flow** (or flow steady in the mean):  
estimated from the time averaging of  $u$

$$\overline{u(x, t)} = \frac{1}{\Delta t} \int_{t-\Delta t/2}^{t+\Delta t/2} u(x, t) dt$$

when  $\Delta t$  is large enough with respect to the turbulence fluctuations

- Ensemble averaging and time averaging satisfy the Reynolds averaging rules, which apply to any two functions  $f$  and  $g$  :

$$(a) \overline{f + g} = \bar{f} + \bar{g} \quad (b) \overline{a f} = a \bar{f} \text{ (a is a constant)} \quad (c) \overline{\frac{\partial f}{\partial s}} = \frac{\partial \bar{f}}{\partial s} \quad (d) \overline{\bar{f} g} = \bar{f} \bar{g}$$



# Averaged equations of motion

- ▶ A turbulent flow instantaneously satisfies the Navier–stokes equations. Therefore turbulent flow could be resolved by obtaining a numerical solution to the unsteady Navier–stokes equation. This approach called DNS (Direct Numerical Simulation) of turbulence is virtually impossible to implement at the reactor scale
- ▶ One practical approach consist on solving the equations of motion for the mean state of the turbulent flow
- ▶ Reynolds Decomposition: the first step to obtain the averaged equations of motion is to separate the dependent–field quantities into components representing the mean and those representing the deviation from the mean:

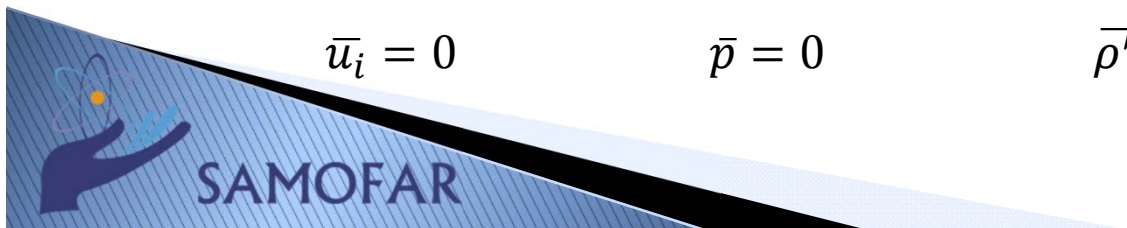
$$\tilde{u}_i = U_i + u_i \quad \tilde{p} = P + p \quad \tilde{\rho} = \bar{\rho} + \rho' \quad \text{and} \quad \tilde{T} = \bar{T} + T'$$

- ▶ The mean quantities are regarded as expected values

$$\bar{\tilde{u}}_i = U_i \quad \bar{\tilde{p}} = P \quad \bar{\tilde{\rho}} = \bar{\rho} \quad \text{and} \quad \bar{\tilde{T}} = \bar{T}$$

- ▶ and the fluctuations have zero mean

$$\bar{u}_i = 0 \quad \bar{p} = 0 \quad \bar{\rho}' = 0 \quad \text{and} \quad \bar{T}' = 0$$



# Averaged equations of the fluid

- ▶ The equations of the mean flow are obtained by:
  - Introducing the Reynolds decomposition into the flow governing equations (continuity, Navier–stokes and energy equations)
  - Averaging the equations and using the Reynolds averaging rules
- ▶ For the case of the Boussinesq set, the mean motion equations are:

Continuity equation:

$$\frac{\partial U_i}{\partial x_i} = 0$$

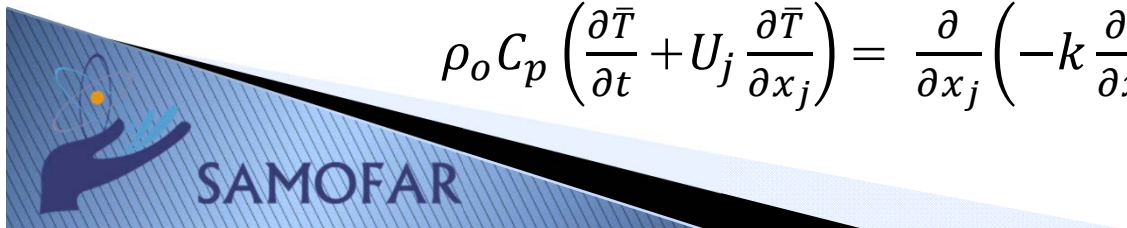
Momentum equation:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = \frac{1}{\rho_o} \frac{\partial}{\partial x_j} (-P \delta_{ij} + 2\mu \overline{S_{ij}} - \rho_o \overline{u_i u_j}) - g_i [1 - \beta(\bar{T} - T_o)]$$

where  $\overline{S_{ij}} = 1/2 (\partial U_i / \partial x_j + \partial U_j / \partial x_i)$  is the mean strain–rate tensor.

Energy equation:

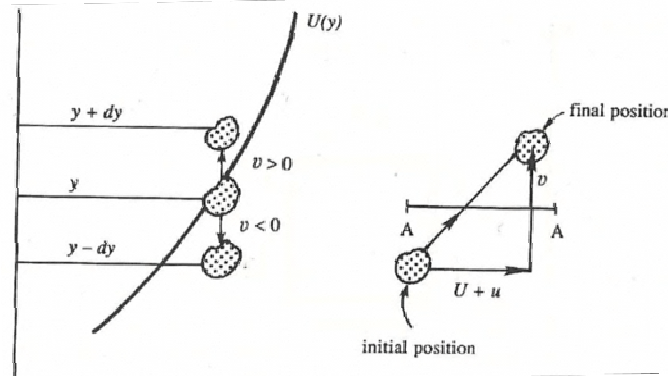
$$\rho_o C_p \left( \frac{\partial \bar{T}}{\partial t} + U_j \frac{\partial \bar{T}}{\partial x_j} \right) = \frac{\partial}{\partial x_j} \left( -k \frac{\partial \bar{T}}{\partial x_j} + \rho_o C_p \overline{u_j T'} \right) + S$$





# Reynolds stresses

- ▶ The correlation tensor  $\overline{u_i u_j}$  is generally non-zero even though  $\overline{u_i} = 0$



$$\overline{uv} < 0$$

- ▶ This new tensor  $(-\rho_o \overline{u_i u_j})$  plays the role of a stress and is called the Reynolds stress tensor
- ▶ The Reynolds stresses are often much larger than viscous stresses except very close to a solid surface (wall) where fluctuations go to zero and mean flow gradient are large
- ▶ The Reynolds stress tensor is symmetric so it has six independent Cartesian components. The diagonal components are normal stresses that augment the mean pressure, while off-diagonal components are shear stresses

# RANS closure modeling

- ▶ As the RANS equations have more unknowns than equations, therefore one possible solution to calculate the Reynolds stress tensor is to use closure equations (RANS closure modeling). Other approaches are DNS and LES.
- ▶ The primary purpose of a turbulent–mean–flow closure model is to relate the Reynolds stresses to the mean velocity fields
- ▶ Typical closure equations are

$$\overline{u_i u_j} = \frac{2}{3} k \delta_{ij} - \nu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad \overline{u_i T'} = -\kappa_t \frac{\partial \bar{T}}{\partial x_i}$$

where  $k$  is the turbulent kinetic energy, and  $\nu_t = \mu_t / \rho_o$  and  $\kappa_t = k_t / \rho_o C_p$  depend on the a characteristic turbulent length and a characteristic turbulent velocity

- ▶ The parameters are numerically estimated using a two–model equations which calculates the turbulent kinetic energy ( $k$  equation) and the rate of the turbulent energy dissipation ( $\varepsilon$  equation)

⇒ A standard two equations model is the  $k - \varepsilon$  model (proposed by Jones and lauder) but many others models exist and may be better suited according to the problem conditions



# Fuel salt RANS equations

Assuming a constant salt density, the RANS equations are:

- Averaged mass conservation equation

$$\frac{\partial \bar{u}_j}{\partial x_j} = 0$$

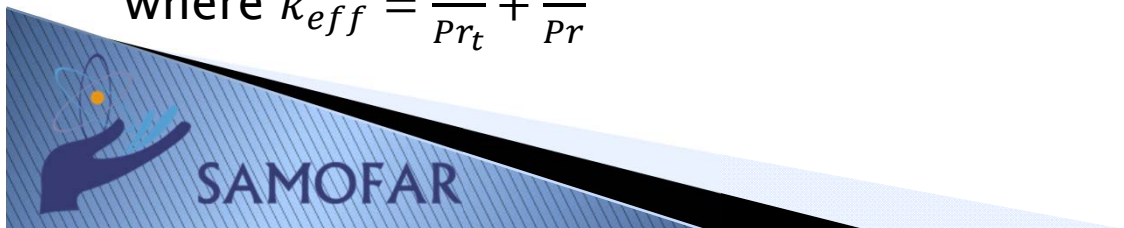
- Momentum conservation equations

$$\frac{\partial \bar{u}_j}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_j \bar{u}_j) = -\frac{\partial}{\partial x_i} \left( \frac{\bar{p}}{\rho_o} + \frac{2}{3} k \right) + \frac{\partial}{\partial x_j} \left\{ (v + v_t) \left( \frac{\partial \bar{u}_i}{\partial x_j} \right) \right\} + g_i [1 - \beta(\bar{T} - T_o)]$$

- Fuel salt energy conservation equation

$$\frac{\partial \bar{T}}{\partial t} + \bar{u}_j \frac{\partial \bar{T}}{\partial x_j} = k_{eff} \frac{\partial}{\partial x_k} \left( \frac{\partial \bar{T}}{\partial x_k} \right) + S$$

where  $k_{eff} = \frac{v_t}{Pr_t} + \frac{v}{Pr}$



# Calculation of the effective viscosity

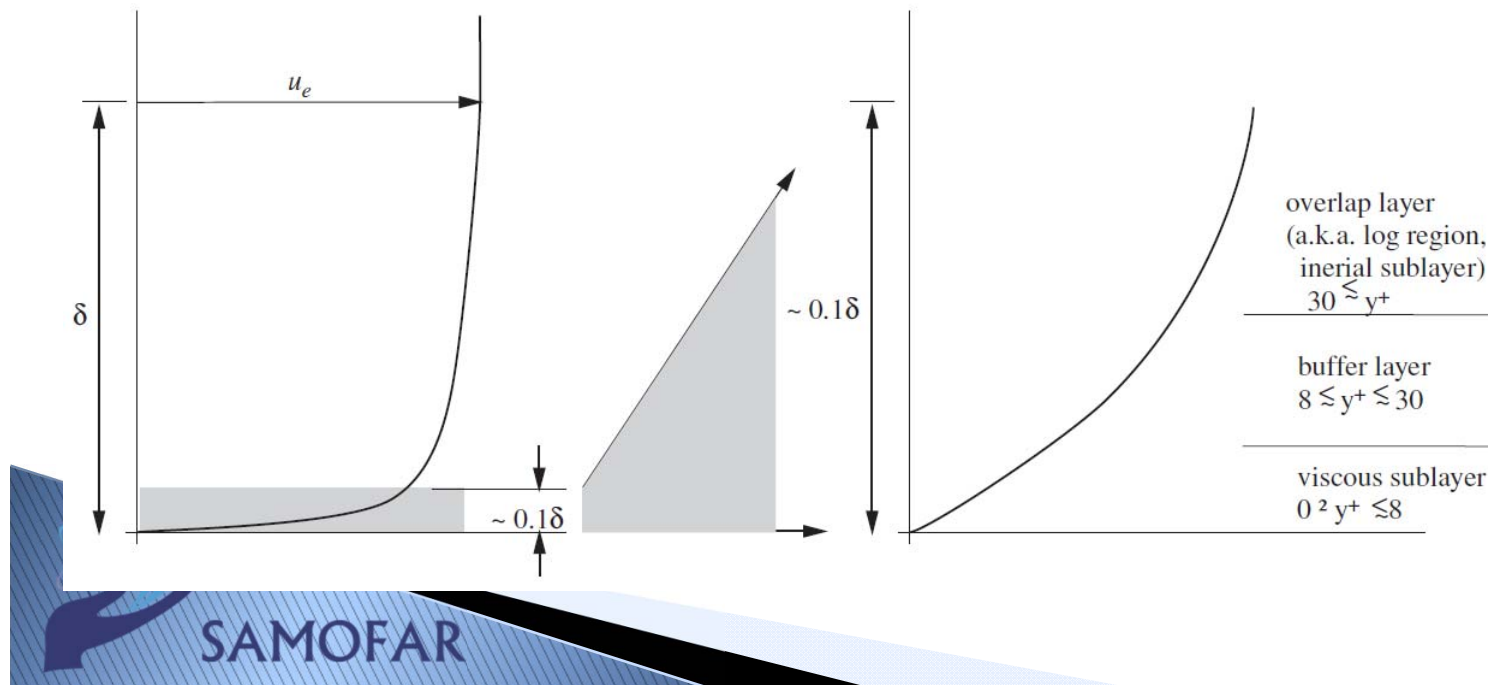
Resolution of the turbulent flow would involve the following iterative steps:

- ▶ Setup and solve equations for the velocities and pressure using the current guess at the effective viscosity
- ▶ Solve the  $k$  and  $\varepsilon$  equations
- ▶ At each point of the flow compute the turbulent viscosity  $\mu_t$
- ▶ Use  $\mu_t$  as appropriate to compute the effective diffusion coefficient for each dependent variable
- ▶ Return to step 1 until convergence



# Wall functions

- ▶ Since velocity and temperature gradients are very steep near the wall, it is often impractical to resolve all the flow details in the near-wall region
- ▶ Wall functions are an economical way (in terms of mesh and CPU time) to bridge between the true wall boundary values and the turbulent core flow
- ▶ Wall functions are derived from a semi-empirical model of the turbulent boundary layer flow called the law-of-the-wall
- ▶ The choice of the wall model has a direct influence on the mesh design



$$y^+ = \frac{u_* y}{\nu}$$

$$u^+ = \frac{u}{u_*}$$

$$u_* = \sqrt{\frac{\tau_{wall}}{\rho}}$$

# COMPUTATIONAL FLUIDS DYNAMICS (CFD)

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- Types of Approaches
- Use of CFD in Nuclear Reactors
- NEA Guidelines for CFD Reactor Studies



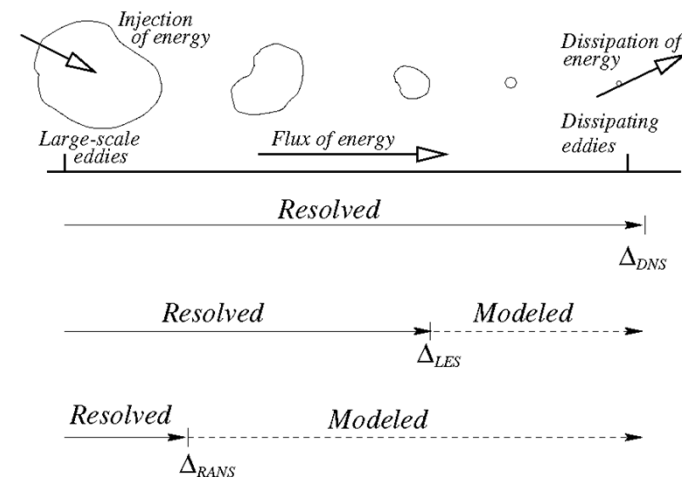
# What is CFD?

- ▶ *CFD (computational fluid dynamics) is a set of numerical methods applied to obtain approximate solutions of problems of fluid dynamics and heat transfer*
- ▶ The advances on computer technology in the last 30 years has transformed CFD codes in a basic tool for engineering design, optimization, and analysis
- ▶ Some of the major commercial or open-source CFD codes are: FLUENT, STAR-CD, CFX, OpenFOAM and COMSOL
- ▶ These codes are basically numerical solvers of partial differential equations with attached physical and turbulent models, as well as modules for grid generation and pre and post-processing



# CFD common approaches

- ▶ **Reynolds-averaged Navier-Stokes equations (RANS):** this approach uses the time-averaged equations of motion for fluid flow (continuity, NS, energy). Time averaging is on a large scale so turbulence is filtered out
- ▶ **Direct numerical simulation (DNS):** computational fluid dynamics simulation in which the Navier-Stokes equations are numerically solved without any turbulence model. Computational mesh should allow to resolve all significant scale of turbulence
- ▶ **Large eddy simulation (LES):** family of method that compromise between RANS and DNS. Large-scale eddies are resolved in the flow equation solution while the effects from the small-scale eddies are obtained from dedicated models (low-pass filtering)
- ▶ **Detached eddy simulation (DES):** further compromise between RANS and LES, to capture key physical phenomena in the lowest possible amount of computer time. Consist in a modified RANS model which switches to a subgrid scale formulation in regions where a LES calculations is needed.



# Use of CFD in nuclear reactors

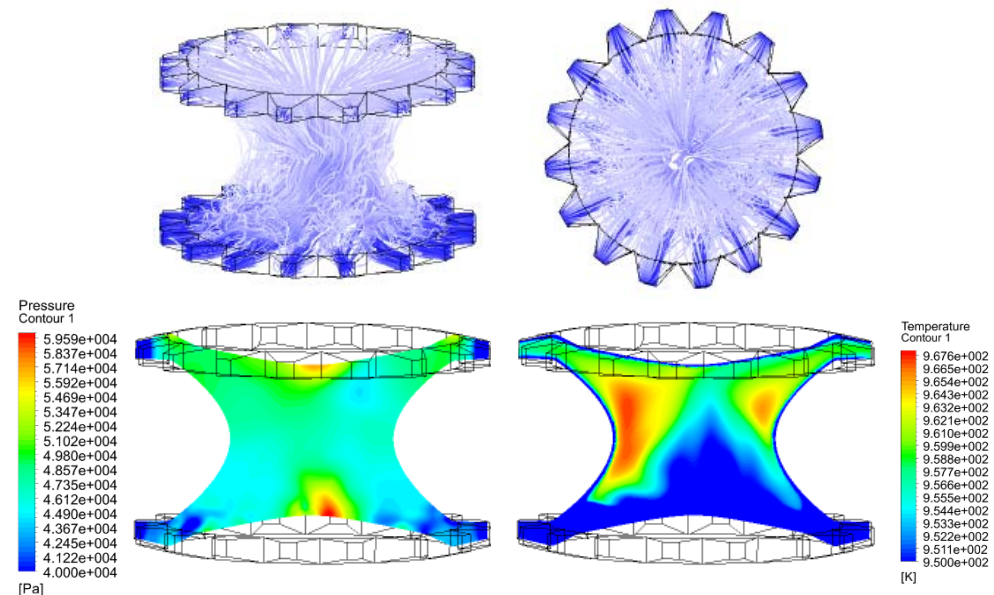
- ▶ The use of CFD in commercial nuclear reactor design applications started about 20 years ago
- ▶ It is currently recommended when there are important 3-D phenomena in a reactor thermal-hydraulics system
- ▶ The implementation of the CFD analysis in the safety studies is still challenging due to licensing issues and significant scrutiny from the nuclear safety authorities
- ▶ Among the existing CFD approaches, RANS equations and the k-Epsilon model are still regarded as the industrial standard turbulence model, simply because they are robust and cheap
- ▶ Current R&D effort is focused in further improving the accuracy of single phase models, fluid-structure interaction, use of CFD in safety analyses and two phases flow modeling (e.G. DNB), coupling with neutronics, etc..





# Use of CFD in nuclear reactors

- Example of problems treated by CFD analyses include:
  - ❑ Flow-induced vibration of in-core components
  - ❑ Boron dilution
  - ❑ Erosion of surface
  - ❑ Mixing and stratification
  - ❑ Thermal fatigue induced by flows
  - ❑ Fuel assembly design
  - ❑ Heterogeneous flow

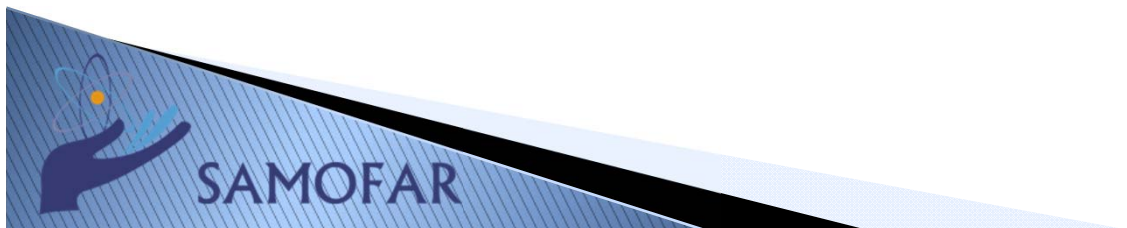


*Velocity streamlines, pressure and temperature distribution during a transient study of the MSFR*



# CFD model development

- ▶ Similarly to others T&H problems the development of a CFD model can be developed as a two step process:
  - Problem isolation: clear definition of the system and the phenomena that are going to be modeled (e.g. force convection versus natural convection)
  - PIRT process : the construction of a PIRT table (Phenomena Identification and Ranking table) is an iterative process that allows to rank phenomena or processes based on their influence on primary design and safety criteria. The model efforts should be focused on the most important
- ▶ The PIRT process can be used to define parameters that should be investigated when performing sensitivity analysis



# Guidelines for reactor studies

1. Mesh requirements
2. Convergence control
3. Transient versus steady state
4. Natural convection
5. Applicability of turbulence models developed and tested for water flows to other fluids
6. Wall resolved or wall approximate modeling



# 1. Mesh requirements

- In a CFD analysis the flow domain is subdivided into a large number of control volumes.
- These control volumes are used to discretize the model equations. The number of mesh cells should then be large to obtain adequate resolution
- Several types of cells (2D or 3D) are possible although they do not have the same efficiency from numerical point of view

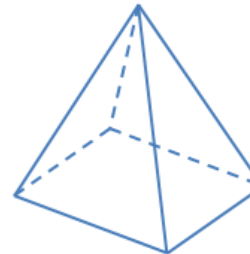


Triangle



Quadrilateral

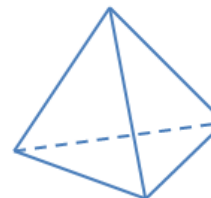
## Example of 2D cells



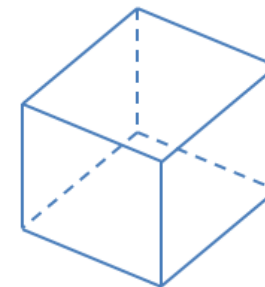
Pyramid



Prism with triangular base



Tetrahedron

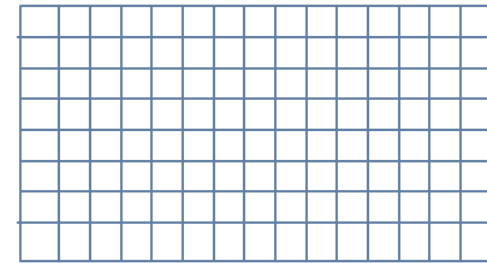


Hexahedron

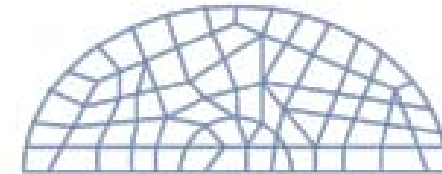
## Example of 3D cells

# 1. Mesh requirements

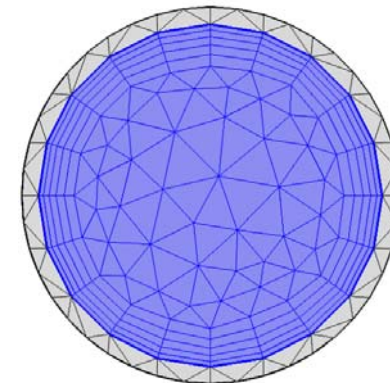
- Three main mesh topologies are commonly used
  - a) Structured grids: consists of hexahedral elements which are theoretically the most efficient element and well suited for the resolution of shear layers
  - b) Unstructured grids: can be generated automatically cell by cell without continuity of mesh lines and thus well suited for complex geometries. Usually employs tetrahedrons as mesh elements. Unstructured meshes require more memory and computing time, and are not efficient for resolution of shear layers
  - c) Hybrid grids: the combination of structured and unstructured grids. For example, tetrahedral elements in the core of the flow domain and prism elements close to the wall is a good alternative to pure hex elements



(a) Structured grid



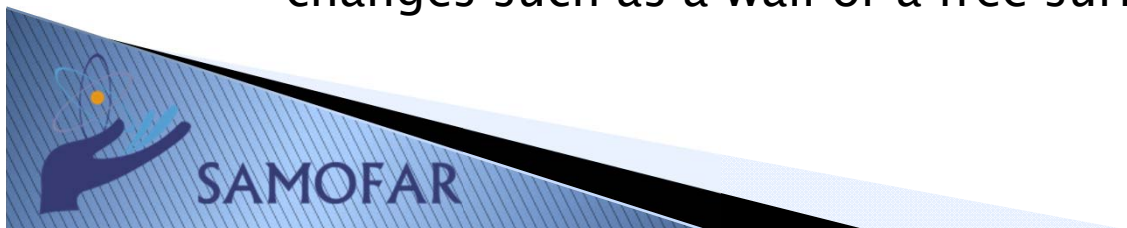
(b) Unstructured grid



Hybrid grid

# 1. Mesh requirements

- ▶ Good mesh quality is essential for performing a good CFD analysis. Most CFD codes contains tools to evaluate the mesh quality
- ▶ High quality mesh usually requires:
  - ✓ Skewness: avoid cells angles below  $20^\circ$  and above  $160^\circ$
  - ✓ Smoothness: avoid jumps in grid density (growth factors  $< 2$ )
  - ✓ Aspect ratio: avoid large cell aspect ratios ( $< 10$  to  $50$ )
  - ✓ Avoid grid lines not aligned with the flow direction
  - ✓ Use finer and regular grid in regions with large gradients or changes such as a wall or a free surface



## 2. Convergence control

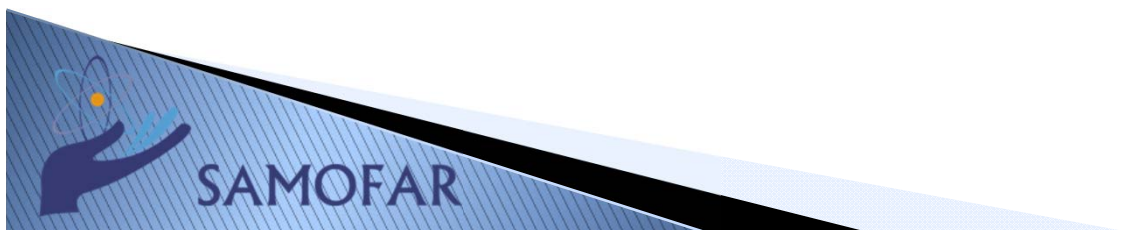
- ▶ Two aspects regarding the convergence control are :
  1. Differential versus discretized equations: convergence of the discretized equations solution to the exact solution. For linear equations systems this is ensured by consistency and stability
  2. Termination of iterative solvers: convergence associated to the criterion used to terminate an iterative process. The use of iterative processes in the numerical resolution of CFD is necessary because of:
    - The use of implicit or semi-implicit time differentiation
    - Non-linear nature of governing equation

The use of an error estimation based on the differences between two successive iterations (measured by an appropriate norm) is not sufficient evidence for solution convergence



### 3. Transient versus steady state

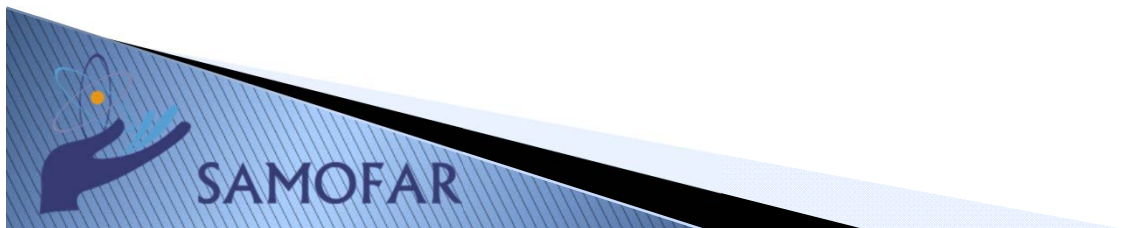
- ▶ The choice between transient and steady-state is only an issue with RANS simulations
- ▶ LES, DES and DNS simulations are transient calculations
- ▶ For a questionable flow the preferred option is to run a transient calculation and inspect the flow patterns
- ▶ A CFD steady-state calculation can be performed by:
  - CFD code achieves steady state solution through pseudo-transient iteration procedure (may not converge if the flow is fundamentally transient)
  - The steady state solution is obtained from an algorithm that calculates the solution of the flow equations without no time derivative terms





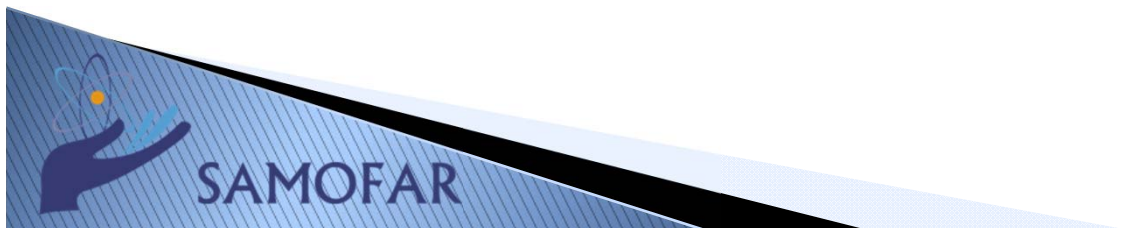
## 4. Natural convection

- ▶ Standard turbulence models assume isotropic Reynolds stresses and the Boussinesq approximation
- ▶ The Boussinesq approximation can be used to account for buoyancy forces until density changes are below 10%
- ▶ Concerning turbulence, models used in a RANS solver can then be applied to flow with Rayleigh numbers ( $Ra_x = Gr_x Pr$ ) up to  $10^5$  or  $10^6$
- ▶ Beyond those values, classic CFD modeling of temperature stratification show deficiencies and it is necessary to consider:
  - ❑ Additional sources in the turbulence equations
  - ❑ Anisotropy of the Reynolds stresses
  - ❑ Use of Large Eddy approach



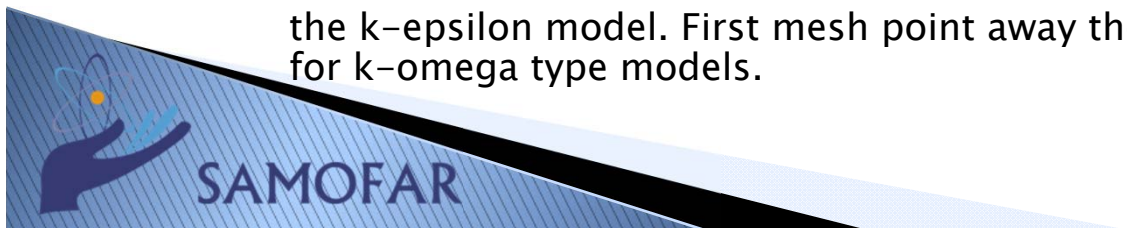
## 5. Applicability of turbulence models developed and tested for water flows to other fluids

- ▶ As long as only an isothermal single-phase flow is considered, which is fully characterized by just a Reynolds number, the usual CFD codes are fully applicable
- ▶ Situation changes if additional phenomena (free surface flows, gas bubble two phase flows, temperature gradients and related buoyancy flows
- ▶ In particular, liquid metals CFD models can not rely on the same water models because of their low Prandtl numbers ( $Pr = \frac{\nu}{\alpha}$ ) and higher surface tension (thermal and momentum boundaries layers have different behavior)



## 6. Wall resolved/Wall approximate modeling

- ▶ The near wall region is usually governed by shear stresses and heat transfer and contains the main turbulence production and dissipation areas
- ▶ These characteristics modify the turbulence structure beyond the assumptions of standard turbulence models
- ▶ Describing the flow behavior in the region near the wall is theoretically possible but requires an extremely refined mesh near the wall
- ▶ This important difficulty is overcome by introducing wall functions which allow avoiding an expensive wall resolution
- ▶ The choice of the wall model has a direct influence on the mesh design
  - Logarithmic wall functions : first mesh point away the wall should comprise between  $30 < y^+ < 500$ . A logarithmic near-wall region does not exist for very small Reynolds numbers.
  - Linear wall functions : linear wall function can be used with special low-Re versions of the k-epsilon model. First mesh point away the wall should verify  $y^+ < 5$ . No restrictions for k-omega type models.



# CURRENT RESEARCH EFFORTS ON MOLTEN SALT T&H MODEL

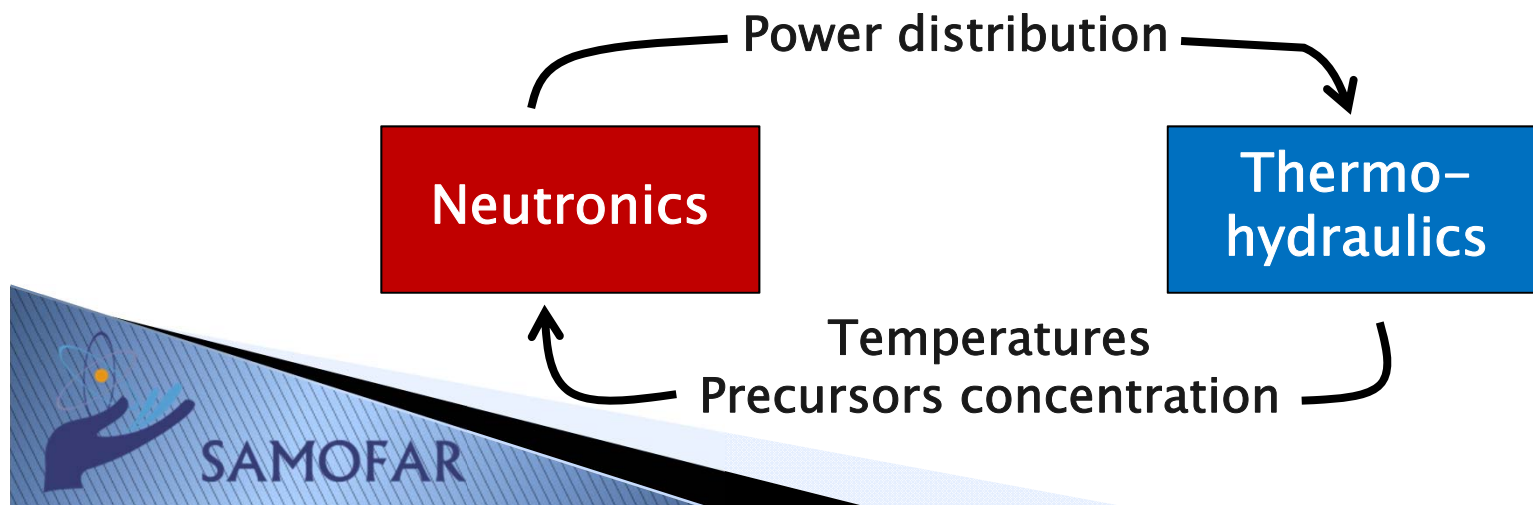
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- Some examples of research work on molten salt Thermo-hydraulics
- SAMOFAR T&H experiments



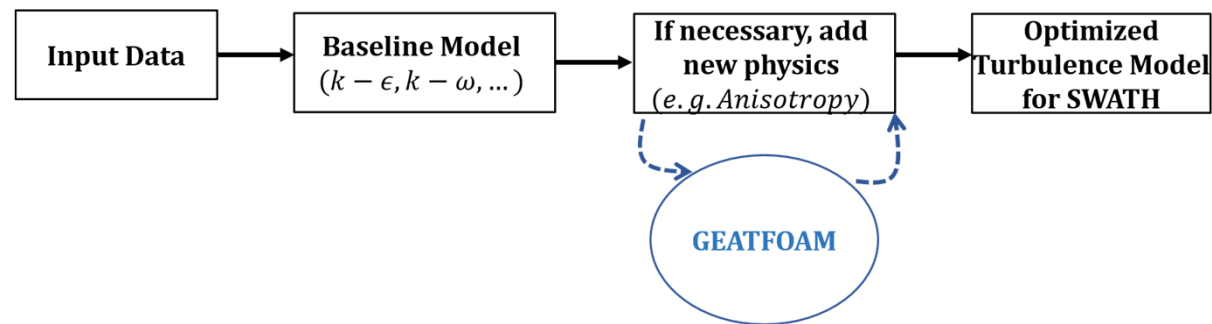
# Neutronics and thermo-hydraulics coupling

- ▶ A strong coupling between fuel power generation and fuel thermal-hydraulics (T&H) exist in the MSFR:
  - Fission power distribution determines the temperature profiles in the fuel salt
  - Feedback effects: the fuel salt temperatures, densities and velocities modify the nuclear properties and thus nuclear reaction rates
  - Delayed neutrons: emitted by some of the fission products transported by the fuel salt
- ▶ Numerical resolution requires a coupled resolution of the reactor neutronics and thermo-hydraulic equations



# Turbulence modeling

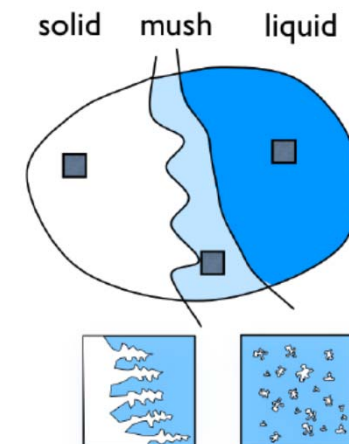
- ▶ Standard RANS models ( $k - \epsilon$ ,  $k - \omega$ , etc.) do not allow obtaining sufficient precision for SWATH modeling ( $\pm 5 - 10\%$ )
- ▶ LES models present further complexities which make them not practical for implementation in a reactor multi-physics model
- ▶ A method to improve the accuracy of RANS models is being developed



- ▶ Accuracy of the RANS closure equations and wall functions for a molten salt will be investigated using a DNS approach

# Salt solidification and melting

- ▶ Salt phase changes has to be considered in the design and safety analyses of Molten Salt Reactors because of its consequences on flow and heat transfer
- ▶ Good estimates of the thermodynamic properties of the solidified fuel salt are also needed for some of these analyses
- ▶ Thermomechanical properties of the solidified fuel salt depends on the solidification process conditions such as
  - ❑ Velocity of the solidification interface,
  - ❑ Undercooling temperature,
  - ❑ Fraction of dissolved gases, etc.
- ▶ Development of both macroscopic and microscopic change models is suitable

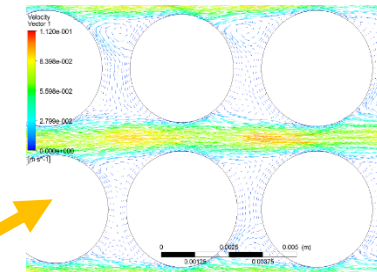
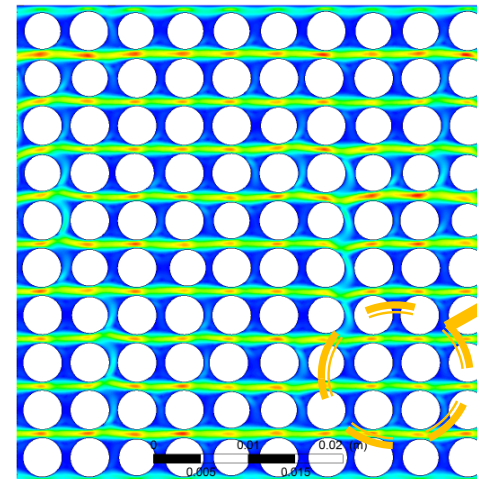
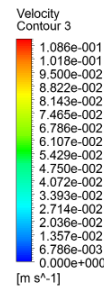
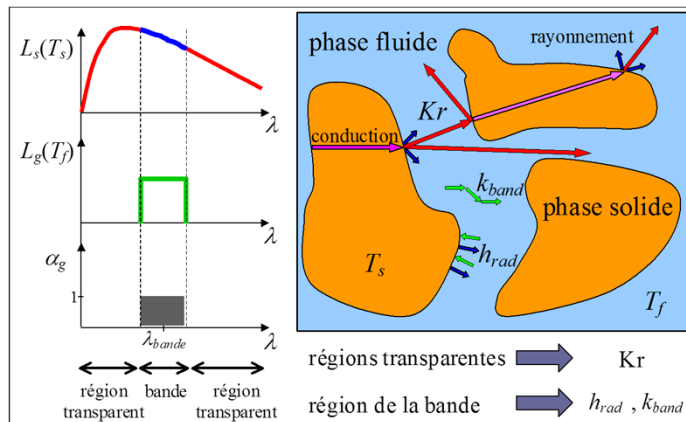




# Salt heat transfer mechanisms

- ▶ Coupled heat transfer mechanisms in various phases (solid, liquid and gas)
- ▶ Complex thermal radiation heat transfer: salt is a semi-transparent medium
- Equation of conservation of energy
 
$$\rho C_P \frac{\partial \bar{T}}{\partial t} + \rho C_P \nabla \cdot \bar{\mathbf{u}} \bar{T} = \nabla \cdot (\mathbf{k} \nabla \bar{T} + \rho C_P \bar{\mathbf{u}}' \bar{T}') + Q_{nuc} + \nabla \cdot \mathbf{S}_R$$
- Challenge: Solving the different interaction scale in the band absorber.
- Radiative flux can be decomposed in an optically thick media (inside the band) + optically thin media (outside the band)

$$\mathbf{S}_R = \mathbf{k}_R \nabla T + \tilde{\mathbf{S}}_{RS2S}$$



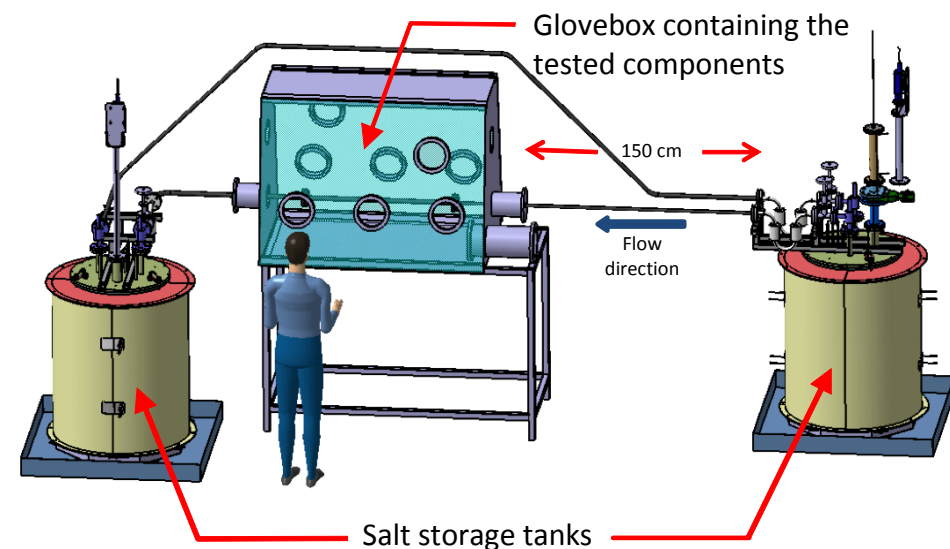
# Salt at Wall: Thermal ExCHanges (SWATH) Experiment

- ▶ Main objectives:
  - Improve molten salt numerical models
  - Demonstrate cold plug working principles
- ▶ Key point: ensure that experimental data uncertainties are smaller than the effects of the studied thermal hydraulics phenomena
- ▶ Phenomena Investigated in SWATH:
  1. Heat transfer in very simple geometries
  2. Evolution of the salt solidification interface with and without forced convection
  3. Solidification along a cold wall after successive molten salt flows (lava flow like)
  4. Flow characteristics in an open channel
  5. Turbulence effects on the flow velocity and temperature profiles near a wall
  6. Radiative heat transfer in the salt



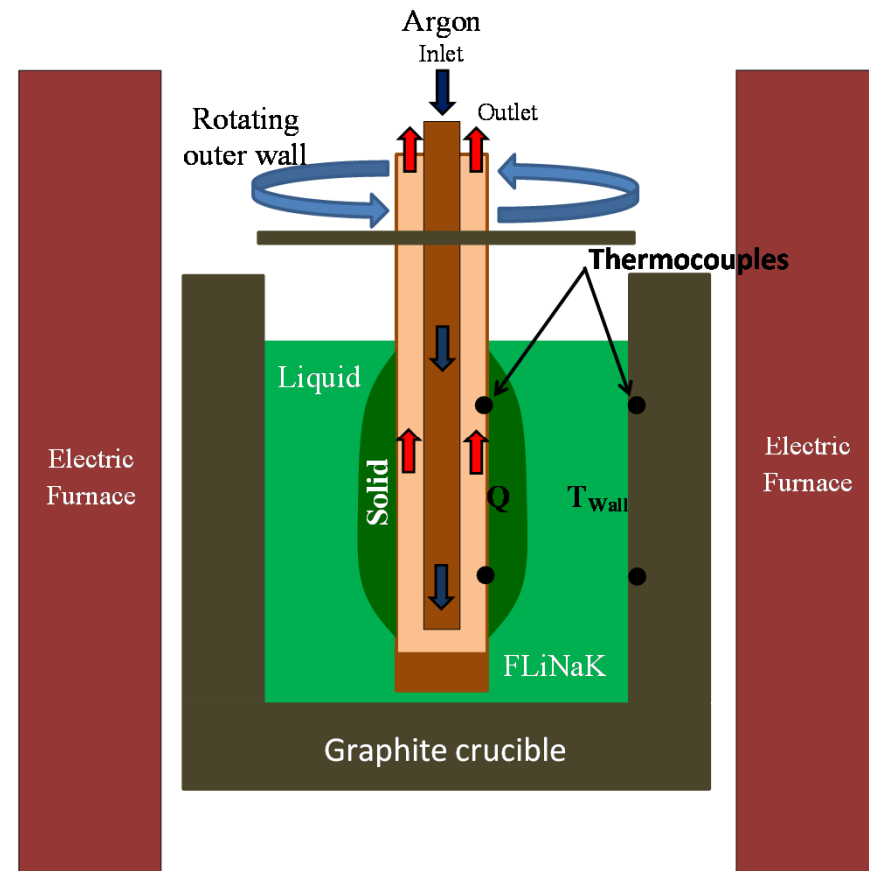
# Salt at Wall: Thermal ExCHanges (SWATH) Experiment

- ▶ SWATH experimental setup is composed of two elements:
  - 1) **SWATH facility**: allows establishing a controlled flow
  - 2) **Tested components**: simple geometries where phenomena are investigated
- ▶ Discontinuous working principle: stable flow is established by regulating pressure difference between two tanks
- ▶ Tank pressure control system relies on pressure drop measurements at specific loop components and on tank level measurements



# SWATH-S solidification experiment

- ▶ Cylindrical annular cavity formed by an inner pipe and graphite crucible
- ▶ The cavity is filled with molten FLiNaK
- ▶ External wall temperature is regulated by the electric resistance
- ▶ Heat is removed by argon flowing inside the inner annular pipe
- ▶ Several temperatures are measured at various elevations on the tube wall and on the crucible wall
- ▶ To investigate solidification in a forced convection environment, the external wall of the annular pipe is rotated (up to 20 rpm)
- ▶ Rotation shaft can be extracted to allow for performing dimensional measurements of the solidified FLiNaK

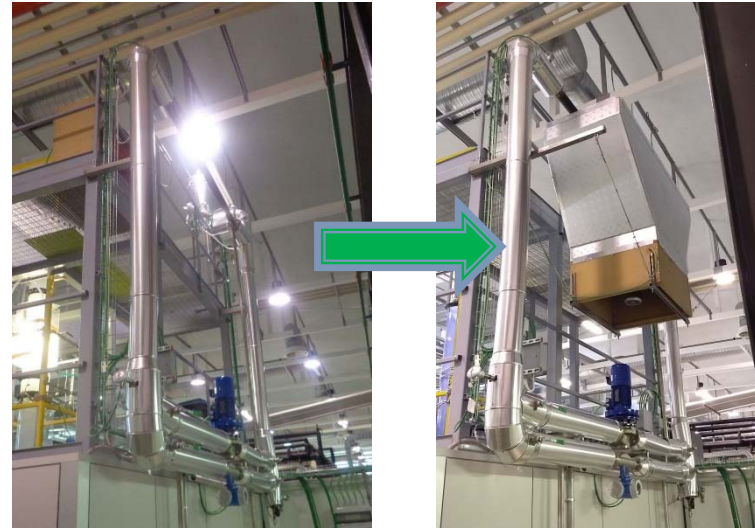


# DYNASTY loop (CIRTEN–Polimi)

- ▶ DYNASTY loop has been built, its data acquisition system is being developed.
- ▶ Some preliminary experiments with water are being carried out for testing purposes.
- ▶ The salt has been produced and its characterization is underway.

## Experiments to be simulated

Experiment	Total power	Cooler temperature
1	0.5 kW	180 °C
2	0.75 kW	190 °C
3	0.75 kW	210 °C
4	0.75 kW	250 °C
5	1 kW	180 °C
6	1 kW	200 °C
7	1 kW	240 °C
8	5 kW	180 °C
9	5.3 kW	190 °C
10	5.3 kW	240 °C

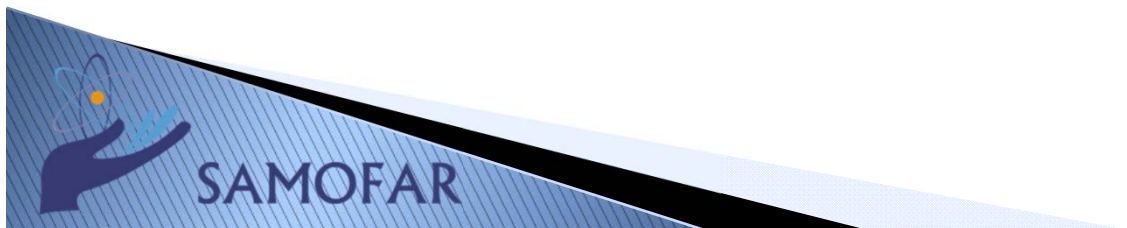


- ▶ Ten cases have been selected for the benchmark and the assessment of the developed models.
- ▶ POLIMI studied the cases by means of stability maps and 1D simulation code. 3D CFD is underway.



# Perspectives

- ▶ Experiments carried-out in SWATH and DYNASTY experiments will be used to improve the current molten salts CFD models
- ▶ Thermodynamics data measured during the SAMOFAR project for molten salts will contribute to improve the accuracy of the numerical models
- ▶ The new thermal-hydraulics models will be integrated in the existing neutronics – thermal hydraulics coupled model of the MSFR to perform the reactor studies
- ▶ These studies will allow to verify that the MSFR meets adequate design and safety requirements



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## Thank You!

