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CFD APPLICATION IN SCWR R&D

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Objectives

Objectives of this Lecture are:

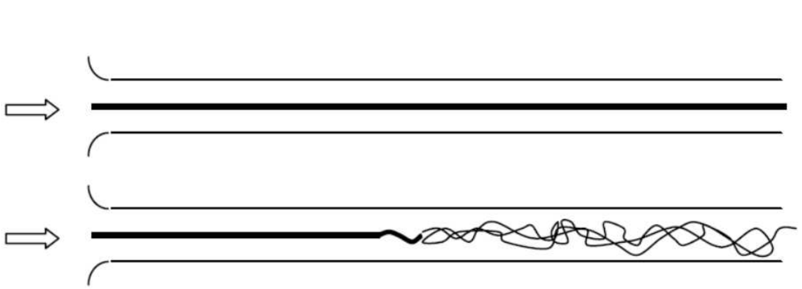
- To make a short summary of the basics of CFD methodologies
- To highlight supercritical fluid issues
- To summarise sample applications to:
  - Heat transfer
  - Stability (summary of the already presented material)
  - Natural circulation

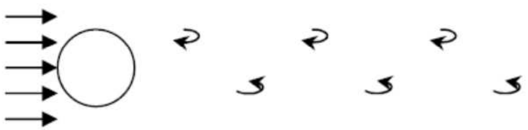
Introduction

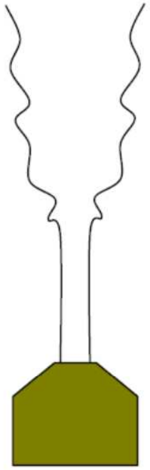
- **Computational Fluid-Dynamics (CFD) is a powerful tool for analysing complex 3D flows**
- **Turbulence is addressed by more basic approaches than the use of global engineering correlations implemented in system codes**
- **The increased power of computers grants nowadays the possibility to afford even relatively complex systems with a reasonable degree of detail**
- **The use of CFD in support to reactor design is a field of increasing interest, though proper code validation processes must be developed to make them reliable for licensing purposes**
- **In this lecture, after reviewing few basic concepts about CFD modelling, examples of application to SCWR research topics from previous work in which the lecturer was involved will be summarised**

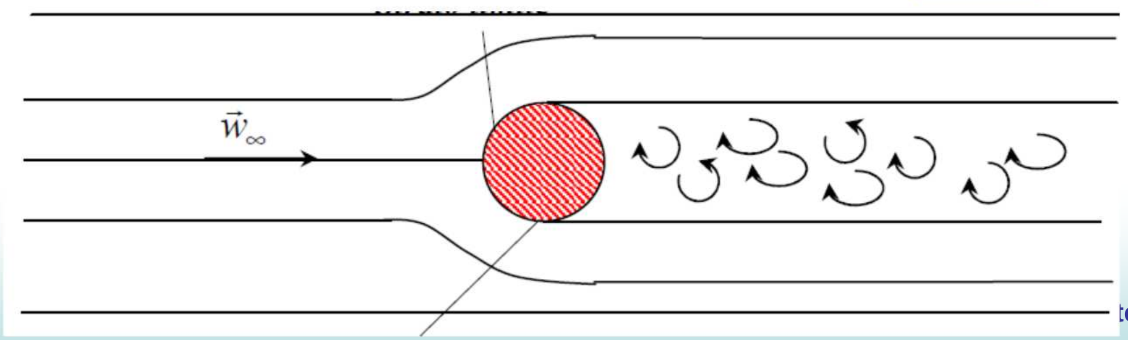
Basic concepts about CFD

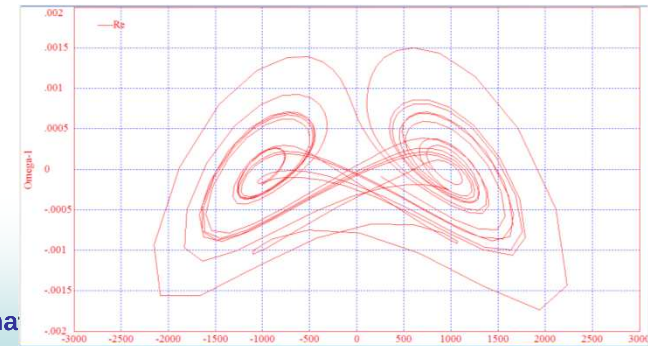
- **Turbulence is known to be a very tough phenomenon to be modelled, as a typical instability showing chaotic behaviour, i.e. a great sensitivity to initial conditions (SIC)**





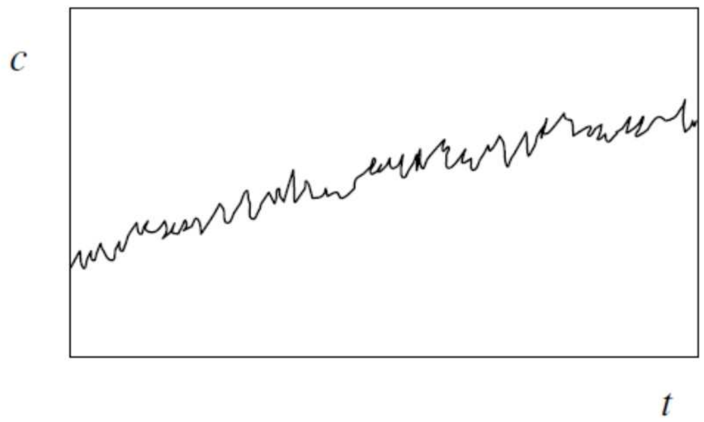






Basic concepts about CFD
Reynolds Averaging

- **Owing to the fluctuating nature of the turbulent flow field, it is customary (after Reynolds) to introduce an appropriate time averaging of any specific value ("intensive") of major "extensive" variables**



$$\overline{c}(t) = \frac{1}{\Delta t}\int_{t-\Delta t/2}^{t+\Delta t/2} c(\tau)\, d\tau$$

$$c(t) = \overline{c}(t) + c'(t) \qquad \int_{t-\Delta t/2}^{t+\Delta t/2} c'(\tau)\, d\tau = 0$$

- **One way of approaching the problem is writing equations in terms of time averaged variables (Reynolds Average Navier-Stokes - RANS), structurally similar to those of laminar flow**
- **This attempt is successful, but fluctuations must be properly accounted for**

Basic concepts about CFD
Turbulence intensity and kinetic energy

- **Time averaging also provides the following quantities having major importance**

$$\sqrt{\overline{w_i'^2}} \qquad \textbf{\textit{turbulence intensity for the i-th velocity component}}$$

$$\sqrt{\overline{w_x'^2} + \overline{w_y'^2} + \overline{w_z'^2}} \qquad \textbf{\textit{turbulence intensity}}$$

$$\overline{w_i' w_j'} \qquad (i, j = x, y, z) \qquad \textbf{\textit{double correlation}}$$

- **Turbulence intensity is strictly related to the turbulence kinetic energy**

$$k = \frac{1}{2}\left(\overline{w_x'^2} + \overline{w_y'^2} + \overline{w_z'^2}\right)$$

- **This is one of the most important quantities adopted in present CFD codes, mostly making use of RANS "two-equation**

Basic concepts about CFD
The RANS equations

- **The general balance equations in local and instantaneous formulation are averaged making use of the above described averaging operator**

$$\boxed{\frac{\partial}{\partial t}(\rho c)+\nabla\cdot(\rho\, c\,\vec{w})+\nabla\cdot\vec{J}_c=\rho\,\phi_c} \Longrightarrow \overline{\frac{\partial}{\partial t}(\rho c)}+\overline{\nabla\cdot(\rho\, c\,\vec{w})}+\overline{\nabla\cdot\vec{J}_c}=\overline{\rho\,\phi_c}$$

- **After classical simplifications, an averaged form is finally reached showing that the attempt to get equations similar to those of laminar flow leaves an additional term**

$$\boxed{\frac{\partial}{\partial t}(\rho\bar{c})+\nabla\cdot\left(\rho\,\bar{c}\,\bar{\vec{w}}\right)+\nabla\cdot\bar{\vec{J}}_c=\rho\bar{\phi}_c-\nabla\cdot\rho\,\overline{c'\vec{w}'}}$$

- **This term, having a clear "advective" nature, points out that fluctuations do play a role in transfers: this role represents a sort of additional "mixing" due to turbulence**

Basic concepts about CFD
Turbulent diffusion in RANS equations

- **In analogy with the molecular motion, the basic idea is therefore to interpret such term as an additional diffusion due to turbulence**

$$\boxed{\frac{\partial}{\partial t}(\rho \overline{c}) + \nabla \cdot (\rho\, \overline{c}\, \overline{\vec{w}}) + \nabla \cdot \left(\overline{\vec{J}_c} + \vec{J}_c^{\,t}\right) = \rho \overline{\phi_c}} \qquad \boxed{\vec{J}_c^{\,eff} = \overline{\vec{J}_c} + \vec{J}_c^{\,t}}$$

- **The momentum and energy balance equations contain such terms that call for a proper modelling**

♦ ***mass***

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

♦ ***momentum***

$$\frac{\partial}{\partial t}(\rho\, \overline{\vec{w}}) + \nabla \cdot (\rho\, \overline{\vec{w}}\, \overline{\vec{w}}) = \nabla \cdot \left(\overline{\overline{\overline{\tau}}} - \overline{p}\vec{\vec{I}}\right) + \rho \vec{g} - \nabla \cdot \left(\rho\, \overline{\vec{w}' \vec{w}'}\right)$$

♦ ***energy***

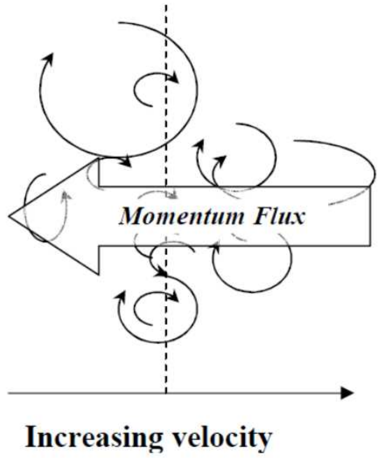
$$\frac{\partial}{\partial t}\left(\rho \overline{u^0}\right) + \nabla \cdot \left(\rho \overline{u^0}\, \overline{\vec{w}}\right) = \nabla \cdot \left[-\overline{\vec{q}''} + \overline{\left(\overline{\overline{\tau}} - p\vec{\vec{I}}\right) \cdot \vec{w}}\right] + \overline{q'''} + \rho \vec{g} \cdot \overline{\vec{w}} - \nabla \cdot \left(\rho\, \overline{u^{0'} \vec{w}'}\right)$$

Basic concepts about CFD
Reynolds stress tensor

- **The "Reynolds stress tensor" appears in momentum equations**

$$\frac{\partial}{\partial t}\left(\rho\,\overline{\vec{w}}\right)+\nabla\cdot\left(\rho\,\overline{\vec{w}}\,\overline{\vec{w}}\right)=\nabla\cdot\left(\overline{\vec{\vec{\tau}}}-\overline{p}\vec{\vec{I}}\right)+\rho\vec{g}-\nabla\cdot\left(\rho\,\overline{\vec{w}'\vec{w}'}\right) \qquad \vec{\vec{\tau}}_{Re}=-\rho\,\overline{\vec{w}'\vec{w}'}$$

- **Its components account for the additional momentum fluxes due to eddies**



$$\frac{\partial}{\partial t}\left(\rho\,\overline{\vec{w}}\right)+\nabla\cdot\left(\rho\,\overline{\vec{w}}\,\overline{\vec{w}}\right)=-\nabla\overline{p}+\nabla\cdot\left(\overline{\vec{\vec{\tau}}}+\vec{\vec{\tau}}_{Re}\right)+\rho\vec{g}$$

Basic concepts about CFD

The Boussinesq approximation and the eddy viscosity

- **It is then customary to adopt the "Boussinesq approximation" based on a definition of "turbulent momentum diffusivity" (eddy viscosity), trying to define a simple constitutive relationship for the Reynolds stress**

$$\left(\vec{\vec{\tau}}_{\mathrm{Re}}\right)_{i,j} = -\left(\rho\, \overline{\vec{w}'\,\vec{w}'}\right)_{i,j} = \rho \nu_T \left[\frac{\partial \overline{w}_i}{\partial x_j} + \frac{\partial \overline{w}_j}{\partial x_i}\right] - \frac{2}{3}\rho k \delta_{ij}$$

- **The quantity ν_T is no more a property of the fluid, but also depends on flow.**
- **Of course, the Boussinesq approximation shifts the toughness of the modelling problem to the definition of the eddy viscosity**
- **There are anyway different "beyond Boussinesq approximation" approaches (e.g., Reynolds Stress Transport models)**

Basic concepts about CFD
The eddy thermal diffusivity

- **The averaged total energy equation and the steady thermal energy equation in terms of temperature can be written as**

$$\frac{\partial}{\partial t}\left(\rho\overline{u^0}\right)+\nabla\cdot\left(\rho\overline{u^0}\,\overline{\vec{w}}\right)=\nabla\cdot\left[-\overline{\vec{q}''}+\overline{\left(\vec{\vec{\tau}}-p\vec{\vec{I}}\right)\cdot\vec{w}}\right]+\overline{q'''}+\rho\vec{g}\cdot\overline{\vec{w}}-\nabla\cdot\left(\rho\,\overline{u^{0'}\vec{w}'}\right)$$

$$\nabla\cdot\left(\rho C_p\overline{T}\,\overline{\vec{w}}\right)=-\vec{\nabla}\cdot\overline{\vec{q}''}+\overline{q'''}+\overline{\Phi}-\nabla\cdot\left(\rho C_p\,\overline{T'\vec{w}'}\right)$$

- **Also in these cases additional terms to be modelled appear, e.g.:**

$$\rho C_p\,\overline{T'\vec{w}'} \qquad\qquad \vec{q}''_{eff}=\vec{q}''+\rho C_p\,\overline{T'\vec{w}'}$$

- **A simple rationale for evaluating the turbulent contribution is similar as in the case of momentum**

$$\rho C_p\left\{\overline{T'\vec{w}'}\right\}_j=-\rho C_p\,\alpha_T\frac{\partial\overline{T}}{\partial x_j} \qquad\qquad \left\{\vec{q}''_{eff}\right\}_j=-\rho C_p\left[\alpha+\alpha_T\right]\frac{\partial\overline{T}}{\partial x_j}$$

where α_T is the "turbulent thermal diffusivity"

Basic concepts about CFD

The eddy thermal diffusivity

- **A simple but effective way to establish this relationship is to define a constant "turbulent Prandtl number", in analogy with the molecular one, assuming that, as a consequence of the Reynolds analogy, this could be in the range of unity**

$$Pr_t = \frac{\nu_T}{\alpha_T} = turbulent\ \ Prandtl\ \ number \approx 1$$

- **The assumption is that the same coherent structures carrying momentum are also responsible of heat transfer**

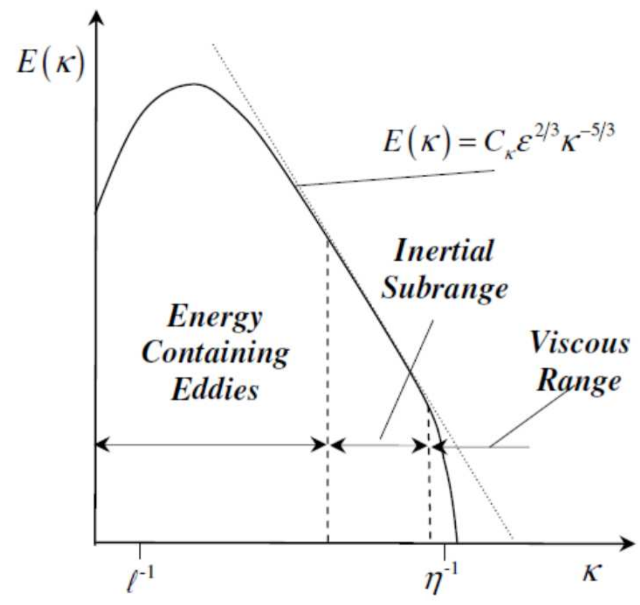
- **However, this assumption holds acceptably for fluids having nearly unity molecular Prandtl number; in the other cases, different approaches should be used: supercritical fluids are characterised by high Pr at the pseudocritical temperature**

Basic concepts about CFD

The energy cascade

- **In turbulent flow an "energy cascade" occurs representing the transfer of turbulence kinetic energy from larger to smaller eddies**
- **As such, turbulence can be considered as a phenomenon characterised by a wide range of lengths at which interesting phenomena do occur:**
  - **→ from the integral length scale, l, at which energy is extracted from the mean flow**
  - **→ to the Kolmogorov length scale, η, at which turbulence kinetic energy is finally dissipated into heat**

$E(\kappa)\,d\kappa = \text{turbulent kinetic energy between } \kappa \text{ and } \kappa + d\kappa$



$$\eta \equiv \left(\nu^3/\varepsilon\right)^{1/4} = \left[\left(\frac{m^2}{s}\right)^3 \left(\frac{s^3}{m^2}\right)\right]^{1/4} = [m]$$

$$\varepsilon = -dk/dt = \left[m^2/s^3\right]$$

Basic concepts about CFD

Different approaches in CFD

Basing on these considerations, it can be concluded that:

- **an adequate representation of turbulence should take into account the phenomena of production and dissipation of turbulence kinetic energy at all the different scales**

- **in this respect, two different strategies can be envisaged:**
  - **→ simulating the transient evolution of vortices of different sizes, putting a convenient lower bound for the smallest scale (e.g., DNS, LES)**
  - **→ simulating turbulence on the basis of the above described statistical averaging approach, introducing appropriate production and dissipation terms to approximately represent the effects of the energy cascade (RANS)**

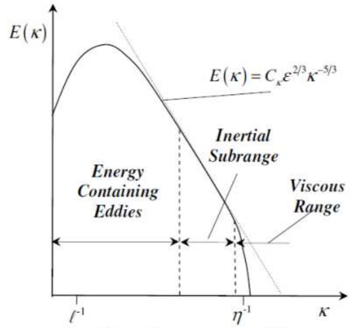
Basic concepts about CFD

Direct Numerical Simulation - DNS

- **This methodology follows the former of the two mentioned routes, trying to simulate with the highest possible space and time detail the evolution of vortices of all relevant sizes**
- **The assumption behind this technique is that the Navier-Stokes equations are rich enough to describe the turbulent flow behaviour with no need of additional constitutive laws; for incompressible flow it is:**

$$\nabla \cdot \vec{w} = 0 \qquad \textit{(continuity equation)}$$

$$\rho \frac{D\vec{w}}{Dt} = \mu \nabla^2 \vec{w} - \nabla p + \rho \vec{g} \qquad \textit{(Navier-Stokes equations)}$$

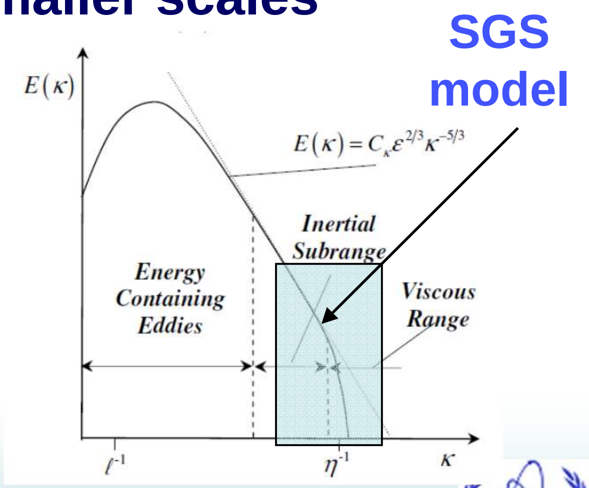


- **The attempt is to simulate the full range of length scales, resulting in a very demanding approach from the point of view of computational resources**

Basic concepts about CFD

Large Eddy Simulation - LES

- **LES is aimed at simulating only larger eddies, while the smaller scales are treated by subgrid-scale (SGS) models**
- **In other words, there are two different length scales:**
  - **→ the large scales that are directly solved as in DNS;**
  - **→ the smaller scales that are treated by SGS models**
- **As such, LES is computationally more efficient than DNS and may be also relatively accurate**
- **Key points in LES are**
  - ✓ **introducing a spatial filtering for the smaller scales**
  - ✓ **adopting a suitable subgrid model**
- **LES is aimed at directly reproducing only the larger length scales in the energy cascade**



Basic concepts about CFD

RANS – k-ω models

- **Two-equation RANS models are mostly based on the definition of a further quantity with respect to k in the form of ε or ω basing on the following relationships that "close" the problem**

  - **for k-ω models it is**

$$\nu_T \sim k/\omega \qquad \ell \sim k^{1/2}/\omega \qquad \varepsilon \sim \omega k$$

in particular for the Wilcox (1998) model it is

$$\frac{\partial k}{\partial t} + \overline{w}_j \frac{\partial k}{\partial x_j} = \tau_{ij} \frac{\partial \overline{w}_i}{\partial x_j} - \beta^* k \omega + \frac{\partial}{\partial x_j}\left[\left(\nu + \sigma^* \nu_T\right)\frac{\partial k}{\partial x_j}\right]$$

$$\frac{\partial \omega}{\partial t} + \overline{w}_j \frac{\partial \omega}{\partial x_j} = \alpha \frac{\omega}{k} \tau_{ij} \frac{\partial \overline{w}_i}{\partial x_j} - \beta \omega^2 + \frac{\partial}{\partial x_j}\left[\left(\nu + \sigma \nu_T\right)\frac{\partial \omega}{\partial x_j}\right]$$

with

$$\tau_{ij} = -\overline{w_i' w_j'}$$

with appropriate values of the constants and, in particular:

$$\varepsilon = \beta^* k \omega \qquad \nu_T = k/\omega \qquad \ell = k^{1/2}/\omega$$

Basic concepts about CFD

RANS – k-ε models

- **for k-ε models it is**

$$\nu_T \sim k^2/\varepsilon \qquad \ell \sim k^{3/2}/\varepsilon \qquad \omega \sim \varepsilon/k$$

the dissipation equation can be derived exactly and has the classical form

$$\frac{\partial k}{\partial t}+\overline{w}_j\frac{\partial k}{\partial x_j}=\tau_{ij}\frac{\partial \overline{w}_i}{\partial x_j}-\varepsilon+\frac{\partial}{\partial x_j}\left[\left(\nu+\frac{\nu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]$$

with

$$\boxed{\tau_{ij}=-\overline{w_i' w_j'}}$$

$$\frac{\partial \varepsilon}{\partial t}+\overline{w}_j\frac{\partial \varepsilon}{\partial x_j}=C_{\varepsilon 1}\frac{\varepsilon}{k}\tau_{ij}\frac{\partial \overline{w}_i}{\partial x_j}-C_{\varepsilon 2}\frac{\varepsilon^2}{k}+\frac{\partial}{\partial x_j}\left[\left(\nu+\frac{\nu_T}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right]$$

The standard k-ε model adopts the definitions

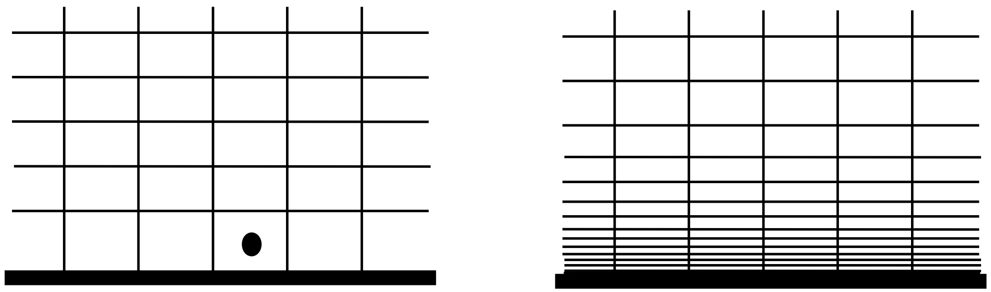
$$\nu_T=C_\mu k^2/\varepsilon \qquad \omega=\varepsilon/\left(C_\mu k\right) \qquad \ell=C_\mu k^{3/2}/\varepsilon$$

$$C_{\varepsilon 1}=1.44 \qquad C_{\varepsilon 2}=1.92 \qquad C_\mu=0.09 \qquad \sigma_k=1 \qquad \sigma_\varepsilon=1.3$$

Basic concepts about CFD

RANS – Near wall treatment

- **When wall phenomena must be dealt with two possible approaches are available:**
  - **use of "wall functions": the logarithmic trend observed for velocity close to a flat surface is assumed to hold approximately near the specific considered wall, together with a corresponding temperature trend; in this case, the value of y+ in the first node close to the wall must be conveniently large (e.g., y+ > 30);**
  - **use of low Reynolds number models: these models are conceived to simulate the actual trend of turbulence close to the wall, by the adoption of damping functions; the value of y+ in the first node must be very small (typically y+<1)**



(a) Wall functions mesh (b) Low-Reynolds number mesh

Specific supercritical fluid issues
Suitability of the different tools for SC fluids

- **As in many other fields of fluid-dynamics, also in the case of supercritical fluids DNS and LES are still used for research purposes, while the only feasible tools in support to design are presently the different forms of the RANS equations**

- **Most of the existing CFD codes can be applied in a straightforward way to supercritical fluids, though the results must be carefully assessed**

- **Though supercritical fluid systems are somehow similar to two-phase flow systems, owing to the changes in fluid properties, the absence of interfaces makes simpler the application of CFD**

- **In principle, fluids at supercritical pressures can be dealt with by the same models adopted for single-phase fluids**

Specific supercritical fluid issues

Quite strange single-phase fluids…

- **However, in this case the large changes in fluid properties must be accounted for:**
  - ✓ **A reasonable representation for each relevant fluid property (density, specific heat, viscosity and thermal conductivity) may require detailed tables or piece-wise polynomial interpolation**
  - ✓ **Light (gas-like) and heavy (liquid-like) fluid regions are unevenly distributed in the cross section giving rise to peculiar phenomena**
  - ✓ **Buoyancy and acceleration effects due to fluid expansion are responsible for damping turbulence production, leading to heat transfer deterioration: catching these phenomena requires sufficient resolution close to the walls, i.e. a low Reynolds approach**
  - ✓ **Turbulence models developed for constant property fluids may not be necessarily applicable to such varying property fluids: there is the need for specific assessment and a broad reconsideration of the suitability of techniques**

Application to Heat Transfer

Frame of the work and first addressed data

- **The work was performed in cooperation with the Universities of Manchester (Prof. J.D. Jackson) and Aberdeen (Dr. S. He)**
- **A purposely developed in-house code was applied by Sharabi (2008) in the prediction of experiments conducted by Pis'menny et al. (2006) at the National Technological University of Ukraine**
- **The experiments investigated turbulent heat transfer in vertical circular tubes for water in a gas-like state or affected by mixed convection in both upward and downward flows, at an operating pressure of 23.5 MPa**
- **The test section was made by thin stainless steel tubes with an inner diameter of 6.28 mm**
- **Uniform heating by direct or alternating electric current was used and thermocouples were placed at the inlet and the outlet of the tube and along its outer surface to measure fluid and wall temperatures**

Application to Heat Transfer

Pis'menny (2006) Water Data

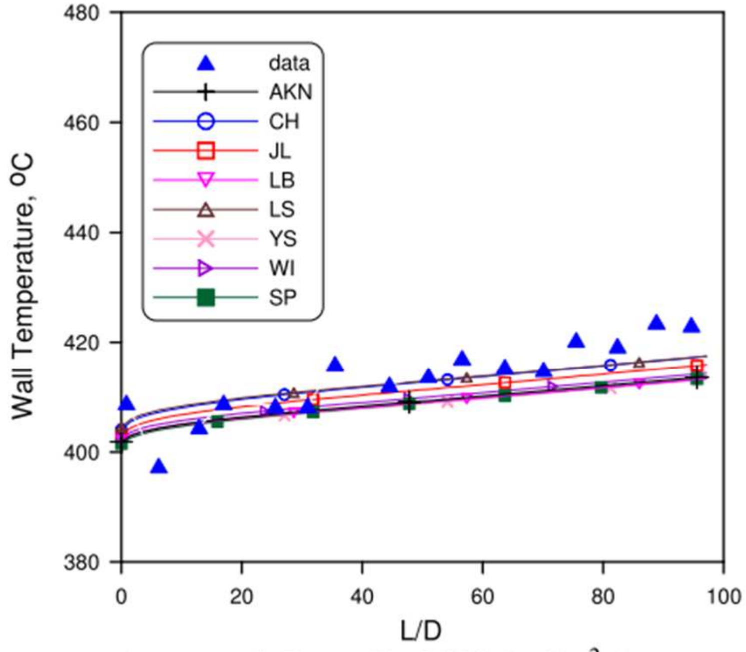
- **The adopted in-house code solved the flow balance equations by different two-equation RANS models in axi-symmetric geometry using the finite volume technique**

- **The turbulence models used were:**
  - **The low-Re k-ε models by Jones and Launder (JL), Launder and Sharma (LS), Lam and Bremhorst (LB), Chien (CH), Yang and Shih (YS), Abe, Kondoh and Nagano (AKN)**
  - **the k-ω model by Wilcox (WI)**
  - **the k-τ model by Speziale (SP)**

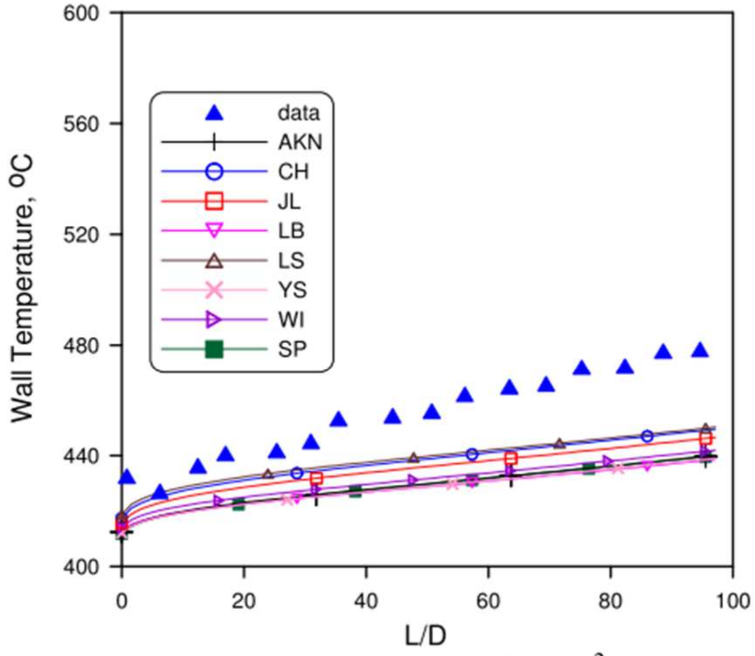
- **The obtained results are shown hereafter**

Application to Heat Transfer

Results for Pis'menny (2006) Water Data by the in-house code - 1



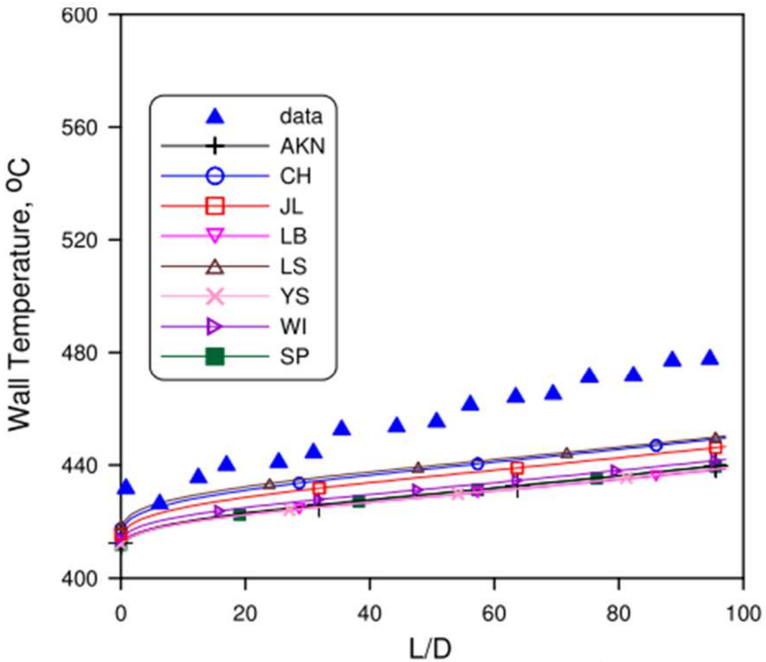
a) upward flow, G=2193 kg/(m²s), q=433 kW/m², T_{in}=391 °C



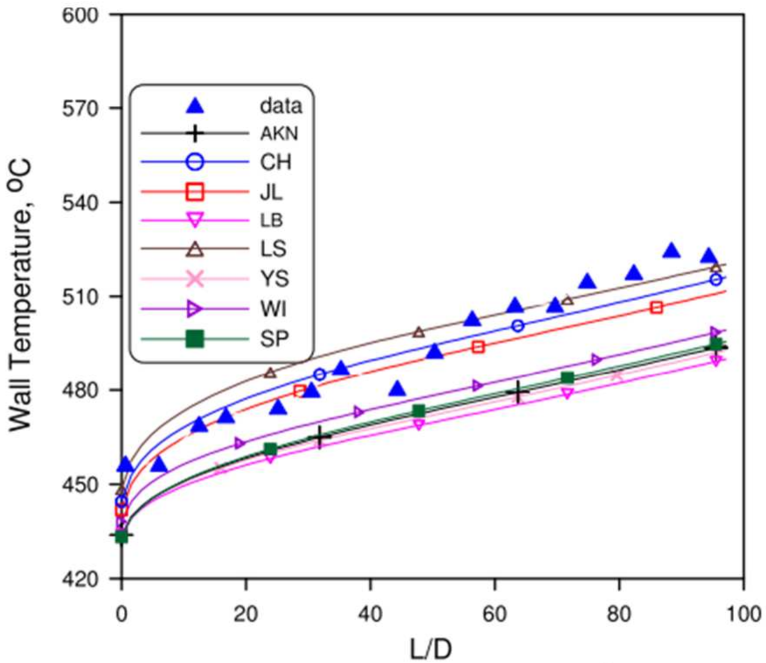
b) upward flow, G=2193 kg/(m²s), q=750 kW/m², T_{in} =391 °C

Application to Heat Transfer

Results for Pis’menny (2006) Water Data by the in-house code - 2

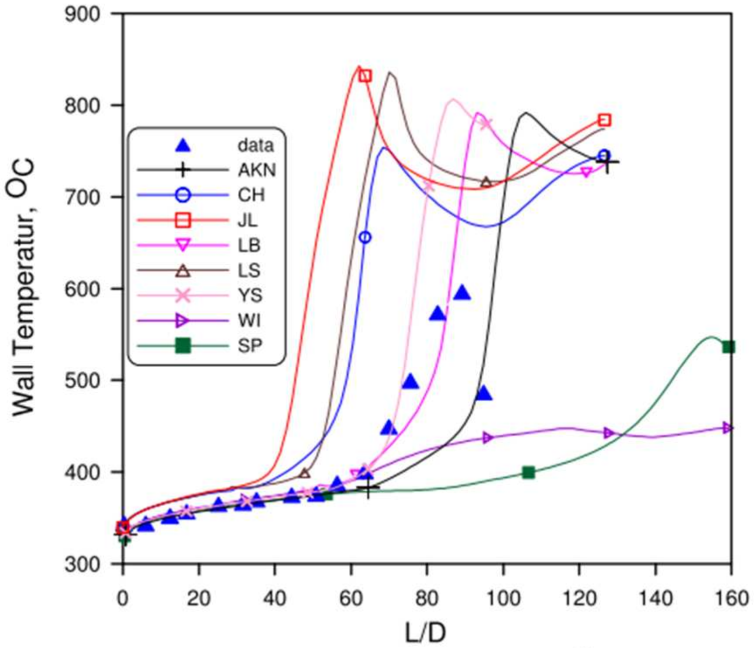


c) upward flow, G=2193 kg/(m^{2}s),
q=750 kW/m^2, T... =391 °C

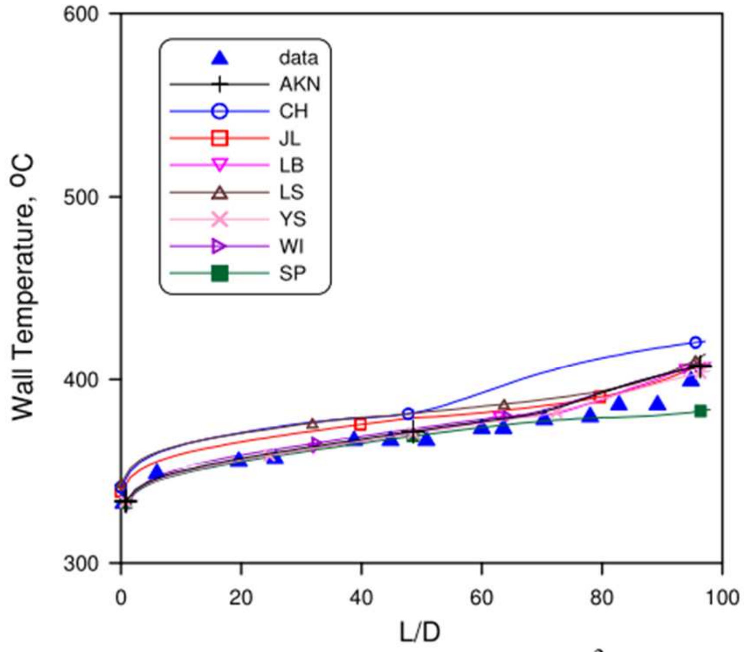


d) upward flow, G=2193 kg/(m^{2}s),
q=1172 kW/m^2, T... =393 °C)

Application to Heat Transfer
Results for Pis'menny (2006) Water Data by the in-house code - 3



e) upward flow, G=509 kg/(m²s),
q=390 kW/m², T_{in} =300 °C

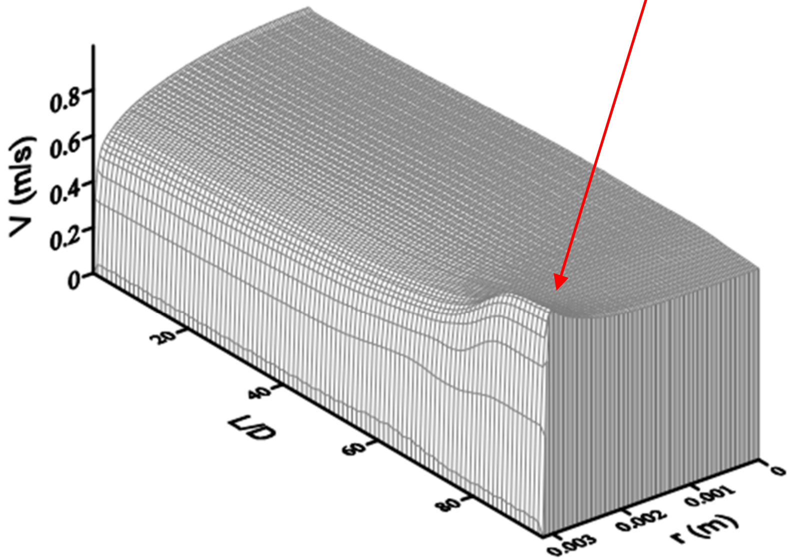


f) downward flow, G=509 kg/(m²s),
q=390 kW/m², T_{in} =300 °C

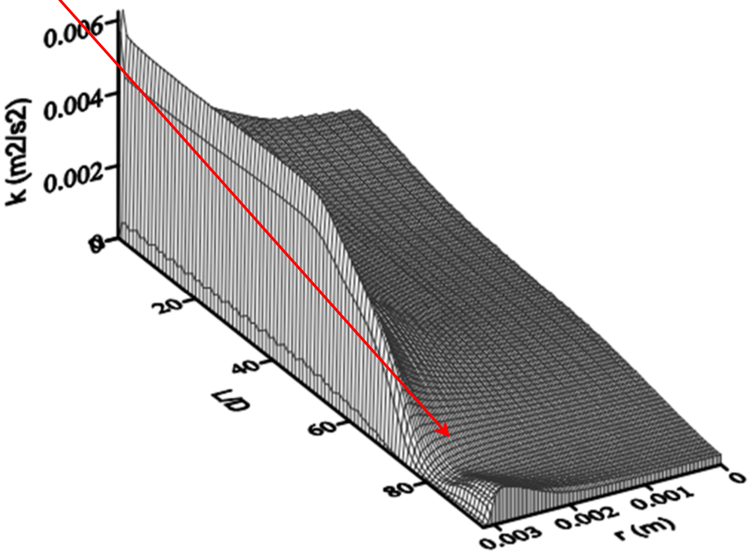
Application to Heat Transfer

Results for Pis'menny (2006) Water Data by the in-house code - 4

Deterioration due to flow laminarisation



a) axial velocity



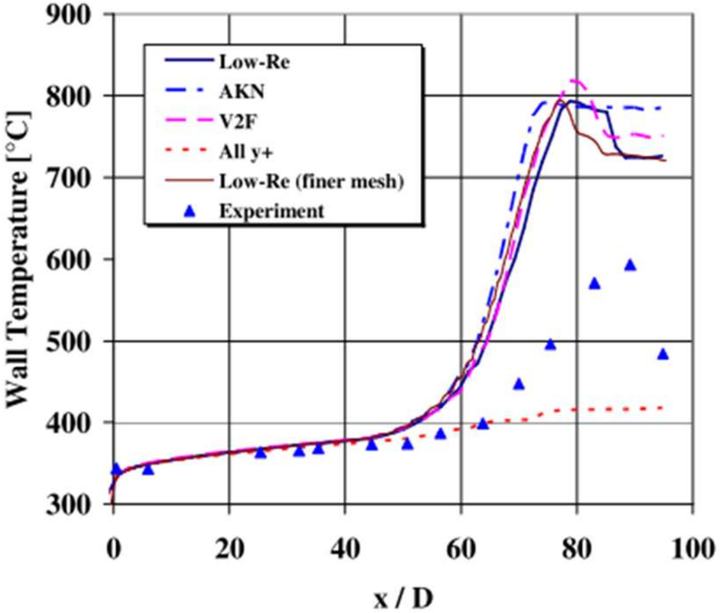
b) turbulence kinetic energy

Application to Heat Transfer

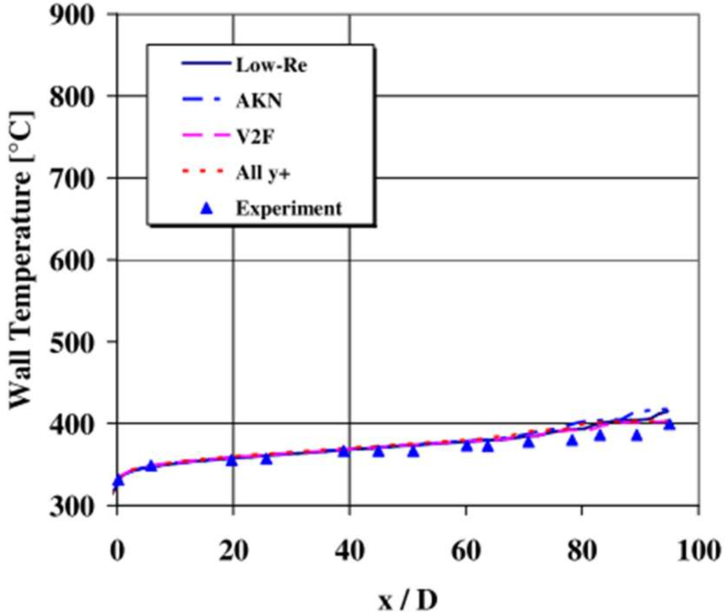
Results for Pis'menny (2006) Water Data by STAR-CCM+ - 1

- **The same data were the subject of analyses by different models implemented in the STAR-CCM+ code**
- **The results showed that the V2F model has also a response similar to the ones of the low Reynolds number k-ε models considered**
- **Expectedly, models making use of wall functions (as the "All y+" one), are not able to reproduce the onset of deterioration**
- **On the other hand, the standard "low-Re" k-ε model implemented in the code produced results similar to the ones observed from other similar models**
- **Later analyses on the same data by STAR-CCM+ showed that the inclusion of a model for the wall was relatively ineffective in improving the predicted behaviour**
- **Finally, a recent application to the same data of the SST k-ω model produced relatively poor results**

Application to Heat Transfer
Results for Pis'menny (2006) Water Data by STAR-CCM+ - 2



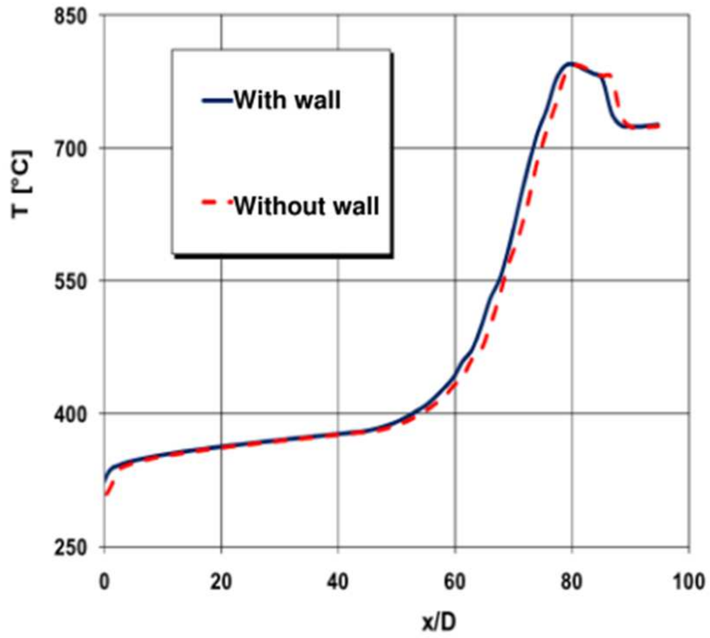
a) $q=390\ kW/m^2$, $G= 509\ kg/(m^2s)$, $T_{in}=300\ °C$, *upward flow [35]*



b) $q=390\ kW/m^2$, $G= 509\ kg/(m^2s)$, $T_{in}=300\ °C$, *downward flow [35]*

Application to Heat Transfer

Results for Pis'menny (2006) Water Data by STAR-CCM+ - 3



c) q=390 kW/m², G= 509 kg/(m²s), T_{in} =300 °C, upward flow [39]

Application to Heat Transfer

Kim et al. (2005) CO_2 Data

- **Kim et al. made use of carbon dioxide at 8 MPa in a 1.2 m long test section heated by DC current and preceded by an adiabatic section of 0.8 m**
- **The flow was upward and conditions of aided mixed convection were established in the channel**
- **The geometry of the tubes varied, including circular, triangular and square cross section pipes with hydraulic diameters of 7.8, 9.8 and 7.9 mm, respectively, made of Inconel 625 with a thickness of 1 mm**
- **Thermocouples were silver-soldered on the outer pipe surface every 30 mm along the heated length**
- **The experimental conditions addressed in the simulations involve an inlet temperature of 15 °C, a mass velocity of 314 kg/m^{2}s and heat fluxes of 20, 23 and 30 kW/m^2**
- **The obtained results with the same in-house tool as for Pis'menny data and FLUENT are described hereafter**

Application to Heat Transfer

Results for Kim et al. (2005) CO_2 Data by the in-house code - 1

The previous conclusions were extended also to other low-Re models (as the Cheng et al. model, CHC; note that SAA has the same meaning as SP in previous plots)

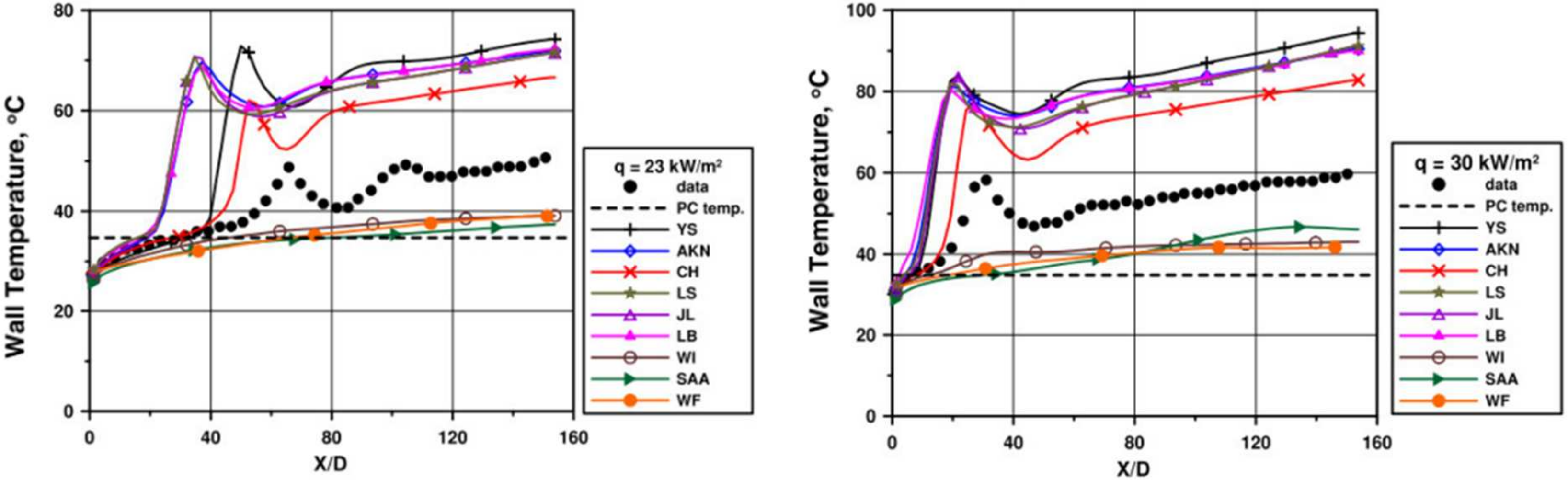
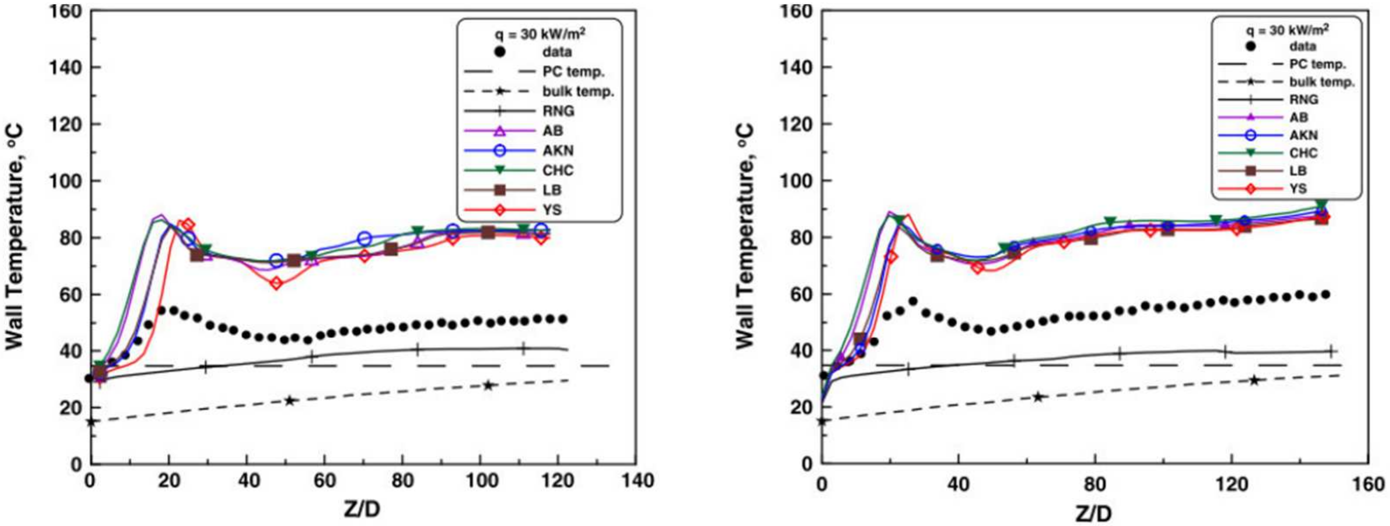


Figure 4. Results obtained by an in-house code for Kim et al. (2005) circular tube data [25]

Application to Heat Transfer

Results for Kim et al. (2005) CO_2 Data by the in-house code - 2

It can be noted that the results confirmed previous findings about the capability of k-ε models in predicting heat transfer deterioration even in 3D conditions and with a different fluid, but <u>with a marked overestimate of wall temperature</u>



a) triangular channel b) square channel

Figure 5. Results obtained by the FLUENT code for Kim et al. (2005) non-circular tube data [26]

Application to Heat Transfer

Watts (1980) Water Data

- **Watts data are the subject of an extensive work being carried out in the frame of the IAEA CRP on "Heat Transfer Behaviour and Thermo-hydraulics Codes Testing for SCWRs"**
- **The interest of these data is in the broad range of conditions over which they were obtained, involving both upward and downward flow and showing deteriorated heat transfer also at temperatures well below the pseudo-critical one**
- **Watts experiments were conducted in a uniformly heated pipe, having a diameter of 25.4 mm and length of 2 m**
- **A unheated length of 0.78 m was located upstream the test section**
- **The operating pressure of the fluid was 25 MPa**
- **A natural circulation loop was used to produce the flow and the test section was heated bv electrical current**

Application to Heat Transfer

Tools adopted for Watts (1980) Water Data and lesson learned

- **In a first phase of the work, the data were simulated extensively by the SWIRL code (S.He, Aberdeen University), allowing to test the performance of the Yang and Shih, the Abe, Kondo and Nagano and the Launder and Sharma models**
- **This revealed again a general capability of these k-ε models to quantitatively reproduce deteriorated heat transfer in upward flow <u>at temperatures lower than the pseudo-critical one</u>**
- **Considering the previous experience, obtained mainly in comparison with deteriorated conditions across the pseudo-critical threshold, <u>this finding represented an interesting additional information</u>**
- **A partial comparison of the results from SWIRL with those obtained by the STAR-CCM+ and the FLUENT codes, with available k-ε models, confirmed these findings, motivating a thorough application of these codes**
- **<u>WARNING:</u> Our results for Watt's data are presently being reconsidered on the basis of more detailed information on boundary conditions: anyway, only minor differences were noted up to now**

Application to Heat Transfer
Results obtained for Watts (1980) Water Data by FLUENT - 1

- **Despite the encouraging behaviour shown by models in such cases, quantitative inadequacies are still present even under non-deteriorated conditions related to upward flows, indicating an incomplete description of turbulence effects**

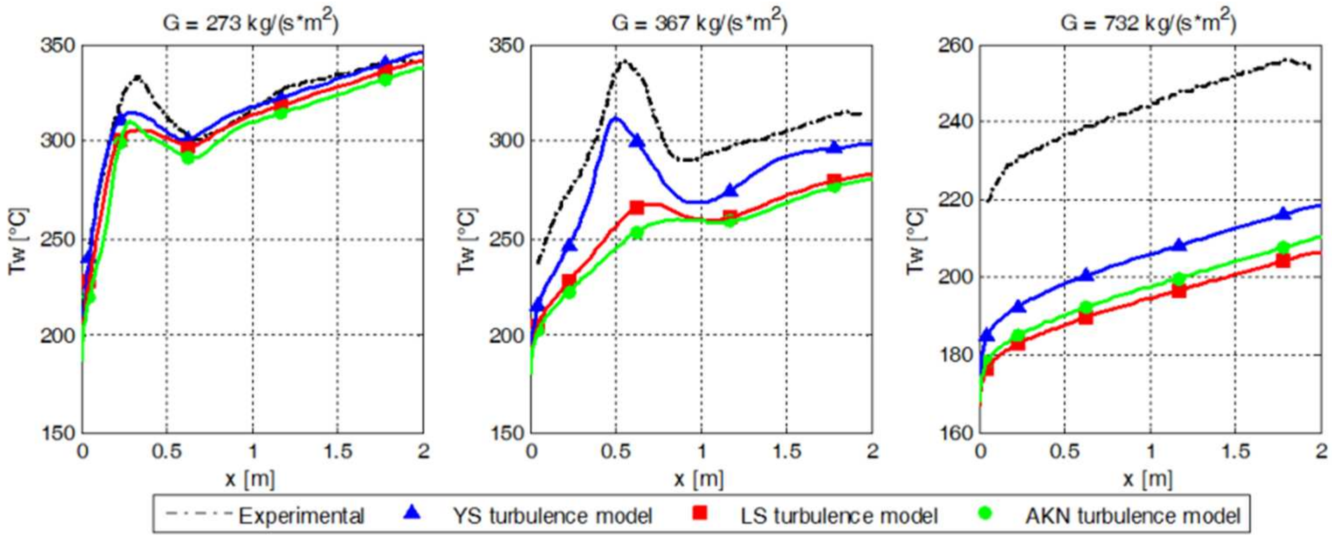


Figure 6. Comparison between experimental and calculated inner wall temperature for Watts (1980) data obtained by the SWIRL code with different turbulence models [23] ($q = 255$ W/m^2, $T_{in} = 150$°C, upward flow)

Application to Heat Transfer

Results obtained for Watts (1980) Water Data by FLUENT - 2

- **As already noted, downward flow seemed easier to reproduce**

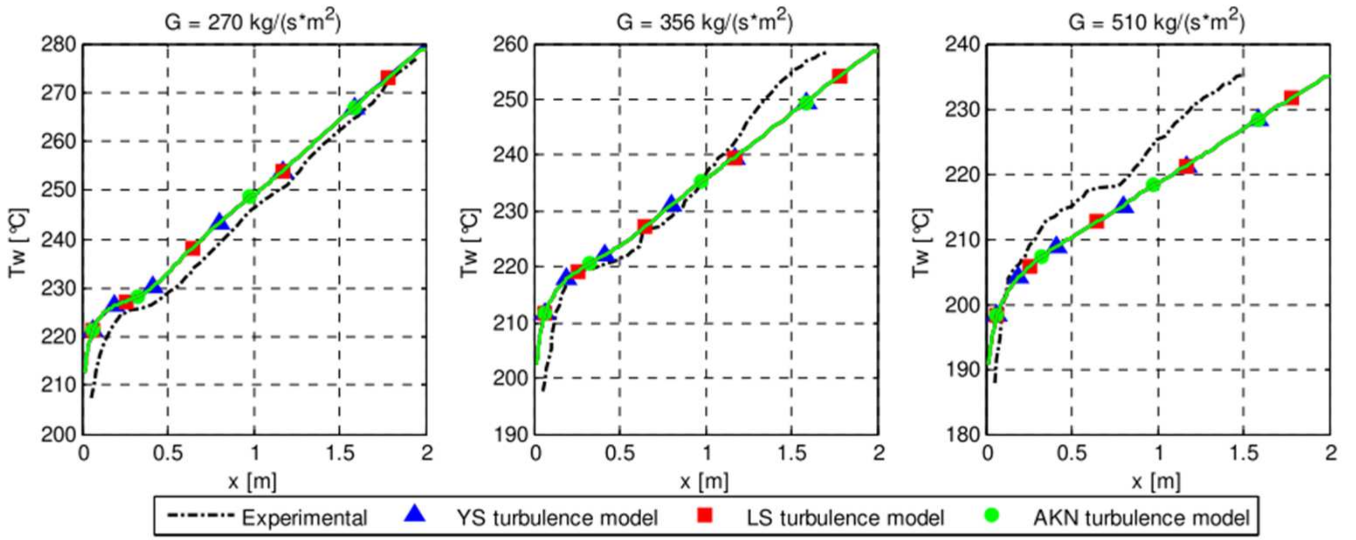


Figure 7. Comparison between experimental and calculated inner wall temperature for Watts (1980) data obtained by the SWIRL code with different turbulence models [23] ($q = 255\ W/m^2$, $T_{in} = 150°C$, downward flow)

Application to Heat Transfer

Results obtained for Watts (1980) Water Data by STAR-CCM+ - 1

- **Also STAR-CCM+ models (the standard low-Re available in the code) provided good results below the pseudocritical temperature and the already observed overestimation of wall temperature beyond it**

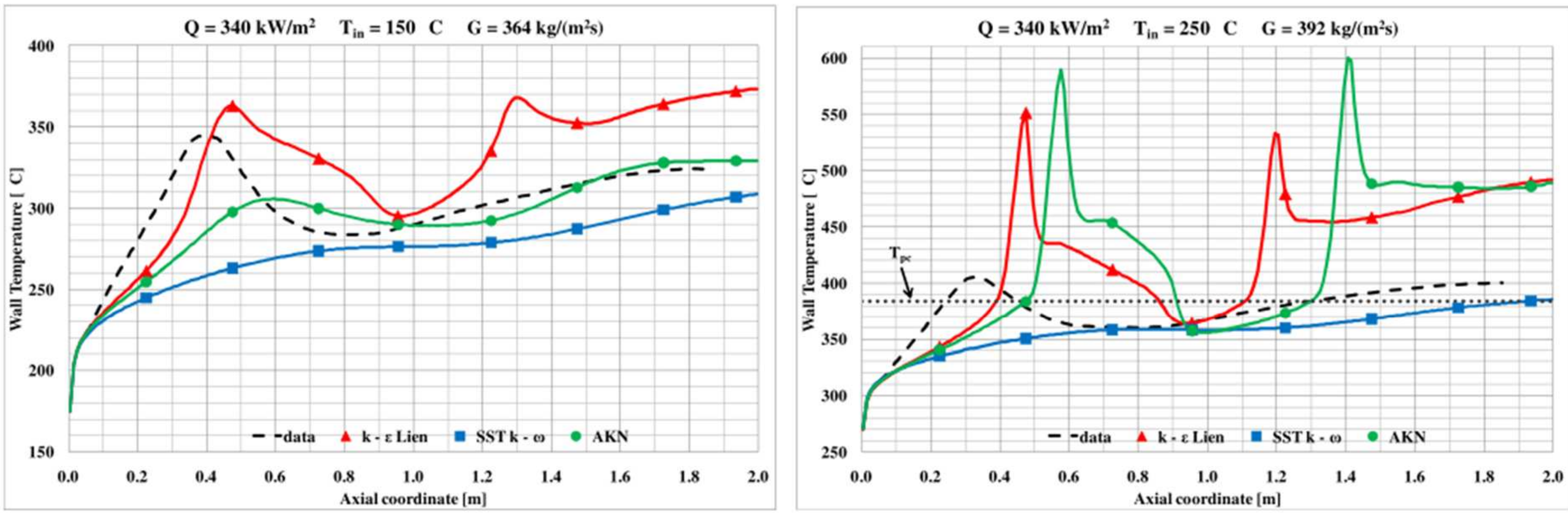
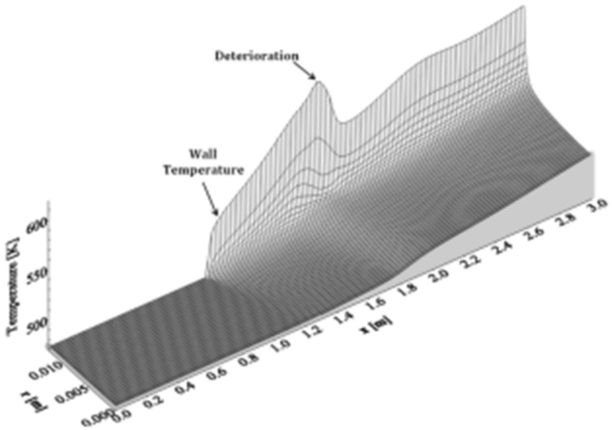


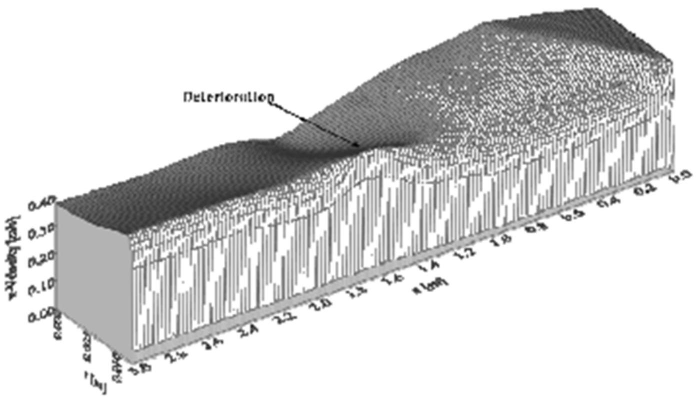
Figure 11. Comparison between experimental and calculated inner wall temperature obtained by the STAR-CCM+ code with different models for upward flow [45]

Application to Heat Transfer

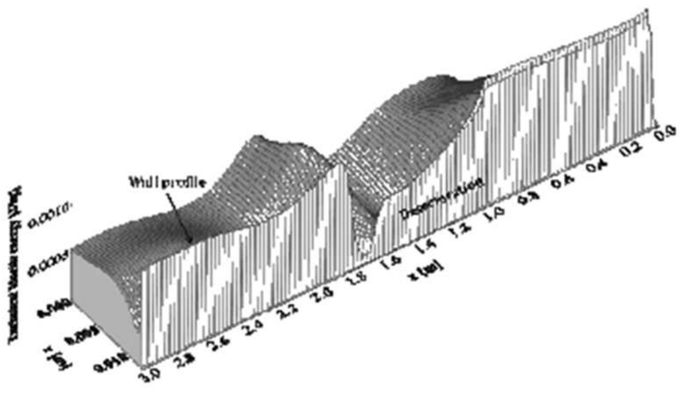
Results obtained for Watts (1980) Water Data by STAR-CCM+ - 2



a) fluid temperature



b) fluid velocity



c) turbulence kinetic energy

Application to Heat Transfer
Summary

- **In summary, most low Re k-ε models tend to over-respond to laminarisation effects when they occur across the pseudo-critical temperature**

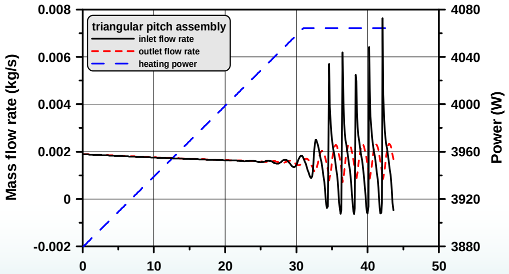
- **Below the pseudo-critical temperature, a better behaviour is observed with a more reasonable representation of wall conditions**

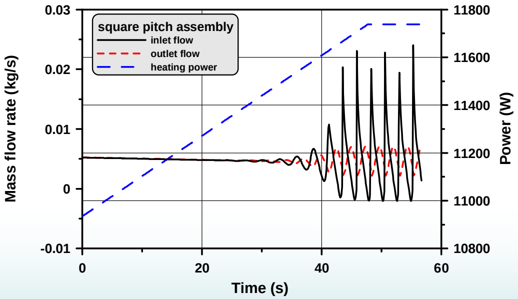
- **Some other models (e.g., k-ω) tend to delay or do not show deterioration**

- **Research is going on to better understand the reasons for this behaviour and propose convenient improvements**

Application to Flow Stability

- **A few aspects related to the analysis of flow stability by CFD have been already mentioned in the previous lecture on this topic**
- **For the sake of brevity, it is here just recalled that:**
  - **Analysis of flow stability by CFD codes was performed for circular channels making use of both wall function and low Reynolds number models (Sharabi et al., 2008)**
  - **Stability was also studied for fuel bundle slices with both square and triangular pitches (Sharabi et al. 2009)**
- **The overall conclusion is that CFD codes provide a description of the instability phenomena which confirm the general features of observations by 1D codes, though with additional detail**





Application to Natural Circulation

BARC CO_2 Experiments

- **In the frame of the ongoing Coordinated Research Project of IAEA on SCWRs, the BhaBha Atomic Research Centre of Mumbai (India) produced interesting experimental data on natural circulation in a closed loop with supercritical carbon dioxide (Vijayan et al., 2010)**

- **A joint effort was made by BARC and the University of Pisa to simulate the observed steady state and transient behaviour by CFD codes: the related paper was submitted at the NURETH-14 Conference (Molfese et al., 2011)**

  The experiments were carried out in an experimental facility installed at the Reactor Engineering Division of BARC, consisting in a uniform diameter (13.88 mm ID & 21.34 mm OD) rectangular loop (SCNCL) with different orientations of heater and cooler

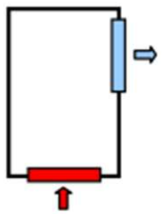
(a) HHHC

- **The tests with carbon dioxide were performed at different power levels, at the supercritical pressures of 8.6 and 9.1 MPa.**

  The steady-state characteristics of the loop were obtained for the horizontal heater and the horizontal cooler configuration (HHHC), and for the horizontal heater and vertical cooler one (HHVC).

  Unstable behaviour was observed only for the HHHC configuration.

(b) HHVC

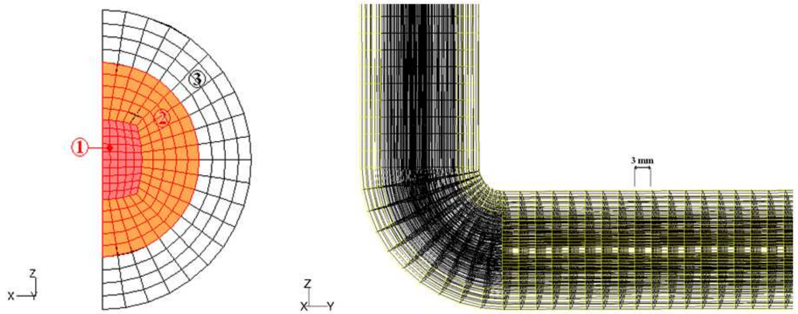


- **The FLUENT and the STAR-CCM+ codes were adopted for reproducing the observed behaviour of the experimental loop in the HHHC configuration**

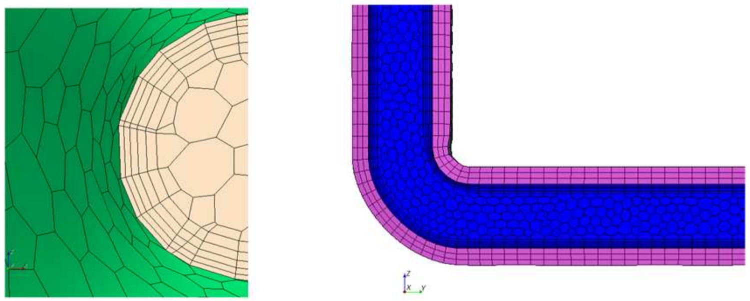
Application to Natural Circulation

Modelling BARC CO_2 Experiments

- **In setting up the spatial discretisation, the symmetry of the SPNCL facility with respect to a middle vertical plane made possible to model only a half of the loop, including heat conduction within the walls**



FLUENT



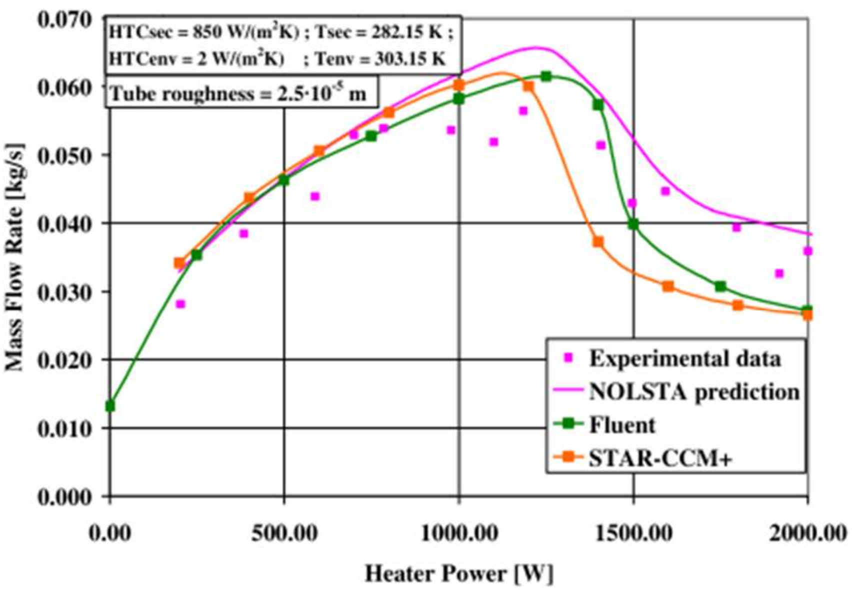
STAR-CCM+

- **Unlike in the case of heat transfer, "wall functions" (i.e., all y+ treatment) were adopted, to avoid the need to considerably refine the meshes close to the walls**
- **A piecewise linear interpolation with 30 point was used for implementing properties in FLUENT, while in STAR-CCM+ cubic spline polynomials were adopted**
- **Wall roughness was assumed, relying on wall functions for its representation**

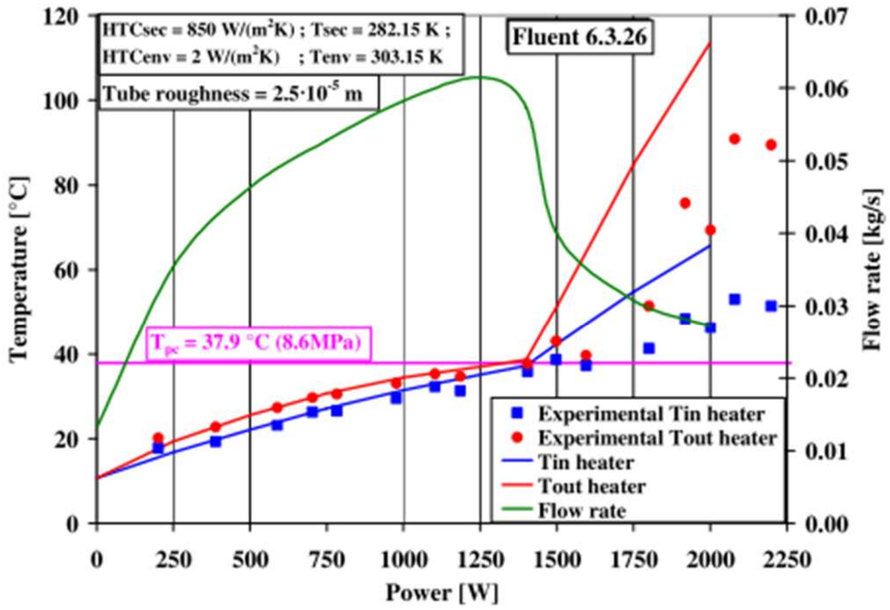
Application to Natural Circulation

Results for BARC CO_2 Experiments - 1

- **The results for the HHHC configuration were consistent with steady state experimental data for both codes**
- **The predictions of the maximum flow (close to the pseudocritical temperature in both the cold and the hot legs) are sensitive to details as pipe roughness and HTC and temperature to the secondary loop and heat losses**

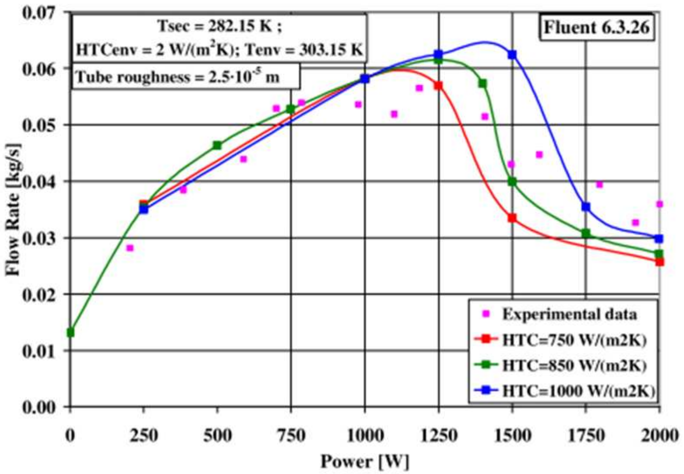


a) flow rate

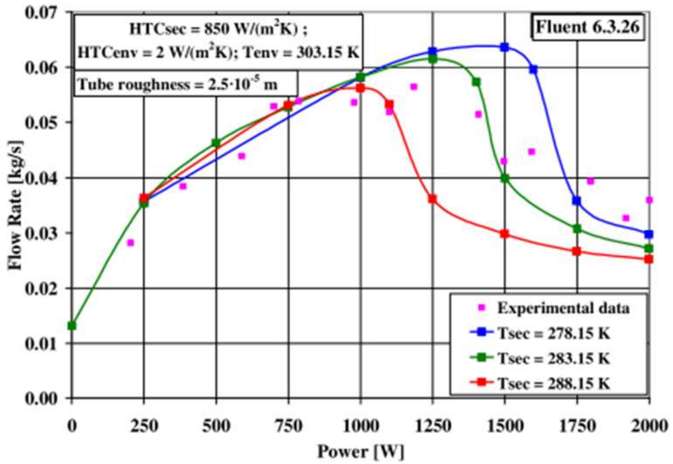


b) fluid temperatures

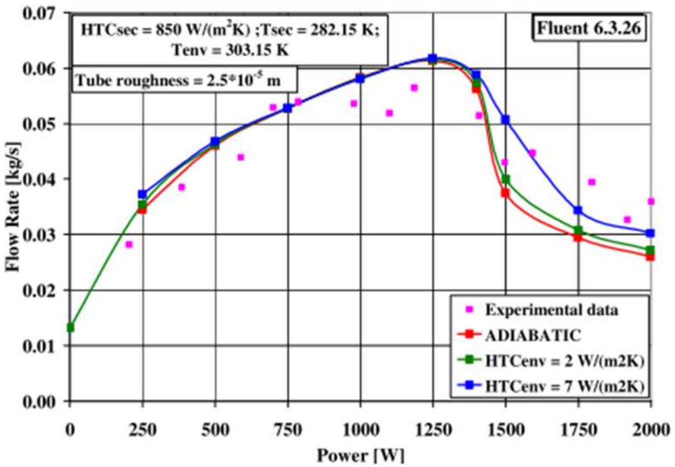
Application to Natural Circulation
Results for BARC CO_2 Experiments - 2



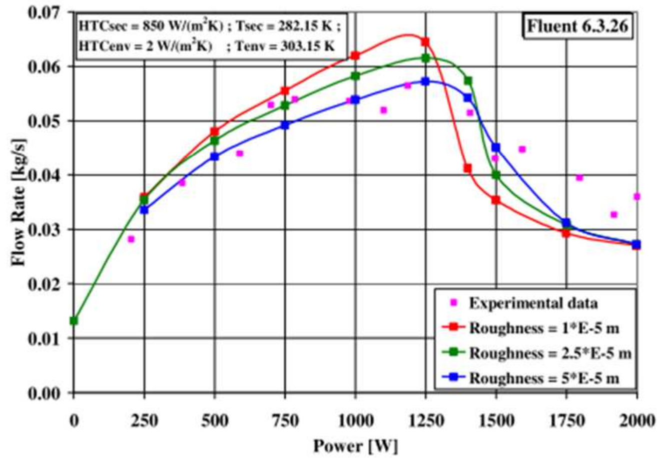
a) HTC with secondary coolant



b) secondary coolant temperature



c) HTC with the environment

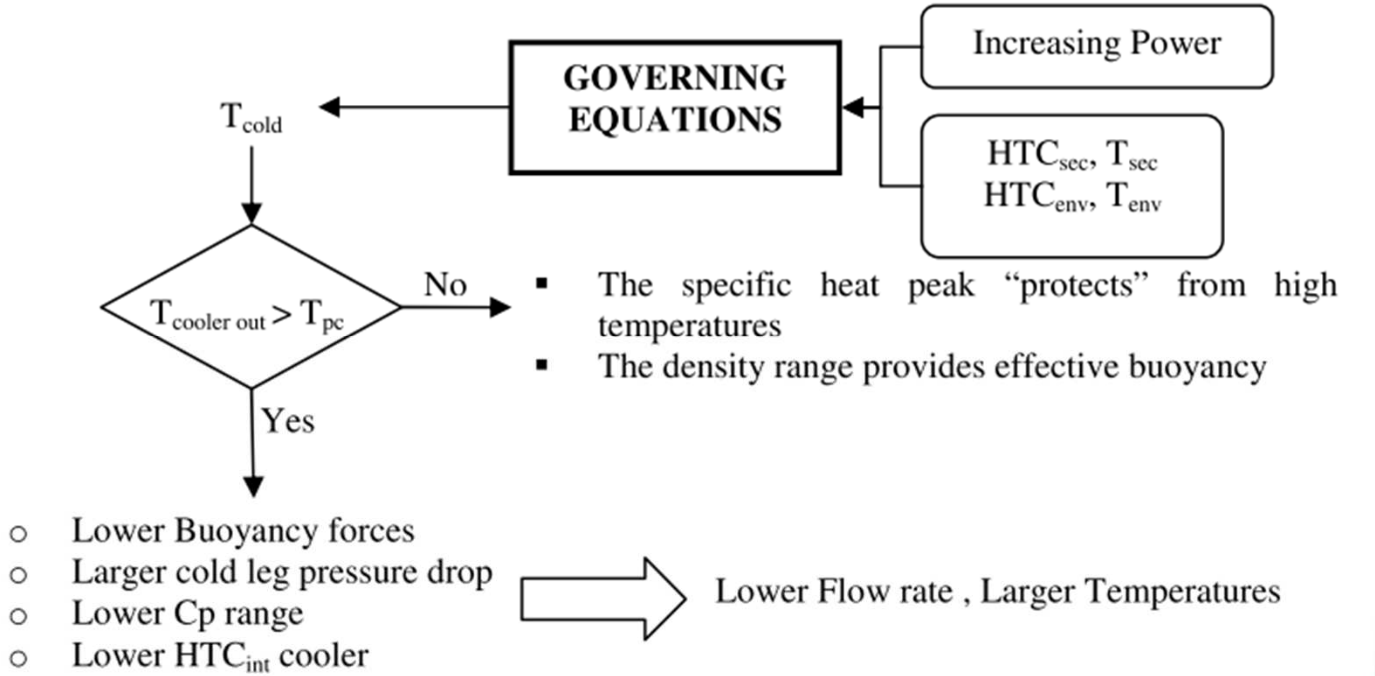


d) pipe roughness

Application to Natural Circulation

Results for BARC CO_2 Experiments - 3

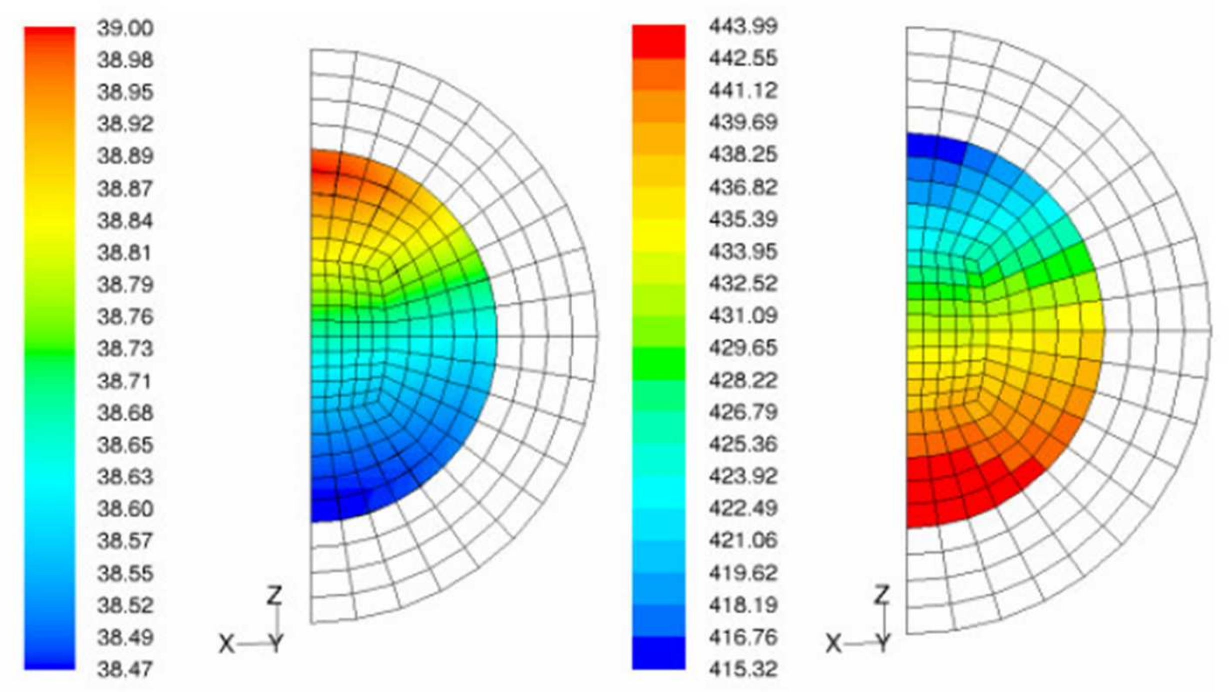
- **The performed sensitivity analyses allowed to highlight the effects leading to the sharp transition to low flow rate after the maximum**
- **In summary, the poorer heat transfer due to the presence of lighter fluid inside the cooler region is responsible for the sharp increase in temperature beyond T_{pc} and for buoyancy decrease**



Application to Natural Circulation

Results for BARC CO_2 Experiments - 4

- **Despite of the small diameter of the pipe, stratification effects take place in the horizontal heater**

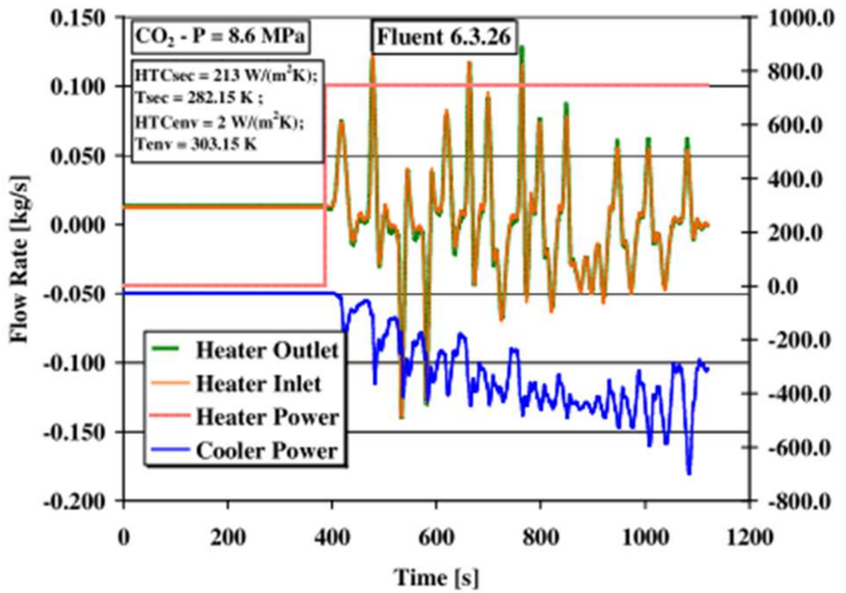


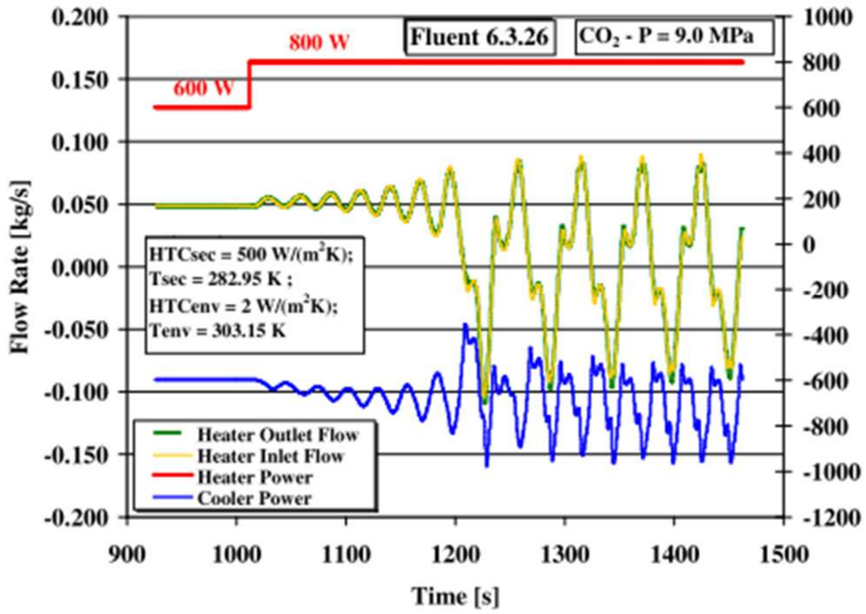
a) temperature [°C] b) density [kg/m^3]

Application to Natural Circulation

Results for BARC CO_2 Experiments - 5

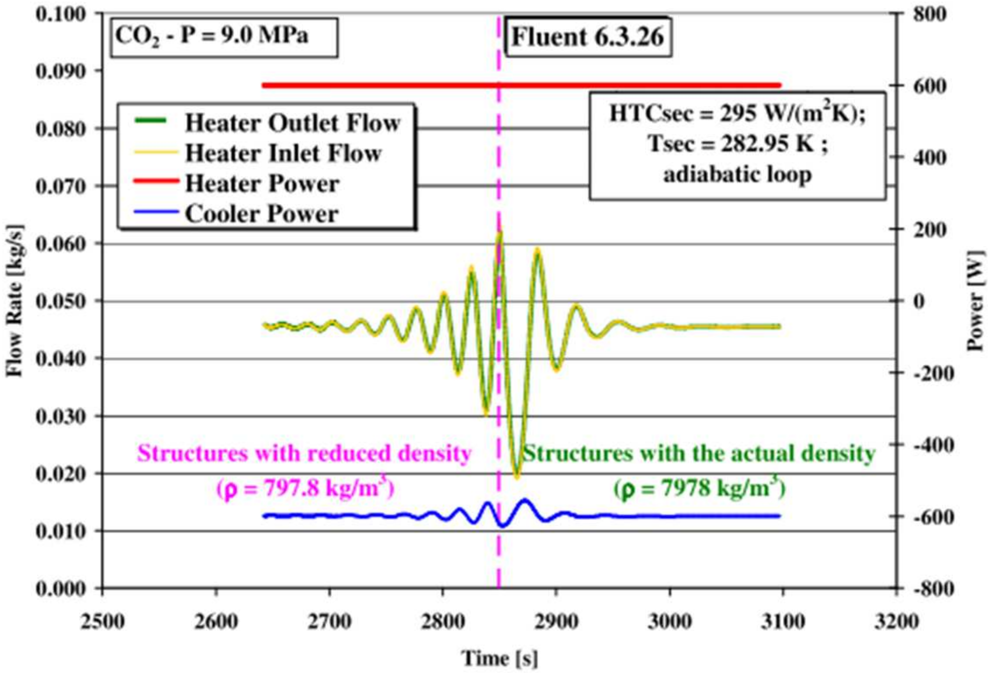
- **Concerning the dynamic behaviour, the observed instabilities could not be predicted by the codes**
- **Sensitivity analyses showed that the representation of the walls has a key role; in fact, artificially decreasing the wall heat capacity it was possible to simulate unstable behaviour**





Application to Natural Circulation
Results for BARC CO_2 Experiments - 6

- **To confirm the important role of heat structures in the model transient calculations were started with FLUENT with reduced heat capacity in the heat structures, later on recovering the physical value of this parameter: the damping effect due to structures is clearly observed**



Conclusion

- **CFD is presently applied to different phenomena of interest for SCWR reactor design**
- **The complexity of supercritical fluid behaviour makes challenging to obtain completely reliable results by the presently available models and research is needed to improve the present capabilities**
- **Among the areas requiring further efforts there is the simulation of deteriorated heat transfer, which is presently described only at a qualitative level, with considerable discrepancies on wall temperature**
- **The stability analyses performed up to now revealed the capability of CFD codes to predict the phenomenon in similarity with what observed with 1D system codes**
- **The experience gained in the application to natural circulation experiments provided a reasonable confidence in the capability to predict steady state conditions, highlighting the need to improve the dynamic predictions**

Thank you for your attention,

Walter Ambrosini

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