*Code Saturne User's Annual Meeting, EDF R&D Chatou FR, Nov. 2007*

# Refined turbulence modelling for reactor thermal-hydraulics

## Part of UK's "Keeping Nuclear Options Open" project

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KNOO
Keeping the Nuclear Option Open

Keeping the Nuclear Option Open
part of the Research Councils UK Energy Programm

http://www.knoo.org/

- to maintain and develop skills relevant to nuclear power generation.
- 4 years, 6M £, 50 PhDs and Post-docs,
- largest commitment to fission reactor research in UK for over 30 years,
- collaboration with industrial and governmental stakeholders and international partners.

Attendees at the KNOO annual meeting at HMS Sultan.

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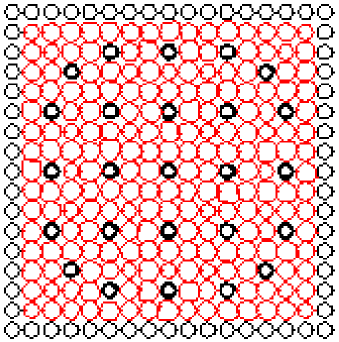
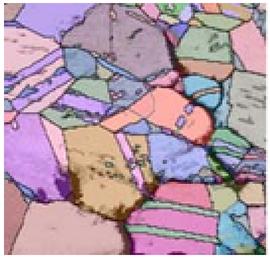
The University of Manchester
University of BRISTOL
Imperial College London
CARDIFF UNIVERSITY PRIFYSGOL CAERDYDD
The Open University
University of Leeds
The University Of Sheffield.

# *KNOO WORKPACKAGES*

## Themes – Work Packages



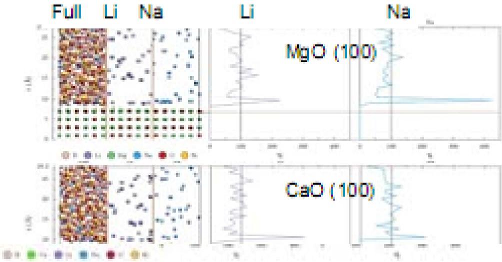
**W/P1. Fuel, thermal hydraulics and reactor systems**
Coupling of multi-pin structural mechanics and three-dimensional transient two phase thermal hydraulic analysis for the study of severe accidents (e.g. pin ballooning under reflood conditions); crud deposition and its thermal hydraulic and neutronic effects; application of advanced CFD to Generation IV systems.

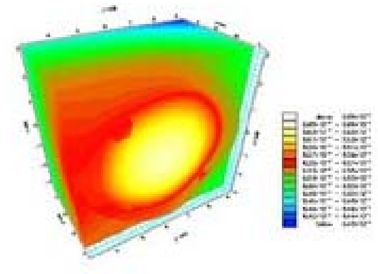


EBSD image of SCC in stainless steel

**W/P 2. Materials performance and monitoring reactor conditions**
Remote structural interrogation and monitoring tools; miniaturised, encapsulated monitoring systems; FE/self consistent models to assess materials; mechanical understanding and predictive models of SCC; mechanical performance of nuclear cladding and structural materials; behaviour of graphite

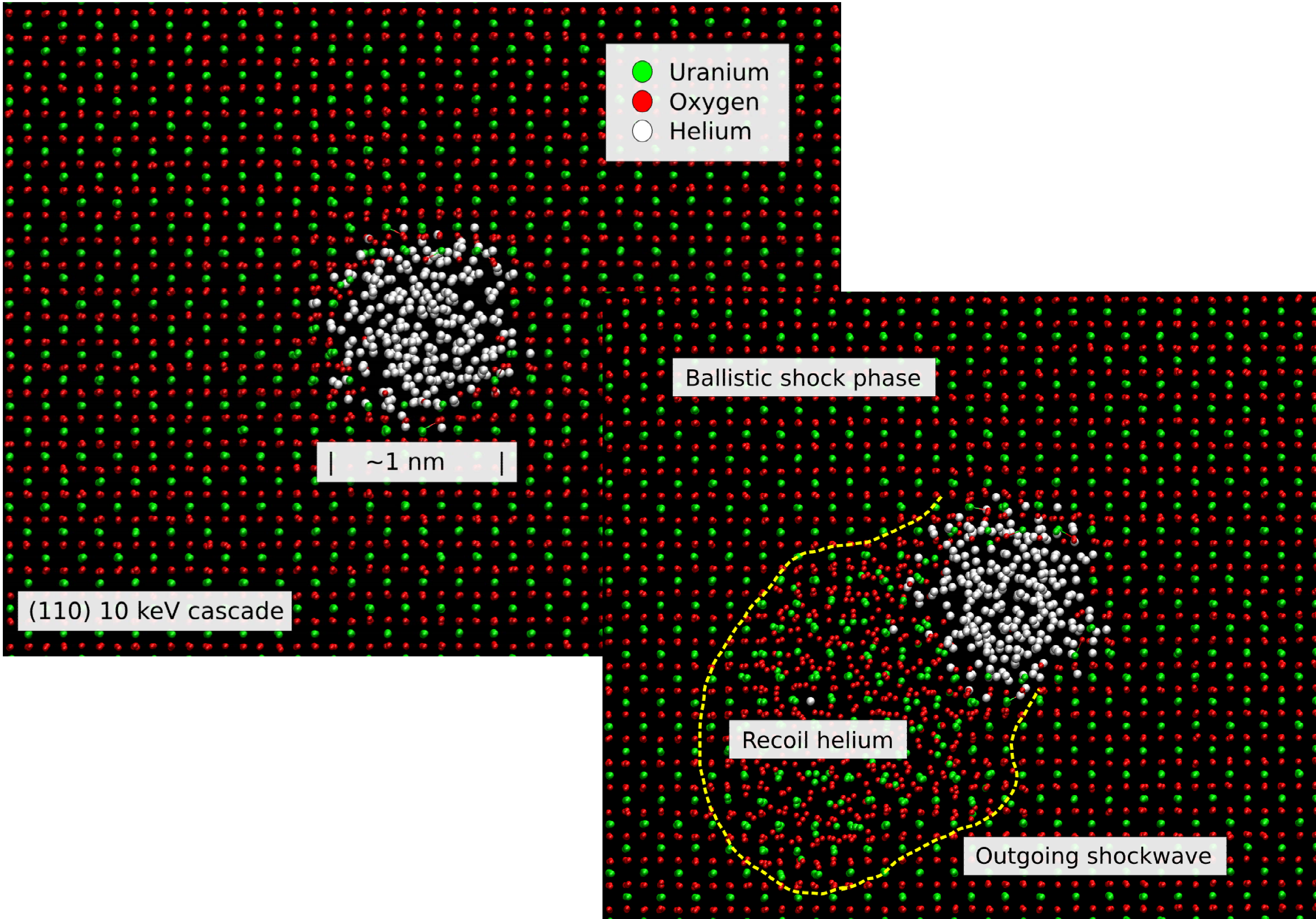
**W/P 3. An integrated approach to waste immobilization and management**
Re-mobilisation, transport, solid-liquid separation, and immobilisation of particulate wastes; develop predictive models for particle behaviour based on atomic scale, thermodynamic and process scale simulations; develop fundamental understanding of selective adsorption of nuclides onto filter systems





**W/P 4. Safety and performance for a new generation of reactor designs**
3D plant fault/severe accident transient studies that match UK industry plans for Generation IV (VHTR, GFR and SFR); assess demands on candidate materials under transient and normal operating conditions; scope safety approaches for the hydrogen production process and systems.

# Ex: Molecular dynamics of radiation enhanced helium re-solution



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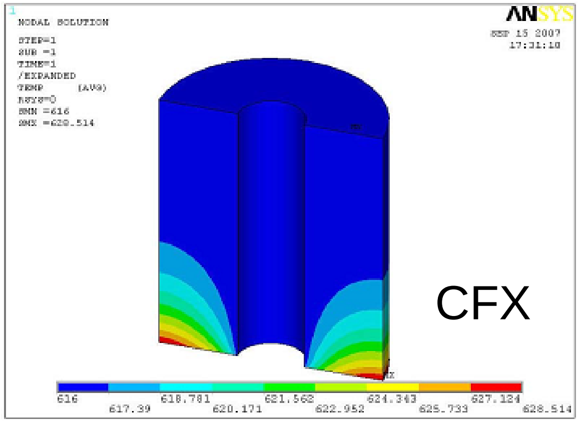
# *CFD @ Imperial College*

eDF

## *Heat transfer through crud*



CFX

Fig: 1 Temperature contours in the porous shell of the crud

## *Droplets on hot solid surfaces: Modelling and Experimentation*

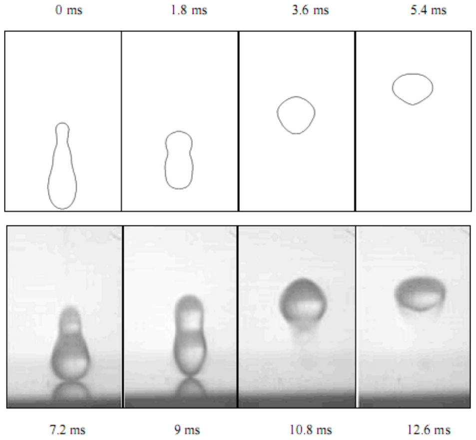
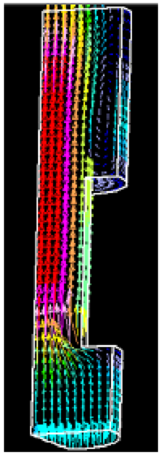


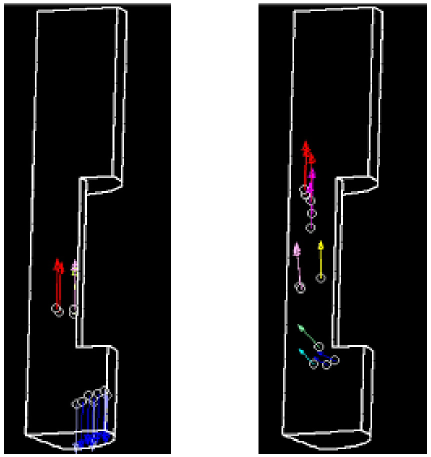
Fig. 1. Comparison between two-dimensional axisymmetric simulation of a millimetric droplet impacting on a 300oC solid surface (We=11) and experimental results by Biance et al (2006) (We=10). The time interval between pictures is 1.8 ms.

## *Ballooning fuel pins*

STAR

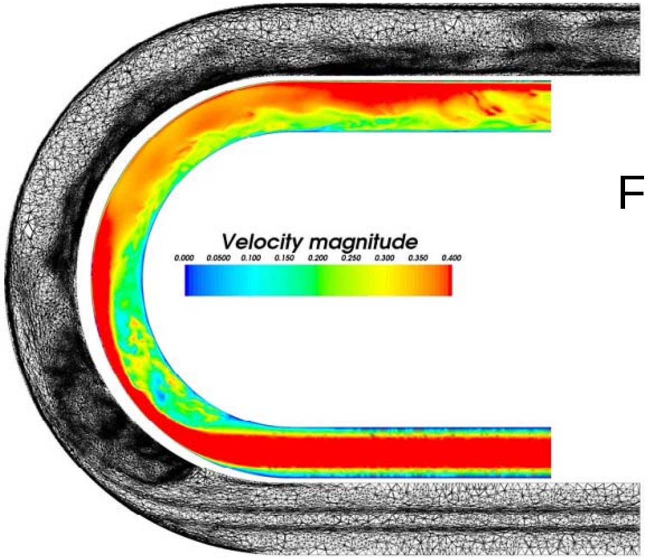


Vapour Flow Velocity Vectors



Droplets Path, (a) Particles of Water Density, (b) Particles of Smaller Density (1.2kg/m$^3$)

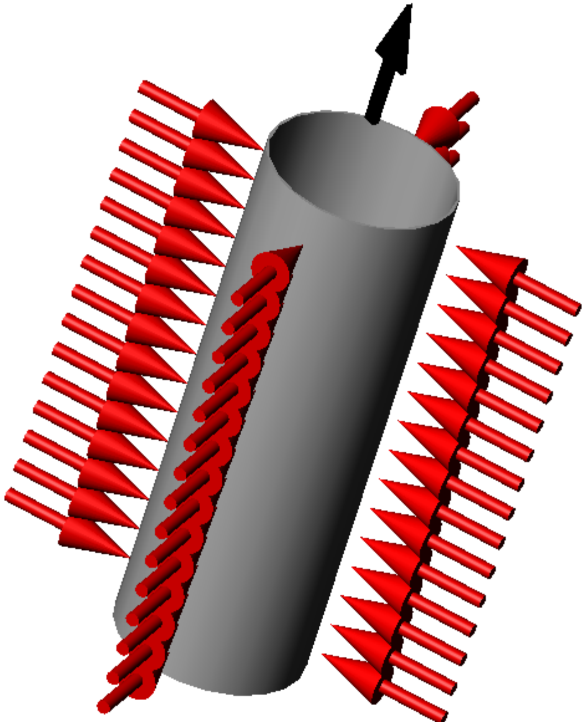
## *LES with adaptive FE meshing*



FE (Fetch

Figure 1 Time snapshot (with a slice through the domain) of flow velocity and adapted mesh for LES modelling of flow through a circular cross section U bend pipe.

# Test Case 1 :
# Mixed convection in vertically flowing heated pipe (buoyancy aiding or opposing)



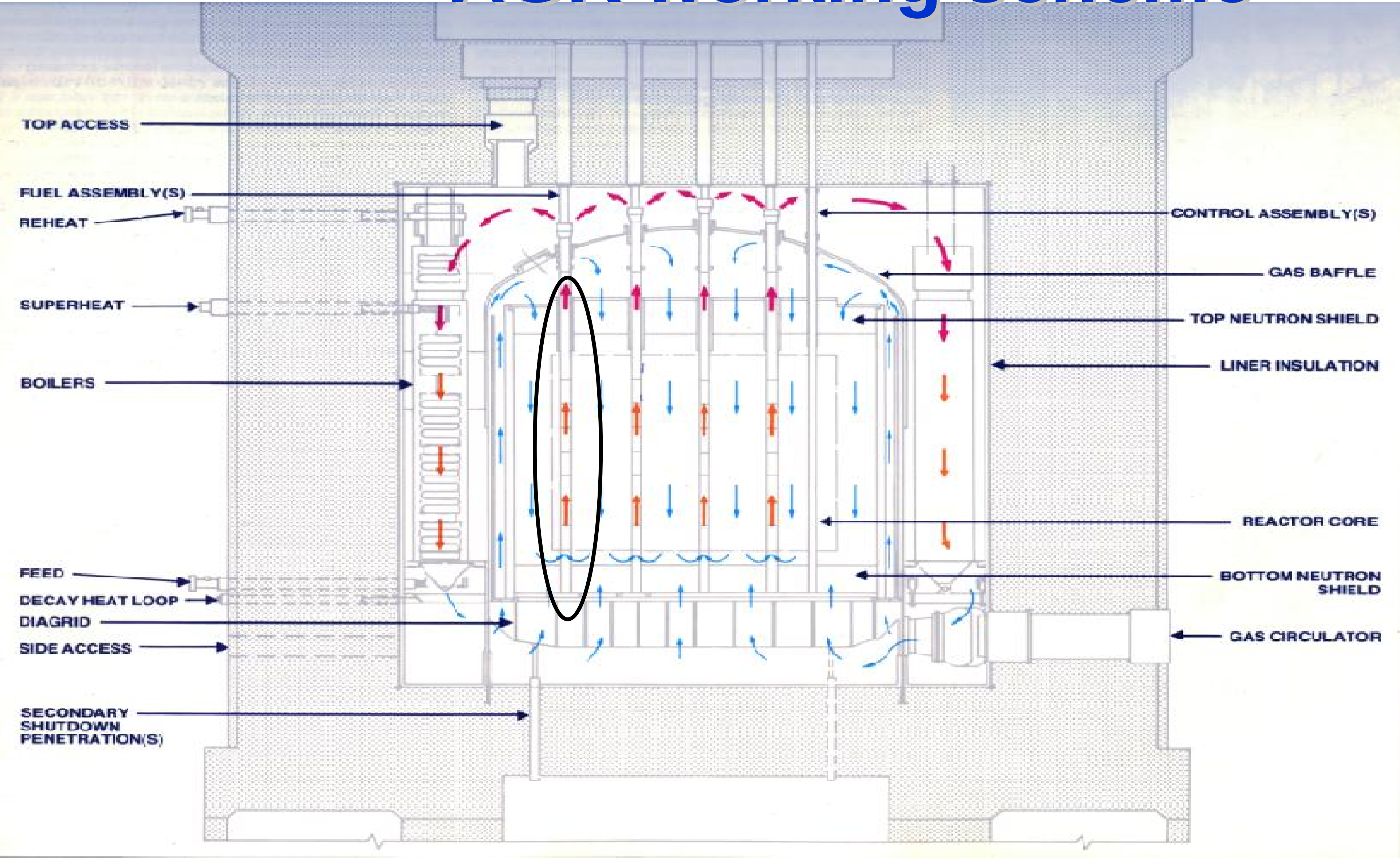
**Problem specifications:**

- Re=2650
- Pr=0.71
- Wall constant heat flux
- Boussinesq approximation

**Heat transfer Regimes:**

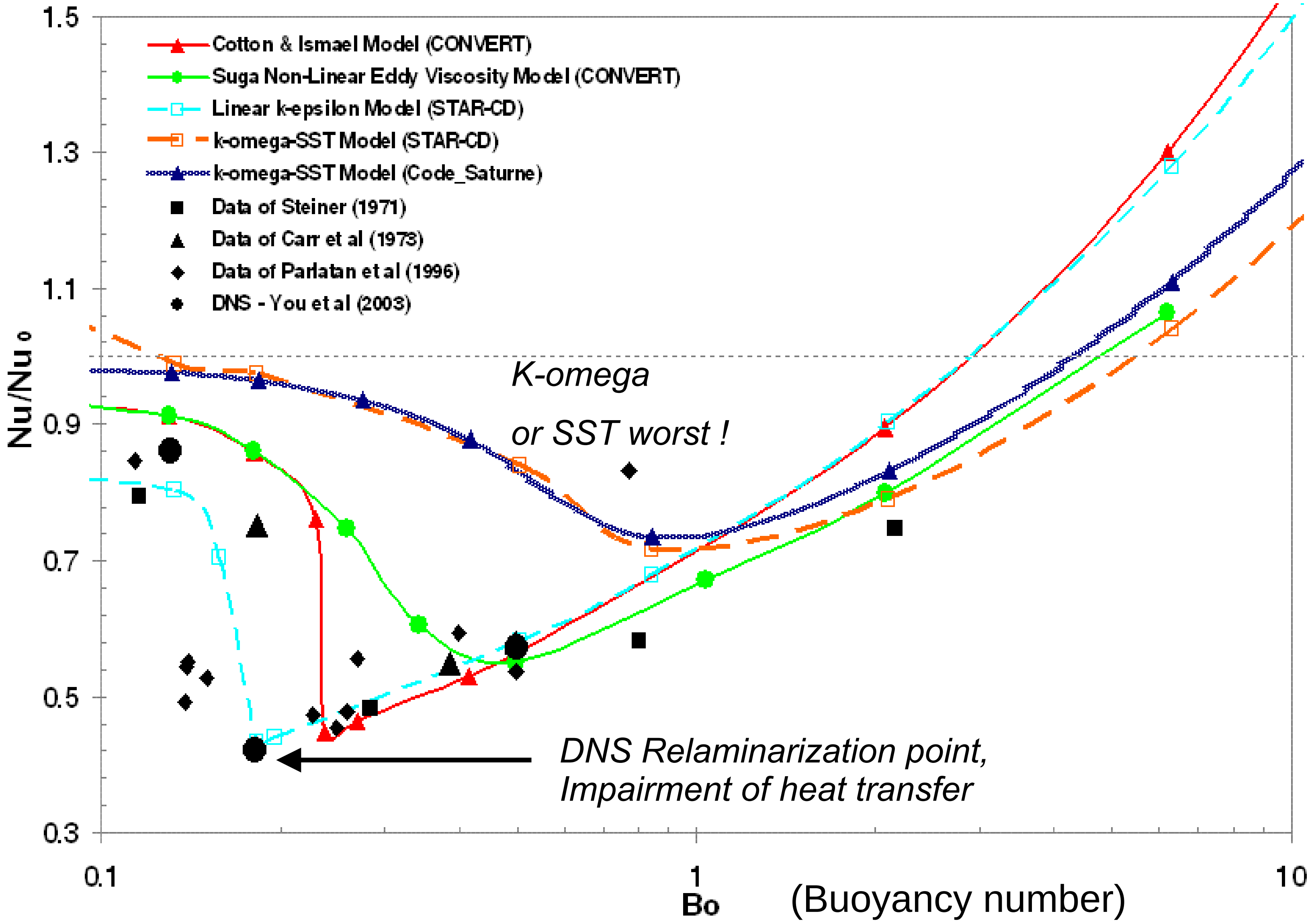
- $Gr/Re^2=0.000$ → Forced Convection
- $Gr/Re^2=0.063$ → Forced/Mixed Convection
- $Gr/Re^2=0.087$ → Re-Laminarization
- $Gr/Re^2=0.241$ → Recovery

# AGR working scheme



# *Buoyancy aided heated pipe flow*

## Range of RANS models



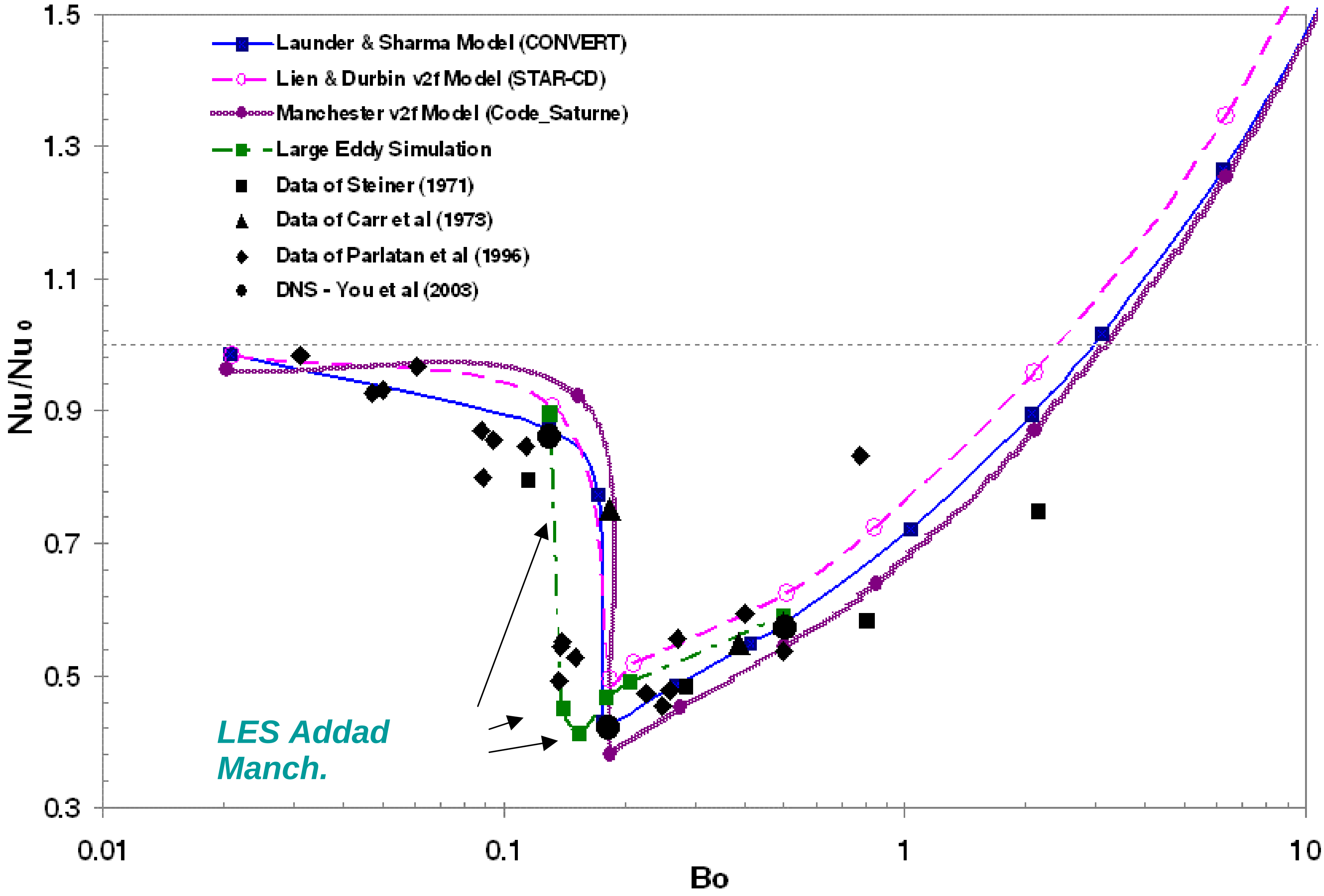
*K-omega*

*or SST worst !*

*DNS Relaminarization point,*
*Impairment of heat transfer*

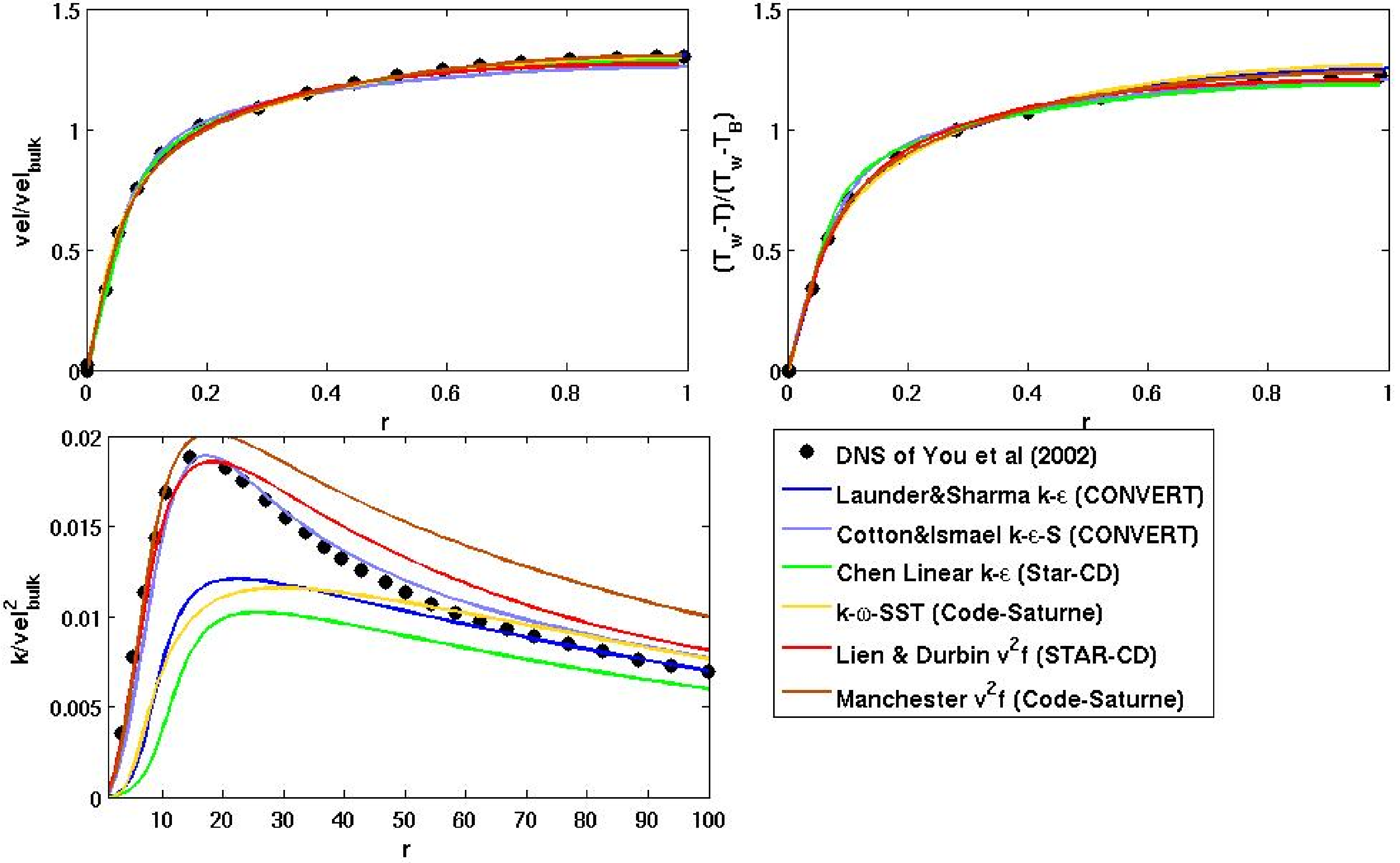
# *Buoyancy aided heated pipe flow*

best models: Launder Sharma, V2F



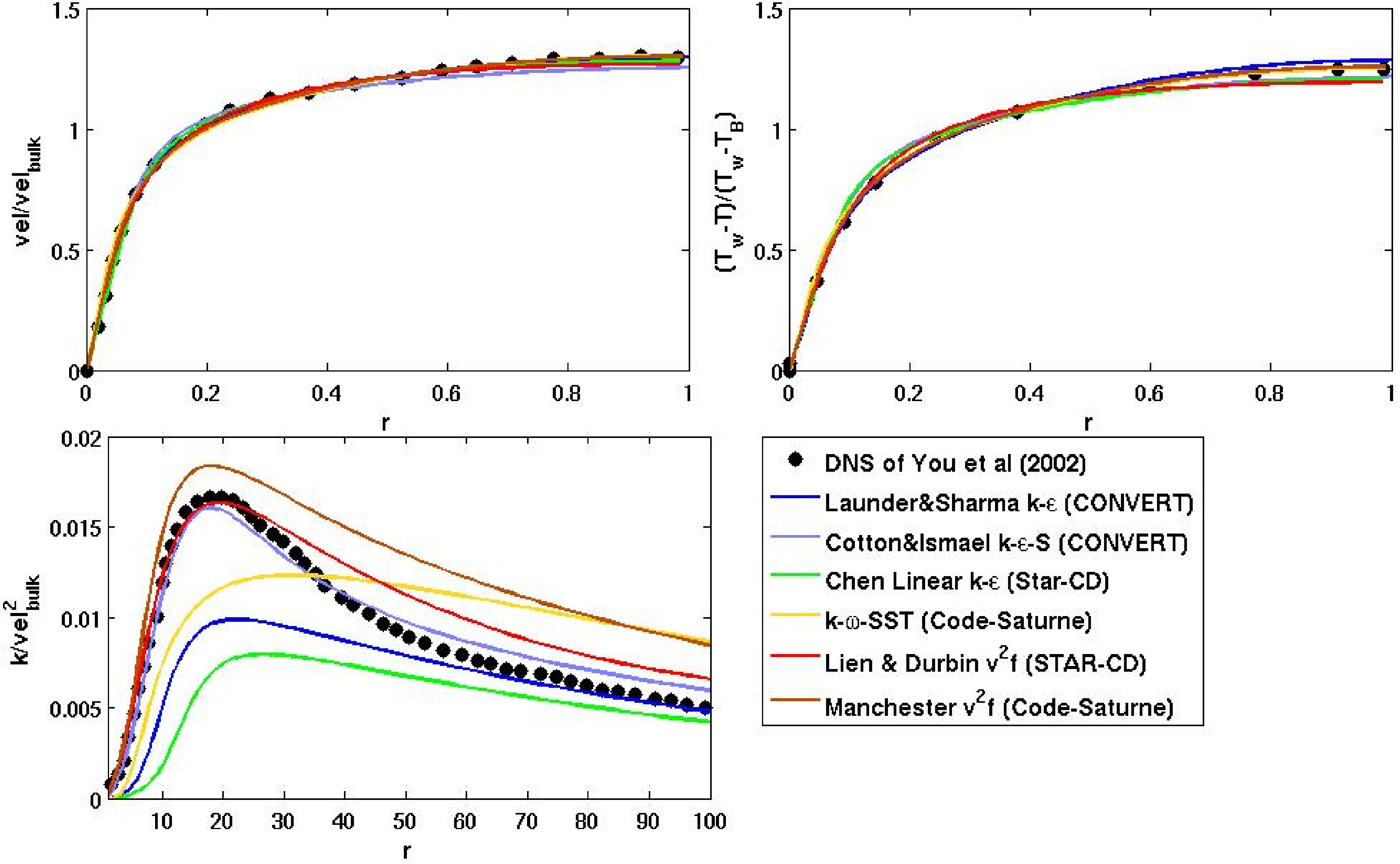
# *Buoyancy aided heated pipe flow*

**Gr/Re**2 = 0.000**



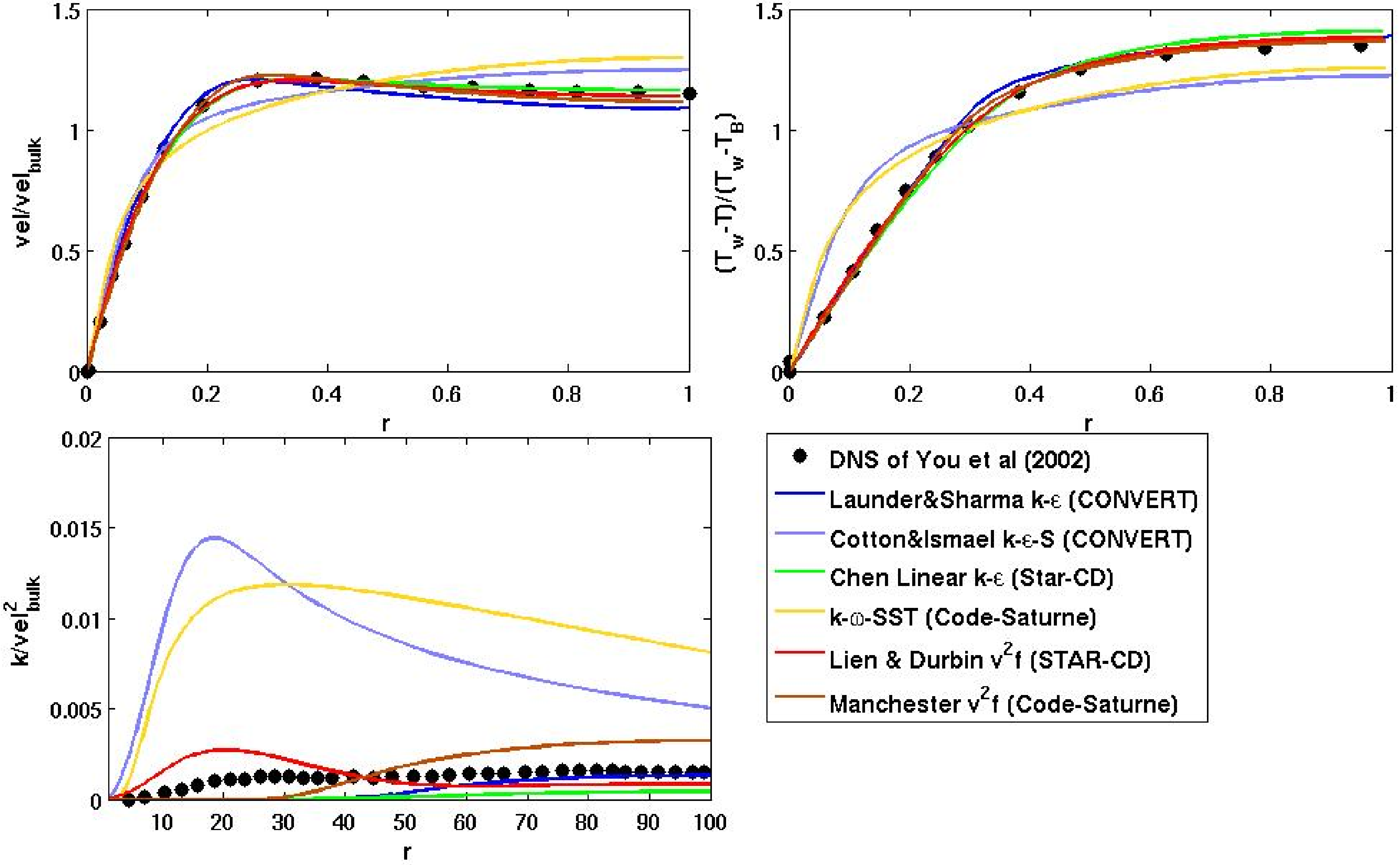
# *Buoyancy aided heated pipe flow*

## Gr/Re**2 = 0.063



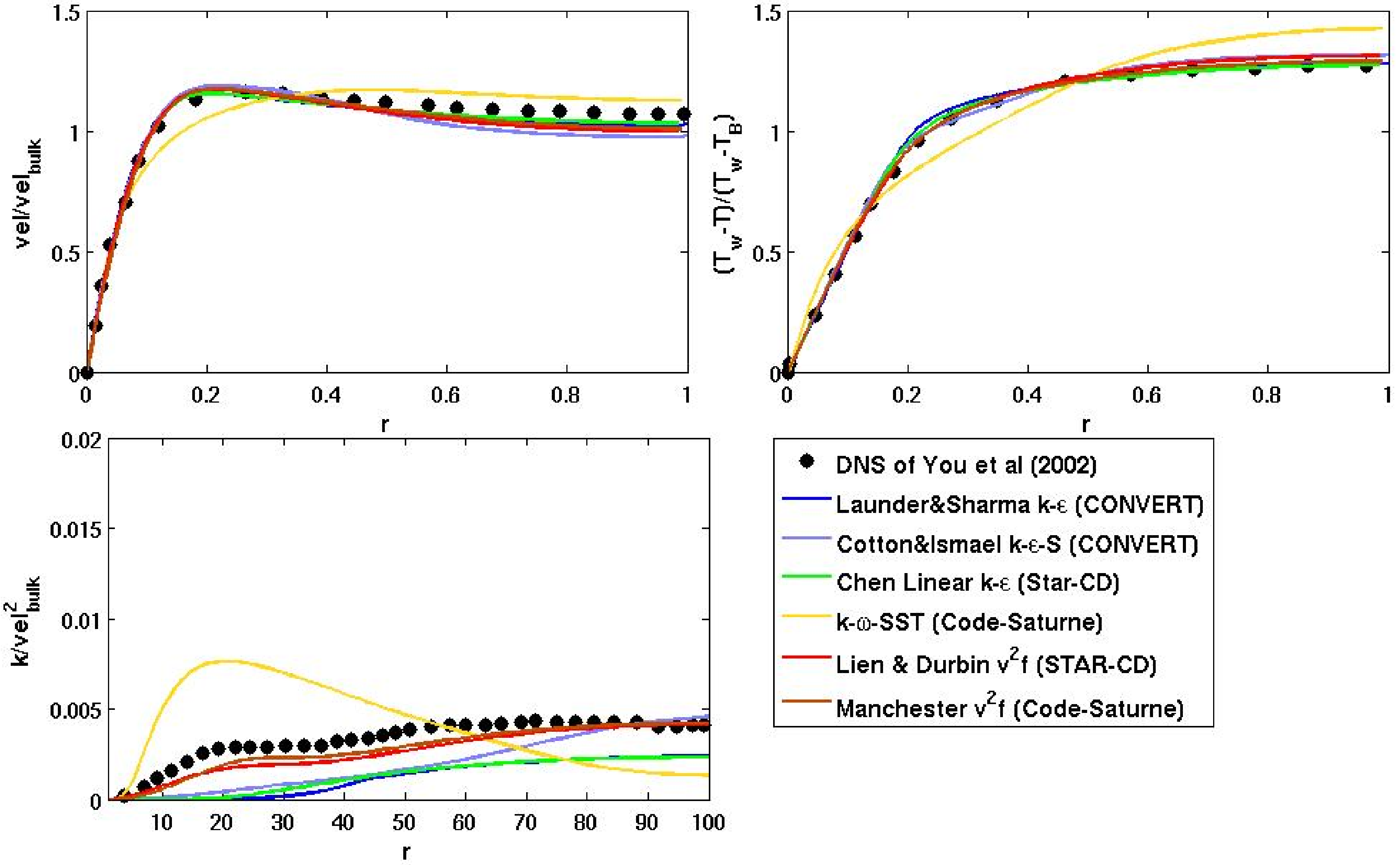
# *Buoyancy aided heated pipe flow*

## Gr/Re**2 = 0.087 (relaminarization)



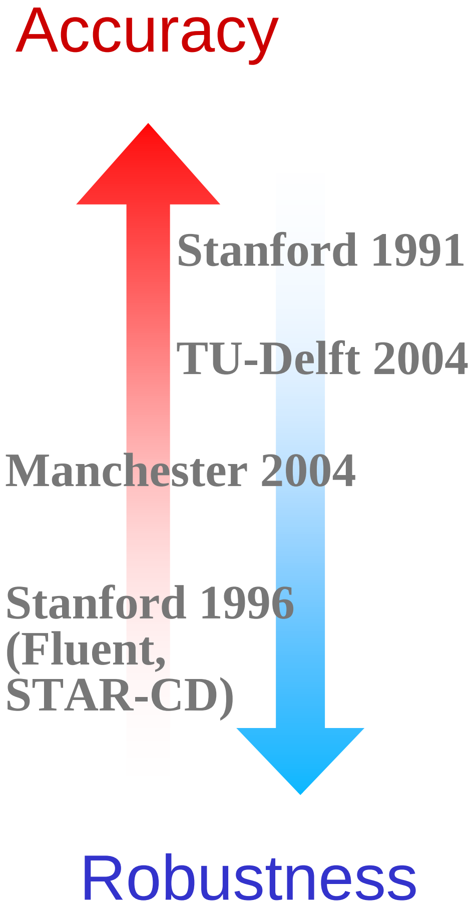
# *Buoyancy aided heated pipe flow*

## Gr/Re**2 = 0.241 (recovery)



# The $\overline{v^2}-f$ model and *Code_Saturne*

- A low-Reynolds (near-wall integration) eddy viscosity model derived from second moment closure models
- No damping functions, no wall functions, less empirical assumptions
- Best results on range of test cases, heat transfer and natural convection in particular.
- The original model is stiff (requires coupled solver or very small time-step)
- Degraded version available in StarCD, Fluent, NUMECA..
- Long collaboration Stanford, Delft, Chatou, Manchester (Durbin, Parneix, Hanjalic, Manceau, Uribe)
  => "several code friendly" versions since 1995.
- Present: Reconsider all historical choices with numerical stability and known asymptotic states as principal objectives



Accuracy

**Stanford 1991**

**TU-Delft 2004**

**Manchester 2004**

**Stanford 1996 (Fluent, STAR-CD)**

Robustness

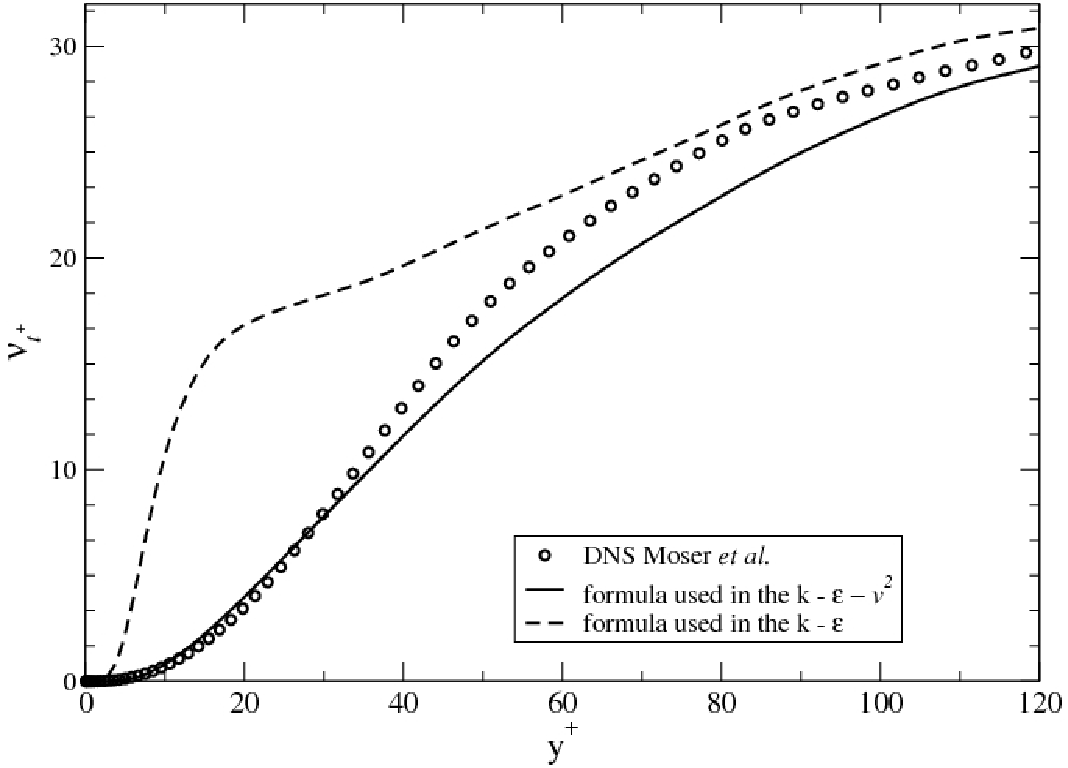
# Durbin's original model

Classic near wall model

$$\nu_t = f_\mu C_\mu k T \quad ; \quad T = k/\varepsilon$$

$$f_\mu = \frac{\nu_t \; you \; want}{\nu_t \; you \; have}$$

$$f_\mu = f(y^+, \nu_t/\nu)$$



Elliptic Relaxation

$$\nu_t = C_\mu \overline{v^2} T$$

$$\frac{D\overline{v^2}}{Dt} = \phi_{22} - \varepsilon_{22} + \nabla((\nu + \nu_t)\nabla\overline{v^2})$$

$$\phi_{22} = -\frac{2}{\rho}\overline{v\,\partial p'/\partial y}$$

the walls affect the whole domain through an elliptic operator : near wall effects (mainly wall echo and wall blocking effect)

# The usual second moment closure

- Usual closure for the source term of $\overline{v^2}$ :

$$\frac{D\overline{v^2}}{Dt} = \underbrace{\phi_{22} - \left(\varepsilon_{22} - \frac{2}{3}\varepsilon\right)}_{\varphi_{22}\ \text{Term to be modelled}} - \frac{2}{3}\varepsilon + Diff_{\nu+\nu_t}\overline{v^2}$$

Model for the dissipation : $\varepsilon_h = \frac{2}{3}\varepsilon$

Launder Reece Rodi (LRR) :

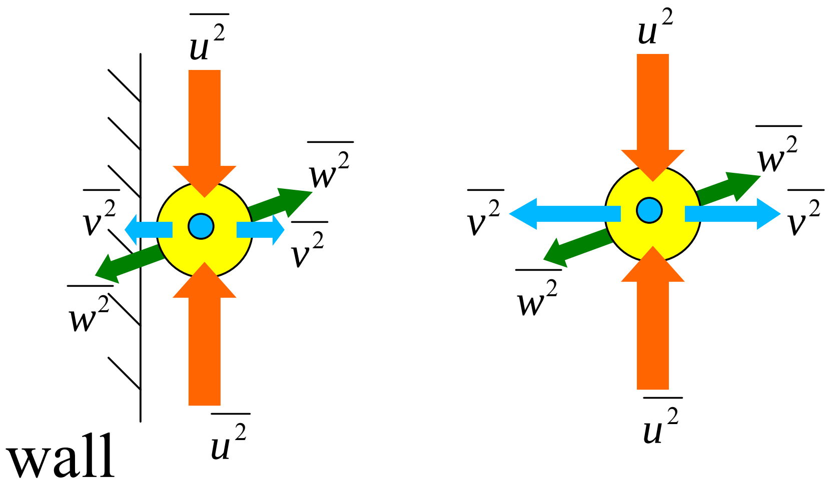
$$\varphi_{22}^h = -\frac{1}{T}C_1\left(\frac{\overline{v^2}}{k} - \frac{2}{3}\right) + C_2\frac{P}{k}$$

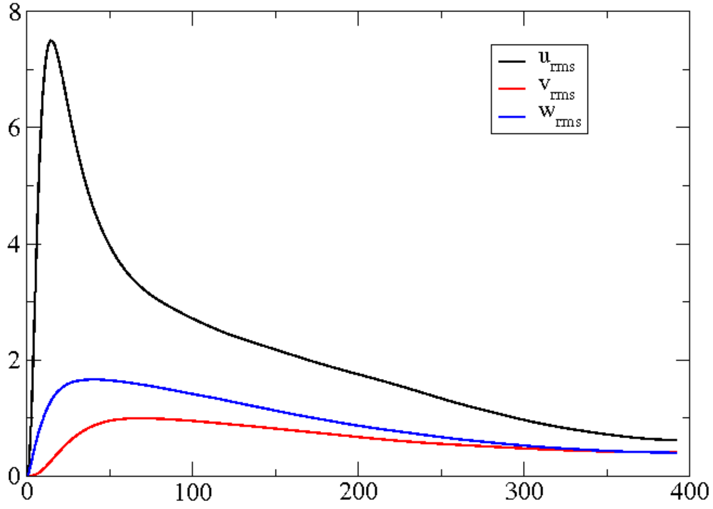
Speziale, Sarkar, Gatski (SSG) :

$$\varphi_{22}^h = -\frac{1}{T}\left(C_1 + C'_2\frac{P}{\varepsilon}\right)\left(\frac{\overline{v^2}}{k} - \frac{2}{3}\right) - \left(\frac{C_4}{3} - C_5\right)\frac{P}{k}$$

Wall blocking effect:

The redistribution is anisotropic near the wall





# The asymptotic behaviour

- Near wall limit of the *k* –eps model $k = O(y^2)$ $\varepsilon = O(1)$

$$\frac{Dk}{Dt} = \underset{(\,O(1)+O(y^3)\,).\Delta O(y^2)}{(\nu+\nu_t)\,\Delta k} + \overset{O(y^3)}{P} - \underset{O(1)}{\varepsilon} \approx \nu\Delta k - \varepsilon \approx \nu\Delta k^{n+1} - \left(\frac{\varepsilon}{k}\right)^{n} k^{n+1}$$

Negative
but implicit
source

**No stability problem**

# The asymptotic behaviour

**two-component limit of the turbulence**

- Taylor series expansion : $\overline{u^2} = O\left(y^2\right)$ $\overline{w^2} = O\left(y^2\right)$ $\overline{v^2} = O\left(y^4\right)$

**term to be modelled**

$$\frac{D\overline{v^2}}{Dt} = \underbrace{\nu\frac{\partial^2 \overline{v^2}}{\partial x_k^2}}_{O\left(y^2\right)} - \underbrace{\frac{\partial \overline{v^2 u_i}}{\partial x_i}}_{O\left(y^5\right)} + \underbrace{\overbrace{\phi_{22}}^{O(y)} + \overbrace{D_{22}^p}^{O(y)}}_{O\left(y^2\right)} - \underbrace{\left(\varepsilon_{22} - \frac{\varepsilon}{k}\overline{v^2}\right)}_{O\left(y^2\right)} - \underbrace{\frac{\varepsilon}{k}\overline{v^2}}_{O\left(y^2\right)}$$

$Ay^2$ $By^2 = k\ f$ $Cy^2$

**The balance between quadratic terms must be ensured**

$$A \ + \ B \ + \ C \ = 0 \quad near\ the\ wall$$

$$(+6) + (-5) + (-1) = 0$$

$$L^2\nabla^2 f - f = f_{\mathrm{hom}} \qquad with \qquad \lim_{y\to 0} f = -20\nu^2 \lim_{y\to 0}\left(\frac{\overline{v^2}}{\varepsilon\, y^4}\right) \quad => \quad = \ -\frac{O(y^4)}{O(y^4)}\ !$$

# Stanford “code friendly” model (1)

Lien and Durbin (1996)

- It involves a change of variable $f = \bar{f} + g$ so that $\lim_{y \to 0} \bar{f} = 0$

Original Durbin : $$0 = Ay^2 + \underset{k\ f}{By^2} + Cy^2$$

Stanford : $$0 = Ay^2 + \underset{k\ f - k\ g}{By^2 - Dy^2} + Cy^2 + \underset{k\ g}{Dy^2}$$

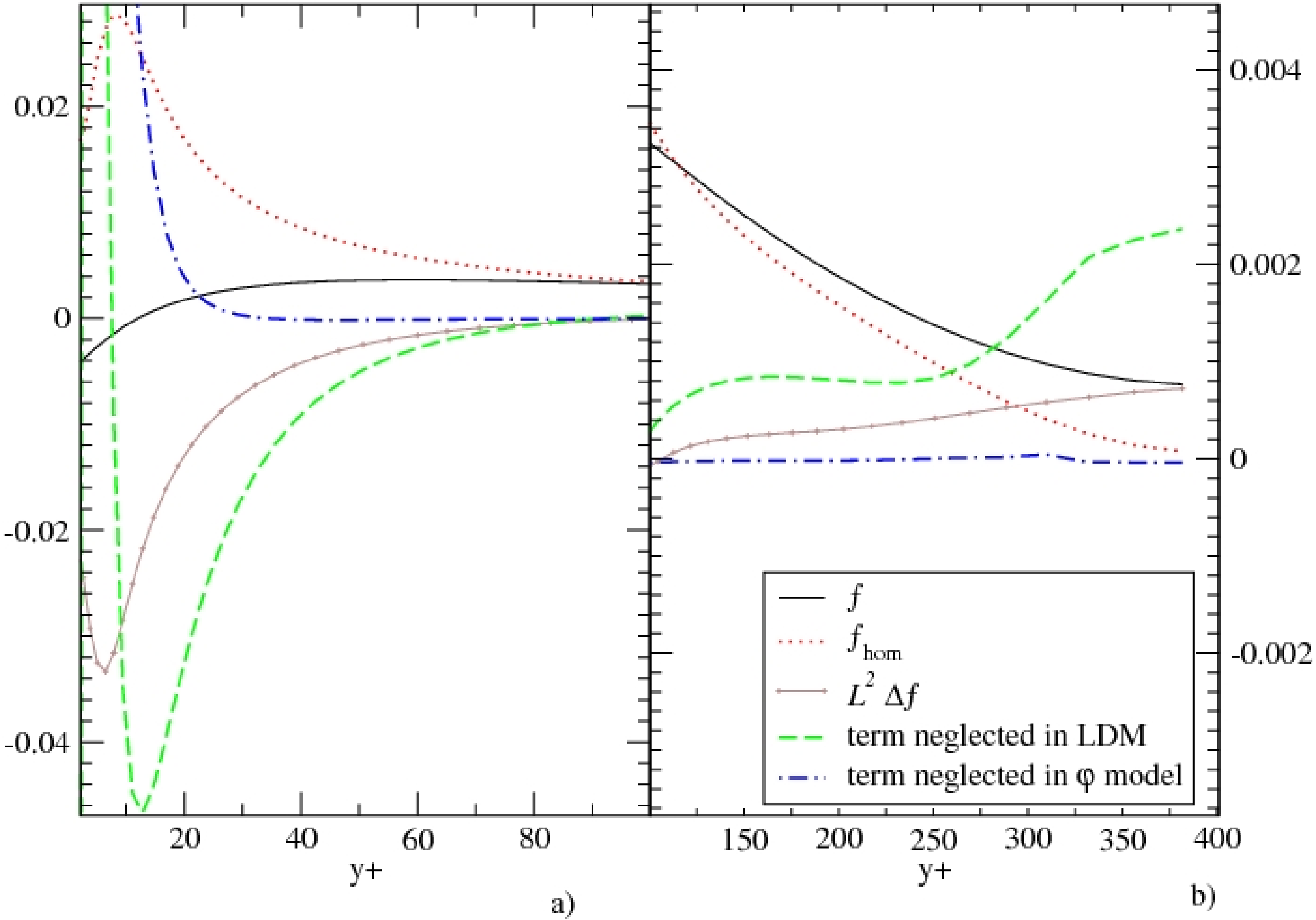
$$B - D = 0$$

- The new equation for f reads :

$$L^2\nabla^2\bar{f} - \bar{f} = \frac{C_1 - 1}{T}\left(\frac{\overline{v^2}}{k} - \frac{2}{3}\right) - C_2\frac{P}{\varepsilon} + g - L^2\nabla^2 g$$

**neglected term**

# Stanford "code friendly" model (2)



# Delft / UMIST approach

UMIST (Laurence *et al.* (2004)) and TU-Delft (Hanjalic *et al.* (2004))

- A new change of variable to reduce the stiffness of the B.C. : $\varphi = \frac{\overline{v^2}}{k} \Rightarrow f_w = -2\varepsilon\frac{\varphi}{y^2}$

$$\frac{D\varphi}{Dt} = \underbrace{f}_{A} - P\frac{\varphi}{k} + \frac{2}{k}\left(\underbrace{\nu}_{B} + \frac{\nu_t}{\sigma_k}\right)\underline{\nabla}\varphi\underline{\nabla}k + \nabla\left(\left(\underbrace{\nu}_{C} + \frac{\nu_t}{\sigma_\varphi}\right)\nabla\varphi\right)$$

$$A = -(B+C) \qquad near\ the\ wall$$

<u>UMIST</u> $\varphi$ model

$$\overline{f} = f + \frac{2}{k}\nu\underline{\nabla}\varphi\underline{\nabla}k + \nu\nabla^2\varphi$$

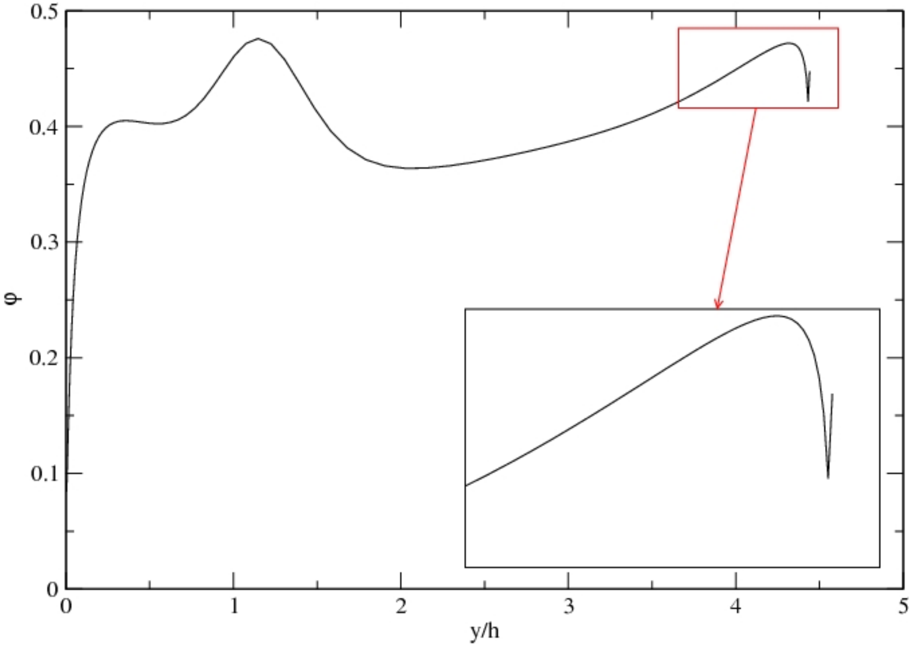
$$f_w = 0$$

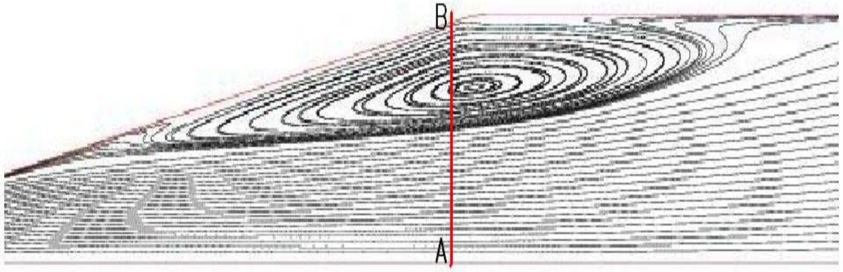
<u>Delft</u> $\varsigma$ model

$$f_w = -2\varepsilon\frac{\varsigma}{y^2}$$

# Numerical stability vs. accuracy

## Numerical instabilities of the $\varphi = \frac{\overline{v^2}}{k}$ model



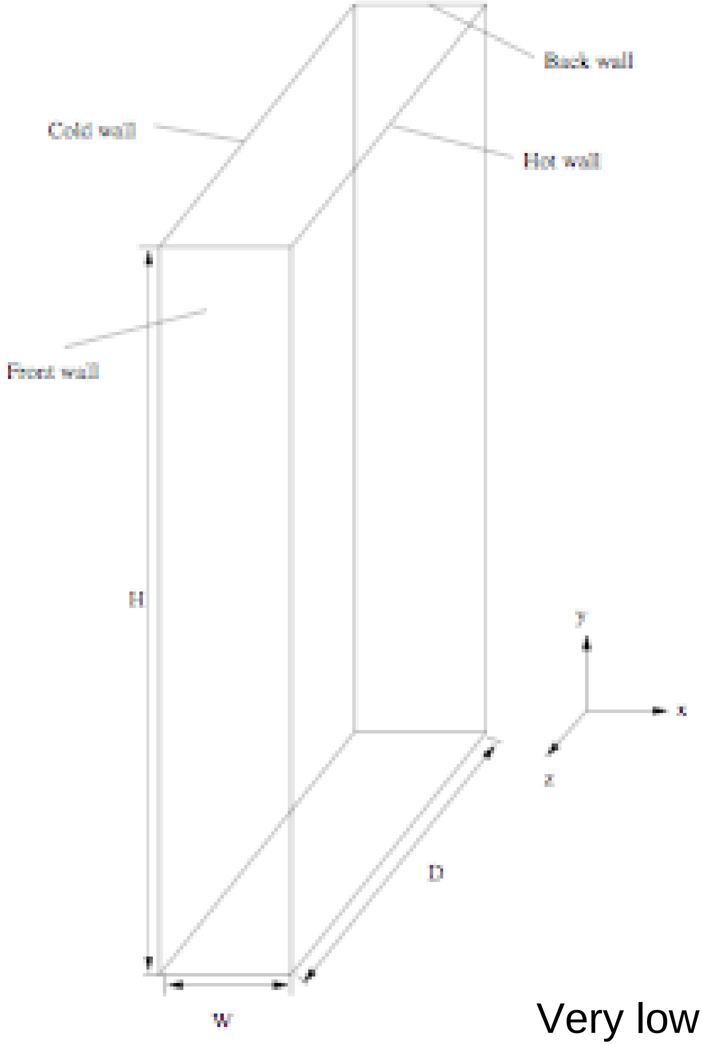


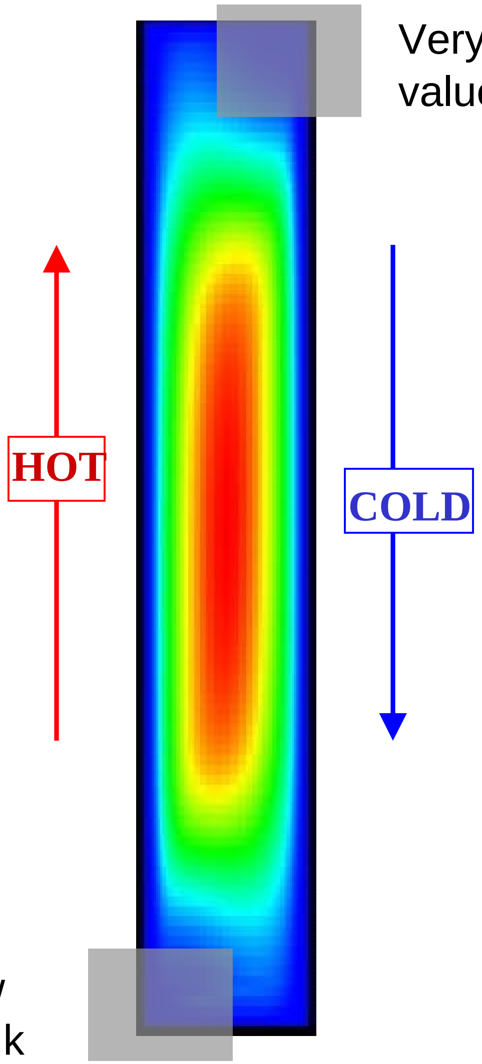
2 options :

- $f$ is forced to be equal to 0 at the wall : excellent robustness, similar to the one of Stanford's model, but bad prediction of the turbulent viscosity near the wall.
- the turbulent viscosity is removed : numerical instabilities

# Natural convection in a heated cavity

*(non convergence in C_S V 1.2 !)*





Very low value of k

Very low value of k

*Code_Saturne*

$\varphi$ model

$$\overline{f} = f + \frac{2}{k}\nu\,\underline{\nabla\varphi}\,\underline{\nabla k} + \nu\nabla^2\varphi$$

## Final model

# The $\varphi - \alpha$ model

- Using the elliptic blending of Manceau and Hanjalic 2002 (with Re stress model)

$$L^2\nabla^2\alpha - \alpha = -1 \qquad \Big| \qquad \alpha_w = 0$$

$$\frac{D\varphi}{Dt} = \alpha^3 f_{hom} + \left(1-\alpha^3\right) f_w - P\frac{\varphi}{k} + \frac{2\nu_t}{k}\underline{\nabla}\varphi\underline{\nabla}k + \nabla\left(\left(\nu + \frac{\nu_t}{\sigma_\varphi}\right)\nabla\varphi\right)$$

$$f_w = -\varepsilon\frac{\varphi}{y^2} \quad \Longrightarrow \quad f_w - \nu\nabla^2\varphi = o(1)$$

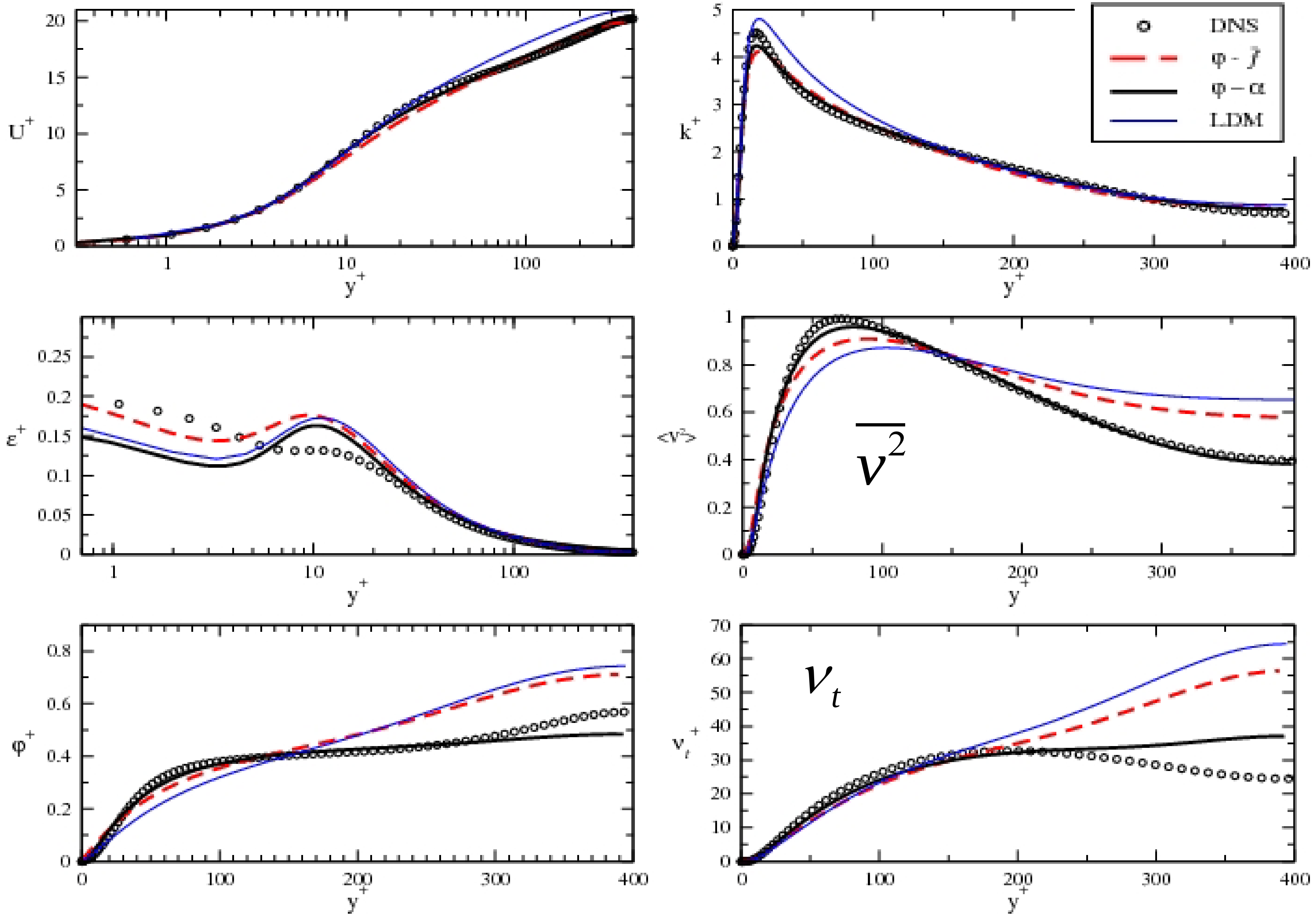
☐ Successfully tested on channel flows for many Re numbers, flow around airfoil trailing edge, heated pipe, heated channel flow, heated cavity

☐ Normal time-step (external flow CFL values as for k-omega)

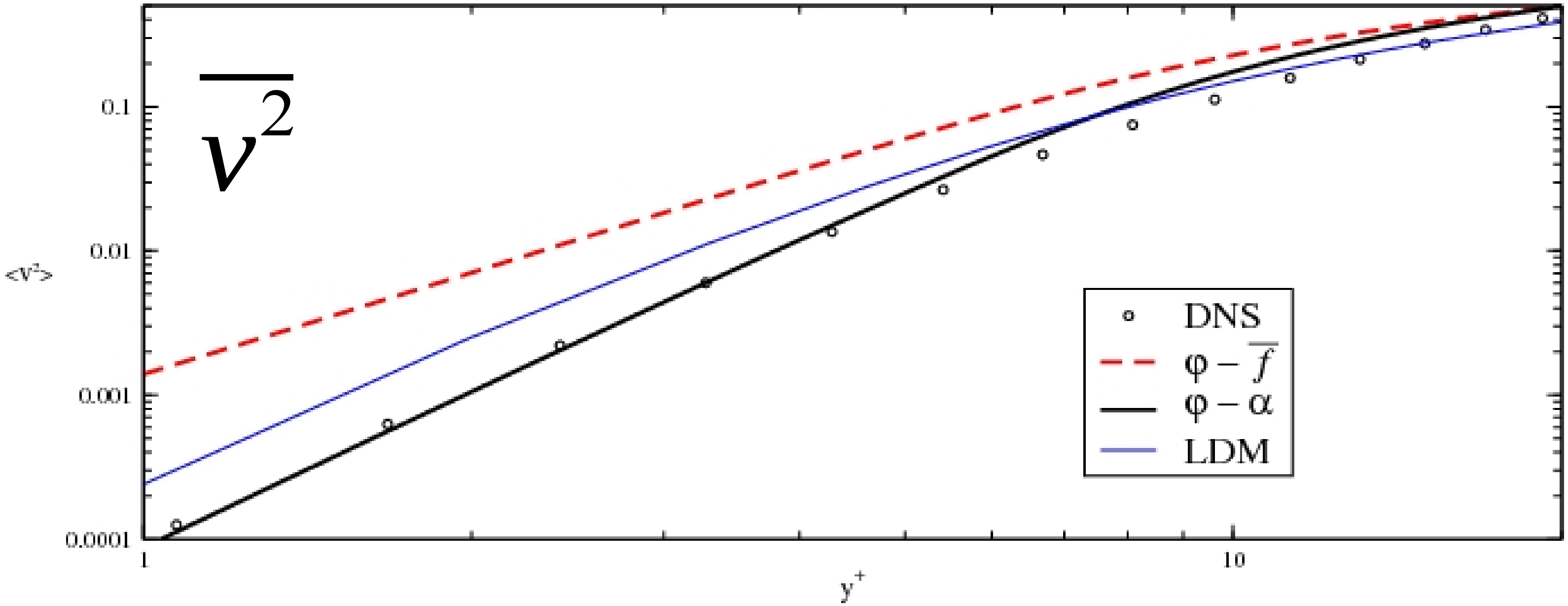
☐ Unlike, code friendly Stanford model, no term has been neglected here

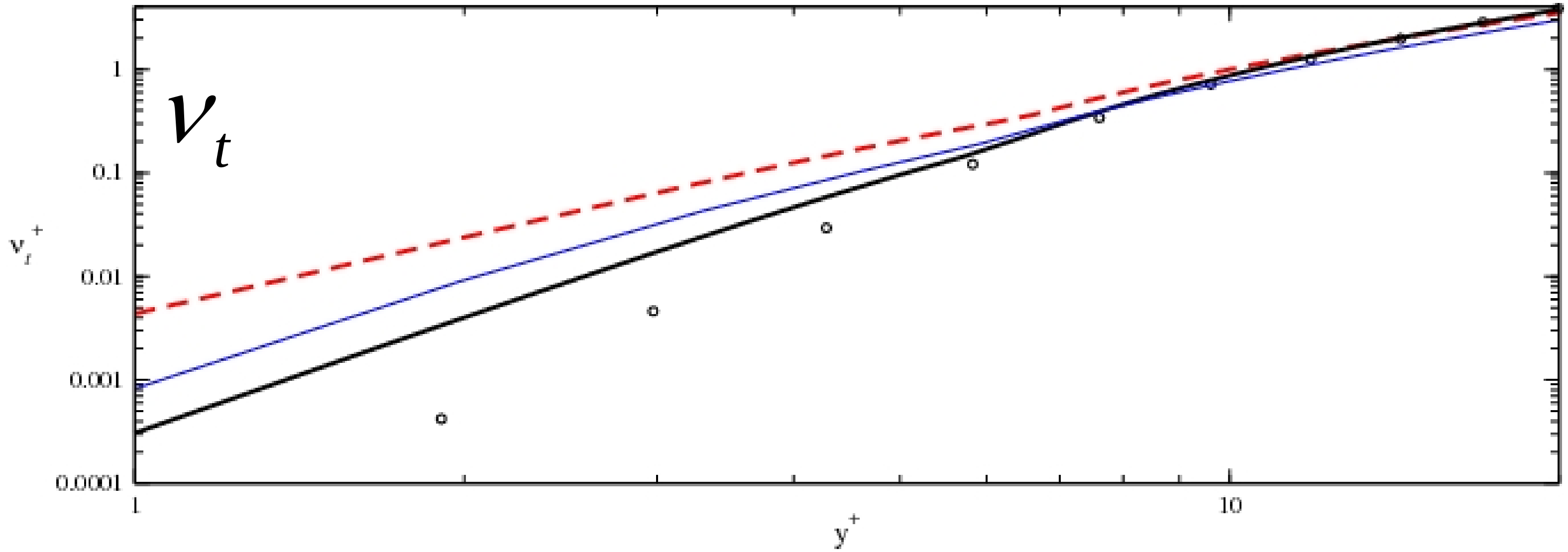
☐ Unlike UMIST and Delft model, the correct asymptotic behaviour of $\overline{v^2}$ and $\nu_t$ is accurately predicted without impairing the numerical robustness

# Results (Channel flow, Re*=395



# Results (Channel flow, Re*=395) (2)





# Conclusions and further work

- 4 different versions of V2F revisited => numerical stability improved while respecting known asymptotic states,

- Relaminarisation OK,
  next: prediction of laminar-turbulent transition,
  input some ingredients of Launder and Sharma model
  (extra viscous source terms in epsilon equation)

- Recalibration of source terms in the $\varepsilon$ equation
  (all literature focuses only on near wall layer
  but prediction of the core region can be improved)

- An accurate and robust near-wall low-Reynolds RANS model also suitable for RANS/LES coupling

[1] Launder, B.E. and Sharma, B.I., 1974, *“Application of the energy dissipation model of turbulence to the calculation of flow near a spinning disc”*, Lett. Heat Mass Transfer, 1, pp. 131-138.
[2] Cotton, M.A., Ismael, J.O., 1998, *“A strain parameter turbulence model and its application to homogeneous and thin shear flows”,* Int. J. Heat Fluid Flow 19, pp. 326–337.
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[4] Wilcox, D.C. 1998, *“Turbulence Modelling for CFD”,* 2nd edition, DCW Industries, Inc.
[5] Durbin, P.A. 1995, *“Separated flow computations with the* $k$-$\varepsilon$-$v2$ *model”* , *AIAA Journal*, 33(4), pp. 659–664.
[6] Laurence, D., Uribe, J.C. and Utyuzhnikov, S., 2004, *“ A robust formulation of the v2-f model”,* Flow, Turbulence and Combustion, 73, pp. 169-185
[7] You, J., Yoo, J.Y. and Choi. H., 2003, *“Direct Numerical Simulation of Heated Vertical Air Flows in Fully Developed Turbulent Mixed Convection”*, Int. J. Heat Mass Transfer, 46, pp.1613-1627