UNIVERSITEIT GENT

FACULTY OF ENGINEERING AND ARCHITECTURE

3D reactor technology for steam cracking: simulation and experimental validation

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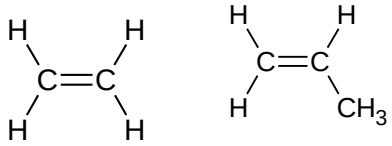
CHEMREACTOR-XXII, London, United Kingdom,
19/09/2016

Steam cracking

Steam cracking

Base chemicals



- Endothermic process
- High temperatures (700 – 900 °C)
- Low partial pressure of hydrocarbons (atmospheric)
- Short residence times (0.1 – 0.5 s)

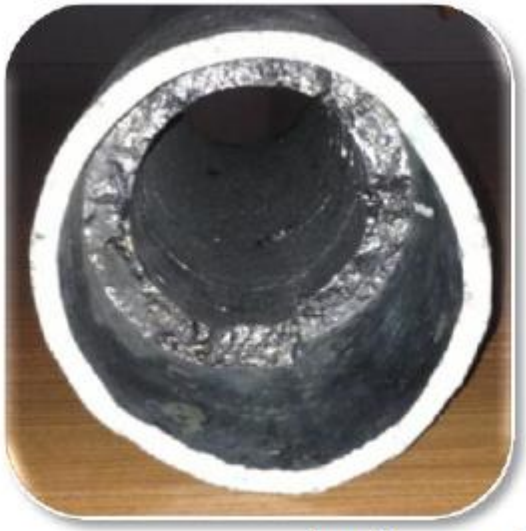
- 1.5 10^6 t/a of ethylene per plant

[1]H. Zimmermann and R. Walzl, "Ethylene," Ullmann's Encyclopedia of Industrial Chemistry, 2009.

Coke formation

Deposition of a carbon layer on the reactor surface

- ☒ Thermal efficiency
- ☒ Product selectivity
- ☒ Decoking procedures



[Muñoz, 2013]

Estimated annual cost to industry: $ 2 billion

Optimization by

- Feed additives
- Metallurgy & surface technology
- 3D reactor technology

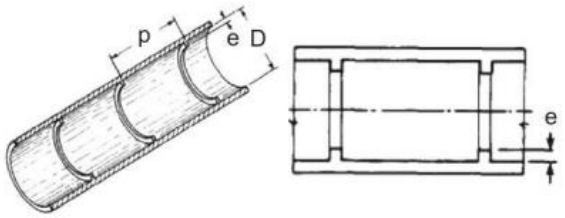
[2]L. Benum, "Achieving Longer Furnace Runs at NOVA Chemicals," in AIChE Spring National Meeting, 14th Annual Ethylene Producers' Conference, New Orleans, Louisiana, 2002.

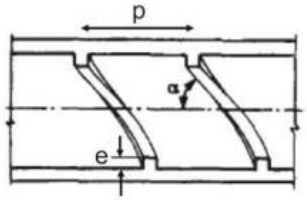
3D reactor technology

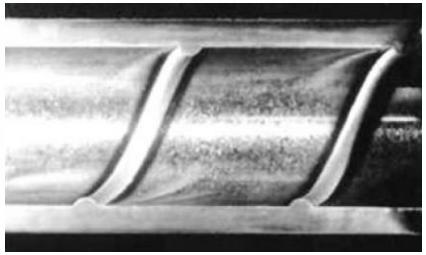
Improve the reactor by decreasing $T_{gas/coke}$

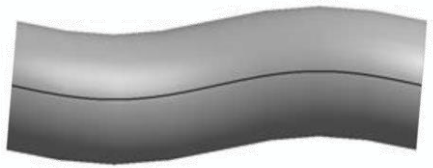
$$Q = U \cdot A \cdot \left(T_{gas/coke} - T_{bulk}\right)$$

- Increase tube area (A)
- Increase heat transfer coefficient (U)



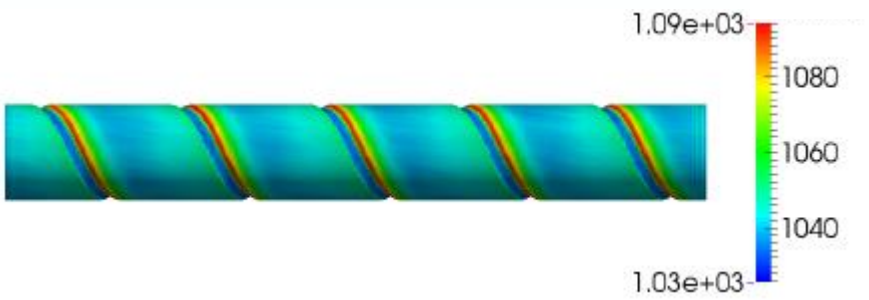


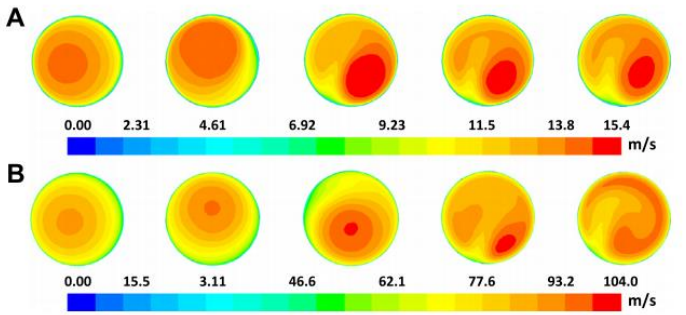


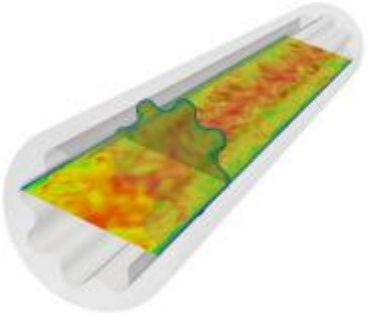


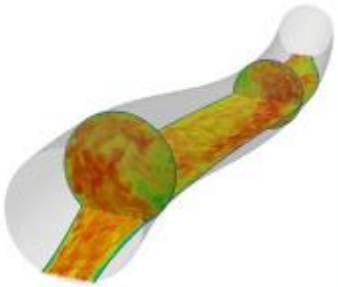
[3]M. Zhu, "Large eddy simulation of thermal cracking in petroleum industry," 2015.

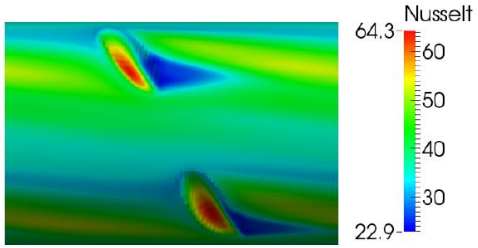
(3D) Simulations are needed



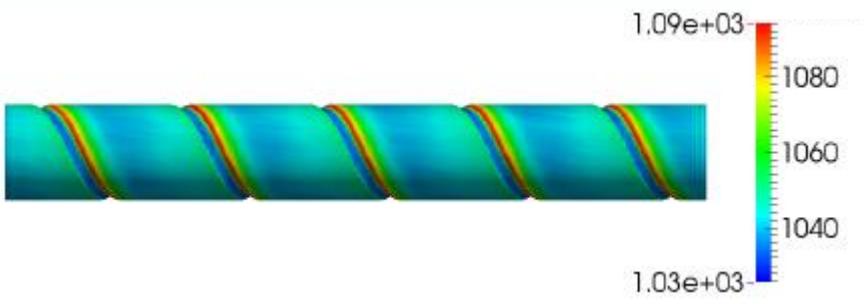


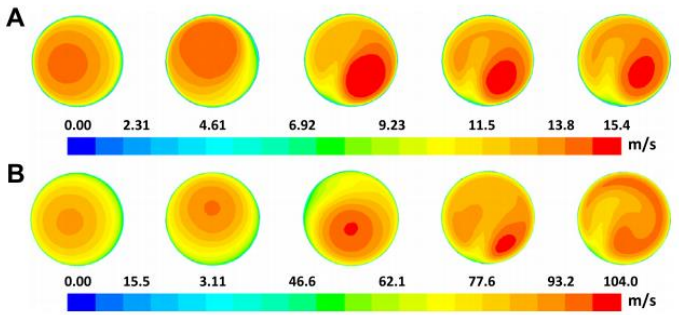


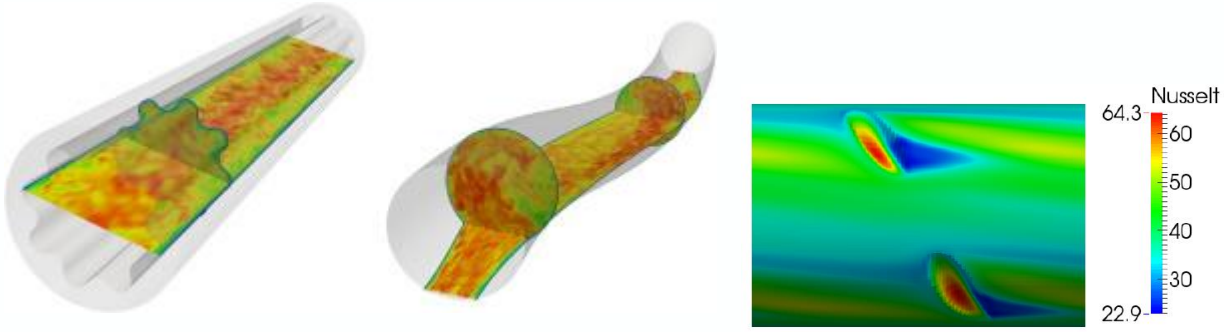




(3D) Simulations need validation



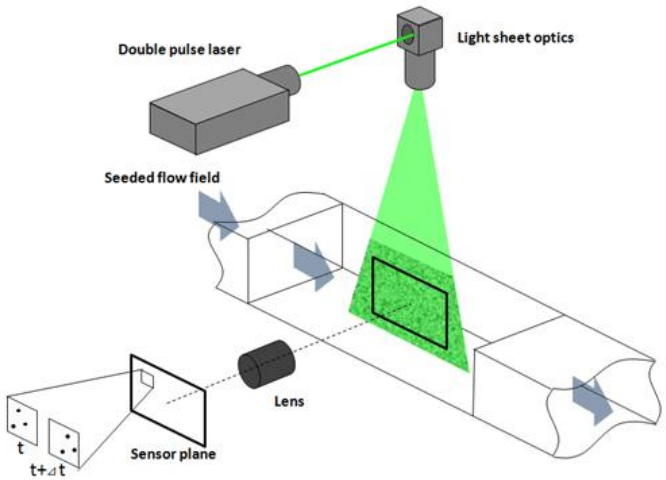




Computational Fluid Dynamics or Completely Flawed Data?

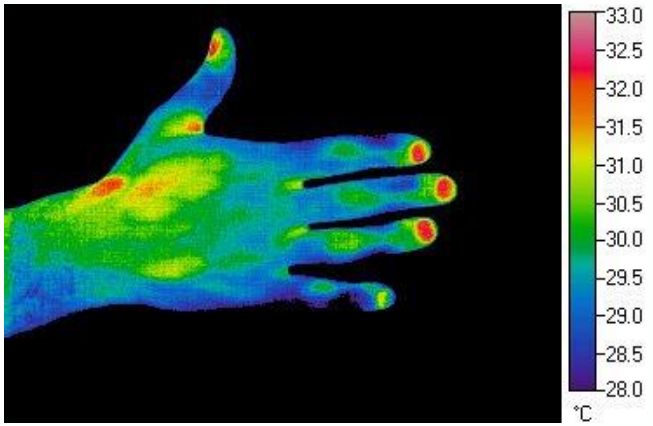
Experiments

PIV



Measuring velocity
and 3D flow profile

Liquid Crystal Thermography

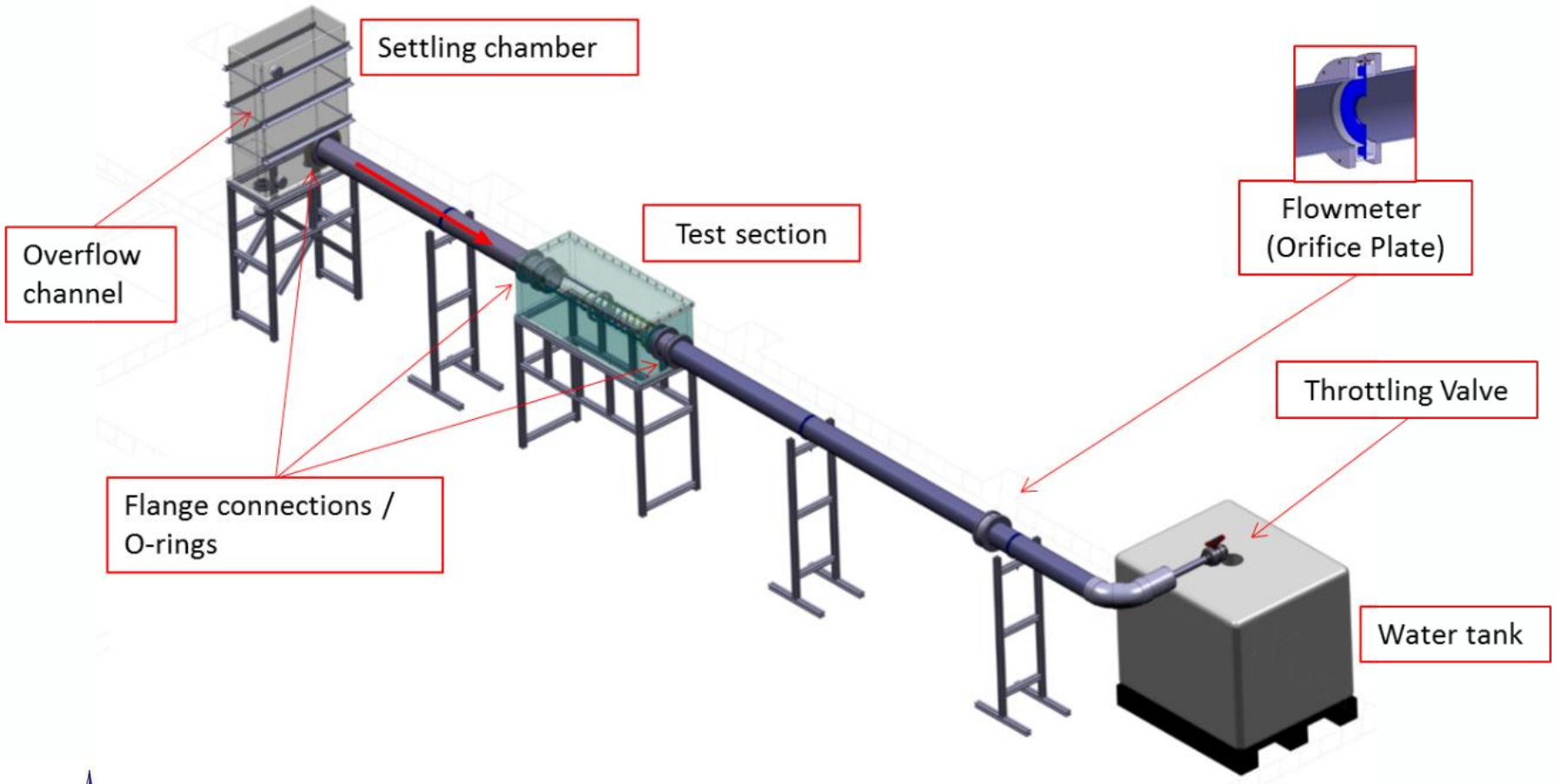


Measuring tube wall temperature
and heat transfer

The von Karman Institute
for Fluid Dynamics

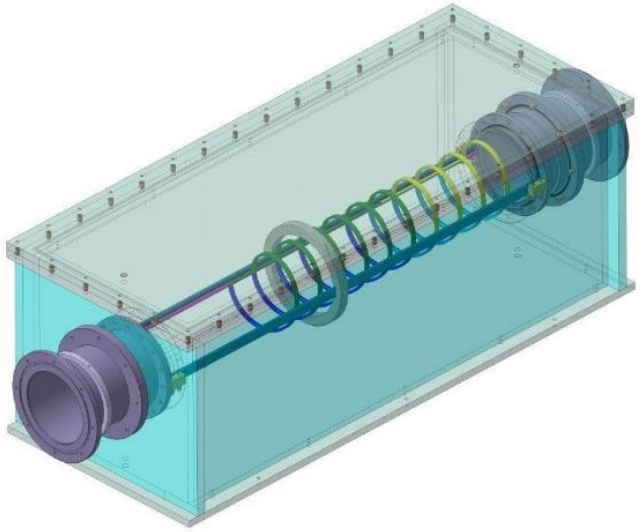
Both experiments were performed at the
von Karman Institute for Fluid Dynamics

PIV setup

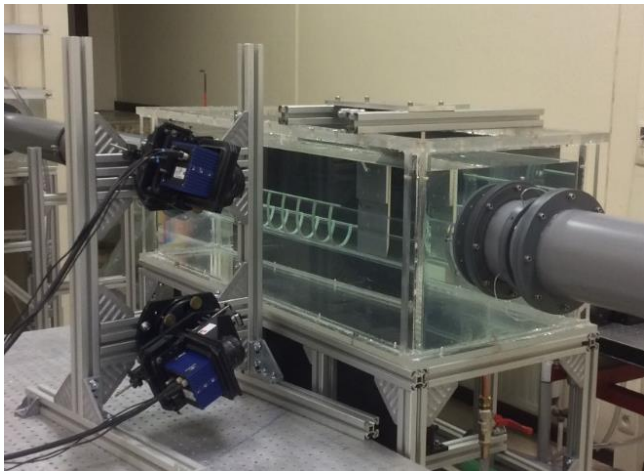


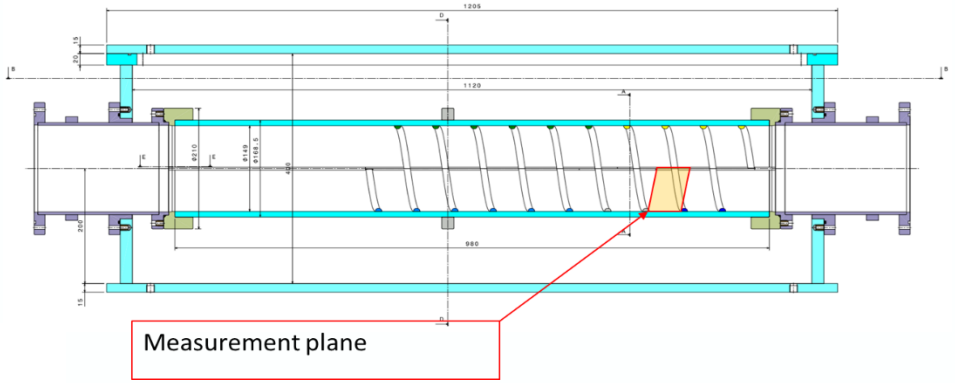
The von Karman Institute for Fluid Dynamics

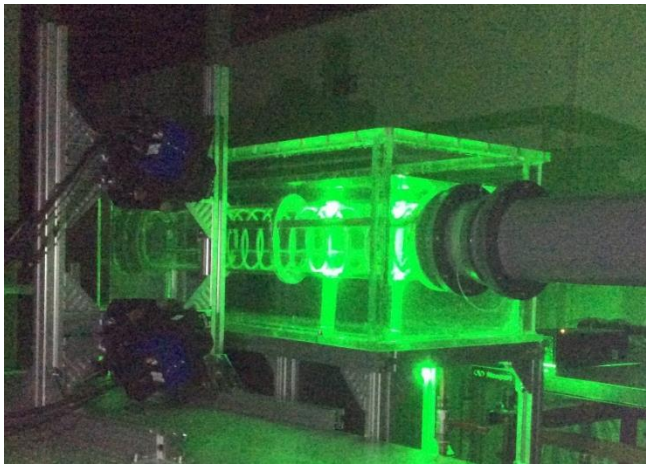
PIV setup



- Length = 980 mm
- D = 150 mm
- e = 5.4 mm
- P = 63 mm
- Re ~ 24000

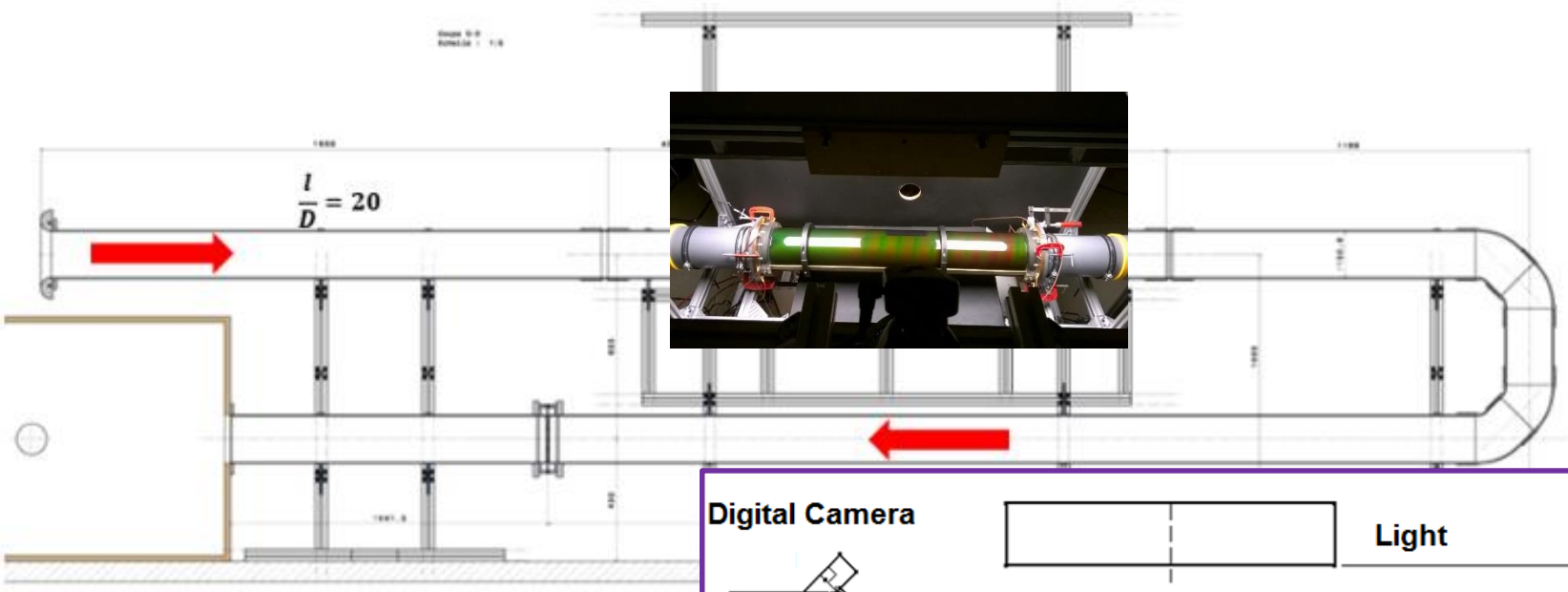


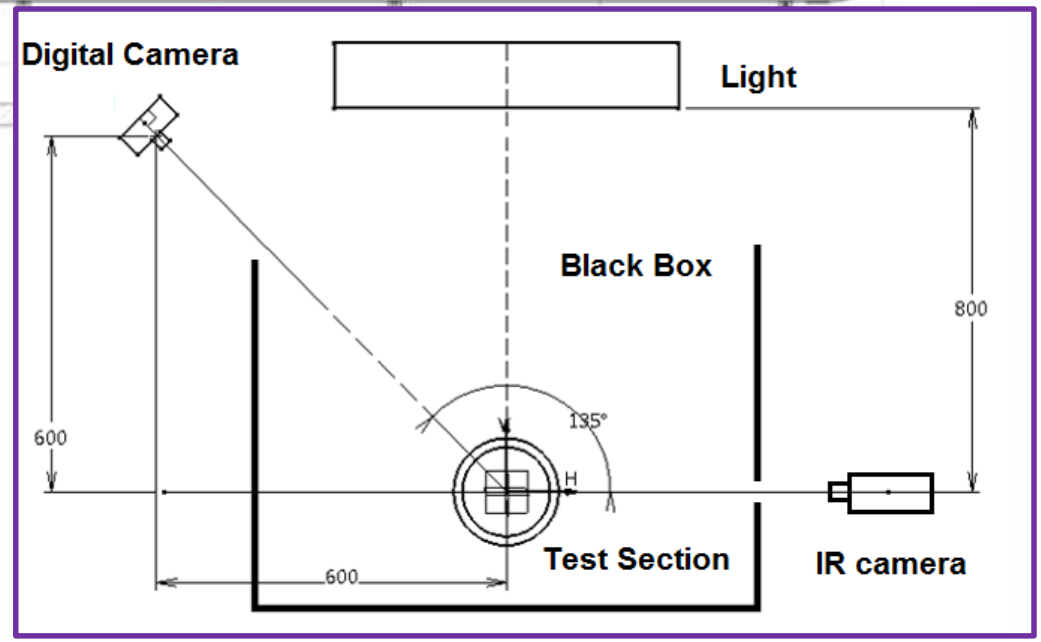




The von Karman Institute for Fluid Dynamics

Liquid Crystal Thermography setup





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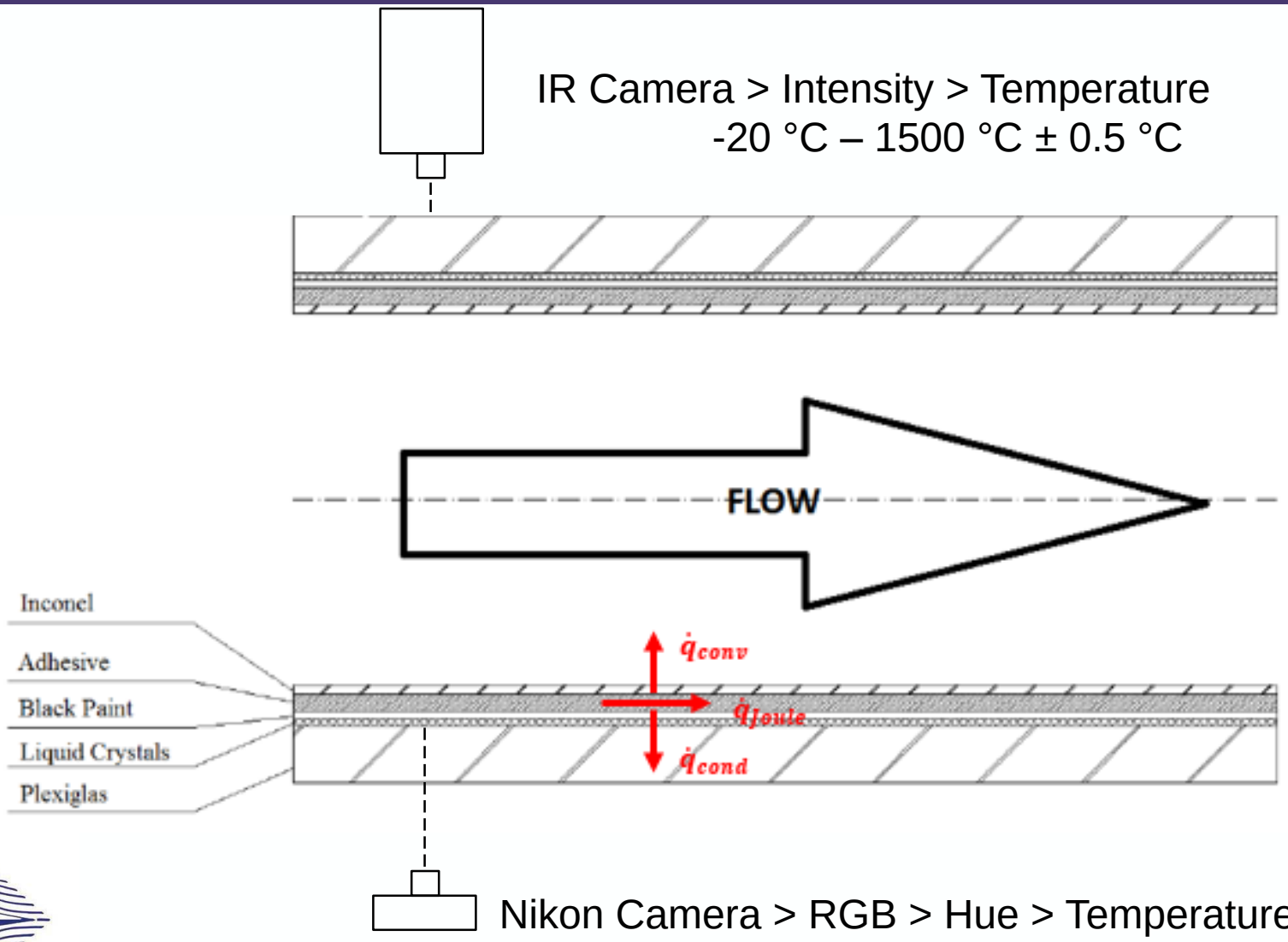
Liquid Crystal Thermography setup



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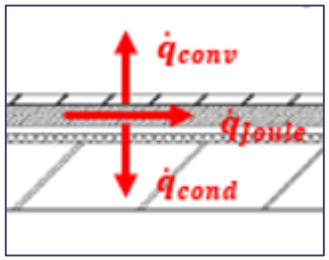
Obtaining Nusselt numbers



$$q_{conv}(z,\theta) = q_{Joule} - q_{cond}(z,\theta)$$

$$q_{Joule} = \frac{V \cdot I}{A}$$

$$h(z,\theta) = \frac{q_{conv}(z,\theta)}{T_{S,int}(z,\theta) - T_b(z)}$$

$$Nu(z,\theta) = \frac{h(z,\theta) \cdot D}{k(T)}$$

$$q_{cond}(z,\theta) = k(z) \cdot (T_{S,int}(z,\theta) - T_{S,ext}(z,\theta))$$

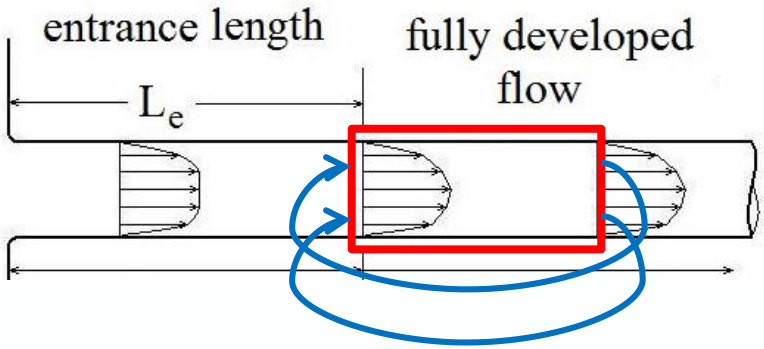
$$T_b(z) = T_{in} + (T_{out} - T_{in}) \cdot \frac{z}{L}$$

$$k(T) = \sum_{i=0}^{4} a_i T_b^i = k(z)$$

The von Karman Institute for Fluid Dynamics

Periodic simulations

Velocity profile independent of axial coordinate

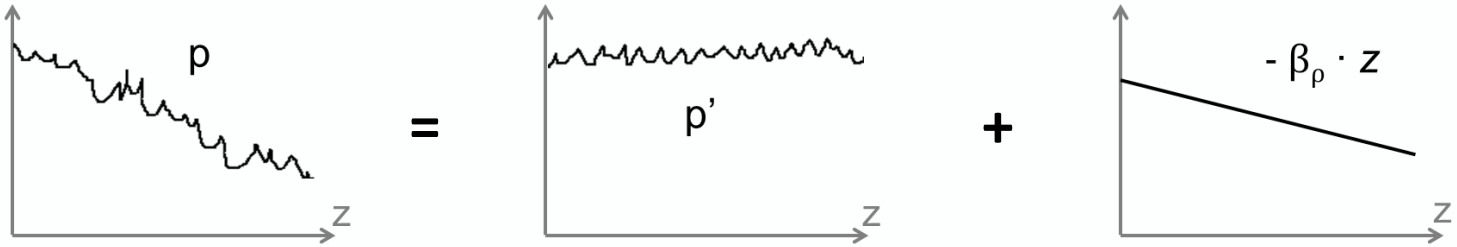


Computational domain can be limited by using
streamwise periodic boundary conditions

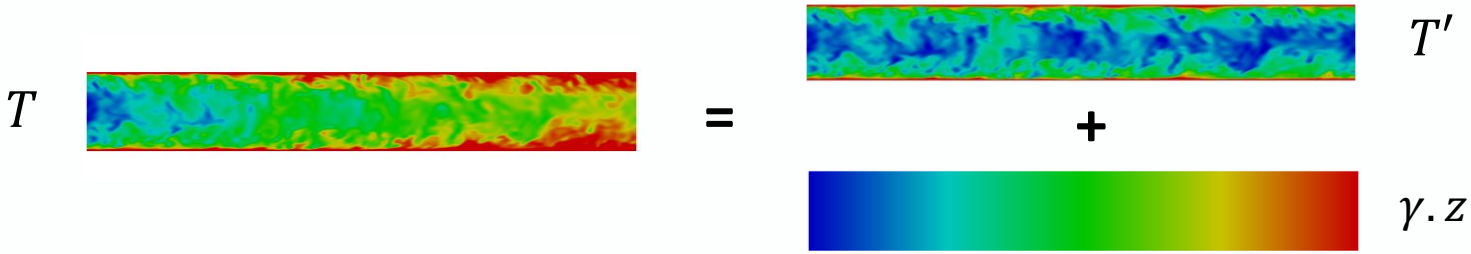
BUT: Pressure, temperature profiles are not periodic by nature

Periodic simulations

Forcing periodicity of pressure profile



Similar for temperature profile



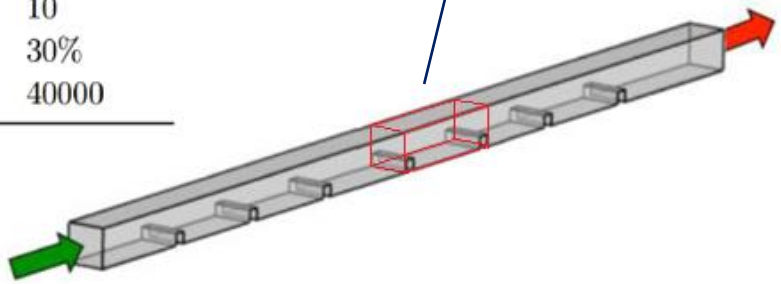
Momentum: $$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial (P'/\rho)}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} + \beta \vec{1}_{flow,i}$$

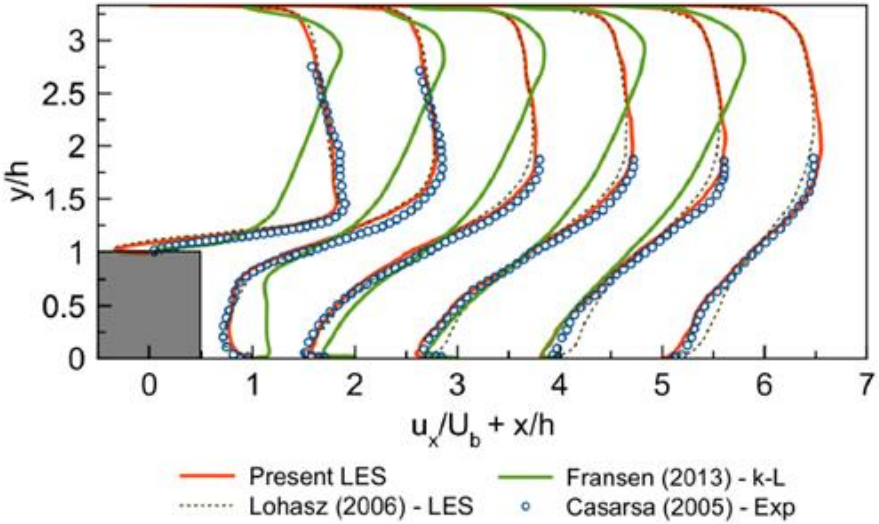
Energy: $$\frac{\partial T'}{\partial t} + U_j \frac{\partial T'}{\partial x_j} = \alpha \frac{\partial^2 T'}{\partial x_j \partial x_j} - U_{flow} \gamma$$

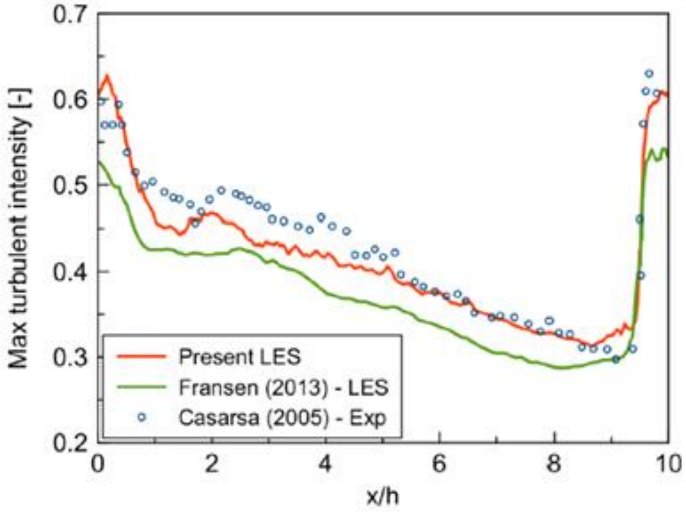
Validation – Ribbed duct (Re = 40000)

Channel section	square	Fluid	*Air*
Hydraulic diameter D_h	0.1 m	Inlet bulk velocity U_b	8.8 m · s^{-1}
Number of ribbed wall	1	Inlet bulk temperature	293 K
Ribs angle	90°	p/h	10
Ribs height h	0.03 m	h/D_h	30%
Ribs pitch p	0.3 m	Re	40000

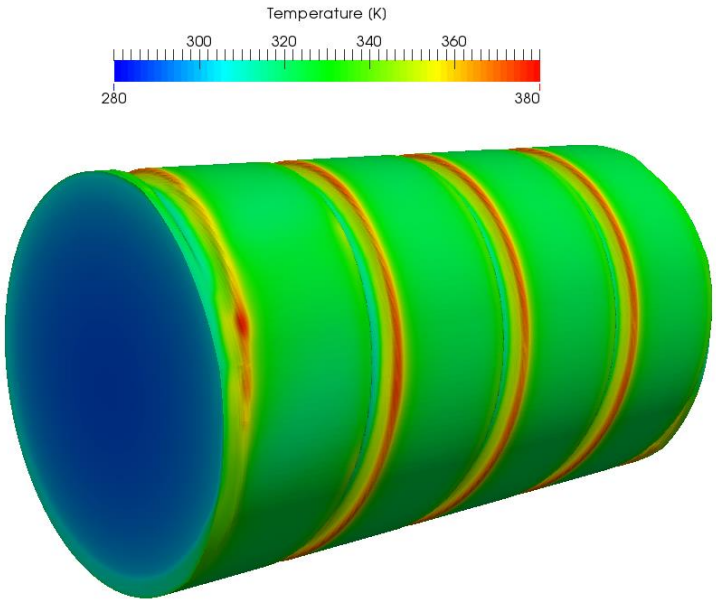
Computational domain
5 000 000 cells

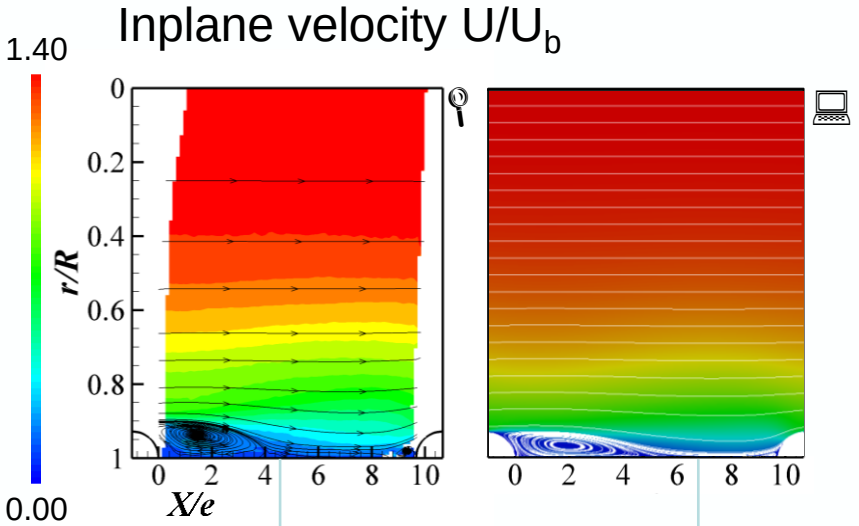






RANS Results



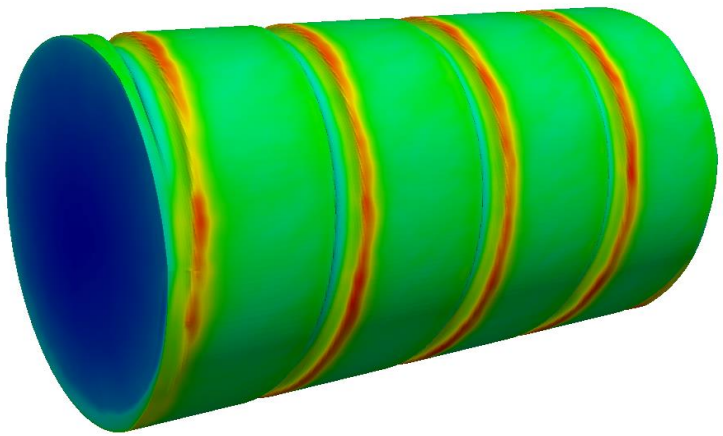


Reattachement point X/e = 4.3

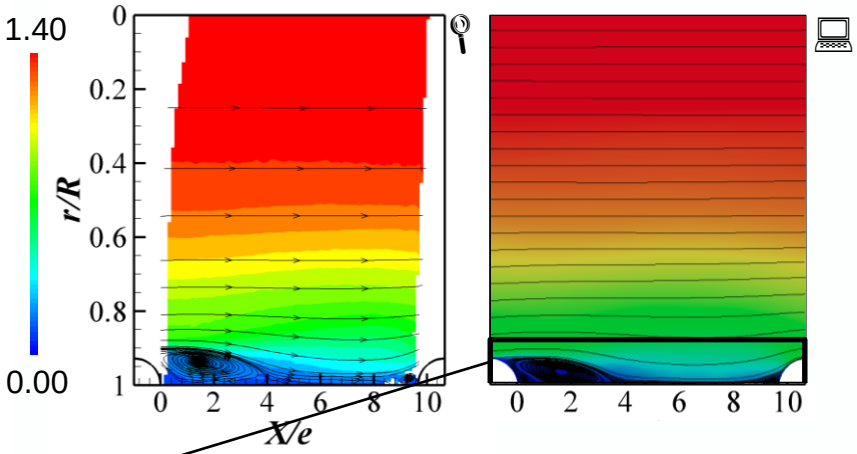
Reattachement point X/e ≈ 7

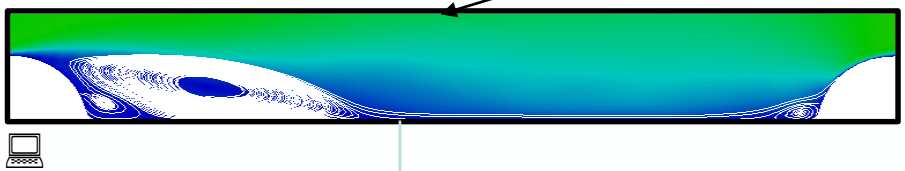
RANS simulations are not accurate enough to fully capture the flow field
➔ heat transfer will not be accurate

From RANS to LES



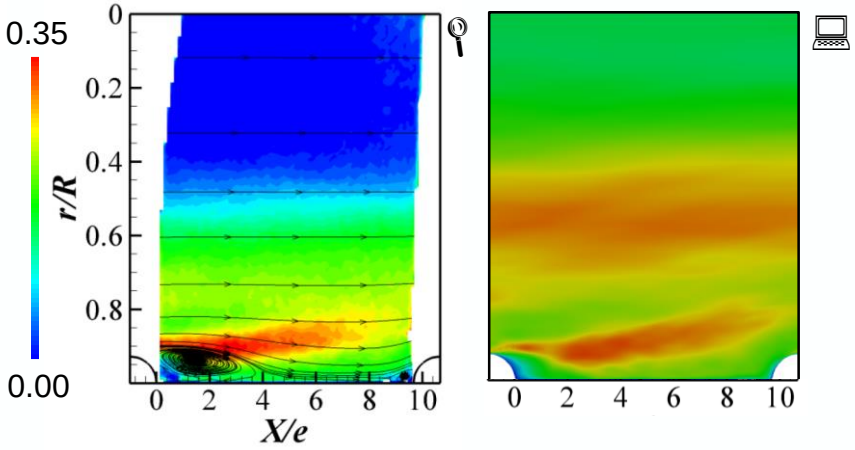
Inplane velocity U/U_b



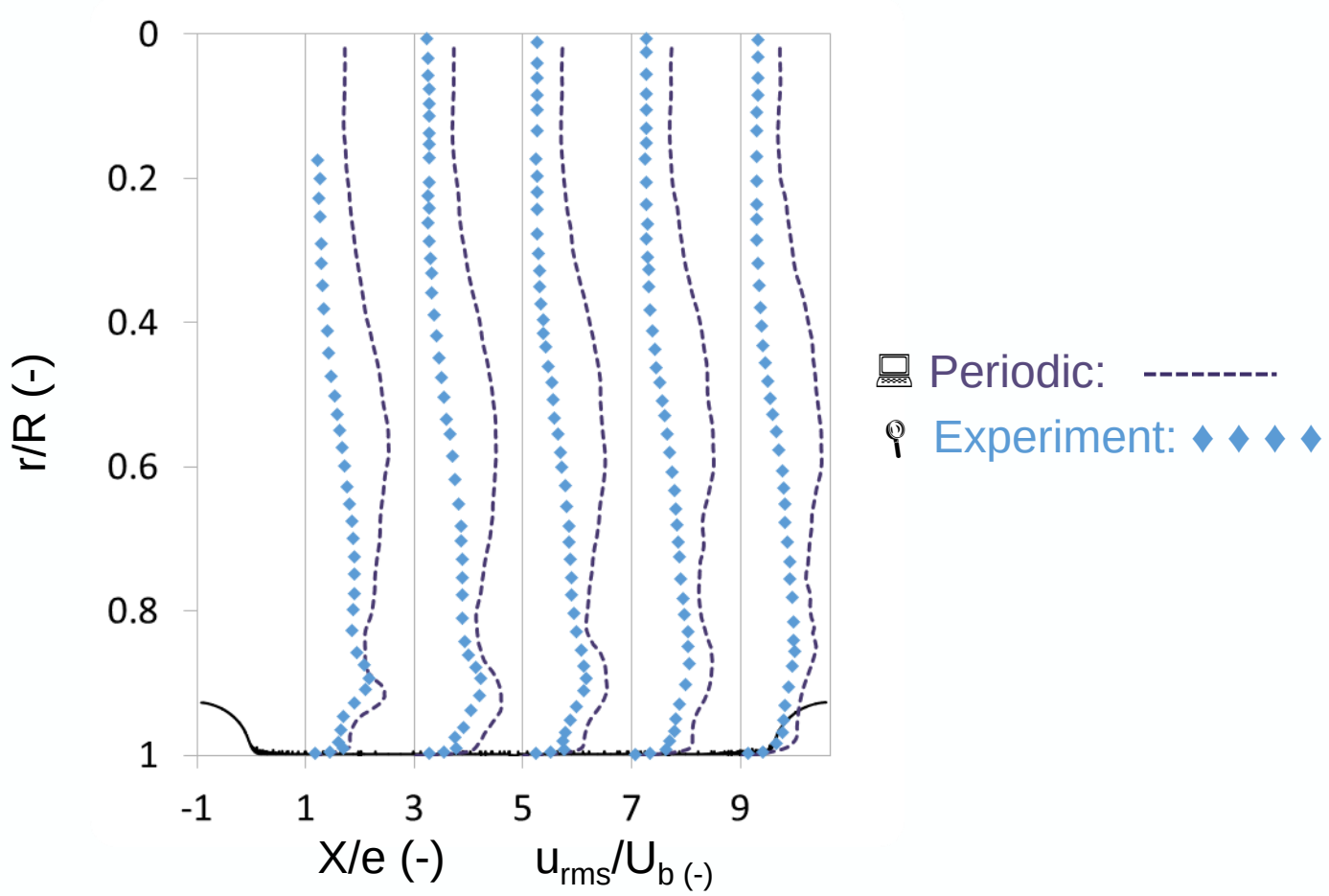


Reattachement point X/e = 4.8

Turbulent velocity fluctuations U_{rms}/U_b



Periodic simulations overpredict turbulence



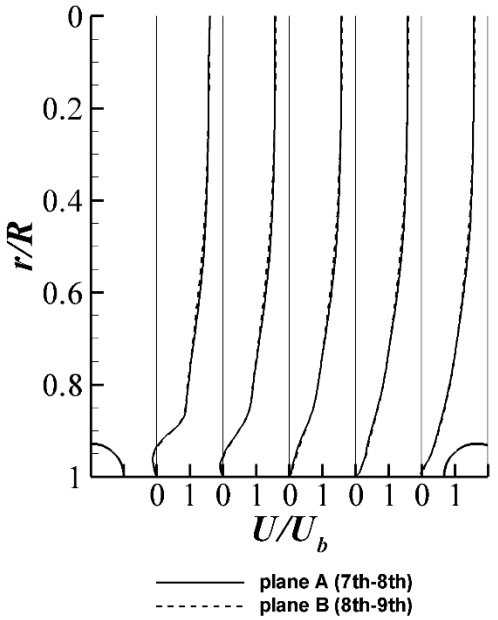
Periodic simulations have difficulties in reproducing the experimental values

Reasons for unsuccessful simulation?

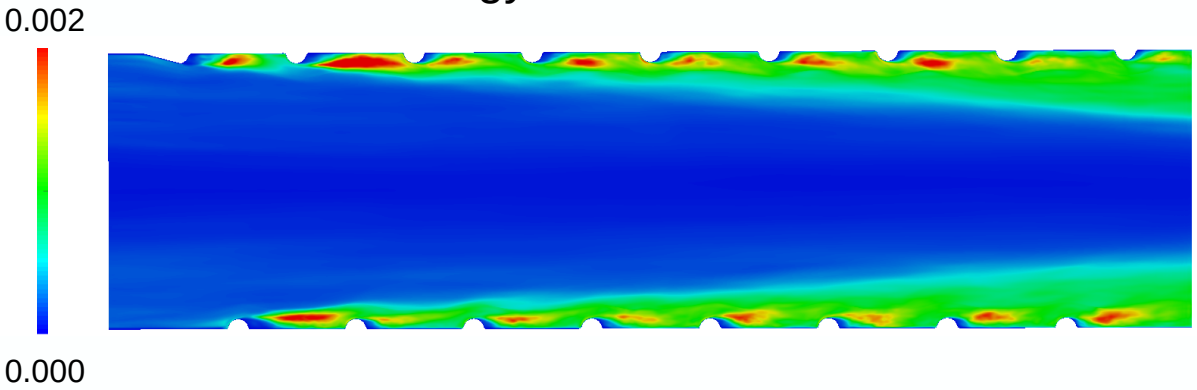
Correct BC? ✓

Wall resolved? ✓

Fully developed flow? ✗



Turbulent Kinetic Energy

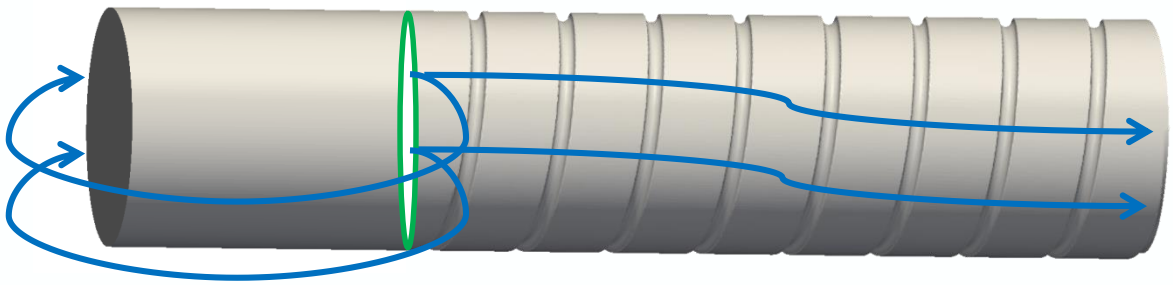


Assumption of fully-developed flow is not met

Current approach

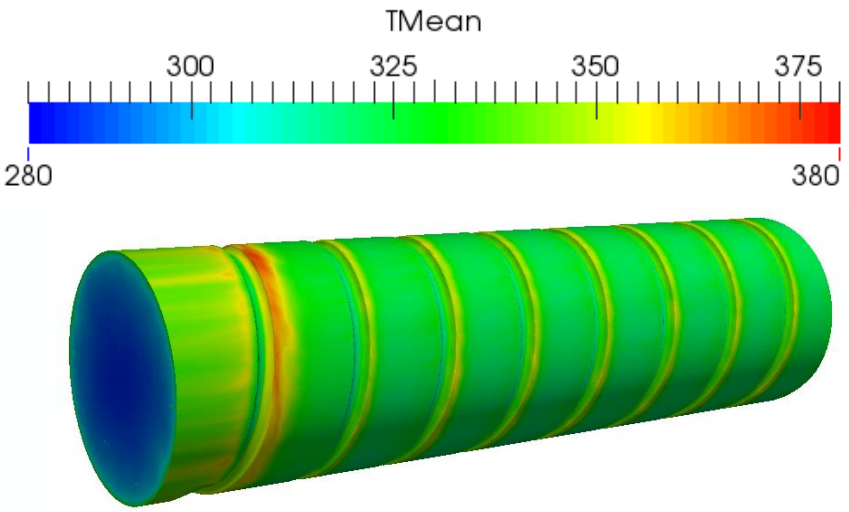
Simulation of the full experimental setup ≈ 30M cells

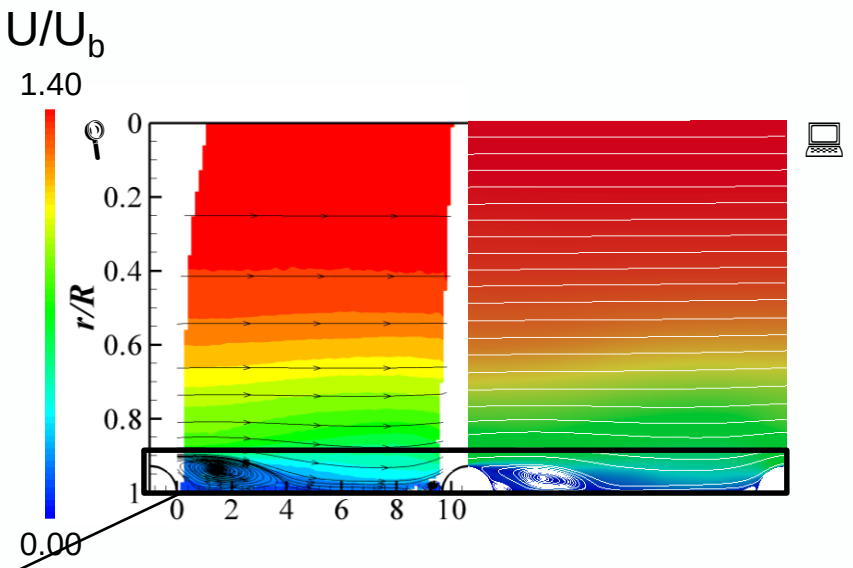
Cyclic boundaries over the bare inlet section, normal outflow conditions over the ribbed section

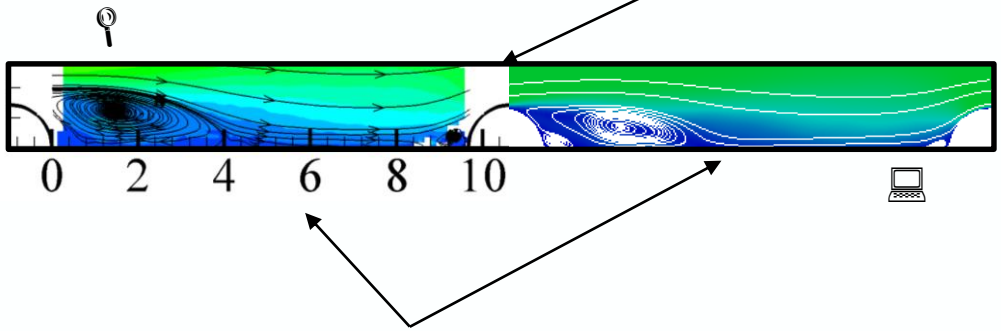


Database of 30 seconds of bare flow profiles, interpolated to the inlet of the ribbed test section

LES simulation of full domain

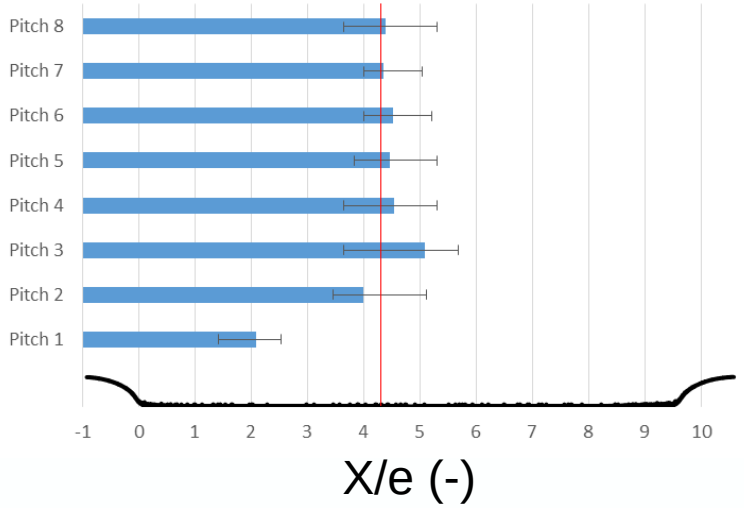




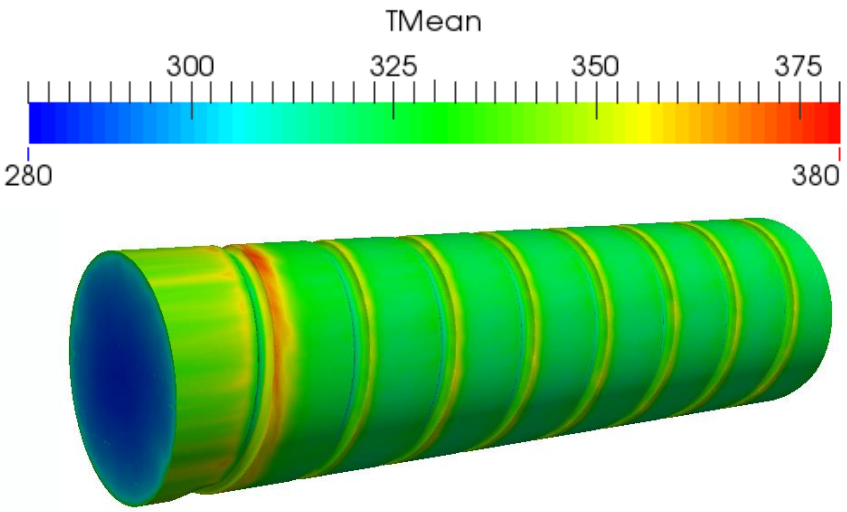


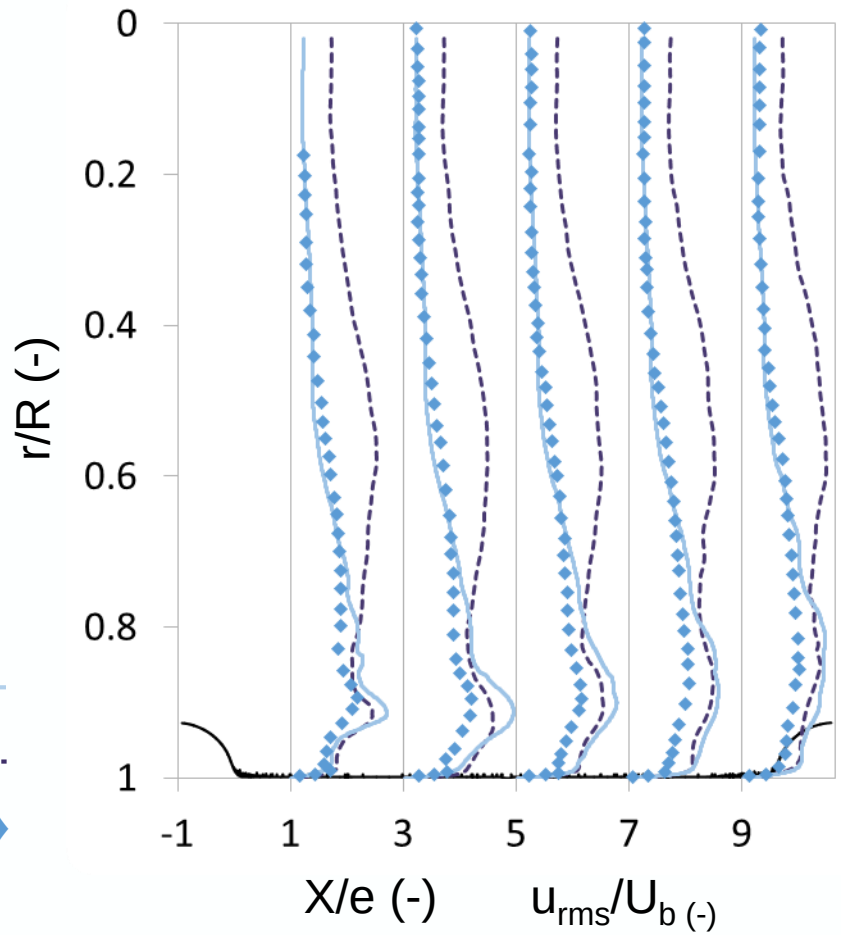
Reattachment behavior differs along the rib

Average reattachement point per pitch



LES simulation of full domain



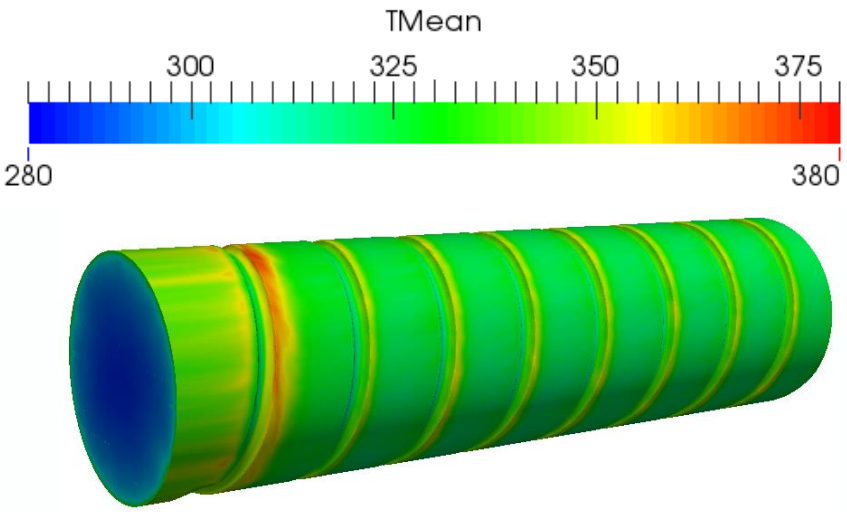


Full domain: ——

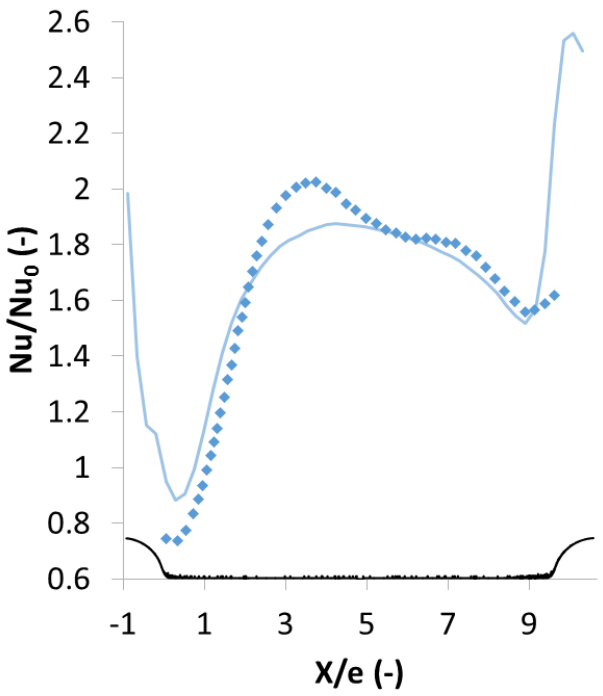
Periodic: --------

Experiment: ♦ ♦ ♦ ♦

LES simulation of full domain



Accurate description of flow is possible and shows more detailed information than experiments

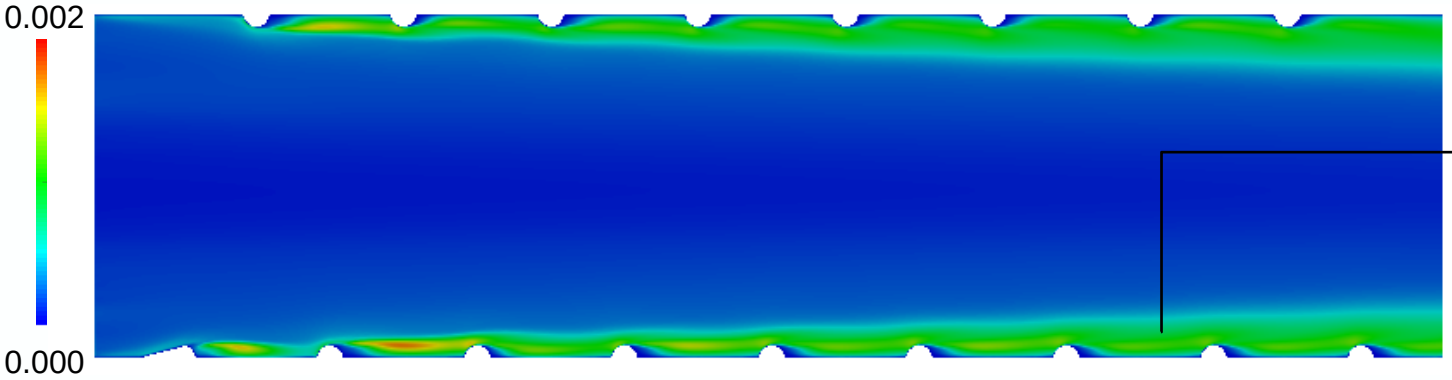


Full domain: ——

Experiment: ♦ ♦ ♦ ♦

RANS simulation of full domain

Turbulent Kinetic Energy

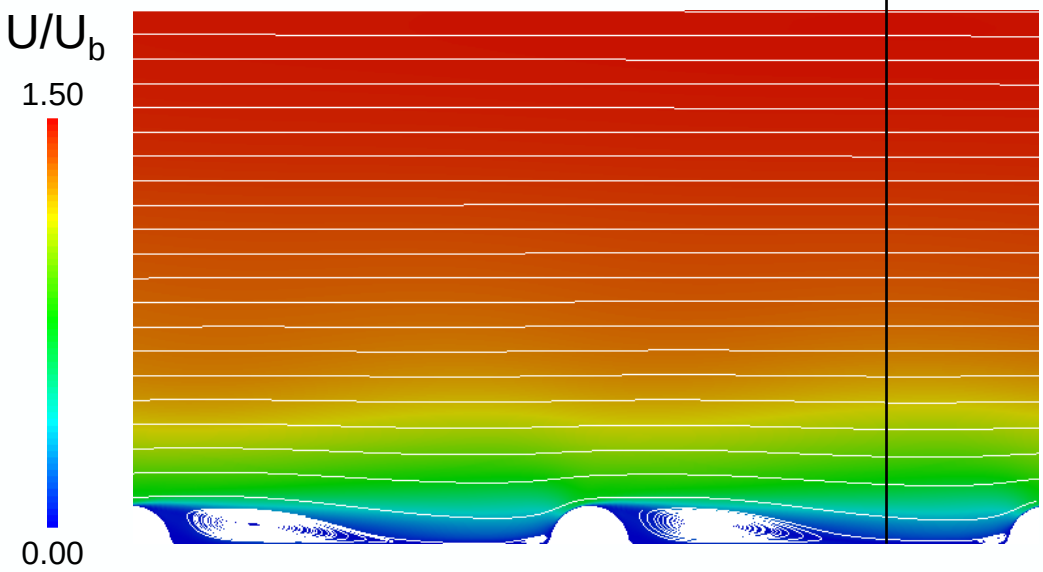


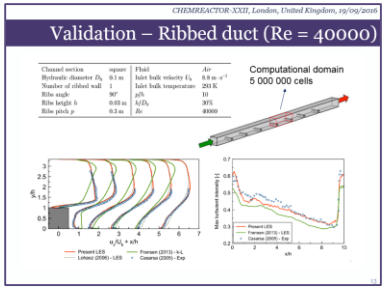
k underpredicted

Average reattachment length

+/- 8 X/e (simulations)

4.3 X/e (experiments)





In this type of geometry RANS does not capture the flow accurately

Conclusions

- ✓ 3D geometries improve heat transfer which can be assessed with 3D simulations
- ✓ CFD simulations are validated with experimental PIV and LCT results
- ✓ Periodicity decreases computational domain but requires fully developed flow
- ✓ Simulations can reveal more detailed information than experiments
- ✓ LES simulations were accurate, RANS failed to accurately predict flow

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3D reactor technology for steam cracking: simulation and experimental validation

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