” Turbulence Modeling, EDC and Finite Rate Detailed Chemical Kinetics for Application to Low Reynolds Number Wall Bounded Reactive Flows”

Andrea Gruber
SINTEF Energy Research

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“Task 3.1C: Experimental and Theoretical Investigation of Interaction Between

Turbulent Structure and Chemical Kinetics in Flows“

PRESENTATION OUTLINE

- Intro / Background
- Modeling assumptions and validation case
- Preliminary results
- Conclusions / Further work

INTRODUCTION

Context: combustion research in the field of high-power micro-sized gas turbines for applications to distributed power generation, robots, drones (Unmanned Aerial Vehicle) etc. Size range: 10^{-1} m - 10^{-3} m.

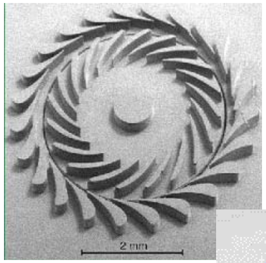
Earlier relevant work: DNS ”numerical experiment” performed in collaboration between SINTEF and Sandia National Laboratories (SNL), (J.H. Chen’s group)

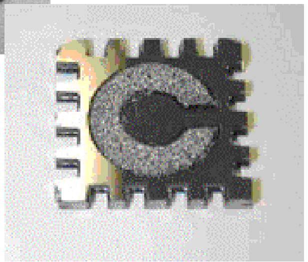
Numerical tools:

SPIDER: Finite-Volume, Computational Fluid Dynamics (CFD) code developed at SINTEF in FORTRAN90 for simulation of 1-D, 2-D and 3-D reactive compressible flows

S3D: massively parallel Direct Numerical Simulation (DNS) Finite-Difference code developed at SNL in FORTRAN90 for simulation of 1-D, 2-D and 3-D reactive compressible flows

RATIONALE





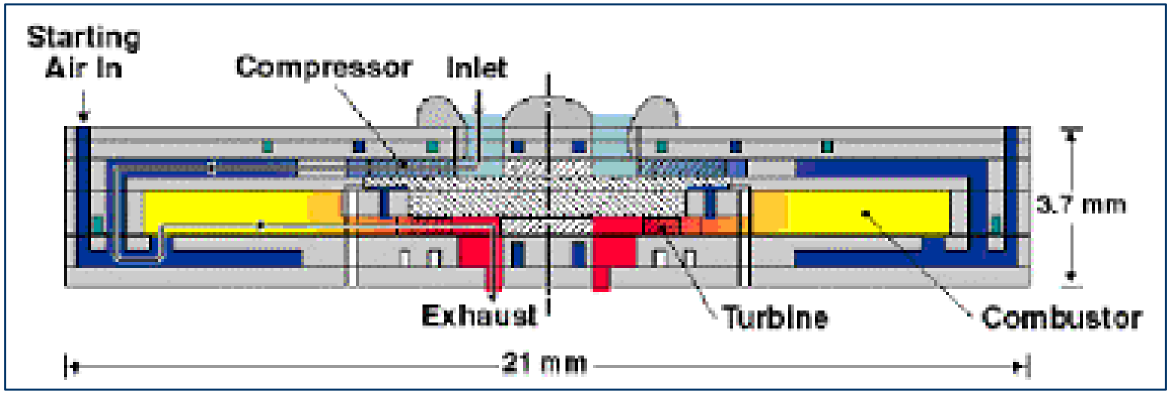


Figure from *"Micropower generation using combustion: Issues and approaches",* Carlos Fernandez-Pello, Proc. Comb. Inst. 2002

- Development of advanced technology for a new generation of small-sized, high power density, energy systems
- Understand and optimize the combustion process within small volume combustors
- Improvement of the environmental friendliness and of the overall efficiency of notoriously inefficient systems

BACKGROUND

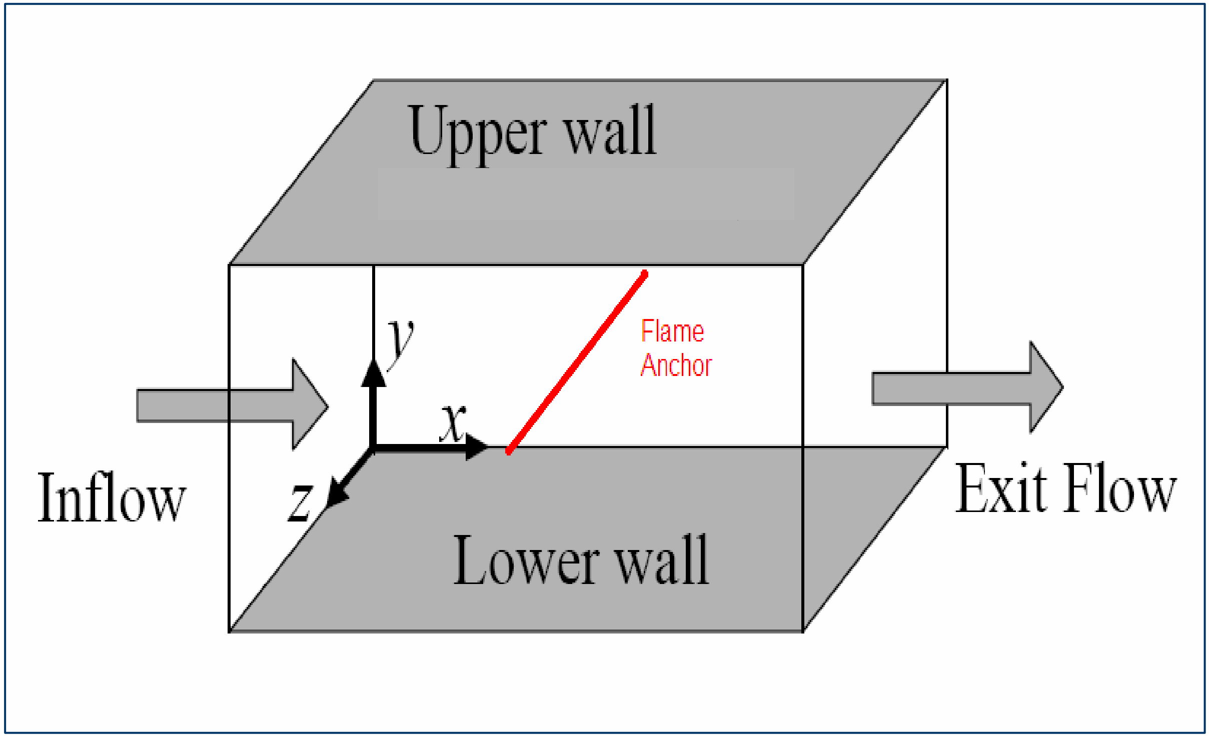
- Turbulent combustion takes place in small, confined volumes for many combustion devices
- Industrial problems require computationally cheap & accurate CFD-estimates which depend on turbulence modeling (k-ε, rsm etc.) and on combustion modeling (EDC, Flamelet, PDF)
- These models are widely used with success in CFD to help designing and investigating relatively large combustors (Re~10^6-10^8)
- These models are presently unable to accurately represent turbulent combustion in *relatively small* combustors: strongly sheared, low-Reynolds number, boundary layer flows (Re~10^3-10^4)

TASK & APPROACH

- Evaluate and possibly enhance predictive capabilities of EDC at low-Reynolds number conditions
- DNS as a ”numerical experiment”
- Improve the understanding of the interaction between flame propagation and near wall turbulence
- Apply the improved models to CFD-analysis of micro-sized combustors*

**N. Iki, A. Gruber, H. Yoshida ”A Numerical and Experimental Study for Optimization of a Small Annular Combustor”, Journal of Power and Energy Systems, Vol. 2, No. 3, 2008.*

ANCHORED V-FLAME IN TURBULENT CHANNEL FLOW



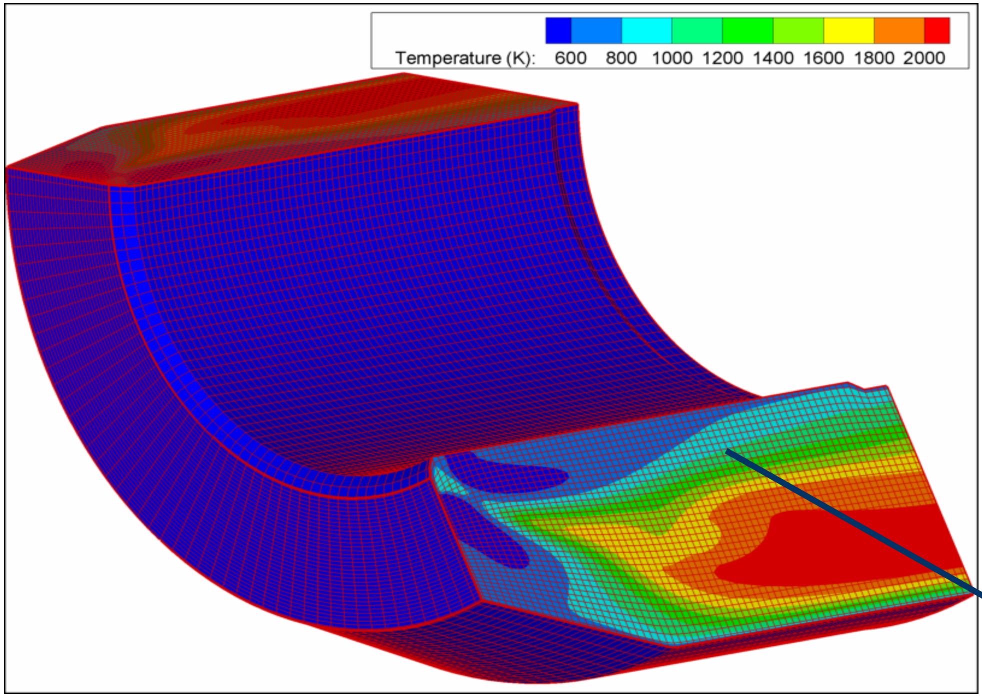
Simple but challenging problem for CFD RANS-simulations!

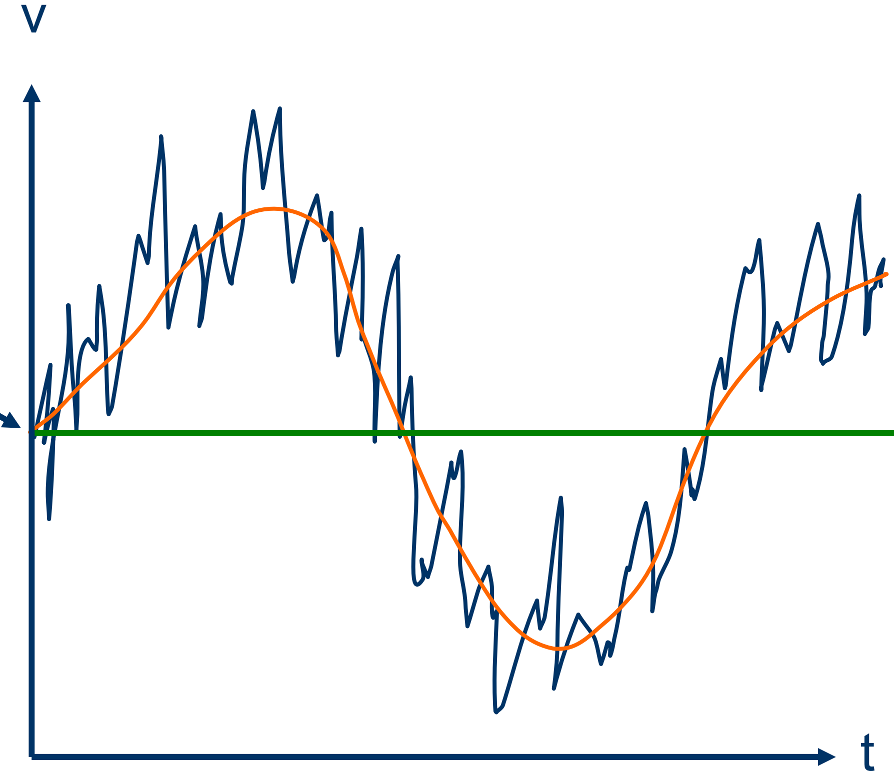
High surface-to-volume ratio combustor → Large fluid-flame-wall effects!

Relatively Low Re ~ 10^3-10^4 → Outside the realm of standard CFD-models (Re~10^6-10^8)!

DNS work shows the importance of detailed kinetics to account for radical recombination at wall

EVALUATING A MODEL: CFD vs. DNS





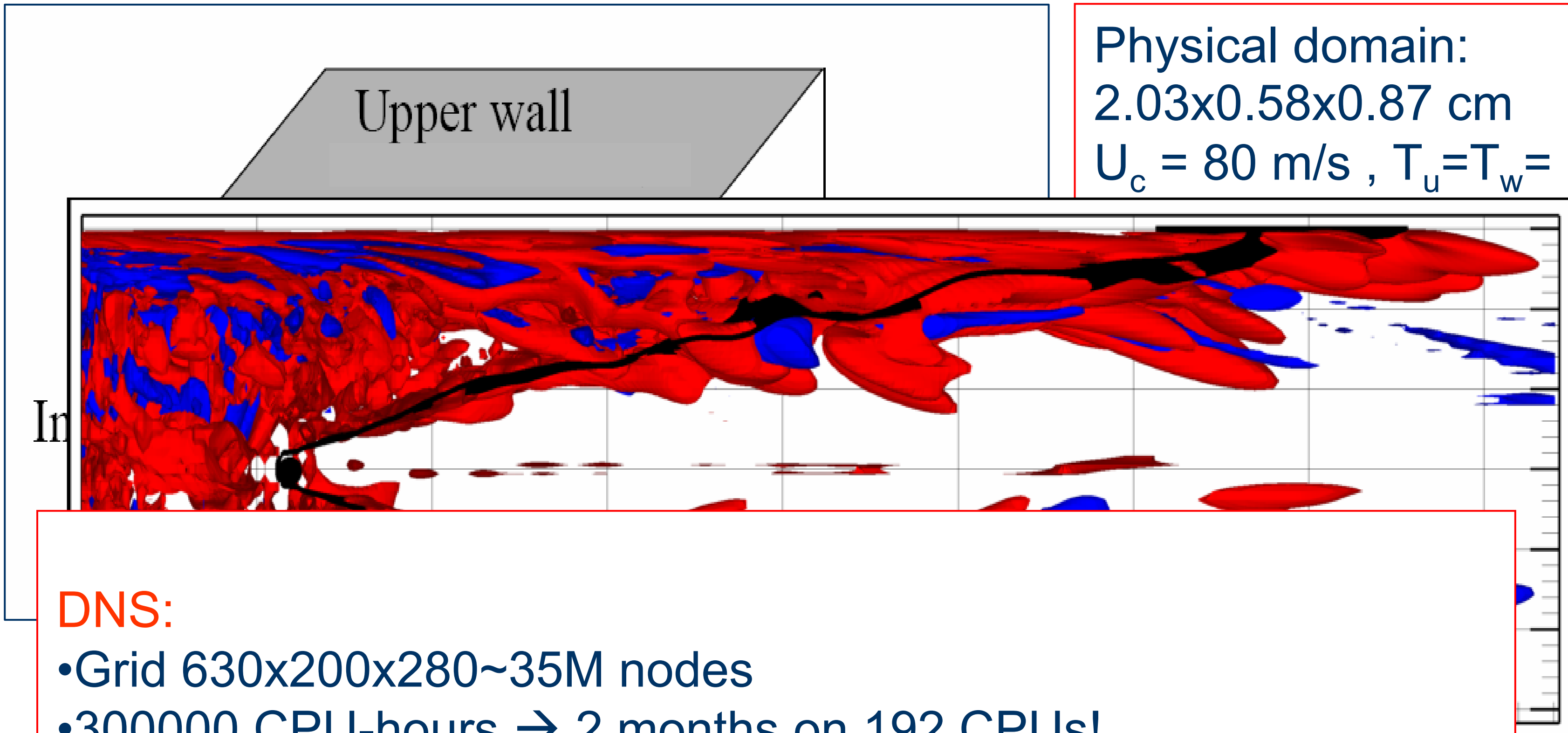
DNS (severely constrained by cost)

LES (CFD codes, more expensive)

RANS (CFD codes, cheap)

DNS Resolves All Spatial and Temporal Scales of a Turbulent Reactive Flow: Very Expensive!

DNS OF PREMIXED V-FLAME ANCHORED IN TURBULENT CHANNEL FLOW



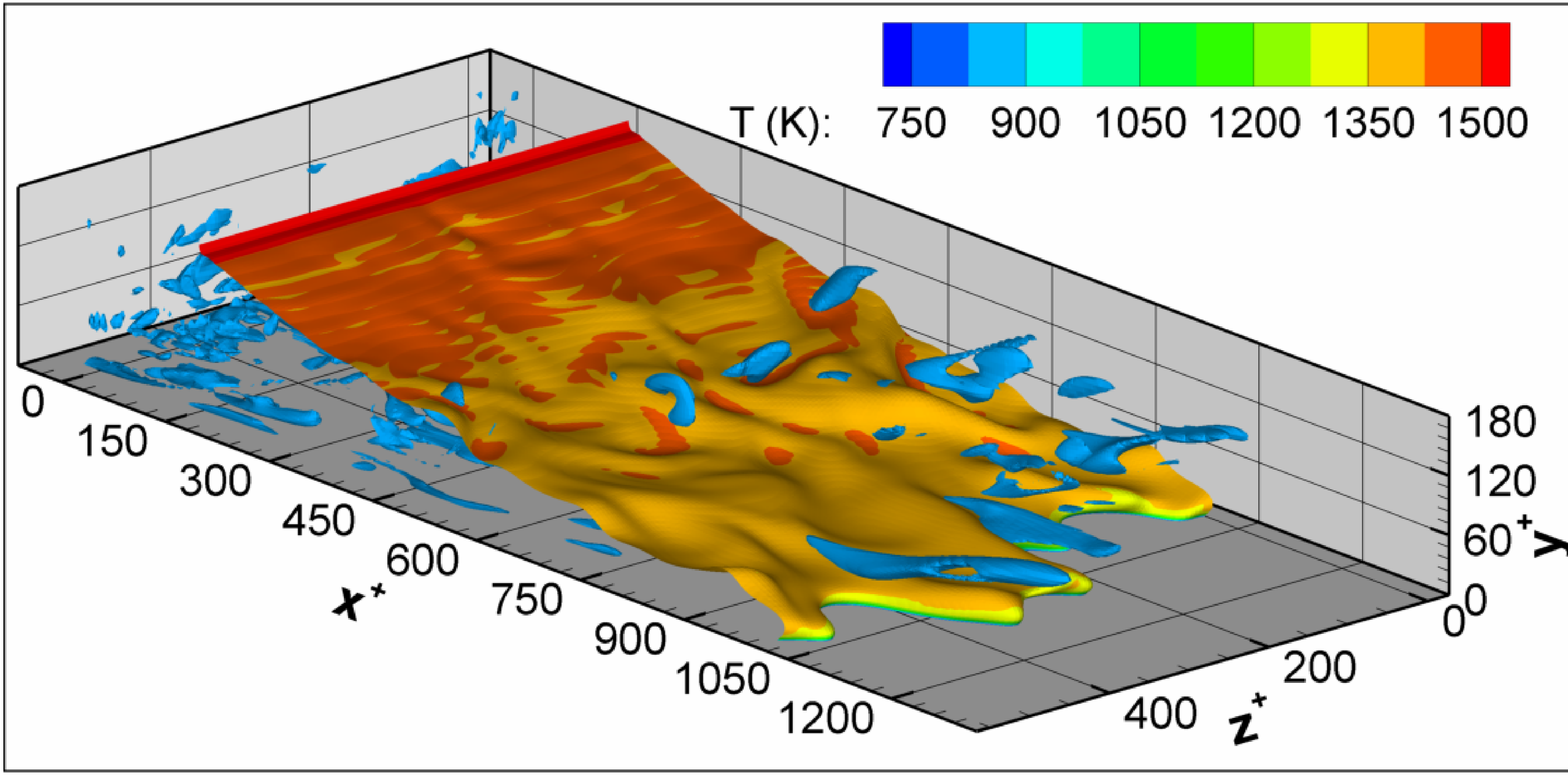
Physical domain:
2.03x0.58x0.87 cm
U_c = 80 m/s , T_u=T_w= 750 K

cs (Li)

DNS:
•Grid 630x200x280~35M nodes
•300000 CPU-hours → 2 months on 192 CPUs!

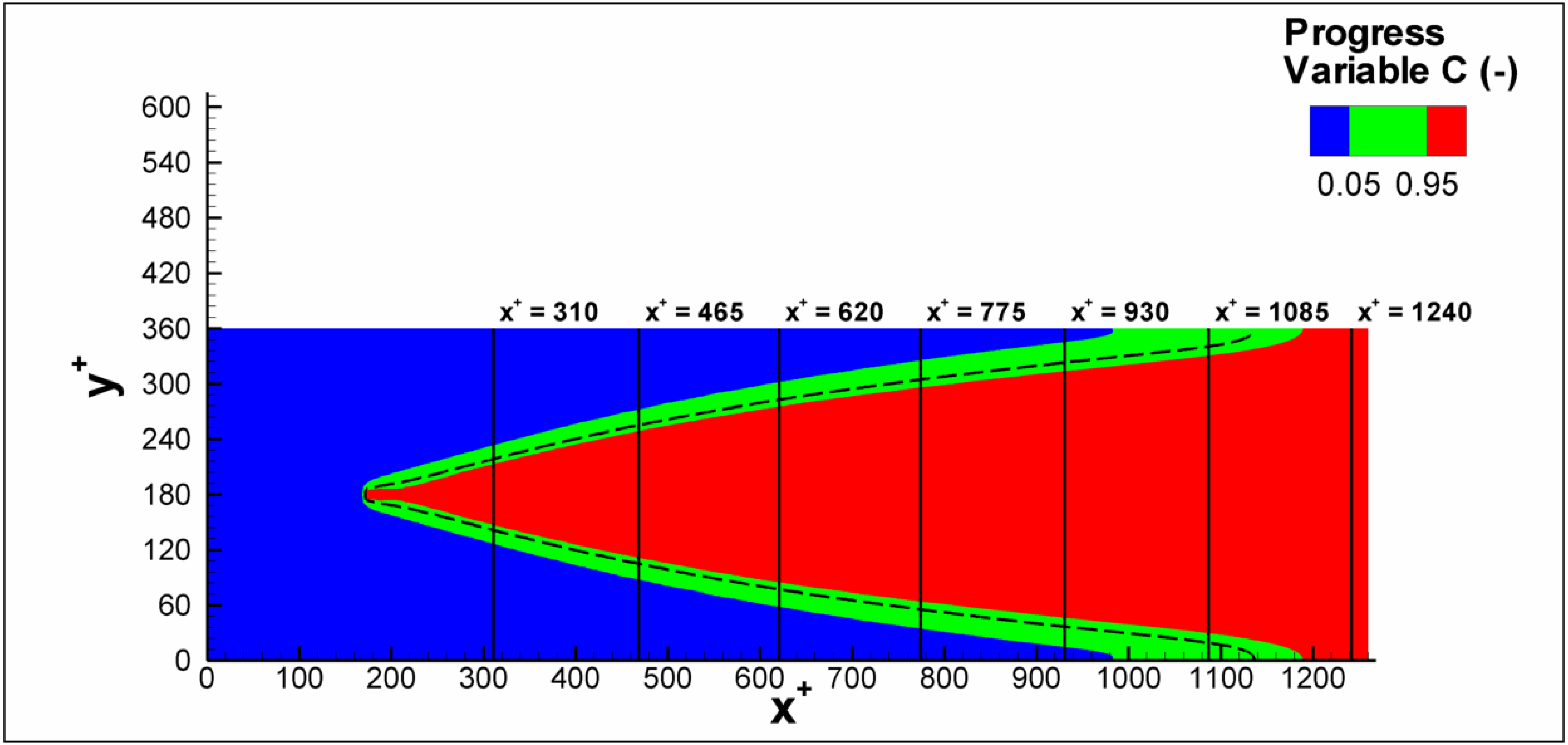
RANS:
•Grid 64x40x15~38K nodes
•5 CPU-hours → 2.5 hours on modern dual core!

TURBULENT FLAME-WALL INTERACTION (1)



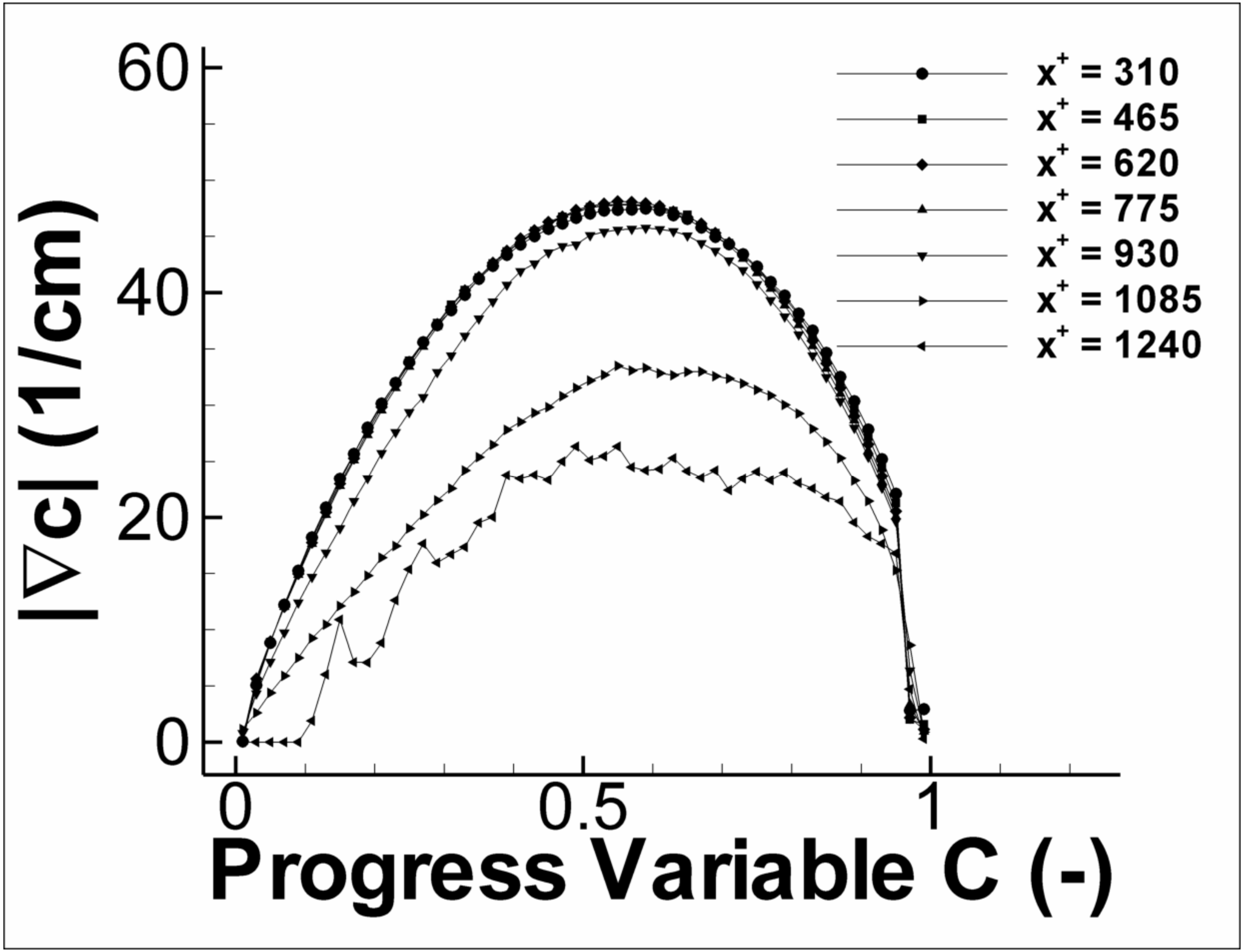
Isosurface of progress variable C=0.5 colored by local temperature / coherent vortical structures of BL

TURBULENT FLAME-WALL INTERACTION (2)



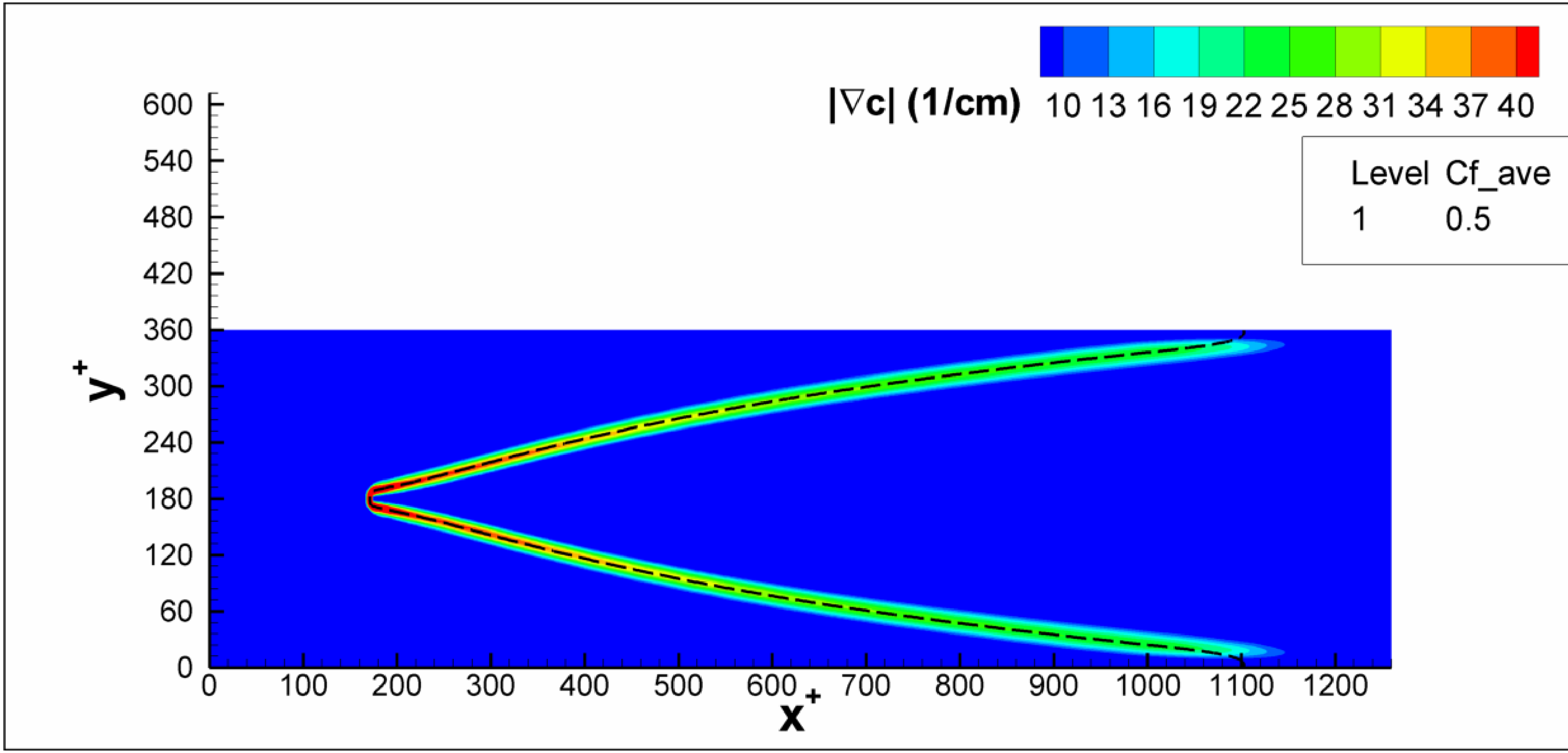
Progress variable C averaged in time and in spanwise homogeneous direction z (dashed line C=0.7)

TURBULENT FLAME-WALL INTERACTION (3)



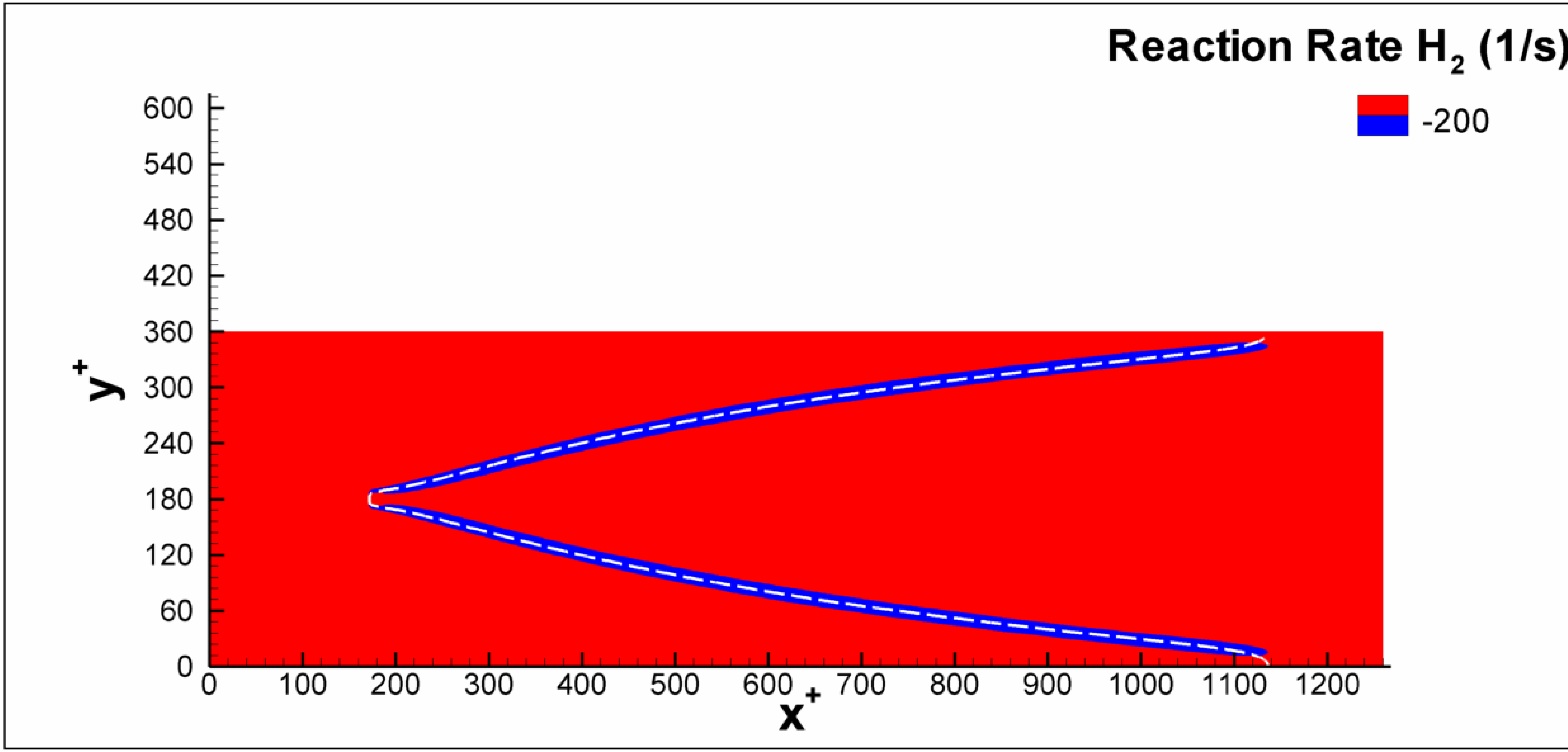
Progress variable C averaged in time and in spanwise homogeneous direction z

TURBULENT FLAME-WALL INTERACTION (4)



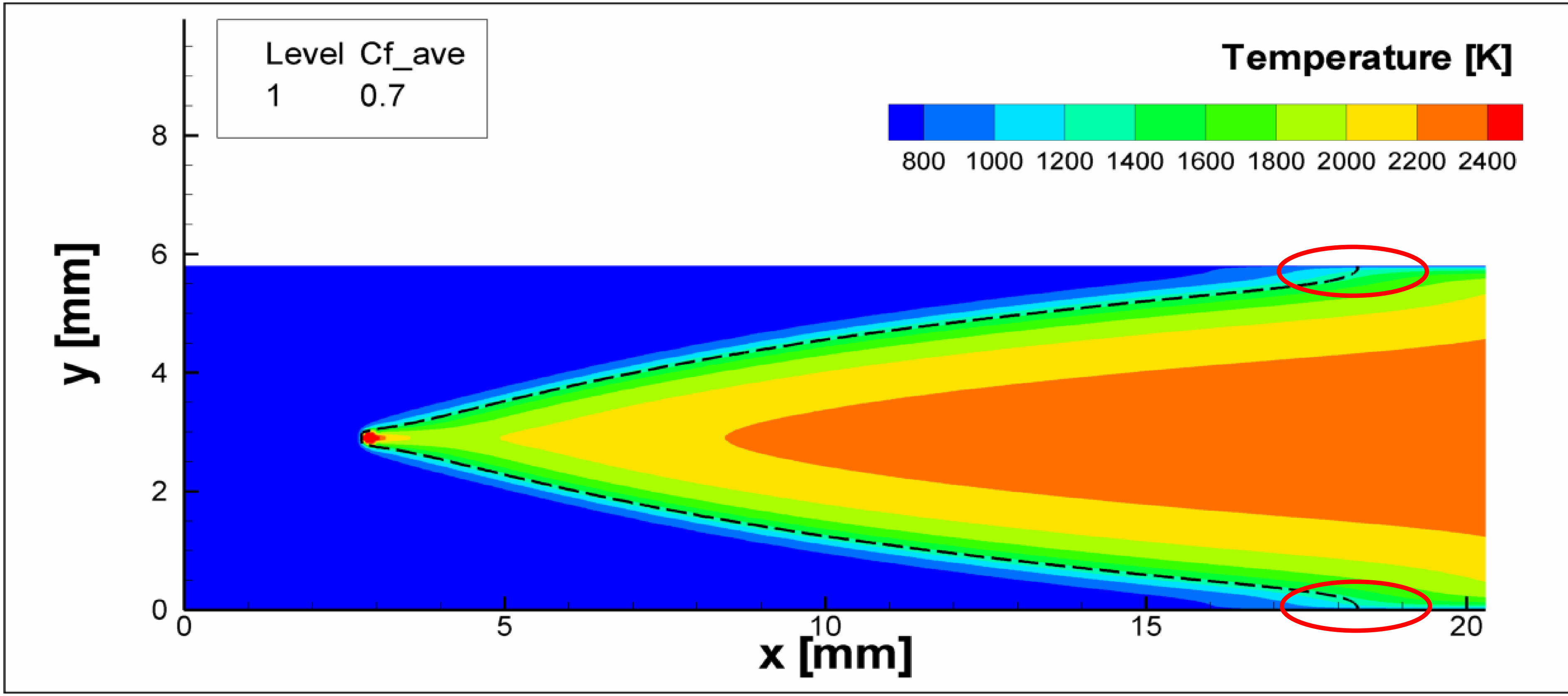
Spatial gradient of progress variable C averaged in time and in spanwise homogeneous direction z

TURBULENT FLAME-WALL INTERACTION (4)



Reaction rate of fuel averaged in time and in spanwise homogeneous direction z

TURBULENT FLAME-WALL INTERACTION (5)



Spatial gradient of progress variable C and of temperature T are not parallel in the near-wall region!
Flame surface normal not defined!
Flamelet model of dubious validity in this region → let's try the EDC!

EDC MODEL, STANDARD & IMPROVED?

1. The EDC turbulent combustion model tries to describe a reacting sub-region of the physical space (called fine structure) in which chemical reaction is assumed to occurr

2. The connection between the fine structure (sub-grid region) and the quantities characterizing turbulence at the grid scale (k,ε) is based on a turbulence cascade model

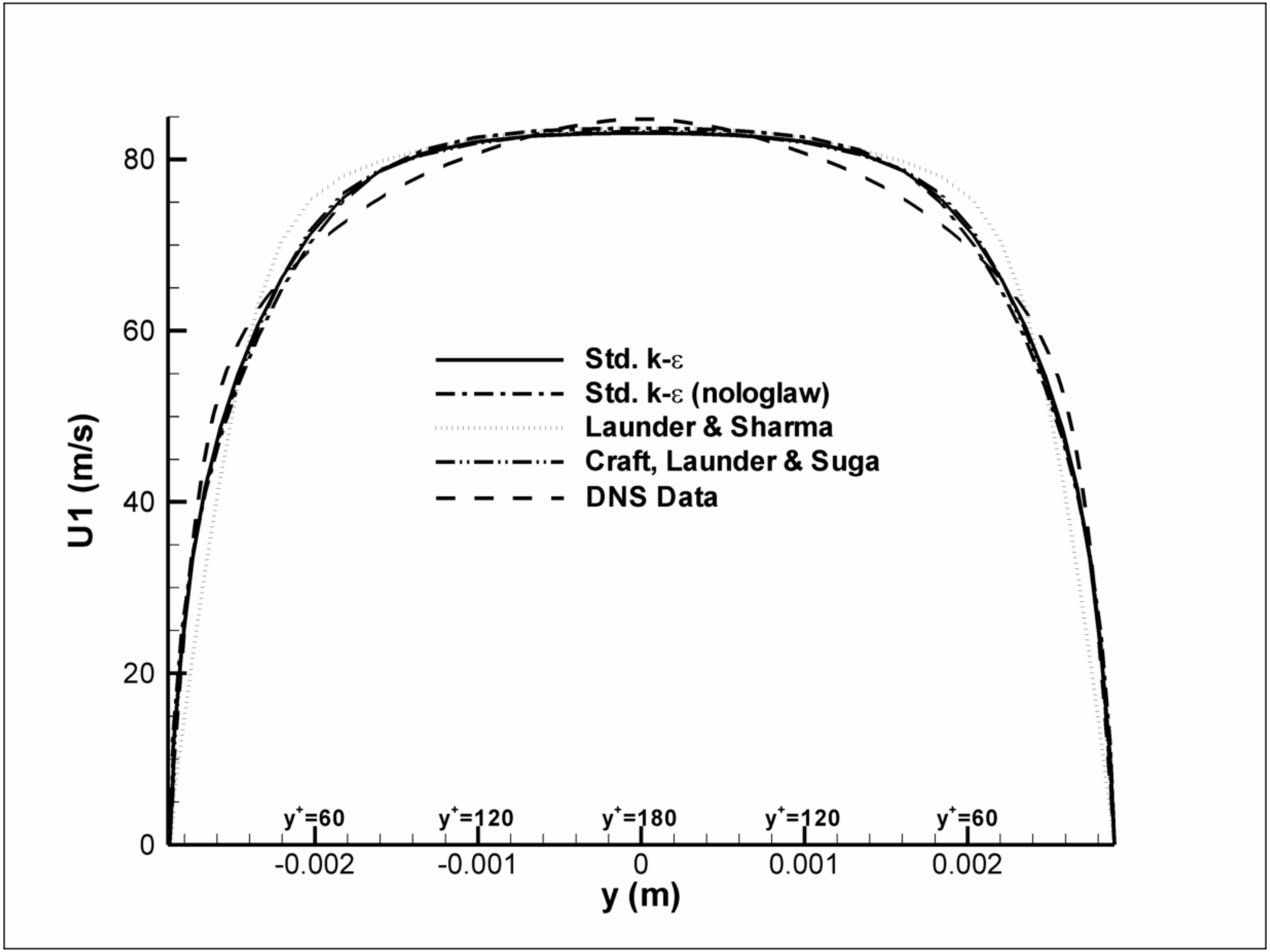
3. $\gamma^* \sim C \times (\nu \times \varepsilon / k^2)$ ^1/2

4. A near-wall fine structure expression is proposed here for FWI region (from the idea of a "generalized" flame sheet)

5. $\gamma_w \sim (L^2 \times \delta_f) / L^3$

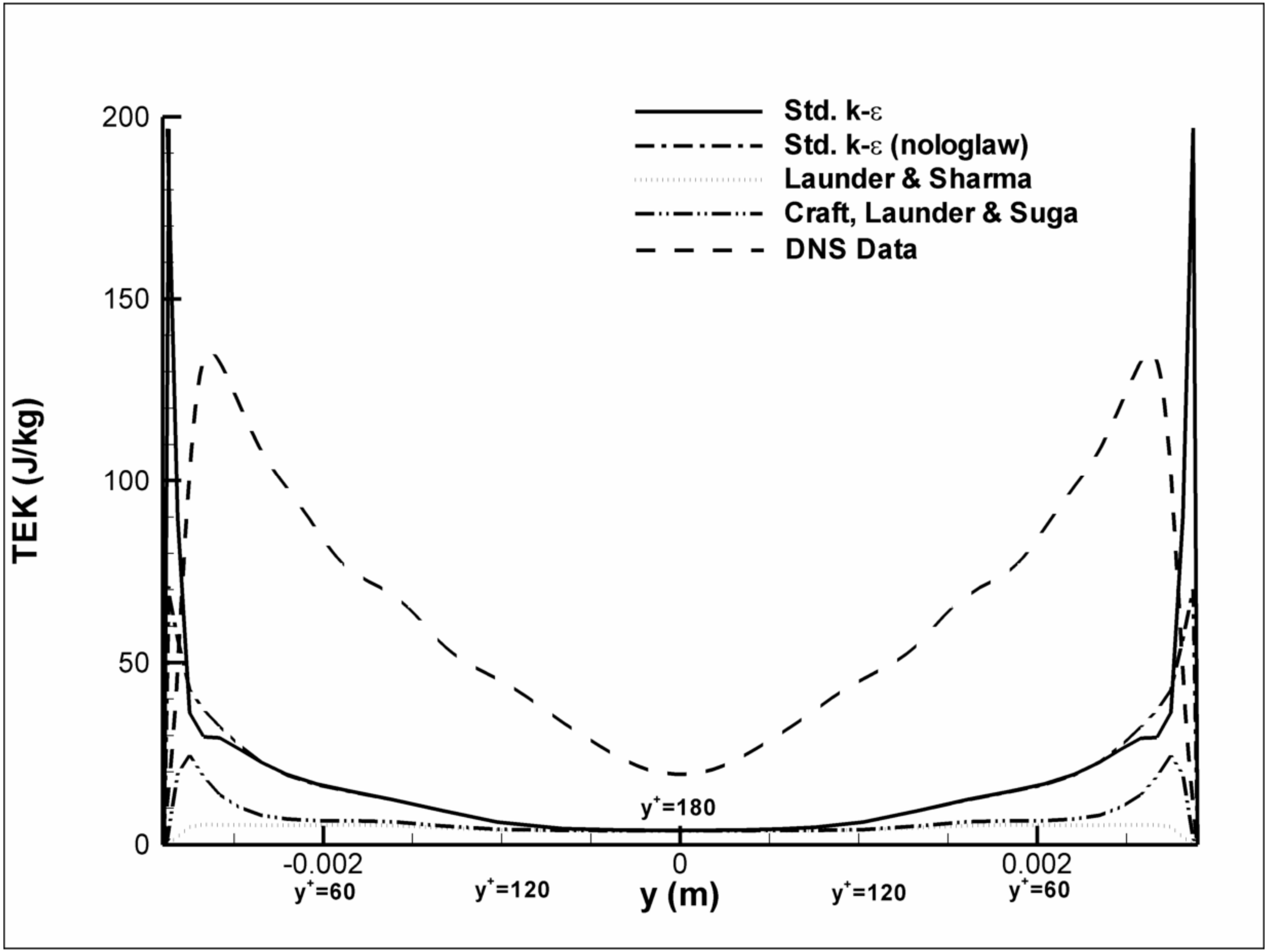
6. A damping function of a locally defined turbulent Reynolds number Re_t is used to transition from γ^* to γw , $f \sim e$^($-Re_t/R$)

TURBULENT PLANE CHANNEL (1)



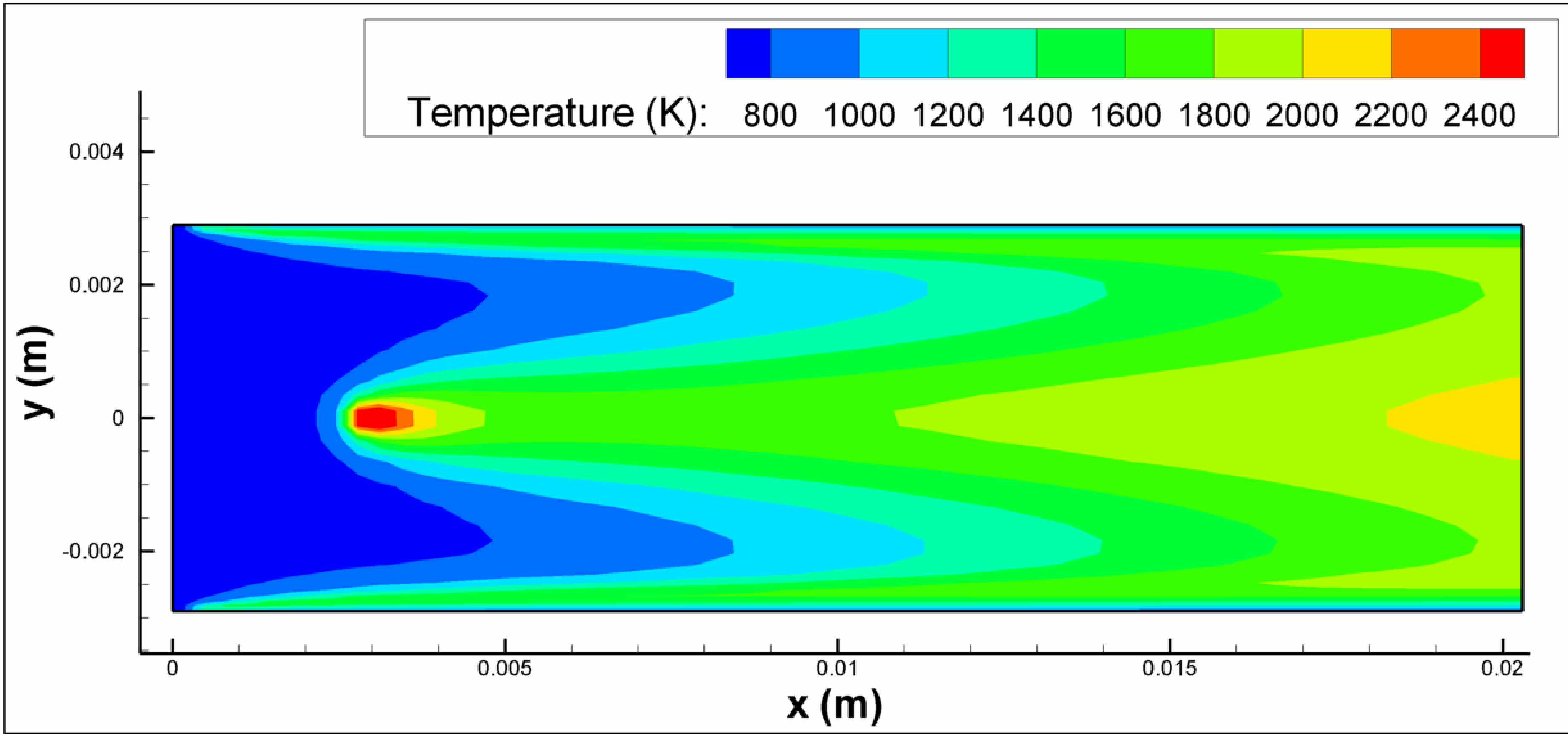
Satisfactory agreement RANS-DNS as for the average streamwise velocity!

TURBULENT PLANE CHANNEL (2)



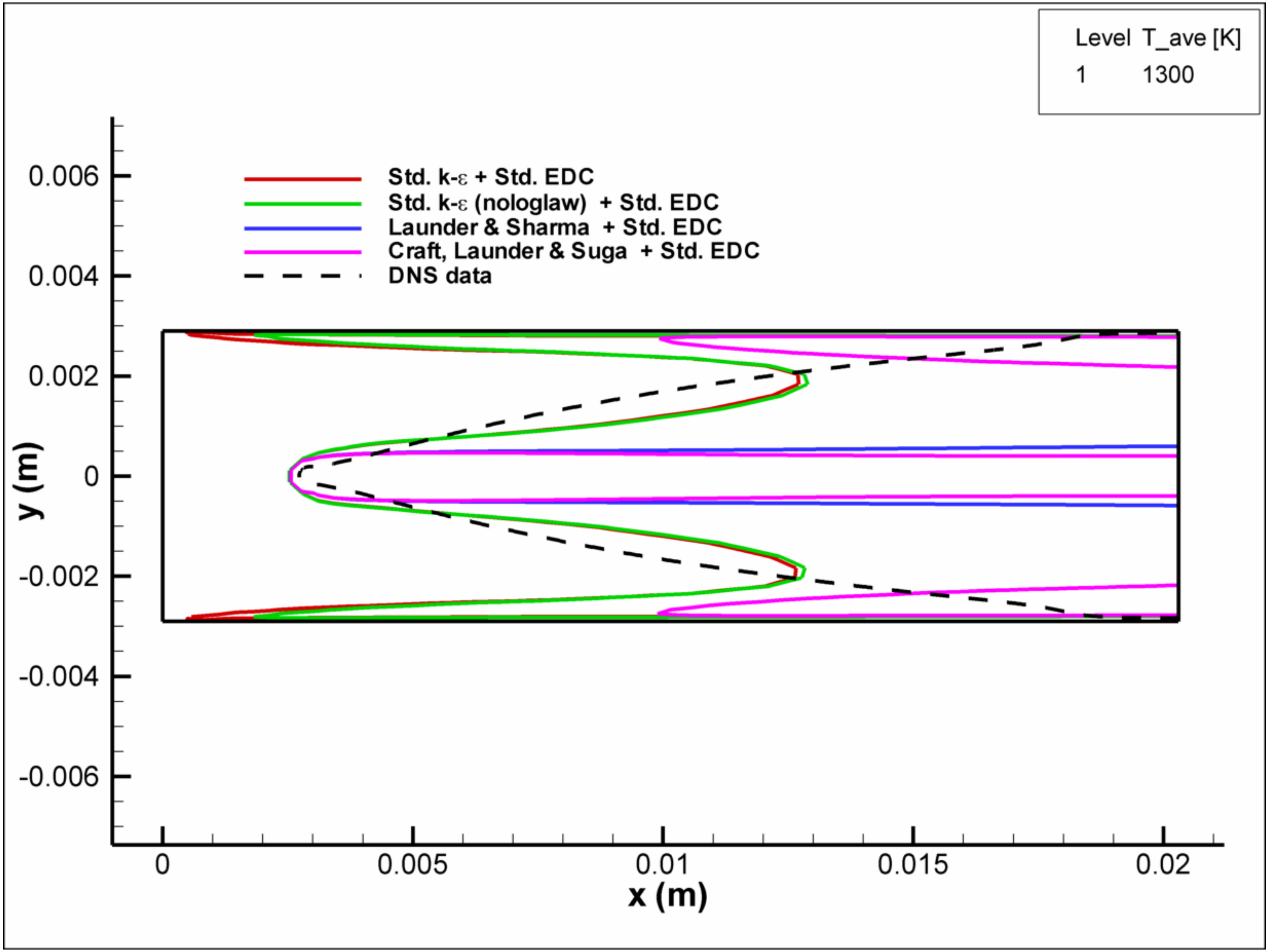
Poor agreement RANS-DNS as for the turbulent kinetic energy level!

RANS OF ANCHORED V-FLAME (1)



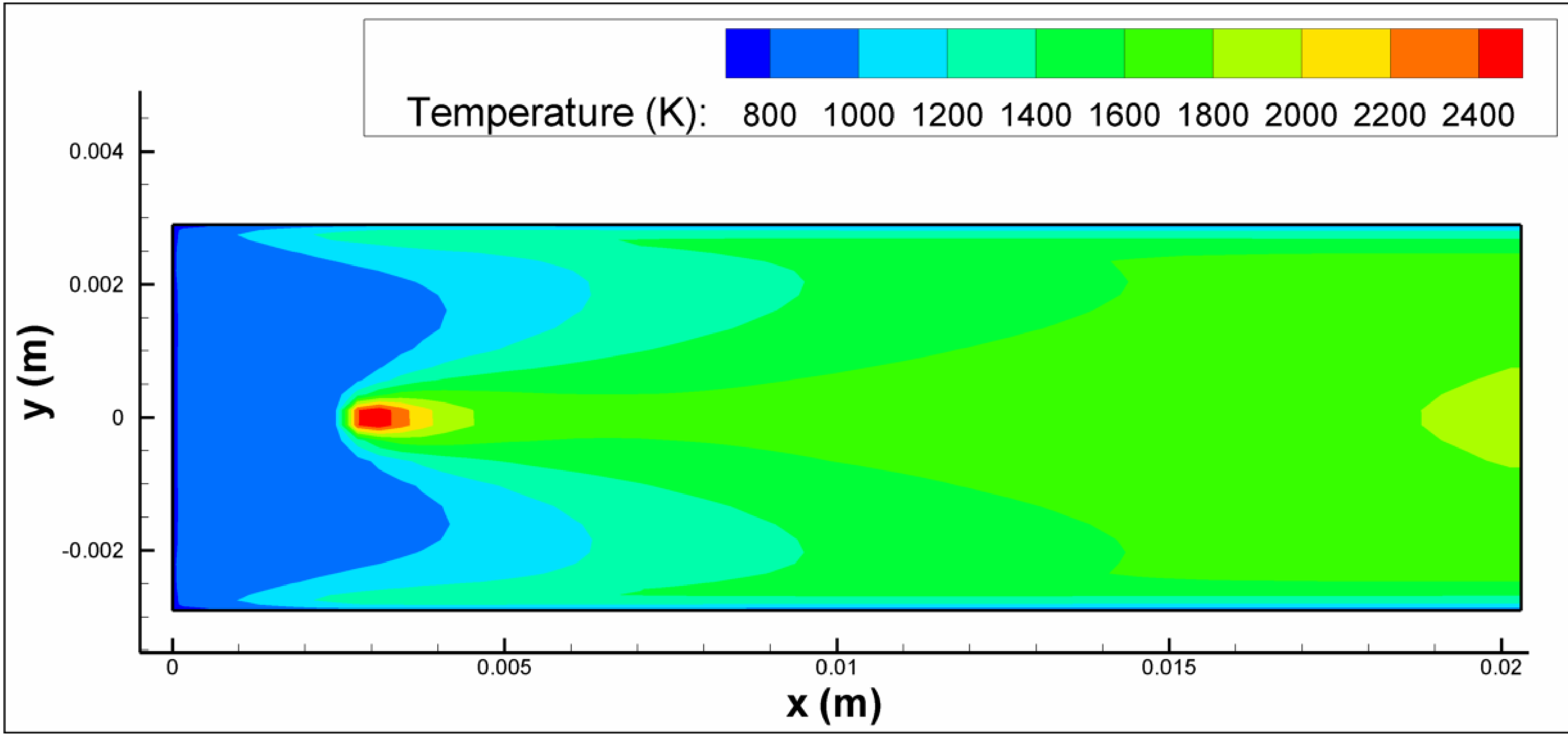
Poor agreement RANS-DNS as for flame temperature, shape & position using std k-ε & EDC models!

RANS OF ANCHORED V-FLAME (2)



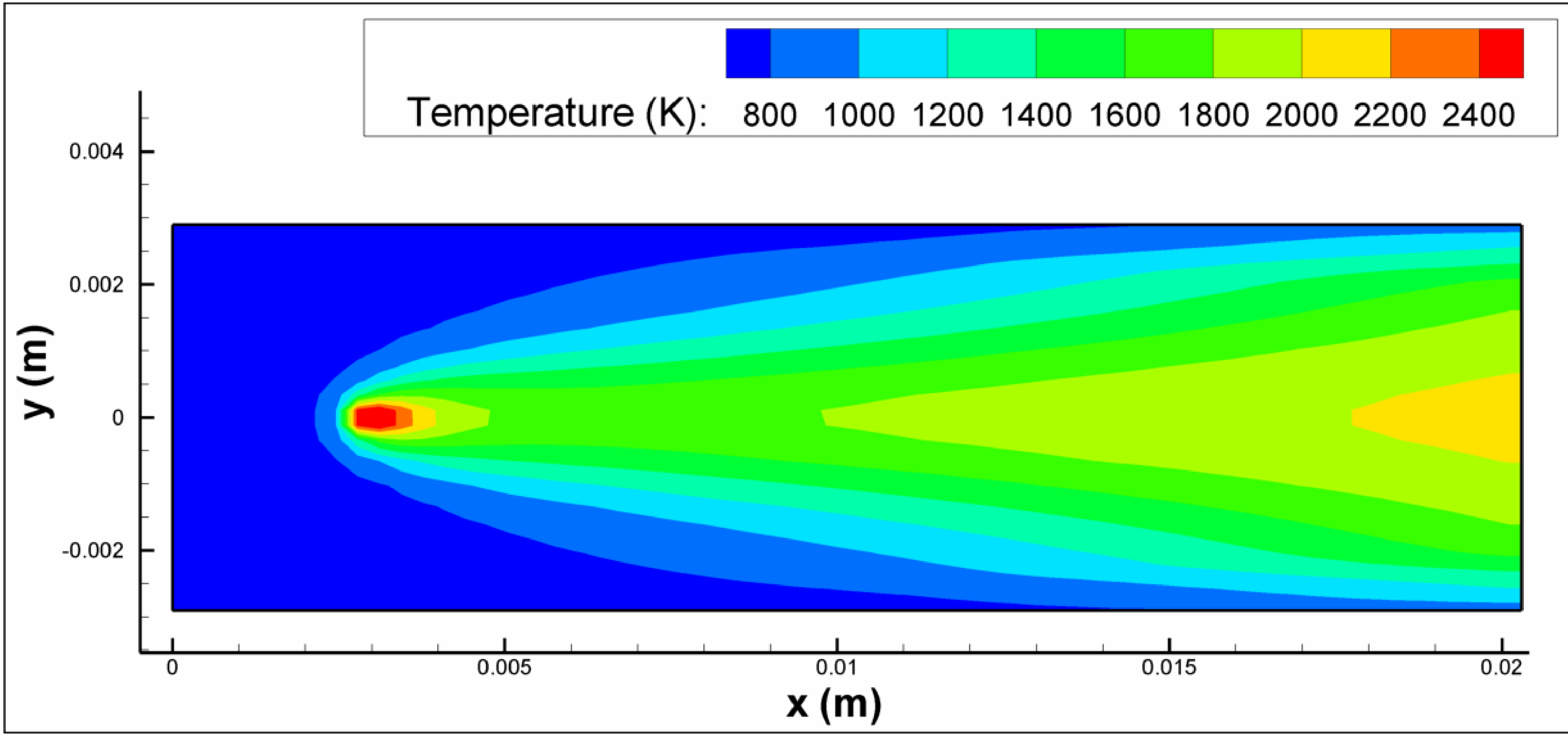
Poor agreement RANS-DNS as for flame temperature, shape & position using other k-ε models!

RANS OF ANCHORED V-FLAME (3)



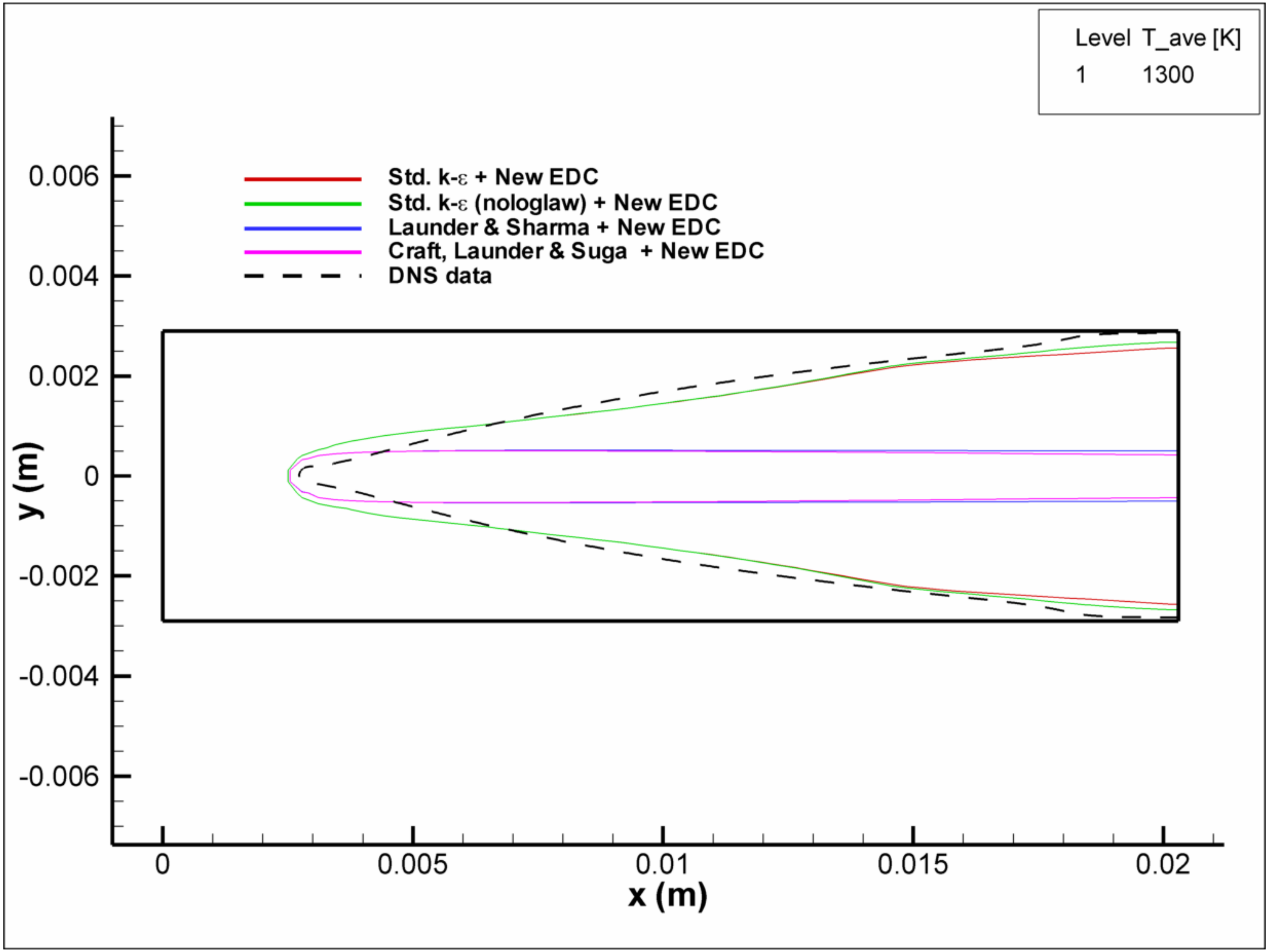
Detailed chemical kinetics does not improve the performance of the turbulence/combustion models!

RANS OF ANCHORED V-FLAME (4)



Modified EDC formulation improves flame shape & position but still underpredicts temperature level!

RANS OF ANCHORED V-FLAME (5)



Modified EDC formulation still performs poorly when coupled with LS and CLS models!

Conclusions and Further Work

1. All flavours of k-ε turbulence models tested perform poorly in predicting turbulence quantities for an apparently simple case

2. The standard EDC model perform poorly in predicting flame temperature level, shape & position

3. The implemented modification to the EDC turbulent combustion model to improve its low Reynolds number behavior is only partially satisfactory

4. Validation against the DNS database suggests that further adjustments to the model is required

Aknowledgements

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Thanks for your attention!

☺

Questions?