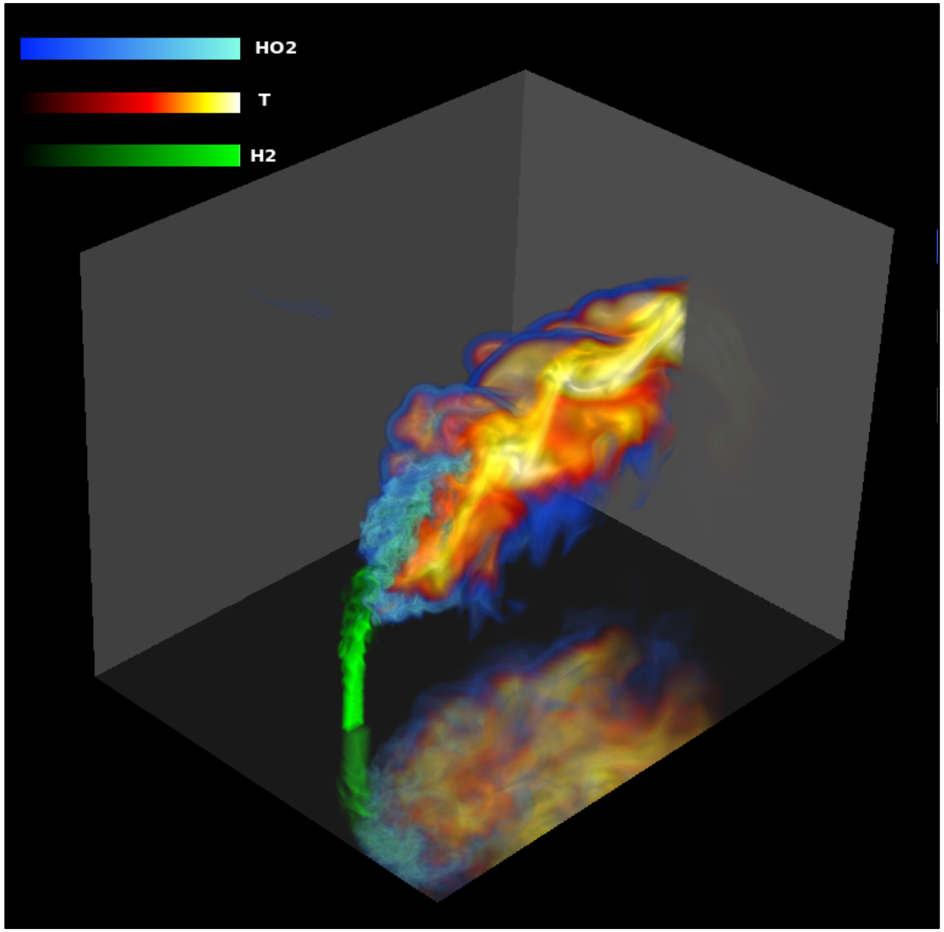
”Direct Numerical Simulations of Atmospheric and Pressurized Hydrogen-Air Flames”



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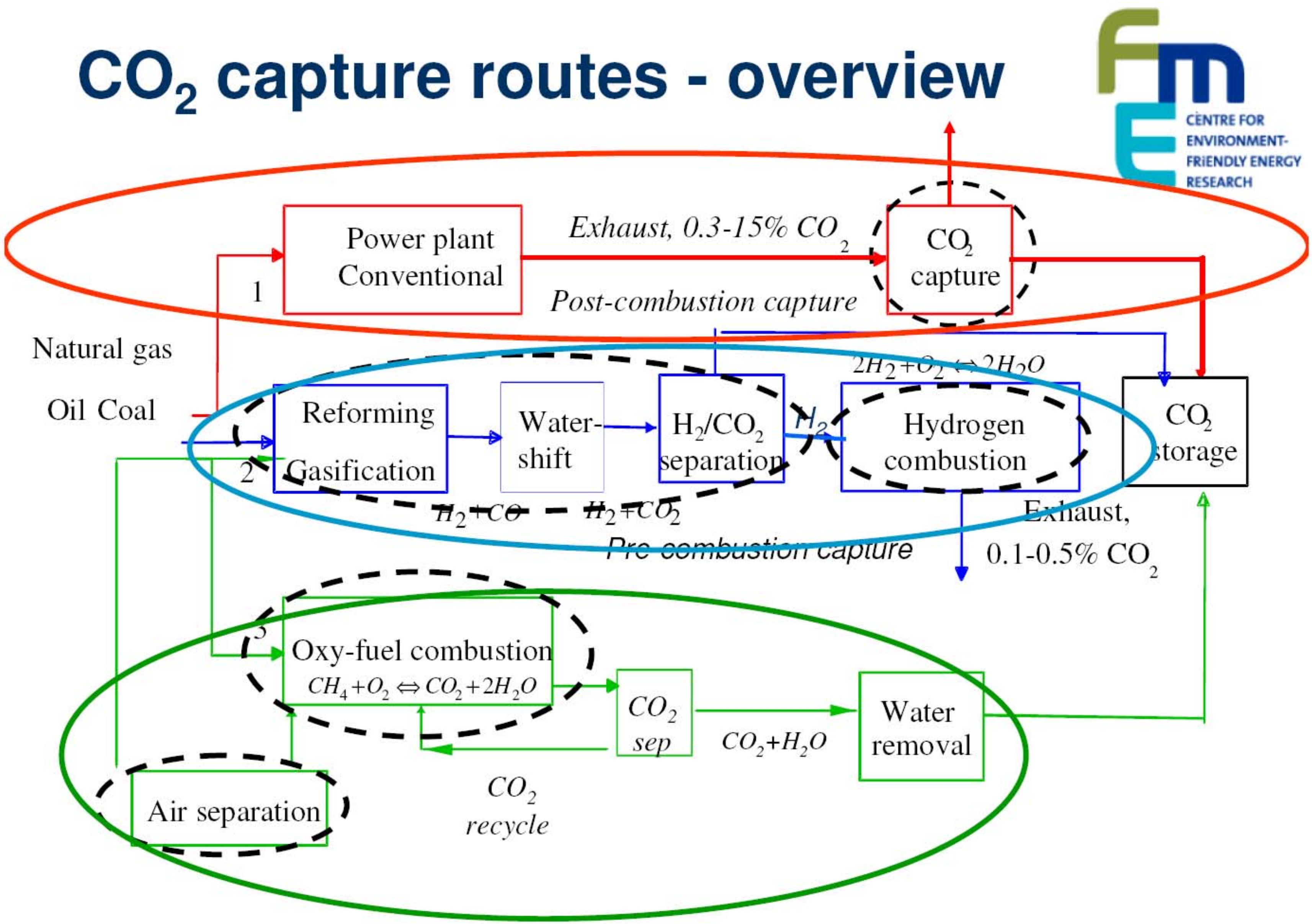
IEA TLM 2010 - Nara - July 28th 2010

Outline of Presentation

- Background & Motivation
- DNS of Reactive Jet in Cross Flow
- DNS of Inert Jet in Cross Flow & Turbulent V-Flames
- Conclusions & Further Work

Background and Motivation (1)



Background and Motivation (2)

Project framework of the present effort:

SINTEF work

- BIGH2 Phase 1/NRC, 10 MNOK (1.6 MUSD), 18 months.
- DECARBIT/EU, 15 MEURO (20 MUSD), 36 months.
- Possible extension: BIGH2 Phase 2/NRC, 30 MNOK (4.8 MUSD)

SNL work

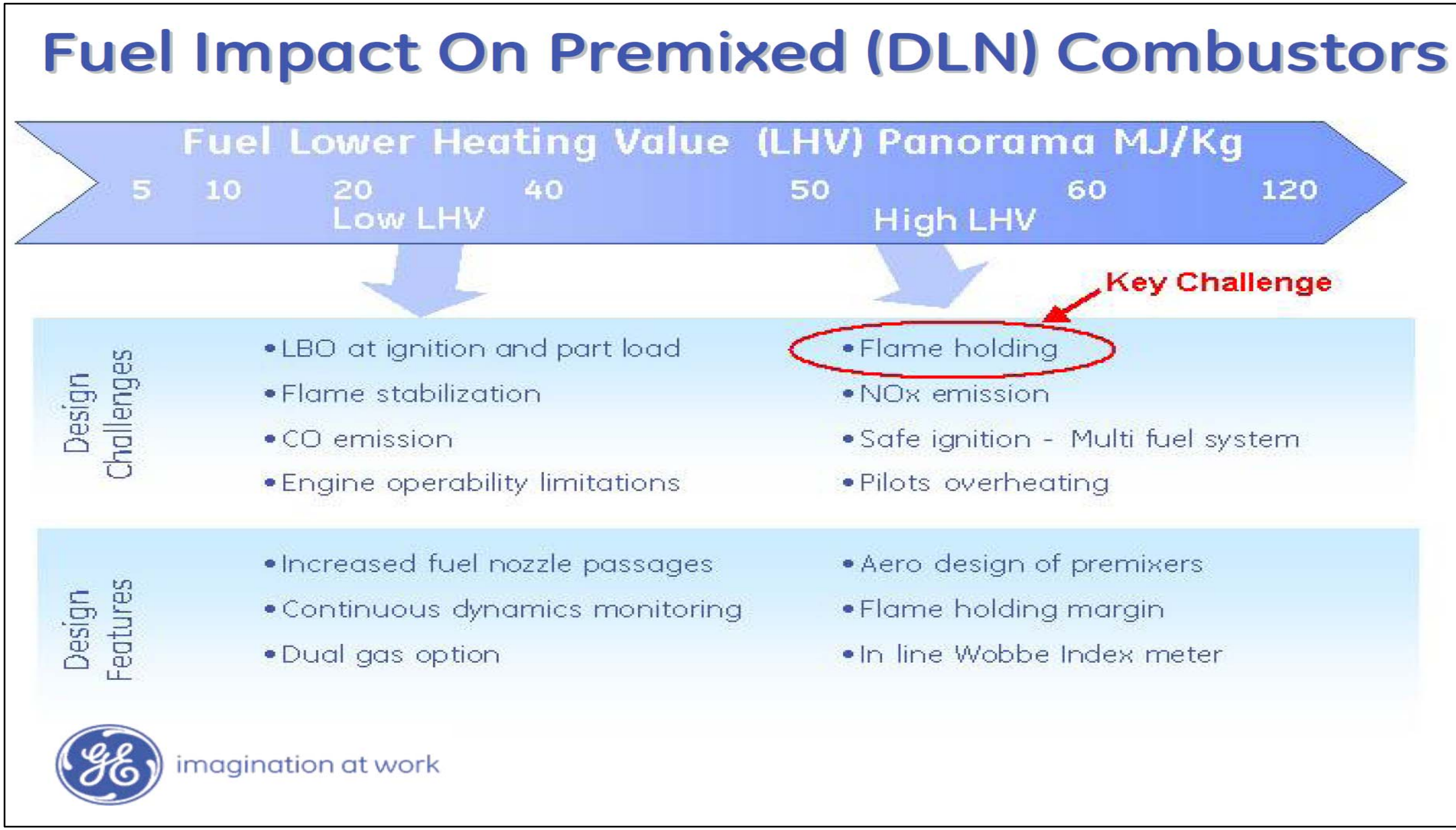
- supported by the Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic Energy Sciences of the US Department of Energy and by the US Department of Energy SciDAC Program.

Background and Motivation (3)

H_2 combustion ”Enabling” for CCS in pre-combustion separation scheme:

- Presently, hydrogen is only burned with nitrogen or steam dilution to contain NO_x emissions within the limits imposed by legislation
- Lean Pre-Mixed (LPM) combustion has proven successful in environmental-friendly, efficient ng & oil firing of gas turbines
- Existing LPM burners fail when burning hydrogen-rich fuels because of important differences between H_2 and HC physical & combustion properties
- Fundamental and applied knowledge has to be aquired in order to achieve successful gas turbine LPM operation with hydrogen-rich fuels

Background and Motivation (4)



"Gas Turbine Fuel Flexibility For A Carbon Constrained World", GE Energy by Bob Jones
Workshop on Gasification Technologies - Bismark, ND (2006)

Background and Motivation (5)

Flame holding is key challenge to design of premixers for high-H_2 fuels

•An unwanted transient brings flame into premixer

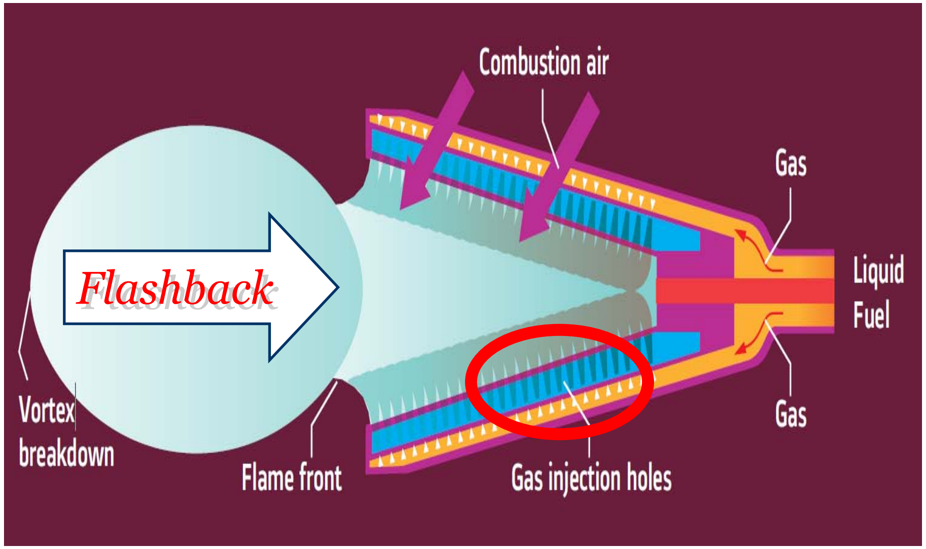
•Flame enters the premixer's bulk flow and "creeps" in low-velocity near-wall regions

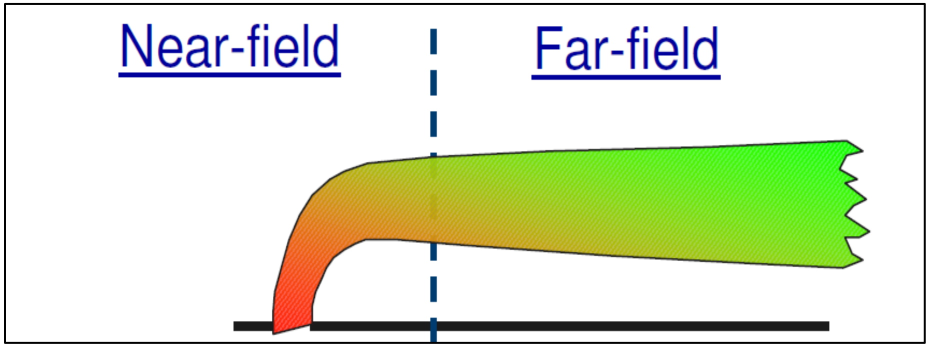
•Regardless of where flashback originates, the near field will ultimately be affected

•Flashback safety criteria implies that flame anchoring in near-field of fuel injector is not acceptable

•Flame must be washed out of premixer as soon as nominal operating conditions are restored

•Blow off is a necessary (but perhaps not sufficient!) condition for flashback safety fuel injection





No "flame holding" at fuel injectors for intrinsic flashback safety!

Flame Stabilization Downstream of Transverse Jet

Cross Flow (in X-direction) from aux DNS :

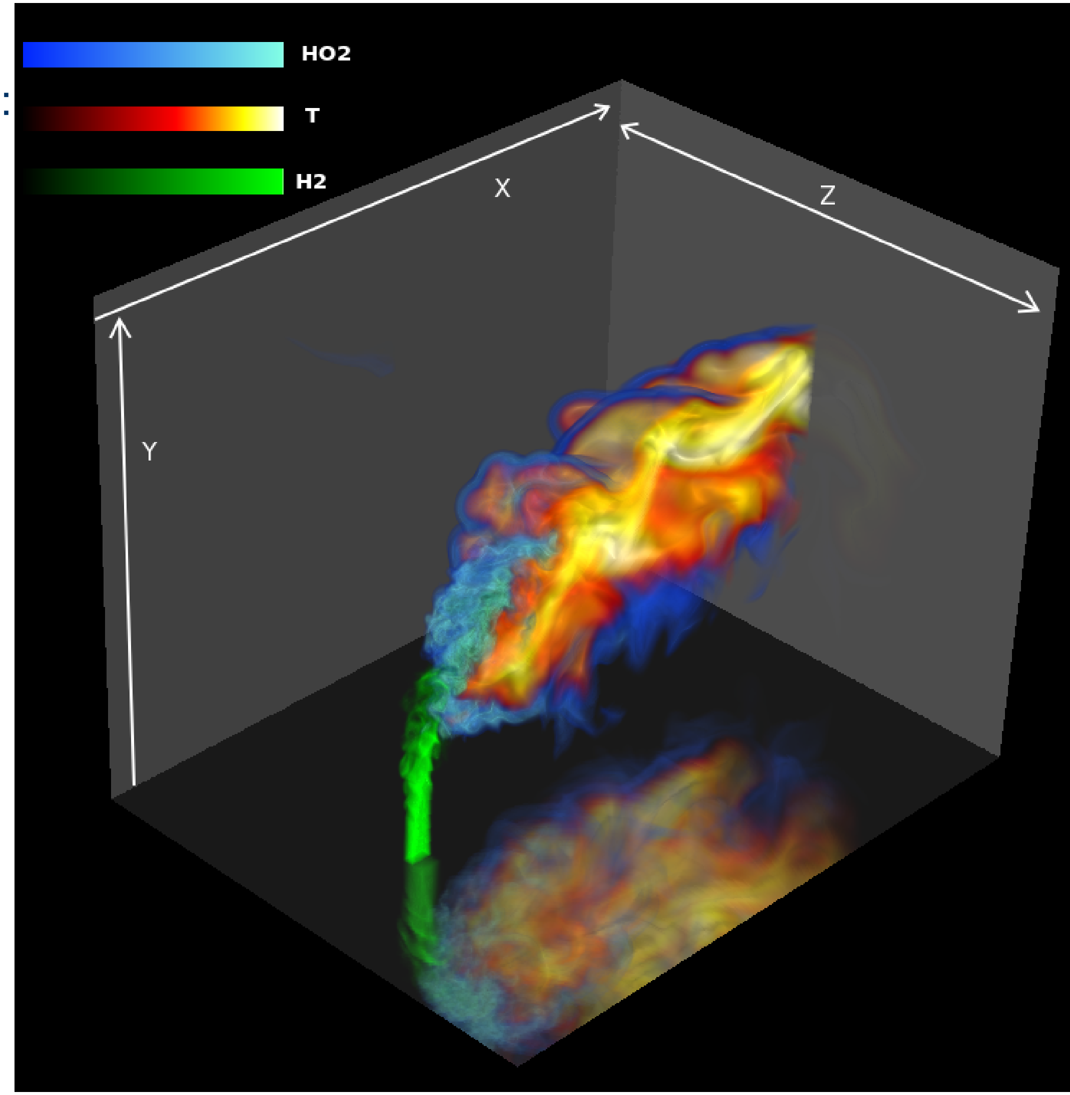
- U_{cf} ~ 55 m/s
- Air at 750 K
- δ_{cf} ~ 3.1 mm (80%)

Jet Flow (in Y-direction):

- U_j ~ 245 m/s
- H2+N2 (70/30) at 423 K
- Characteristic lenght d_j = 1 mm
- Parabolic laminar profile (Re~2700)

Case Parameters (Pressure = 1 bar):

- Assuming full chemical kinetics
- $R_v = U_j / U_{cf} \sim 4.4$
- $R_m = \rho_j U_j\text{^}2 / \rho_{cf} U_{cf}\text{^}2 \sim 10.6$
- Lx ~ $25{*}d_j$, Ly ~ $20{*}d_j$, Lz ~ $20{*}d_j$
- d_j = 1 mm
- Resolution 10 – 20 µm ($\Delta x^+ = \Delta z^+ \sim 0.5$, $\Delta y+ \sim 0.3\text{-}0.7$)
- Grid = 1408x1080x1100 ~ 1.6*10^9
- Total CPU time ~ 3.7 Mhrs (Jaguar @ ORNL)



Mathematical Model & S3D

$$\frac{\partial(\rho \boldsymbol{u}_\alpha)}{\partial t} = -\nabla_\beta \cdot (\rho \boldsymbol{u}_\alpha \boldsymbol{u}_\beta) + \nabla_\beta \cdot (-p\delta_{\alpha\beta} + \tau_{\beta\alpha}) + \rho \sum_{i=1}^{\mathrm{N_g}} Y_i \boldsymbol{f}_{i\alpha}$$

$$\frac{\partial \rho}{\partial t} = -\nabla_\beta \cdot (\rho \boldsymbol{u}_\beta)$$

$$\frac{\partial(\rho e_t)}{\partial t} = -\nabla_\beta \cdot (\rho e_t \boldsymbol{u}_\beta) + \nabla_\beta \cdot (-p\boldsymbol{u}_\beta + \tau_{\beta\alpha} \cdot \boldsymbol{u}_\alpha - \boldsymbol{q}_\beta) +$$

$$\rho \boldsymbol{u}_\beta \cdot \sum_{i=1}^{\mathrm{N_g}} Y_i \boldsymbol{f}_{i\beta} + \sum_{i=1}^{\mathrm{N_g}} \boldsymbol{f}_{i\beta} \cdot \boldsymbol{J}_{i\beta}$$

$$\frac{\partial(\rho Y_i)}{\partial t} = -\nabla_\beta \cdot (\rho Y_i \boldsymbol{u}_\beta) - \nabla_\beta \cdot \boldsymbol{J}_{i\beta} + W_i \dot{\omega}_i$$

$$\dot{\omega}_i = \frac{W_i}{\rho} \sum_{n=1}^{\mathrm{N_r}} \left(\nu''_{in} - \nu'_{in}\right) k_n \prod_{i=1}^{\mathrm{N_g}} c_i^{\nu'_{in}}$$

$$k_n(T) = B_n T^{a_n} exp\left(\frac{E_{an}}{\mathscr{R}T}\right)$$

S3D Numerics

Spatial Differencing: 8th order explicit centered FD in the interior domain

Spatial Differencing: 3rd order explicit one-sided FD at the boundaries

Temporal Integrator: 4th order 6-stage explicit Runge-Kutta

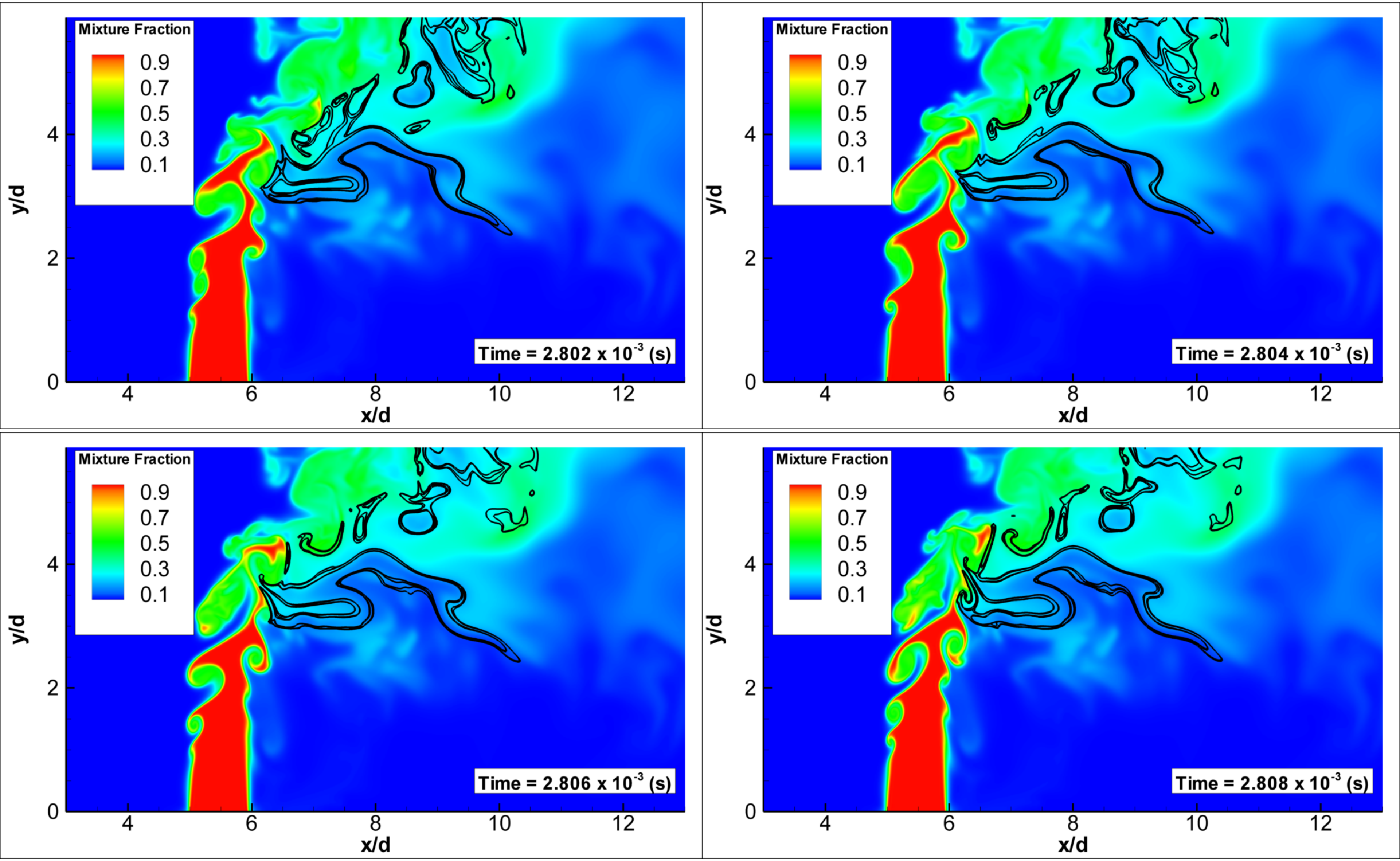
n	Reaction	B	a	E_a
1	O2 + H <-> OH + O	3.547e+15	-0.406	1.6599E+4
2	H2 + O <-> OH + H	0.508E+05	2.67	0.629E+04
3	OH + H2 <-> H + H2O	0.216E+09	1.51	0.343E+04
4	H2O + O <-> 2 OH	2.97e+06	2.02	1.34e+4
5	H2 + M <-> 2 H + M	4.577E+19	-1.40	1.0438E+05
6	2 O + M <-> O2 + M	6.165E+15	-0.50	0.000E+00
7	H + O + M <-> OH + M	4.714E+18	-1.00	0.000E+00
8	OH + H + M <-> H2O + M	3.800E+22	-2.00	0.000E+00
9	O2 + H (+M) <-> HO2 (+M)	1.475E+12	0.60	0.00E+00
10	H + HO2 <-> O2 + H2	1.66E+13	0.00	0.823E+03
11	H + HO2 <-> 2 OH	7.079E+13	0.00	2.95E+02
12	O + HO2 <-> OH + O2	0.325E+14	0.00	0.00E+00
13	OH + HO2 <-> O2 + H2O	2.890E+13	0.00	-4.970E+02
14	2 HO2 <-> O2 + H2O2	4.200e+14	0.00	1.1982e+04
15	H2O2 (+M) <-> 2 OH (+M)	2.951e+14	0.00	4.843E+04
16	H + H2O2 <-> OH + H2O	0.241E+14	0.00	0.397E+04
17	H + H2O2 <-> H2 + HO2	0.482E+14	0.00	0.795E+04
18	O + H2O2 <-> HO2 + OH	9.550E+06	2.00	3.970E+03
19	OH + H2O2 <-> H2O + HO2	5.800E+14	0.00	9.557E+03

Li et al. (2004)

Reactive JICF, Instantaneous Temperature Field in XY-plane

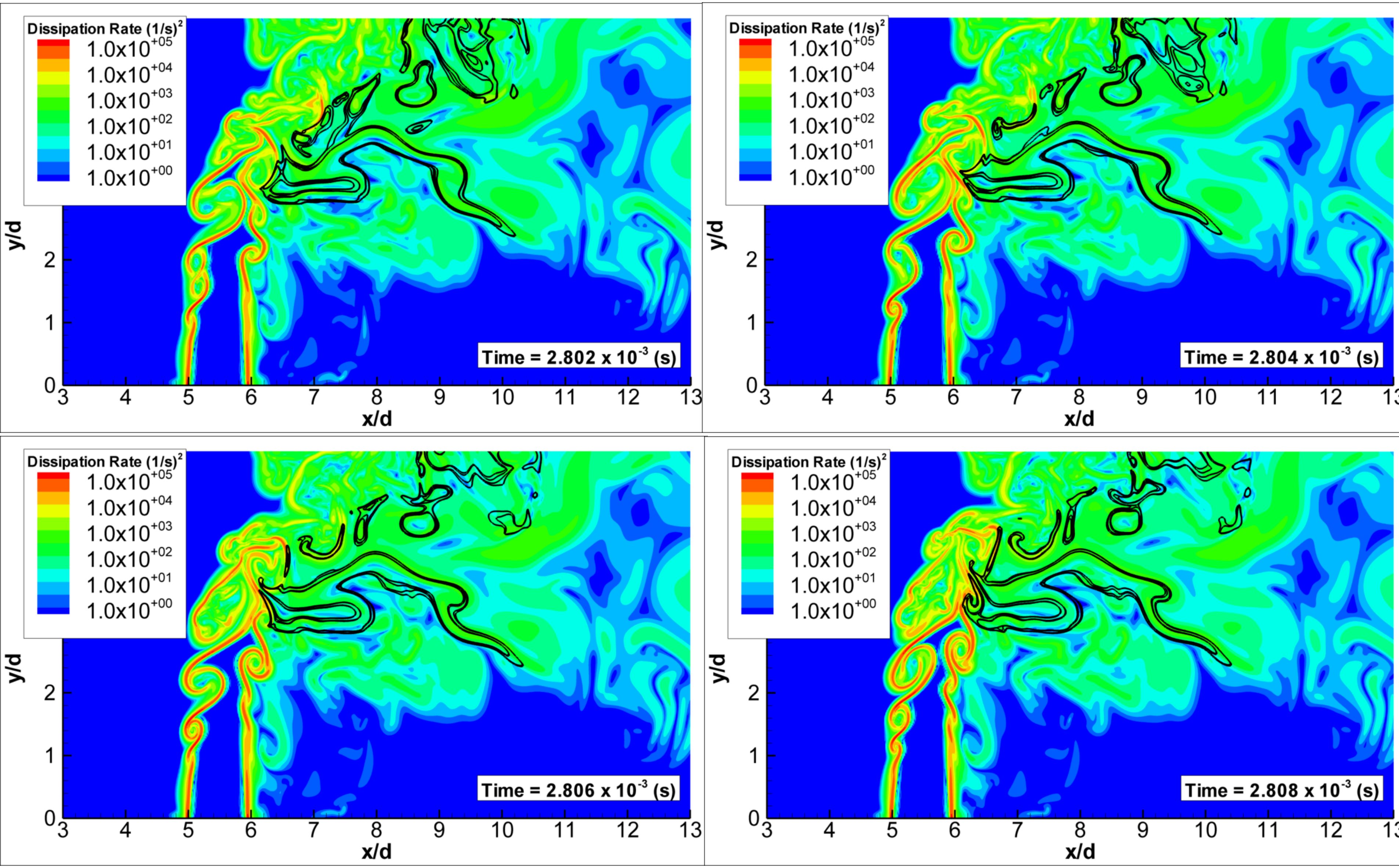
Reactive JICF, Instantaneous Temperature Field in YZ-plane

Reactive JICF, flame anchoring (1)



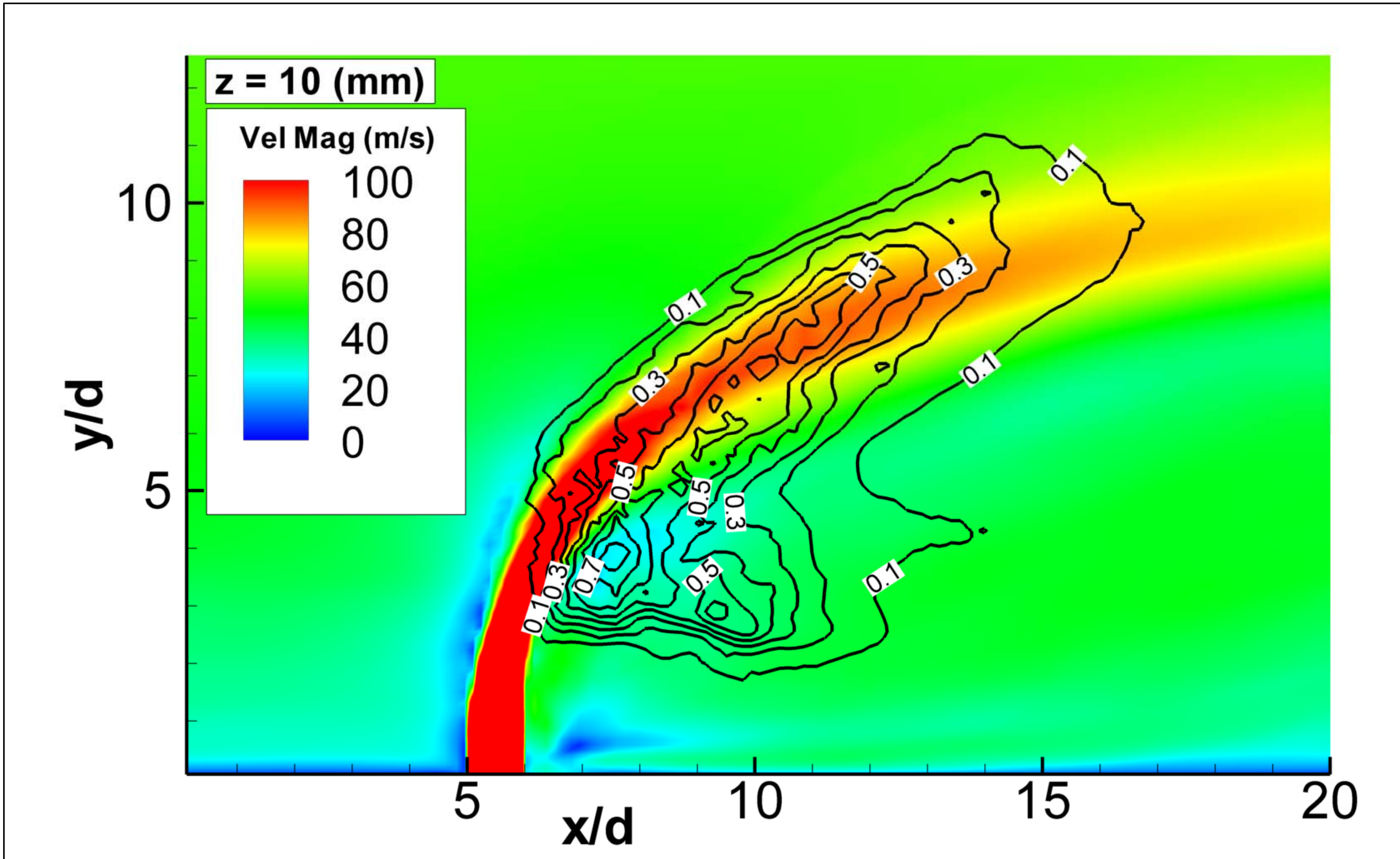
Maximum heat release rate (black lines) mark flame tongues entraining vortex shedded in shear layer

Reactive JICF, flame anchoring (2)



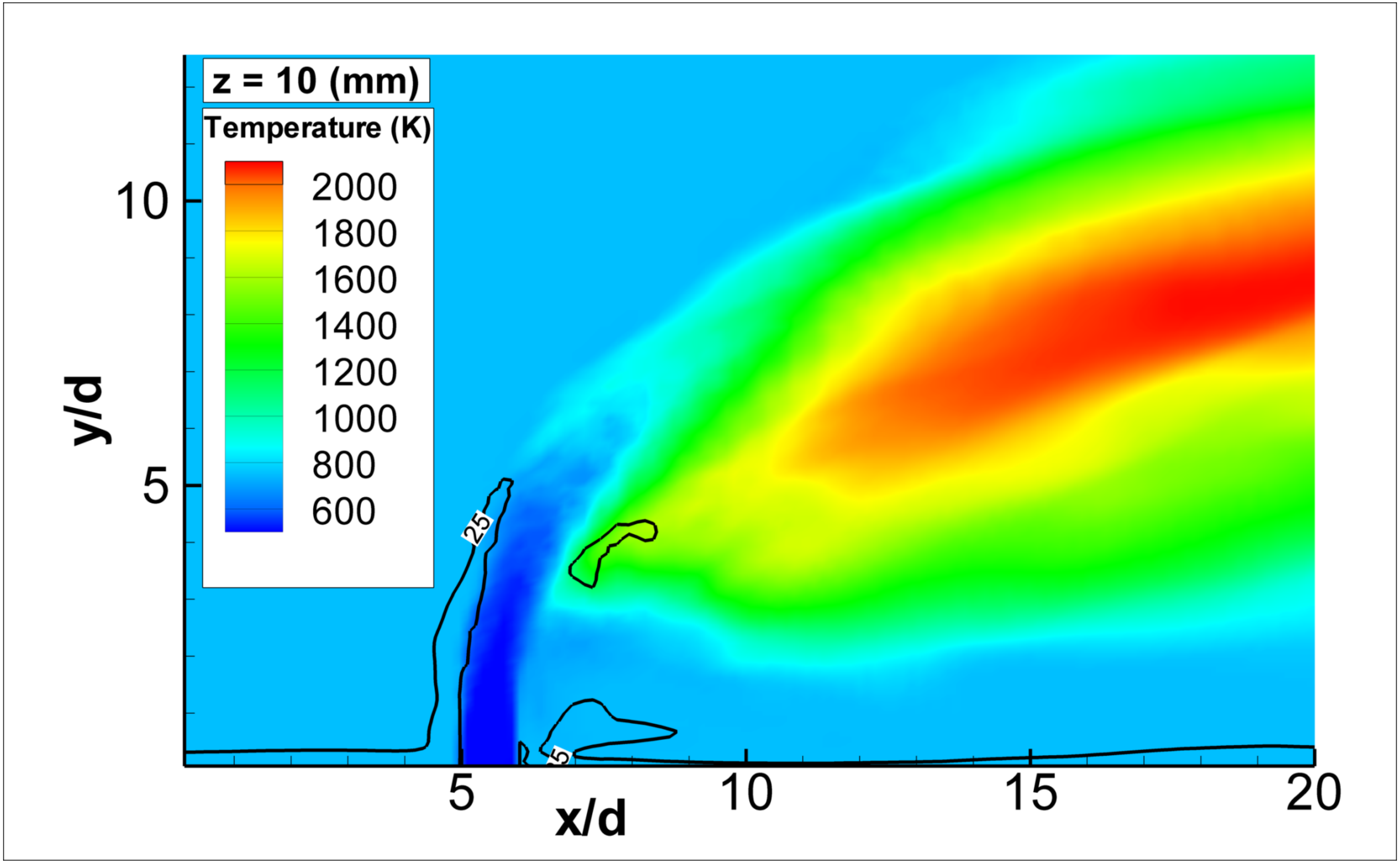
Maximum heat release rate (black lines) mark flame tongues entraining vortex shedded in shear layer

Reactive JICF, velocity and heat release rate averaged fields



Flame is ”Anchored” in Low Velocity Region Downstream of Jet (~4d from wall)

Reactive JICF, averaged temperature and ”low-velocity” zones



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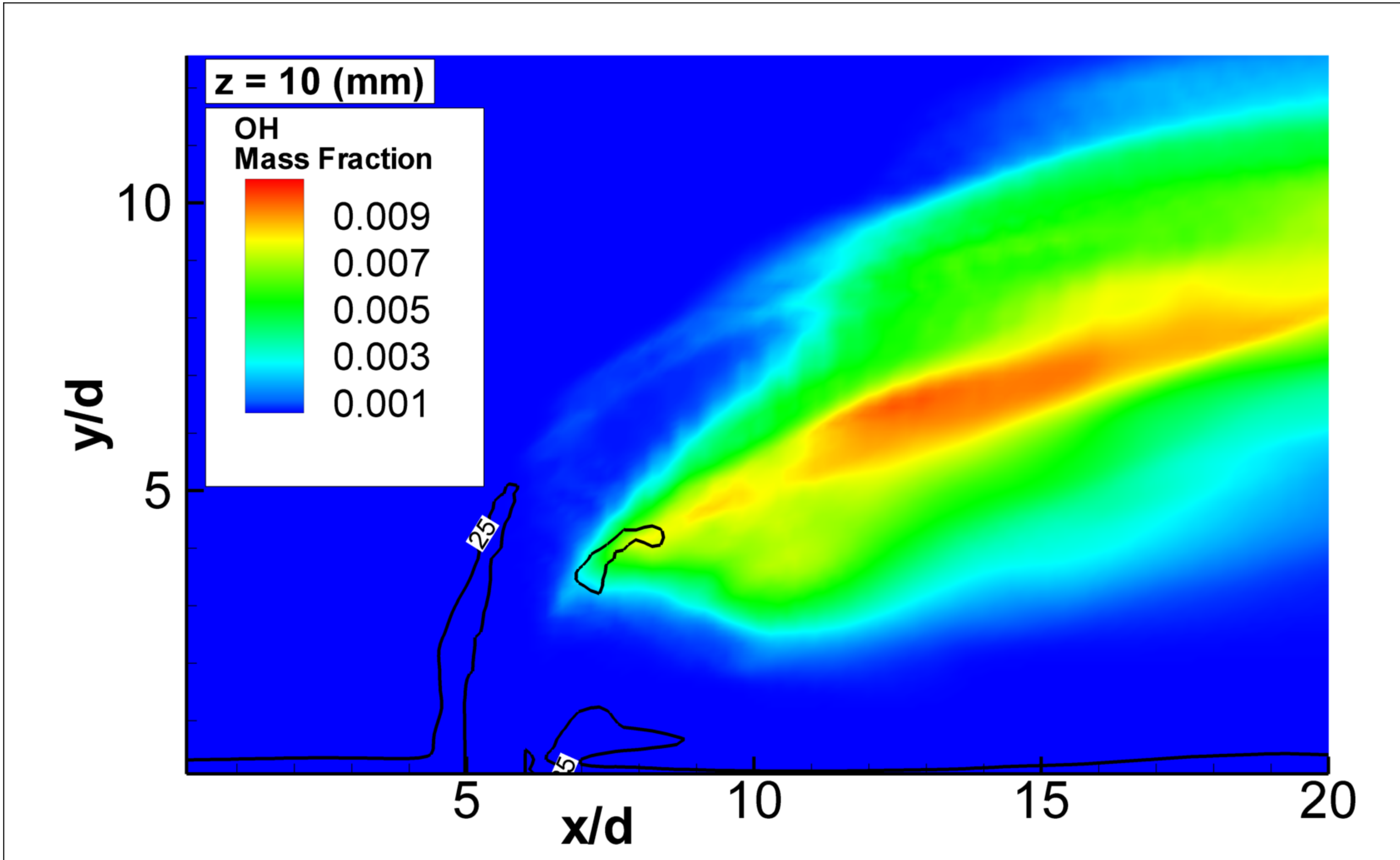
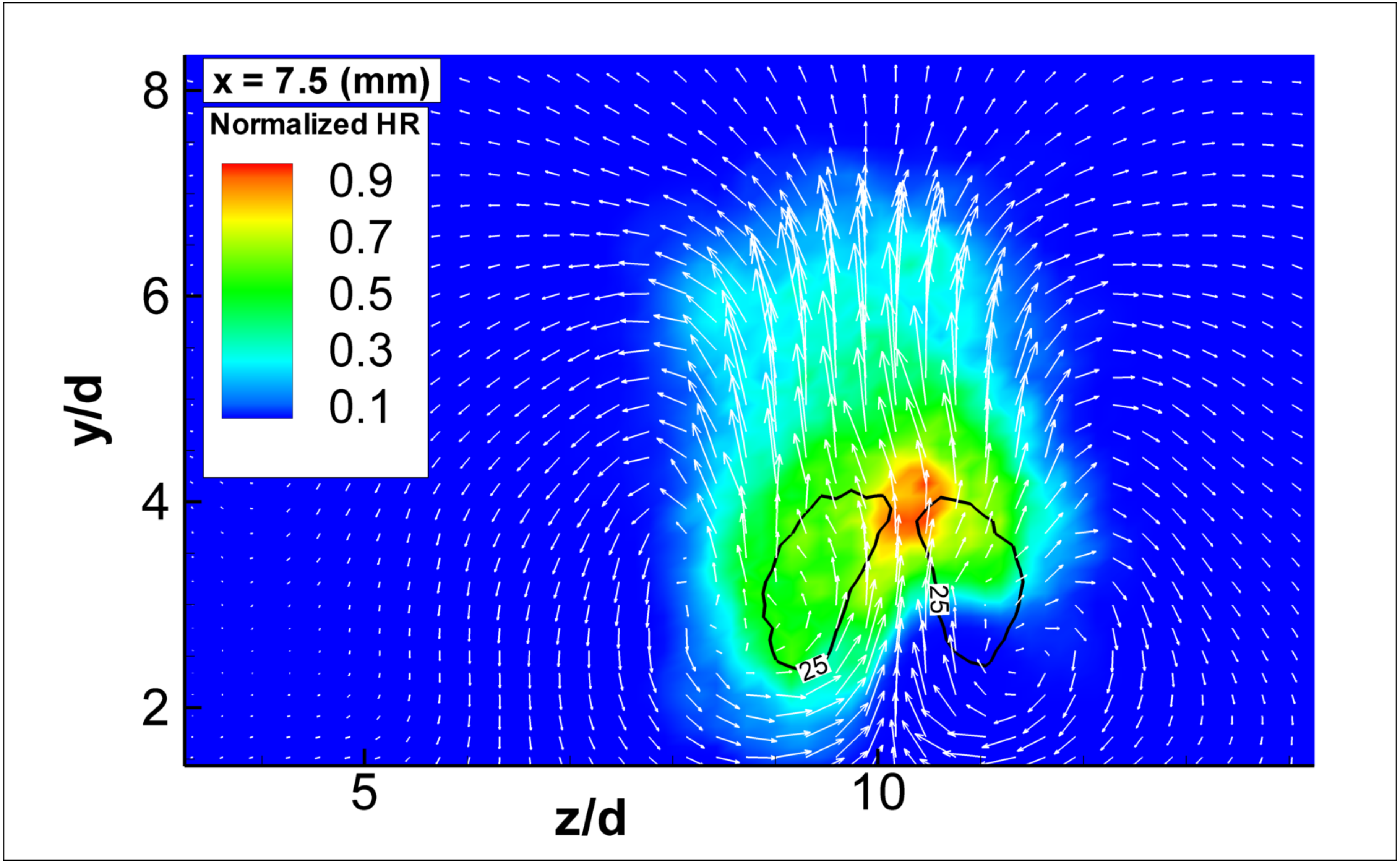


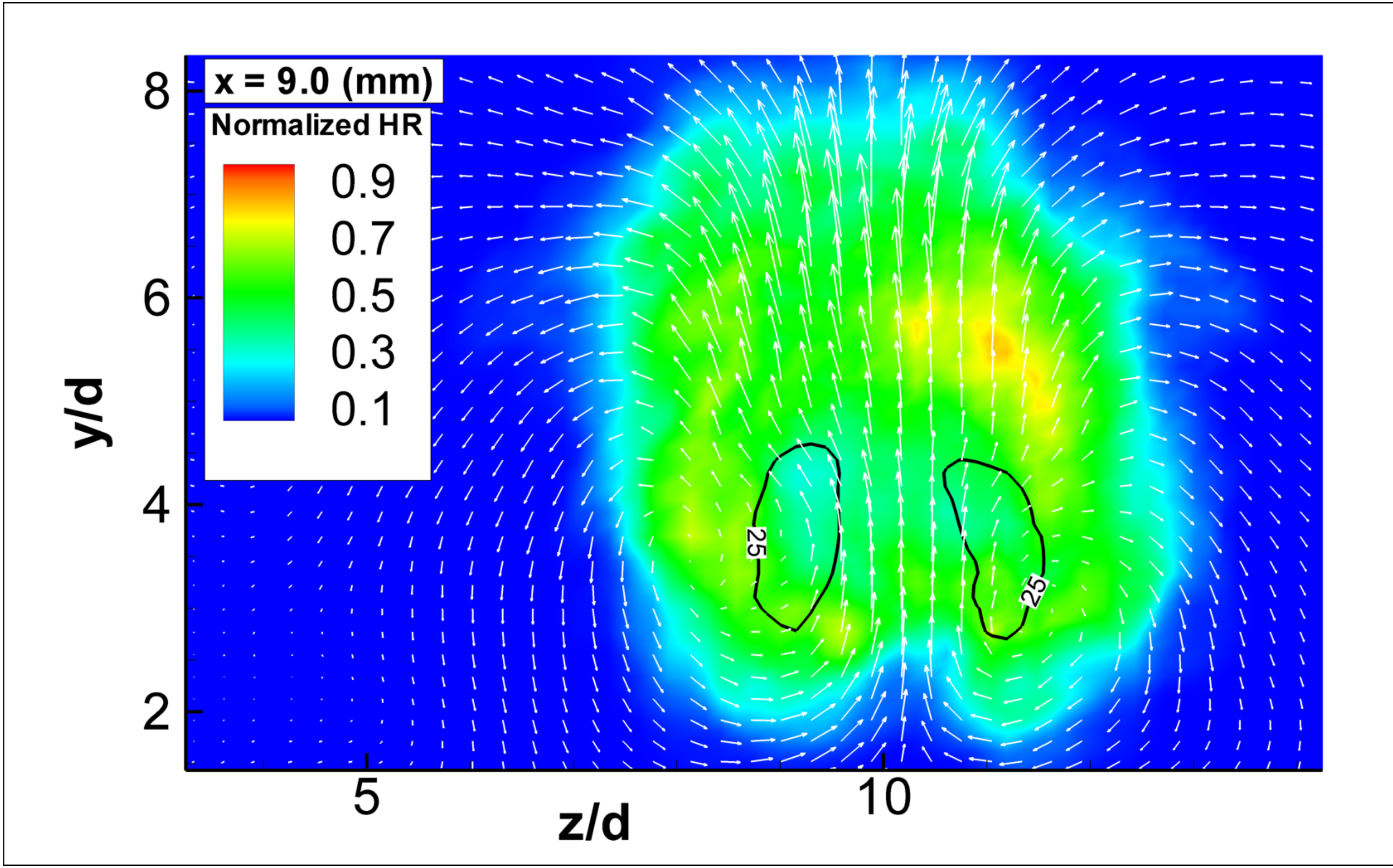
Flame is ”Anchored” in Low Velocity Region Downstream of Jet (~4d from wall)

Reactive JICF, counter-rotating vortex pair (CVP)



Upstream region of high heat release rate stabilized between the CVP

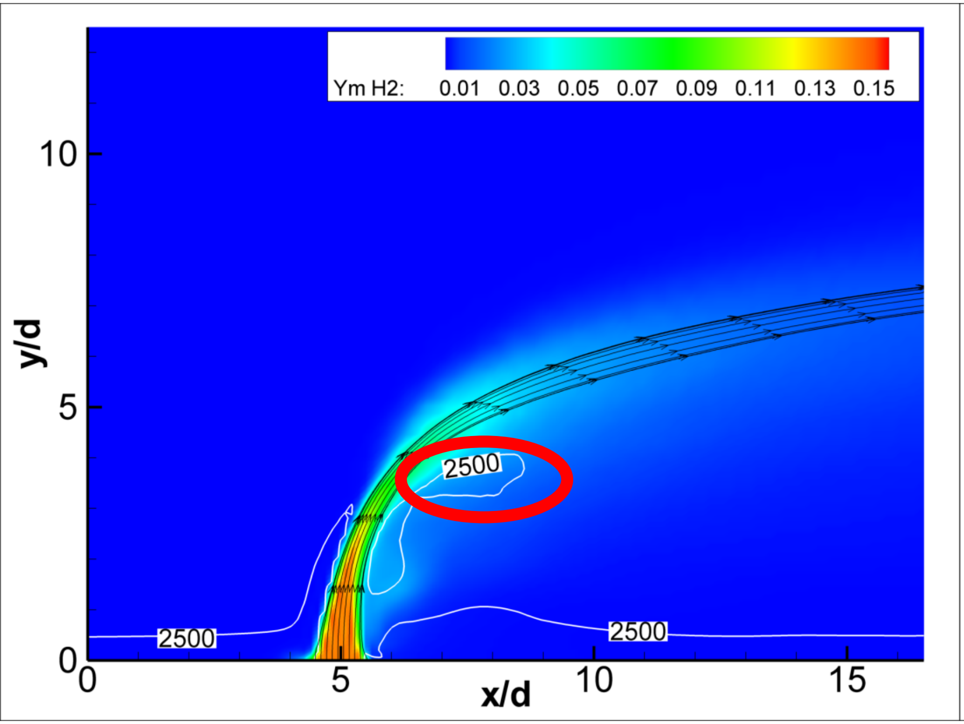
Reactive JICF, counter-rotating vortex pair (CVP)



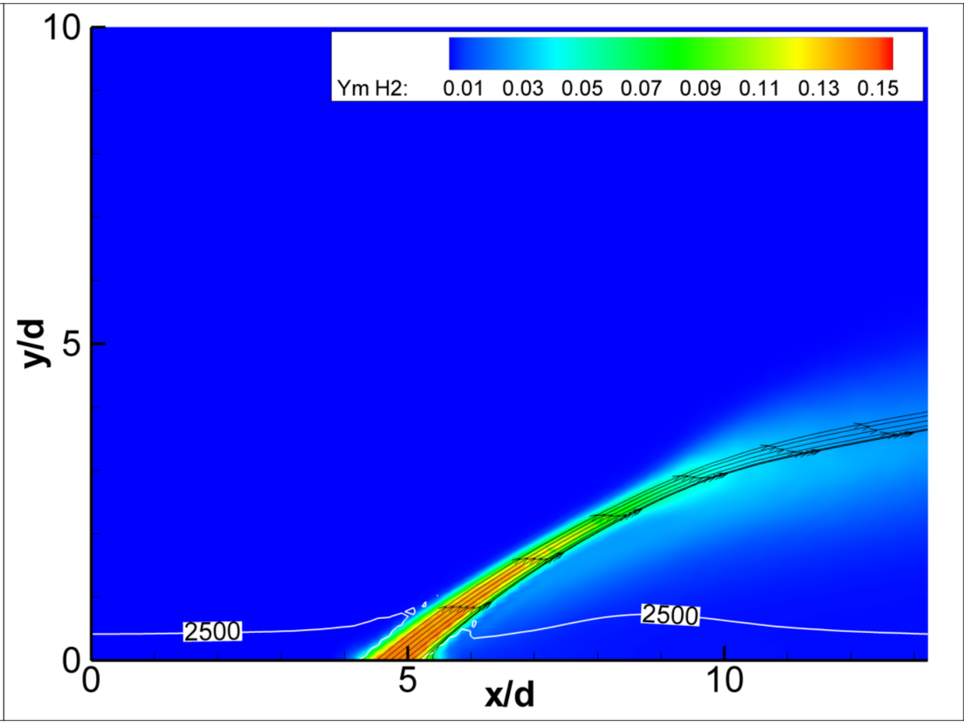
Downstream region of high heat release wraps around CVP (lower in between)

Inert JICF, parametric study (ongoing)

Non-reactive DNS of fuel injection (CPU cost ~ 2x10^5 hrs for each simulation)



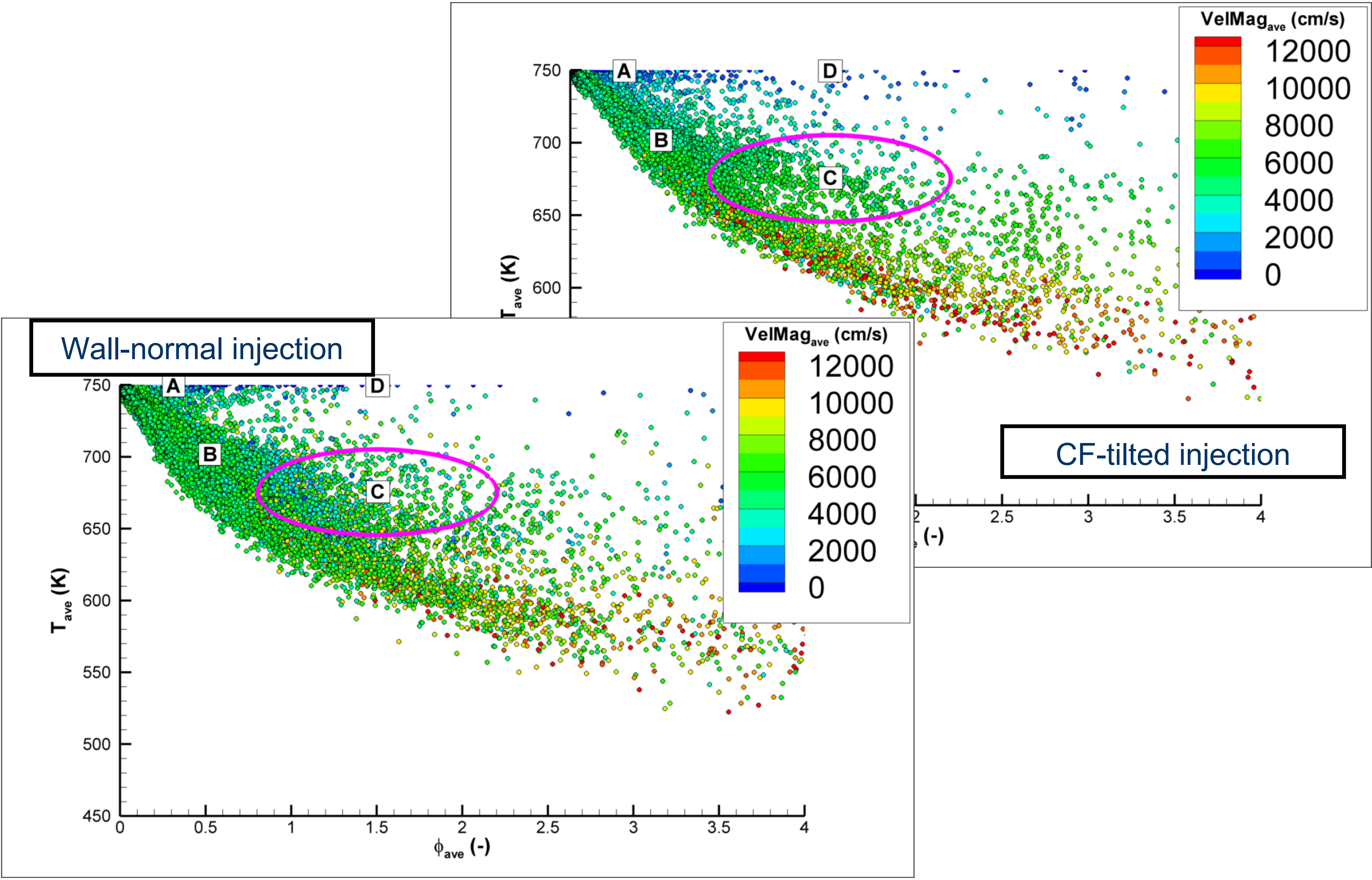
DNS of inert mixing case (wall-normal injection)



DNS of inert mixing case (CF-tilted injection)

- **Criteria is formulated to predict likehood of flame holding: co-located low mean flow speed and high fuel concentration (corollary → outside wall thermal boundary layer)**
  - **Probable flame holding locations can be indicated for specific fuel injection configurations after parametric study varying injection angle, nozzle shape etc.**

Inert JICF, parametric study: flame anchoring assessment



- **Knowledge of turbulent flame speed is required!**

Behavior of laminar flames

Laminar flame speed decrease for increasing pressure…

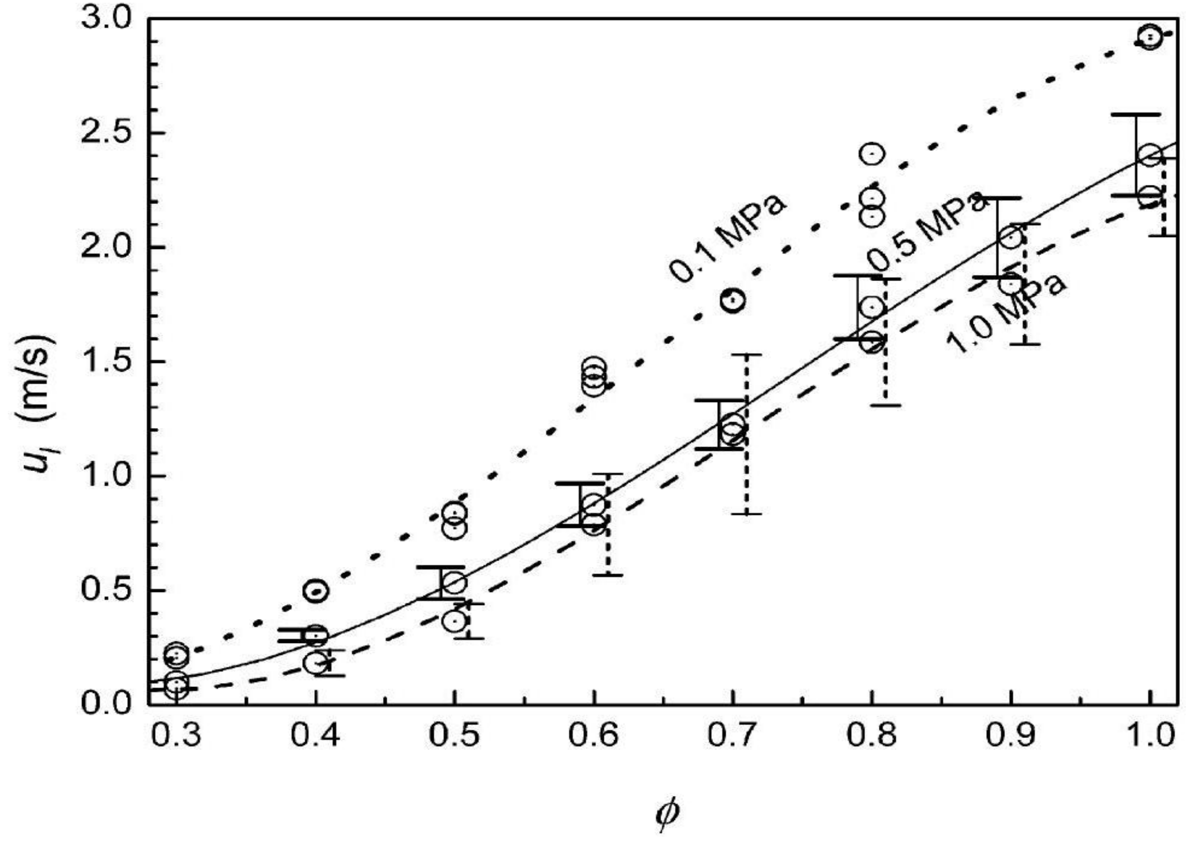
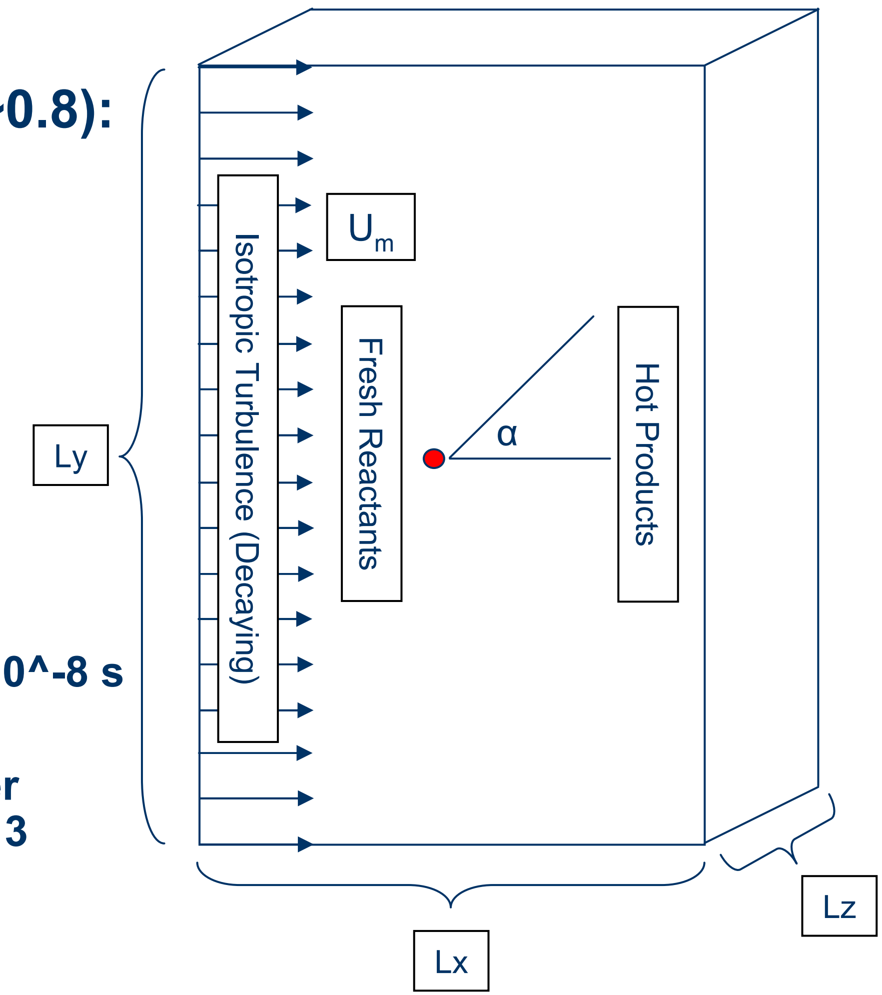


Fig. 10. Present experimental values of u_1 for different ϕ for $p = 0.1$, 0.5, and 1.0 MPa, $T = 365$ K.

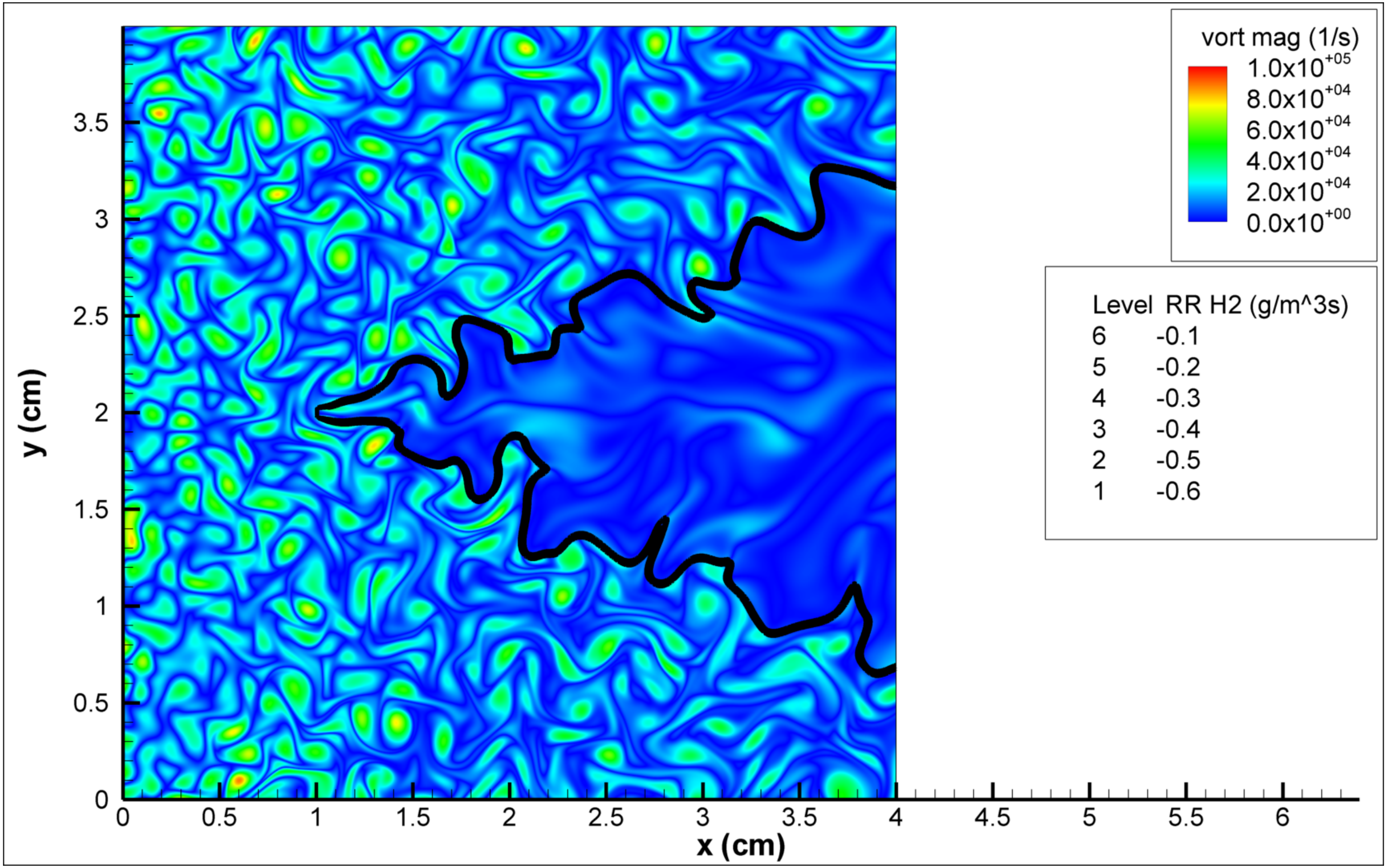
Experiments of Bradley et al. 2007

DNS of Turbulent V-flames (ongoing)

- **Typical 2-D case (1, 5 & 10 bar, φ~0.8):**
  - Full chemical kinetics (9 species, 19 reactions, Li et al. 2004)
  - Lx * Ly ~ 4.0 cm * 4.0 cm
  - Resolution 18 μm
  - Grid ~ 2240x2240 ~ 5.0*10^6
  - U_m ~ 60 m/s
  - U' ~ 7.4 m/s
  - Re_t ~ 400
  - Da = t_t / t_f ~ 5.6
  - CPU cost pr. node&timestep τc ~ 1.0*10^-8 s
  - Typical timestep τs ~ 2-10 ns
  - Useful physical simulation time T (after initial transient of 1 ”transit times”) → 3 ”transit times” ~ 3*(Lx/ U_m) = 2 ms
  - Turbulent flame speed estimated as:
    - S_t ~ sqrt(U_m^2 * tan^2(α)/(1+ tan^2(α)))

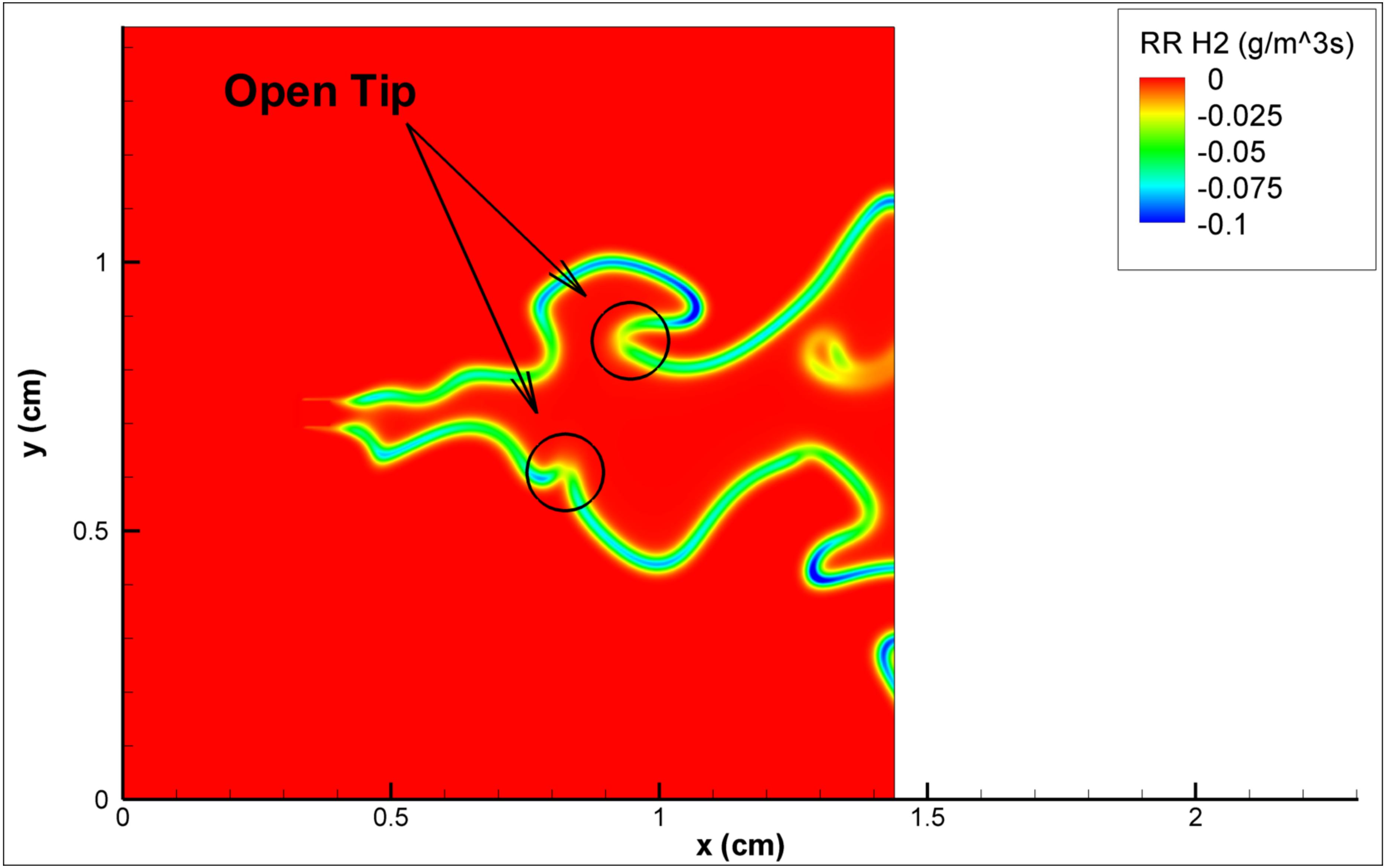


DNS of Turbulent V-flames: P=1 bar, φ=0.8



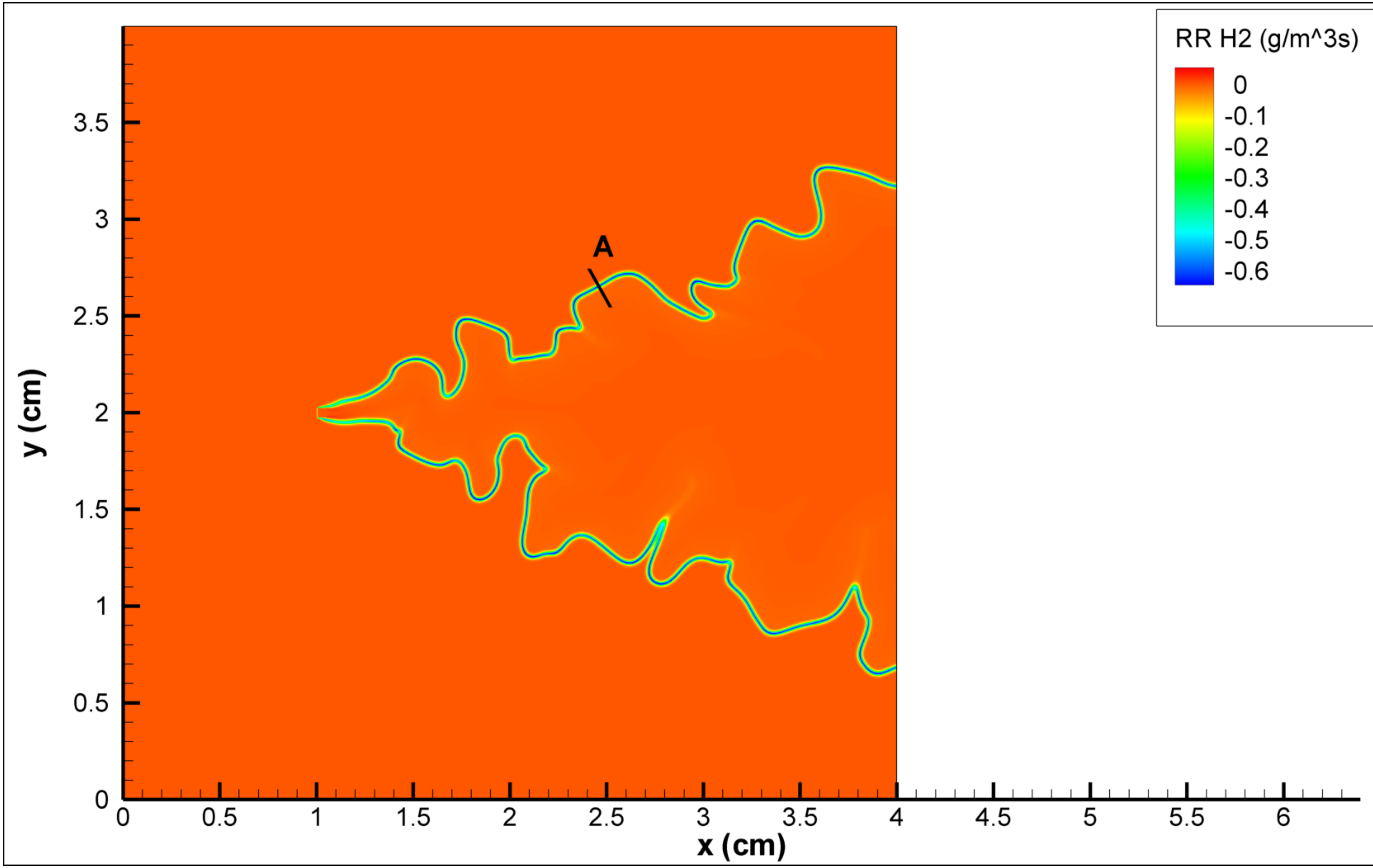
Semi-laminarization past the flame surface and turbulence decay towards domain exit!

DNS of Turbulent V-flames: P=1 bar, φ=0.3

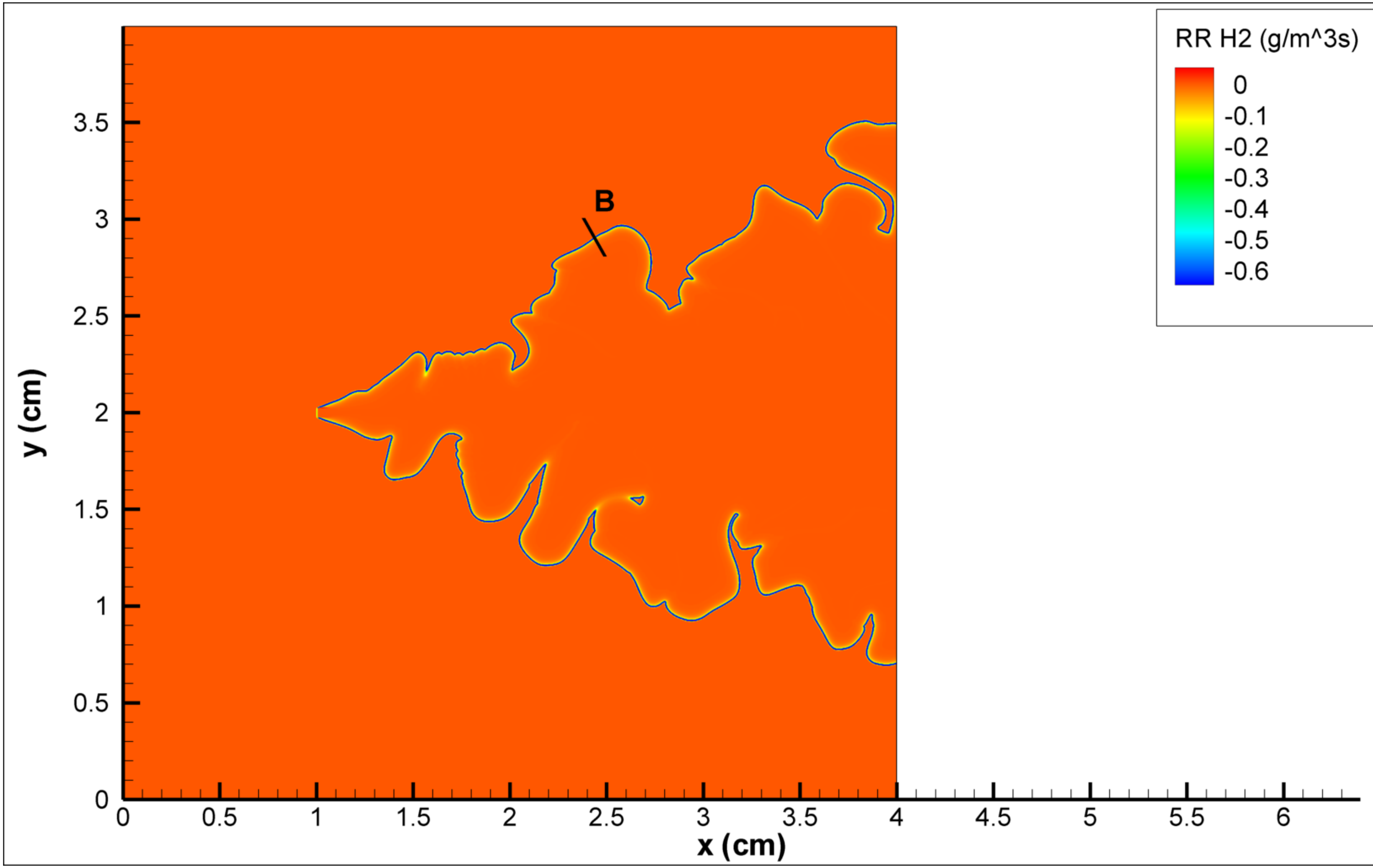


Characteristic ”open tip/cusp” and highly reactive ”domes” for ultra-lean case!

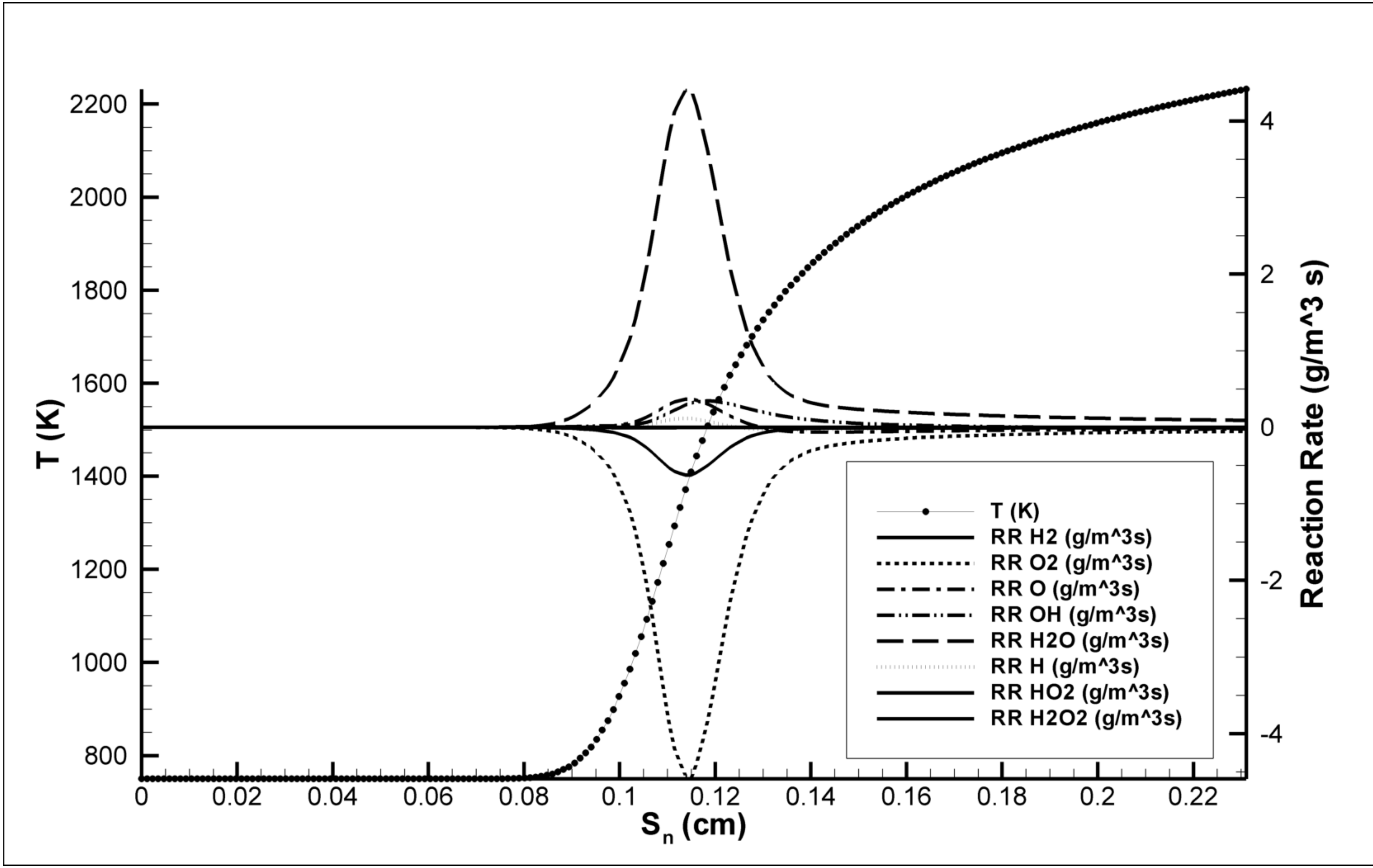
DNS of Turbulent V-flames: P=1 bar, φ=0.8



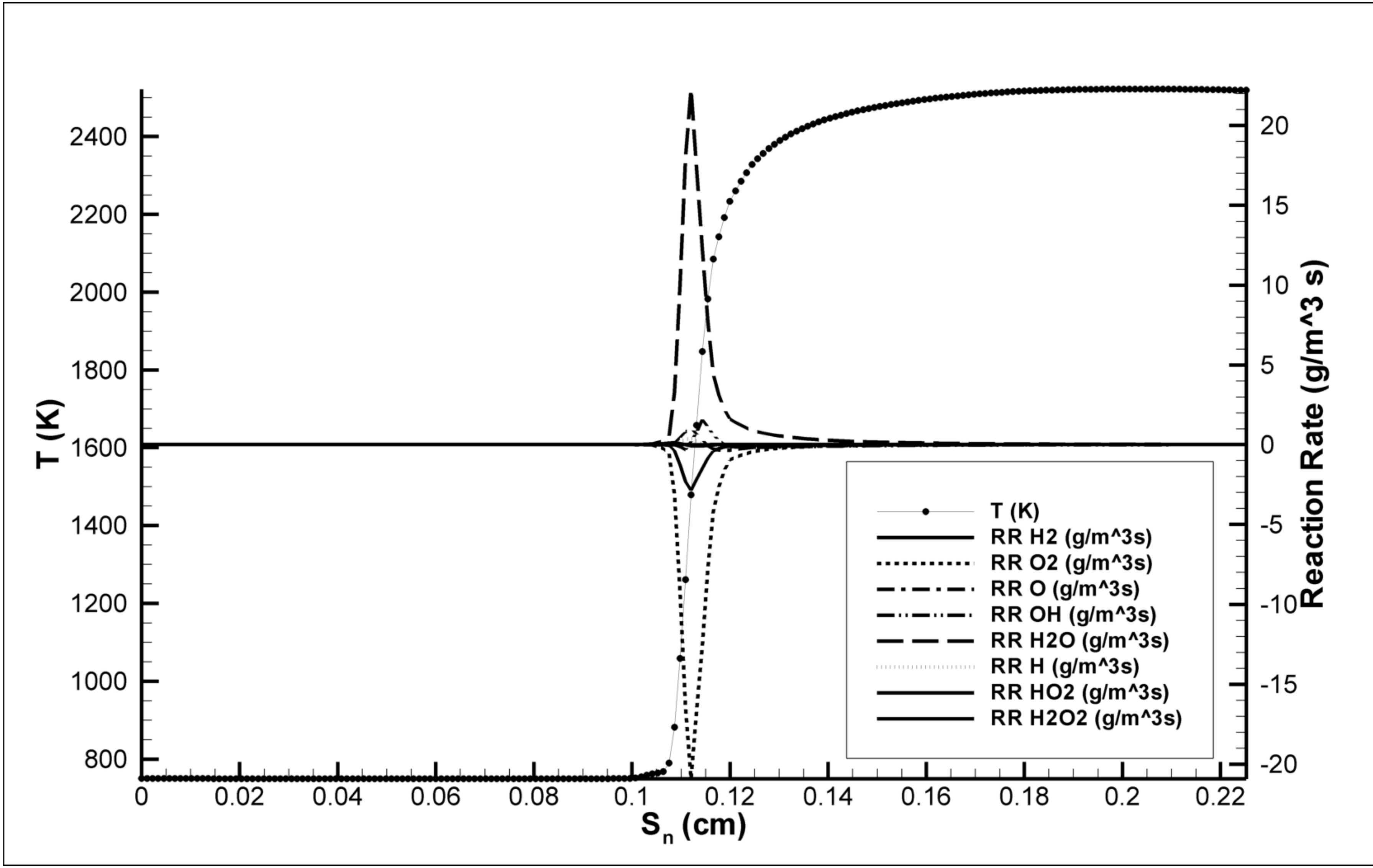
DNS of Turbulent V-flames: P=5 bar, φ=0.8



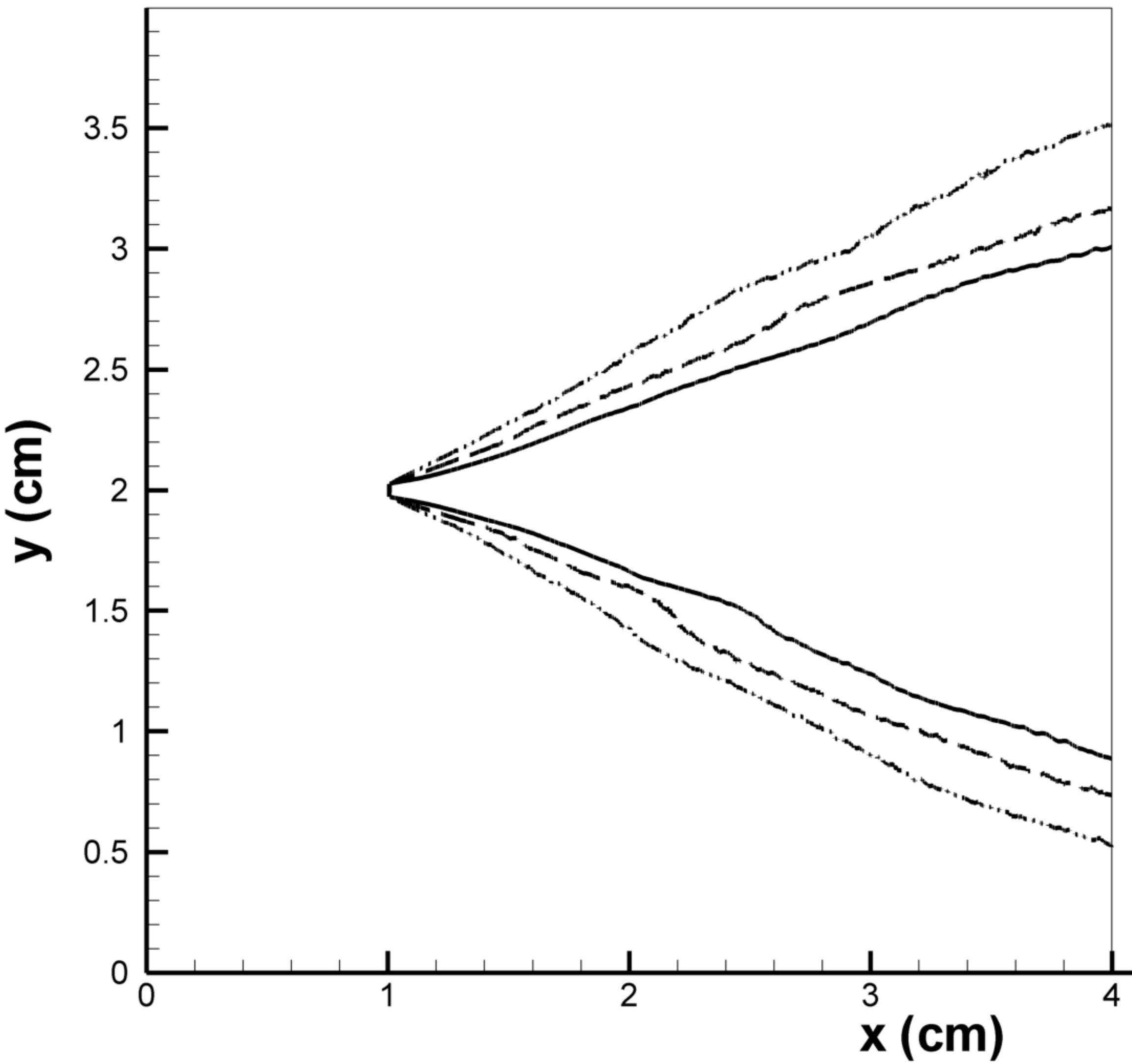
DNS of Turbulent V-flames: P=1 bar, φ=0.8



DNS of Turbulent V-flames: P=5 bar, φ=0.8



DNS of Turbulent V-flames: S_t comparison



Progress variable C=0.7 (avg)

P = 1 bar

P = 5 bar

P = 10 bar

Case parameters:

U_m ~ 60 m/s

u' ~ 7.4 m/s

l_t ~ 5*10^-3 m

η_k ~ 7*10^-5 m

Re_t ~ 300

ϕ = 0.8 , T_u = 750K

Estimated turbulent flame speed:

S_t ~ 18 m/s (1 bar)

S_t ~ 22 m/s (5 bar)

S_t ~ 27 m/s (10 bar)

DNS of Turbulent V-flames: S_t overview

Pressure/φ	0.3	0.5	0.8	1.5
1 bar	11.0 m/s	15 m/s	18 m/s	23 m/s
5 bar	9.5 m/s	13 m/s	22 m/s	28 m/s
10 bar	?	10 m/s	27 m/s	?

Opposite behavior is observed in the lean and rich case!

Conclusions & Further Work

1. ”Flame holding” in the near field of fuel jets in cross flow of air appear to be closely related to the vortex shedding of the jet shear layer and not to flame propagation in the boundary layer.*
2. Analysis and data mining of the DNS results are needed to quantitatively relate flame anchoring and propagation to the complex flow field.
3. Further work includes also:
   - investigation of the effects of boundary layer turbulence, nozzle shapes, injection angles on fuel injection configurations
   - detailed mapping of turbulent flame speeds at GT conditions and comparison with experimental investigations (AIST? PSI? Others…)

* This work is scheduled for oral presentation at the 33rd International Symposium on Combustion in Bejing.