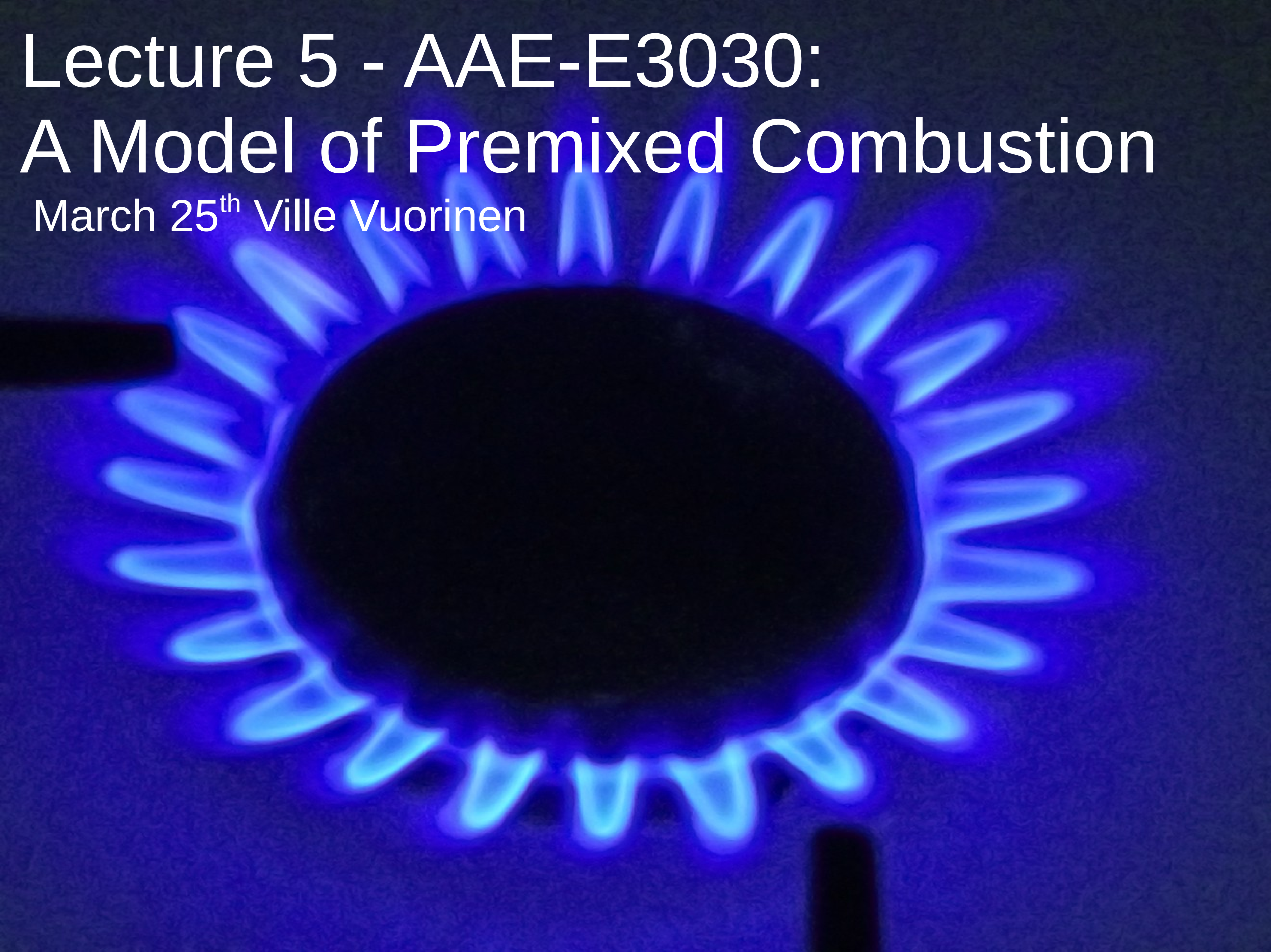

Lecture 5 - AAE-E3030:
A Model of Premixed Combustion

March 25th Ville Vuorinen

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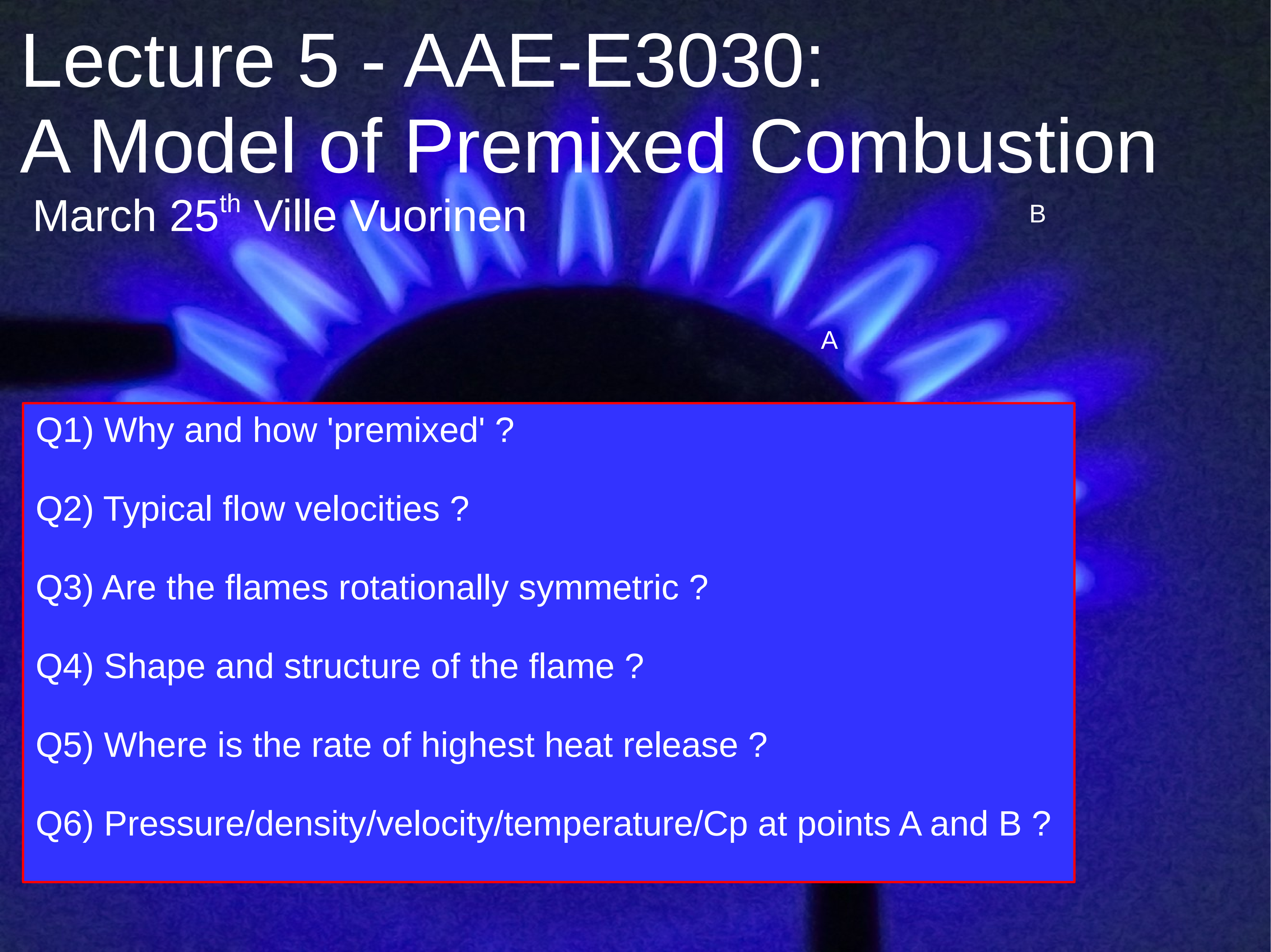


Q1) Why and how 'premixed' ?

Q2) Typical flow velocities ?

Q3) Are the flames rotationally symmetric ?

Q4) Shape and structure of the flame ?

Q5) Where is the rate of highest heat release ?

Q6) Pressure/density/velocity/temperature/Cp at points A and B ?

Lecture 5 in the Multiphase Course Timetable

- Lectures 1-2 → Fuel drops/multiphase flows
- Lectures 3-4 → Premixed 0d chemistry
- Lecture 5 → Premixed combustion 1d & 2d
- Lectures 6-7 → Premixed 1d chemistry
- Lecture 8 → Non-premixed combustion

Warnatz
Ch. 8, 10, 15

Motivation

Combustor (partially premixed ?)

https://www.youtube.com/watch?v=B7OajNkGp80

Acoustics and flames (acoustic modulation)

https://www.youtube.com/watch?v=EQXcOqH_Drs&list=PLxAI1X0qwonL1OyfLgfjonQSVFH8AdXnT

Flame blowoff and flashback (influence of inflow rate)

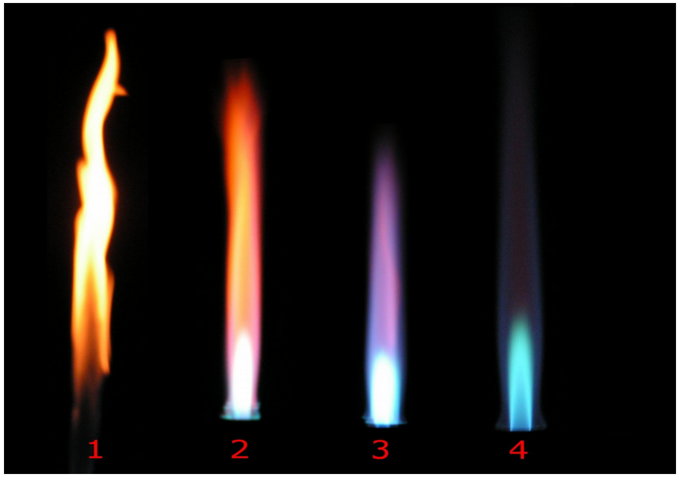
https://www.youtube.com/watch?v=KmyGR6mSPe0&list=PLxAI1X0qwonL1OyfLgfjonQSVFH8AdXnT&index=2

LES of premixed combustor (influence of swirl and recirculation techniques)

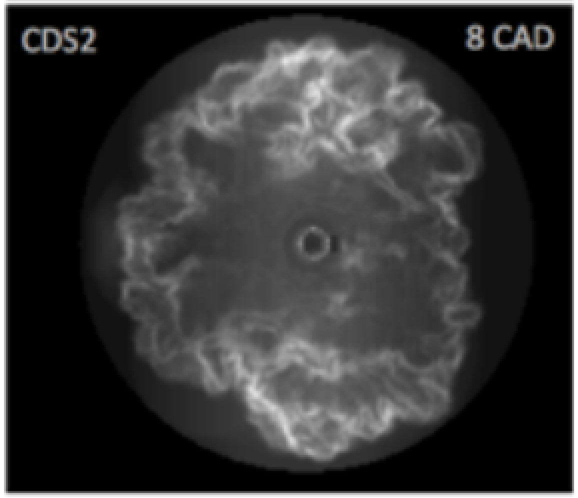
https://www.youtube.com/watch?v=Mim33CvQTUQ

Spark ignition of premixed gas (advantages of mixture uniformity thanks to premixing)

https://www.youtube.com/watch?v=xg3Ri1-1rCE

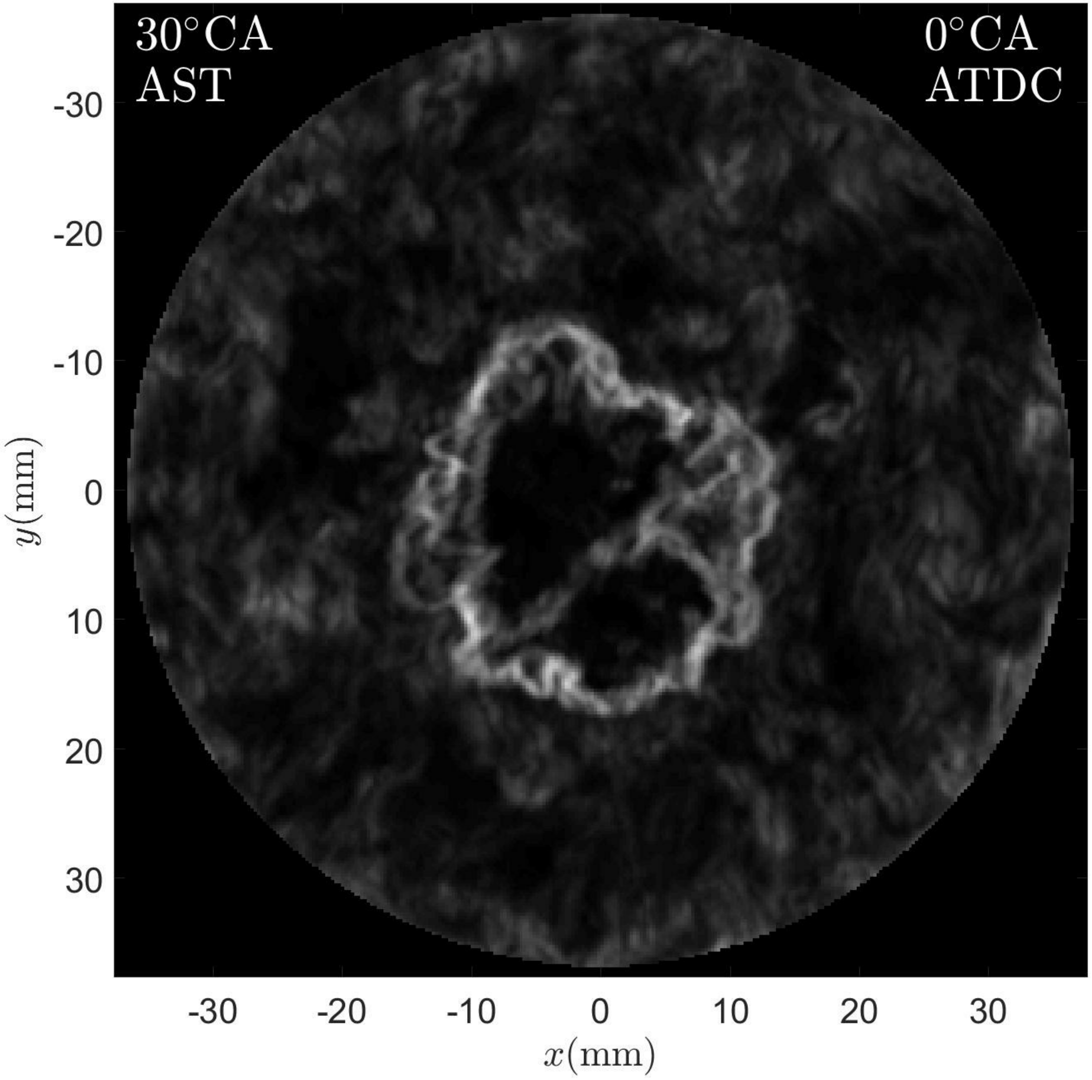


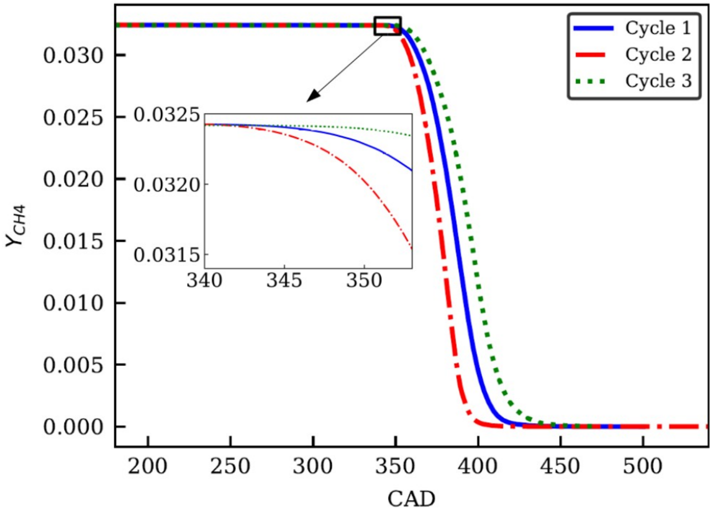
LES simulation of spark ignited fuel

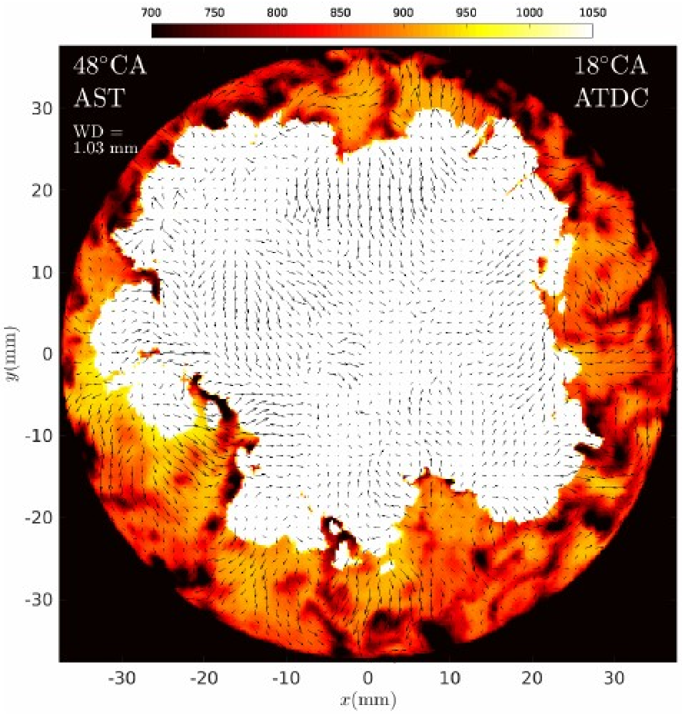


Courtesy of: Nguyen and Kempf, LES4ICE conference (2016)

Large-Eddy Simulation (LES CFD method) on Spark-Ignited (SI), Premixed Methane-Air Combustion

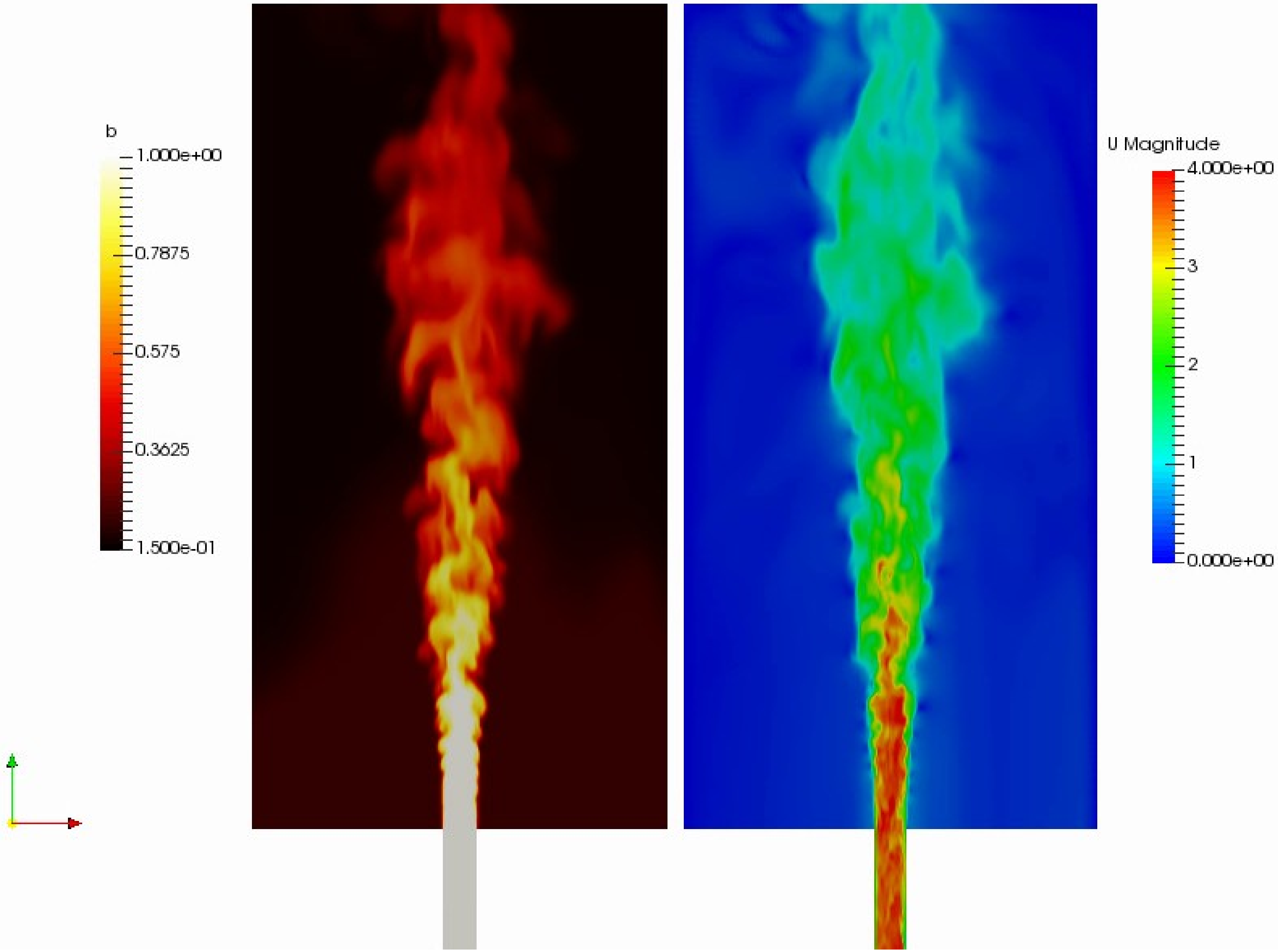




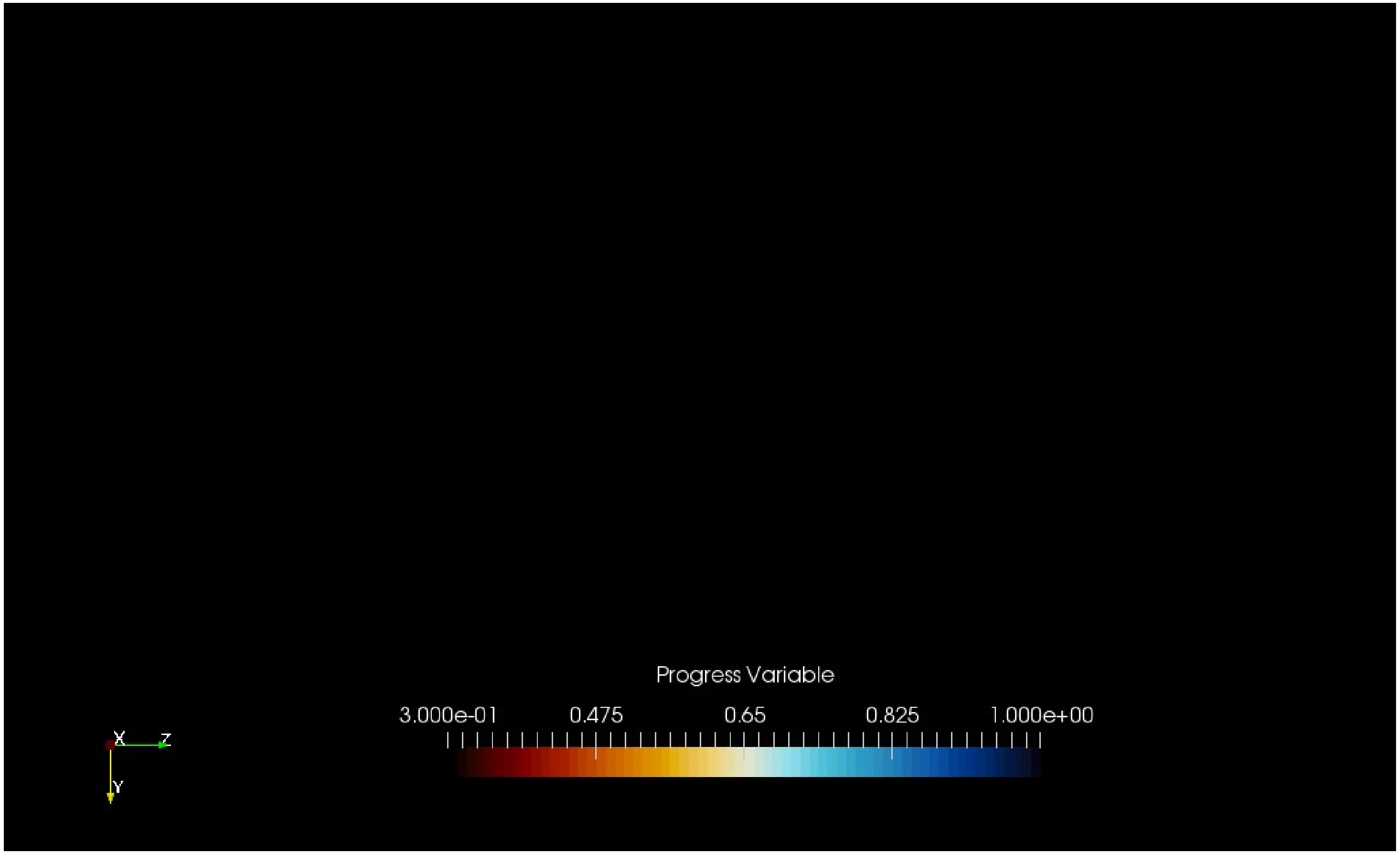


CFD-simulation of premixed gas combustion (G-equation) in Spark Ignited gas engine. M.Ghaderi-Masouleh, Vuorinen et al. Applied Energy (2018)

Typical scalar (e.g. concentration of incoming gas A) and velocity fields in a turbulent jet



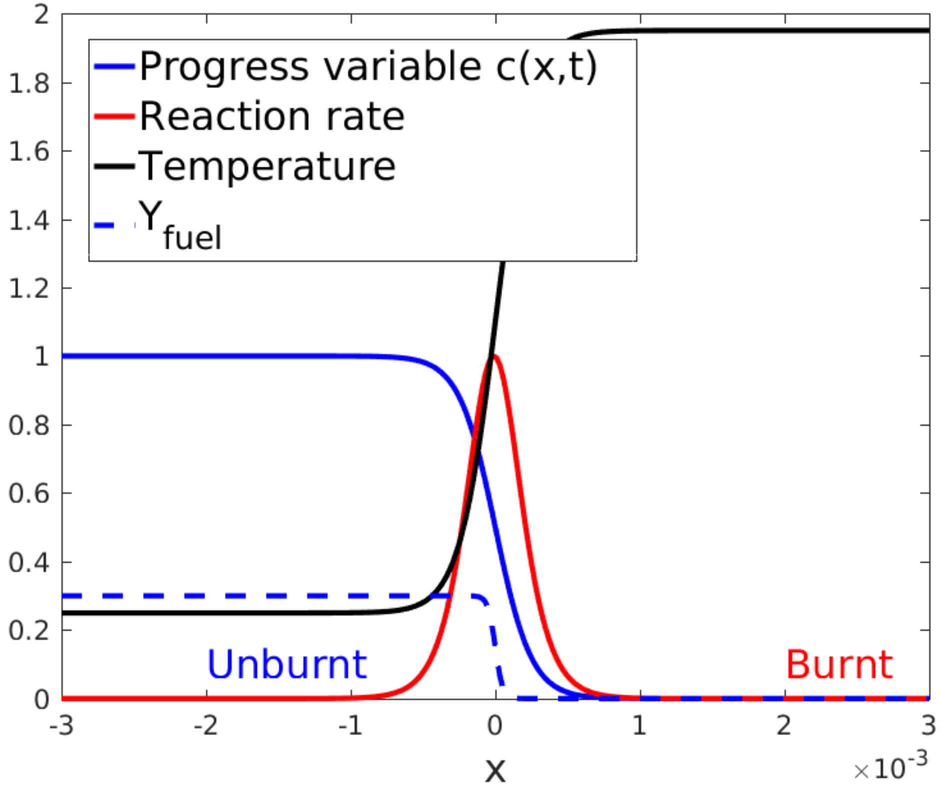
Simulation of premixed flame for different flame speeds



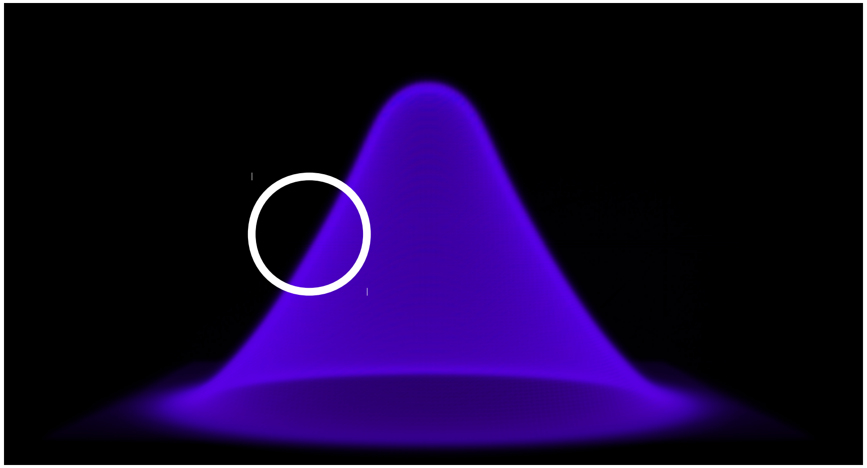
Courtesy of B.Tekgul (2017)

We look next on a simplified model on premixed flame and imagine how the flame would look like locally

Simplified view on flame structure



Locally, flame is considered to be 1 dimensional in the direction of flame surface normal



Important concept: S_L = laminar flame speed

Some assumptions

Single step reaction of premixed fuel and air either lean, stoichiometric or rich. For example:

$$CH_4+2\left(3.76\,N_2+O_2\right)\rightarrow CO_2+2\,H_2O+7.52\,N_2$$

The deflagration type flame front thickness is thin, simple scaling estimates:

$$\delta=\frac{\lambda_{therm}}{\rho\,c_p S_L}=\frac{D_{therm}}{S_L} \qquad \mathrm{Re}_{flame}=\frac{S_L\,\delta}{D_{therm}}=1$$

A progress variable describes flame evolution:

$$c=\frac{Y_f^b-Y_f}{Y_f^b-Y_f^u}$$

$c=1$ → unburnt
$c=0$ → burnt

$$T\approx\left(1-c\right)T_b+cT_u$$

1d Convection-Reaction Equation for c i.e. c-equation

$$\underbrace{\frac{\partial \rho \overset{\text{Progress variable}}{\overset{\downarrow}{c}}}{\partial t}}_{\overset{\uparrow}{\text{Time derivative}}} + \underbrace{\frac{\partial \rho c \overset{\text{Velocity}}{\overset{\downarrow}{u}}}{\partial x}}_{\overset{\uparrow}{\text{Convection term}}} = \underbrace{\boxed{-\overset{\text{Unburnt density}}{\overset{\downarrow}{\rho_u}} \overset{\text{Laminar flame speed}}{\overset{\downarrow}{S_L}} \left|\frac{\partial c}{\partial x}\right|}}_{\overset{\uparrow}{\text{Reaction source term}}} \longleftarrow \text{High at burnt/unburnt interface}$$

Progress variable approach in general (1D, 2D and 3D)

$$\frac{\partial \rho c}{\partial t} + \nabla \cdot \rho c \boldsymbol{u} = \boxed{-S_d \rho_u |\nabla c|}$$

Interplay of thermal diffusion and global reaction
rate consumes fuel

$$S_d = displacement\, speed$$

$$S_d = S_L \left(1 \boxed{- L_M \kappa - S}\right)$$

Correction terms for curved and strained plane fronts (deviation from plane flame, uniform ambient flow Assumption).

Markstein length

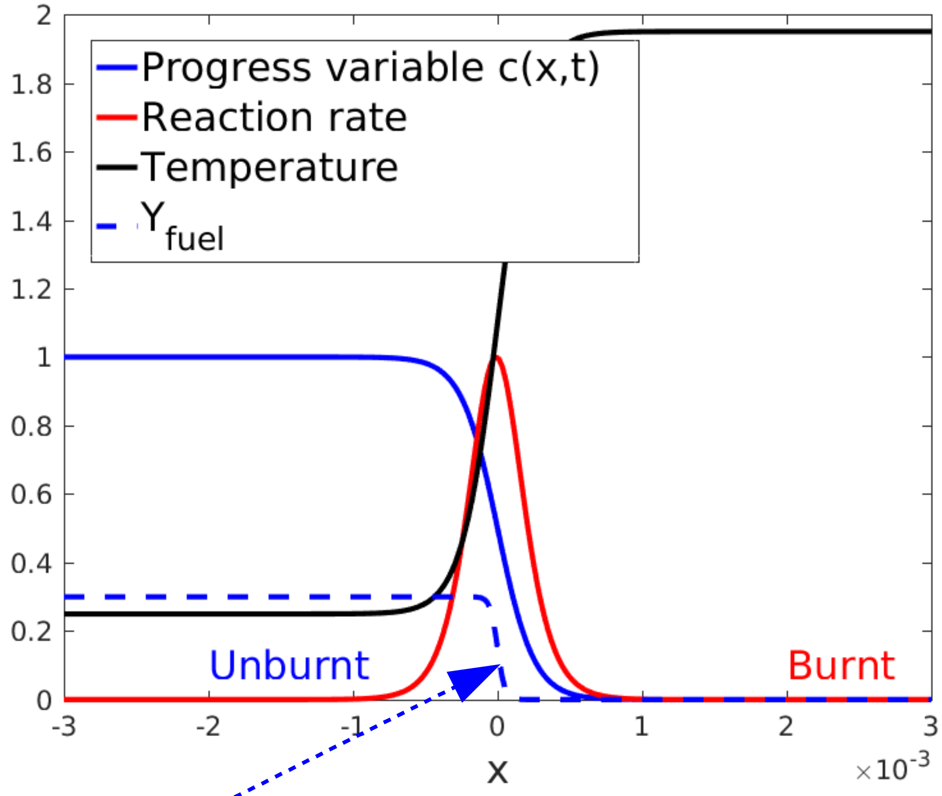
Curvature

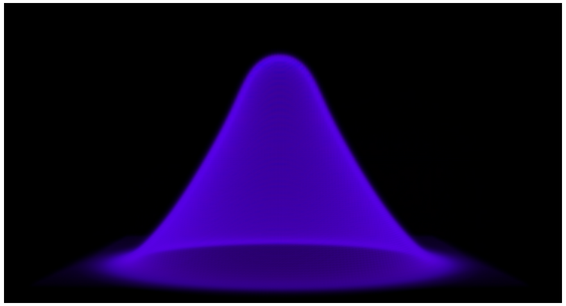
Strain

$$\kappa = \nabla \cdot \boldsymbol{n}$$

$$\boldsymbol{n} = \frac{\nabla c}{|\nabla c|}$$

C-equation says: “We look at an averaged flame on scales much larger than flame thickness. To describe flame propagation we need model for 1) reaction rate, 2) flame speed, and 3) burnt/unburnt thermodynamics.”



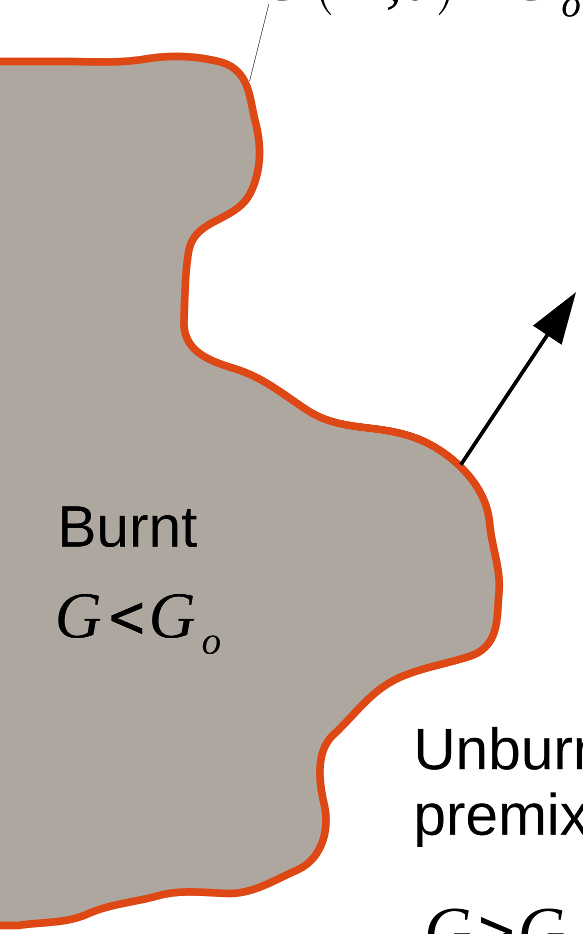


The real fuel mass fraction profiles are not captured.

$$\delta \ll \Delta x$$

$$\Delta x = grid\ spacing$$

Premixed Combustion as Flame Propagation Phenomenon
G-equation (Markstein 1964, Williams 1985)



$G(\boldsymbol{x},t)=G_o$

$\boldsymbol{n}=\frac{\nabla G}{|\nabla G|}$

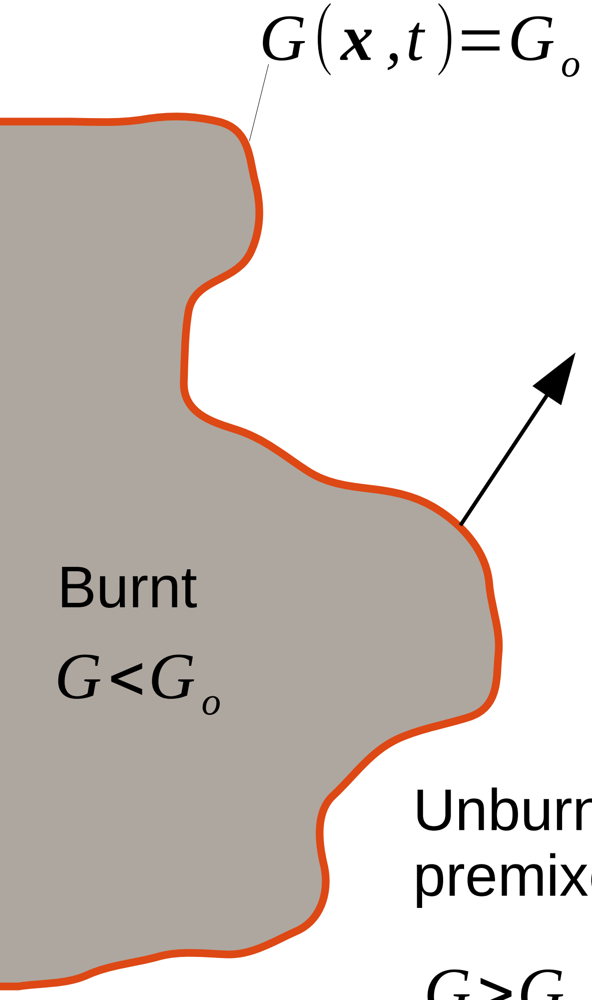
Burnt

$G<G_o$

Unburnt,
premixed fuel-air mixture

$G>G_o$

Premixed Combustion as Flame Propagation Phenomenon
G-equation (Markstein 1964, Williams 1985)



$$G(\boldsymbol{x},t)=G_o$$

$$\boldsymbol{n}=\frac{\nabla G}{|\nabla G|}$$

Burnt

$$G<G_o$$

Unburnt,
premixed fuel-air mixture

$$G>G_o$$

$$\frac{dG(\boldsymbol{x},t)}{dt}=\frac{\partial G}{\partial t}+\frac{d\boldsymbol{x}_f}{dt}\cdot\nabla G=0$$

$$\frac{d\boldsymbol{x}_f}{dt}=\boldsymbol{u}+S_f\boldsymbol{n}$$

$$\frac{\partial G}{\partial t}+\boldsymbol{u}\cdot\nabla G=-S_f|\nabla G|$$

$-S_f|\nabla G|$ Reaction source term

$\boldsymbol{u}\cdot\nabla G$ Convection term

$\frac{\partial G}{\partial t}$ Time derivative term

Some Available Options as Premixed Combustion CFD Model (May Apply to Non-Premixed as Well)

Model family/concept	**Some assumptions**	**What the model typically needs?**	**Benefits**	**Some Drawbacks**
G-equation (Markstein 1964, Williams 1985)	- physical flame thickness $\delta << \Delta x$ - flame at G = const. i.e. level-set approach - separation to **burnt** and **unburnt** regions	- Correlation S_L - an algorithm to find the flame position	- single equation to describe premixed combustion	- G=G(x,y,z,t) has no physical meaning elsewhere than at flame - level set approach so the flame really needs to be tracked → compications for implementation
Flame surface density (c-equation)	- Thin flame $\delta << \Delta x$ - c is defined everywhere in contrast to level-set -	- Correlation S_L - Correlation for flame surface density (effect of unresolved flame deviation from planar)	- single equation to describe premixed combustion - rather simple to implement	-assumption of single step chemistry -a particular link between emissions and c needed - possibly even extra eqn for surface density needed
Flamelet method	- flame=ensemble of 1d flames	- pre-calculated chemistry look-up tables	- fast in runtime with accurate description of species from tables	- pre-tabulation can be a tedious task
Direct chemistry	- full Navier-Stokes + species eqs solved - flame is resolved DNS	- low Reynolds number - accurate diffusion model	- computational 'experiment' with all possible data available	- very heavy and limited to small mechanisms
Thickened flame	- flame artificially thickened to numerically resolve the flame - reaction rate scaled by L and thermal diffusivity by 1/L while S_L is const.	- reduced or accurate chemical mechanism which gives correct flame speed and IDT	- flame front is really resolved with important species	- is the physics still the same ?

Assumptions of this eqn?

$$\rho U \sin(\alpha) = \rho_u S_L$$

Bunsen Flame – Background

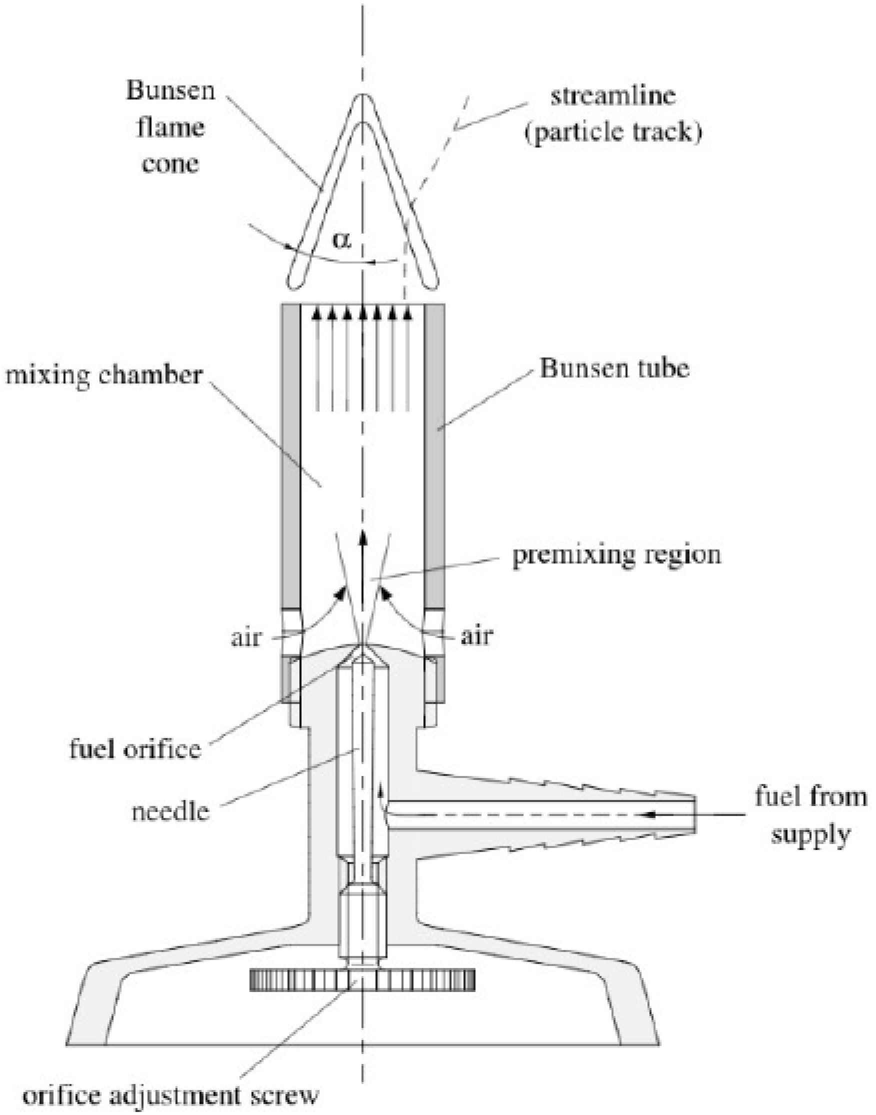


Figure 1 : Typical Bunsen burner. *(Peters. Turbulent combustion)*

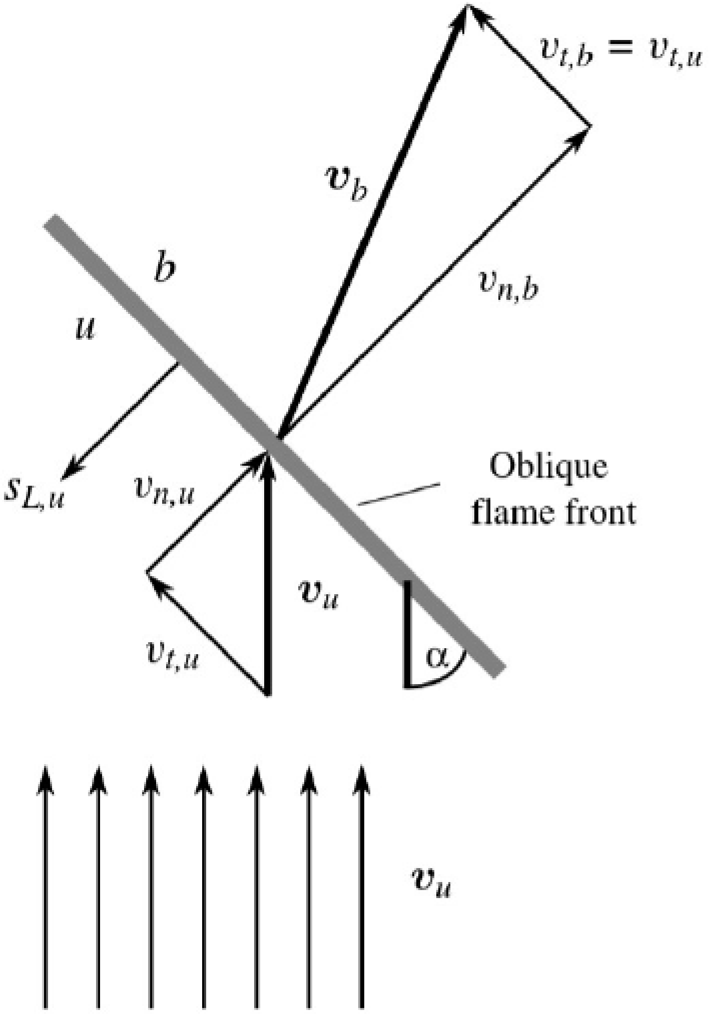


Figure 2 : Kinematic balance for a steady oblique Bunsen flame. *(Peters. Turbulent combustion)*

Compressible fluid flows: Full Navier-Stokes Equations

$$\frac{\partial \rho}{\partial t}+\frac{\partial \rho u_j}{\partial x_j}=0$$

Mass conservation

Viscous stress tensor

$$\sigma_{ij}=\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\mu\frac{\partial u_i}{\partial x_j}\delta_{ij}$$

$$\frac{\partial \rho u_i}{\partial t}+\frac{\partial \rho u_i u_j}{\partial x_j}=-\frac{\partial p}{\partial x_i}+\frac{\partial \sigma_{ij}}{\partial x_i}$$

Momentum conservation

Internal energy

$$e=c_v T+\frac{1}{2}u_i^2$$

$$\frac{\partial \rho e}{\partial t}+\frac{\partial(\rho e+p)u_j}{\partial x_j}=\frac{\partial u_i \sigma_{ij}}{\partial x_i}+\frac{\partial}{\partial x_i}\lambda\frac{\partial T}{\partial x_i}$$

Energy conservation

$$p=\rho R T$$

Note: 1 + 3 + 1 equations, the set is closed by the equation of state

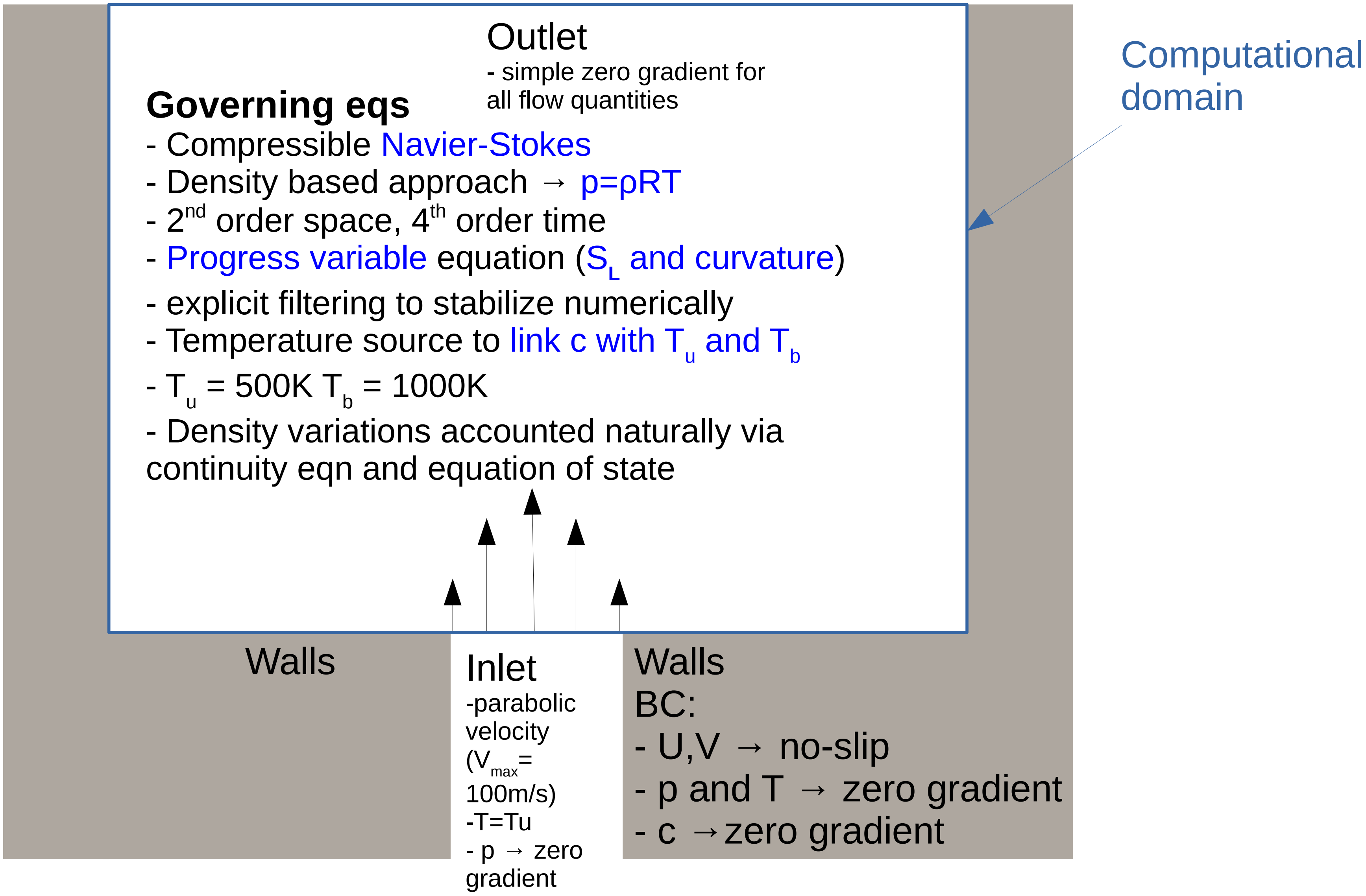
Note 1: Possible viscosity model: Sutherland

Note 2: Specific heat is in general temperature dependent

Simplified Matlab Code for Simulating Premixed Slot Burner

- 2d Navier-Stokes equations of gas dynamics i.e. mass, momentum, and energy conservation
- c-equation to describe burnt/unburnt region
- Runge-Kutta 4 time integration
- Premixed combustion of a prototype “fuel” with $T_u = 500K$ $T_b = 1000K$
- Density effect accounted for via NS-eqs (continuity, momentum eqs)
- Ideal gas law $p=\rho RT$
- The code can simulate 1) Bunsen burner, 2) Flame propagation in 2d “quasi-turbulence”

Bunsen Flame – Domain Modeled as a 2d “Slot” Burner in the Matlab Code



Outlet

- simple zero gradient for all flow quantities

Governing eqs

- Compressible Navier-Stokes
- Density based approach → $p=\rho RT$
- 2nd order space, 4th order time
- Progress variable equation (S_L and curvature)
- explicit filtering to stabilize numerically
- Temperature source to link c with T_u and T_b
- T_u = 500K T_b = 1000K
- Density variations accounted naturally via continuity eqn and equation of state

Walls

Inlet

-parabolic velocity (V_{max}= 100m/s)

-T=Tu

- p → zero gradient

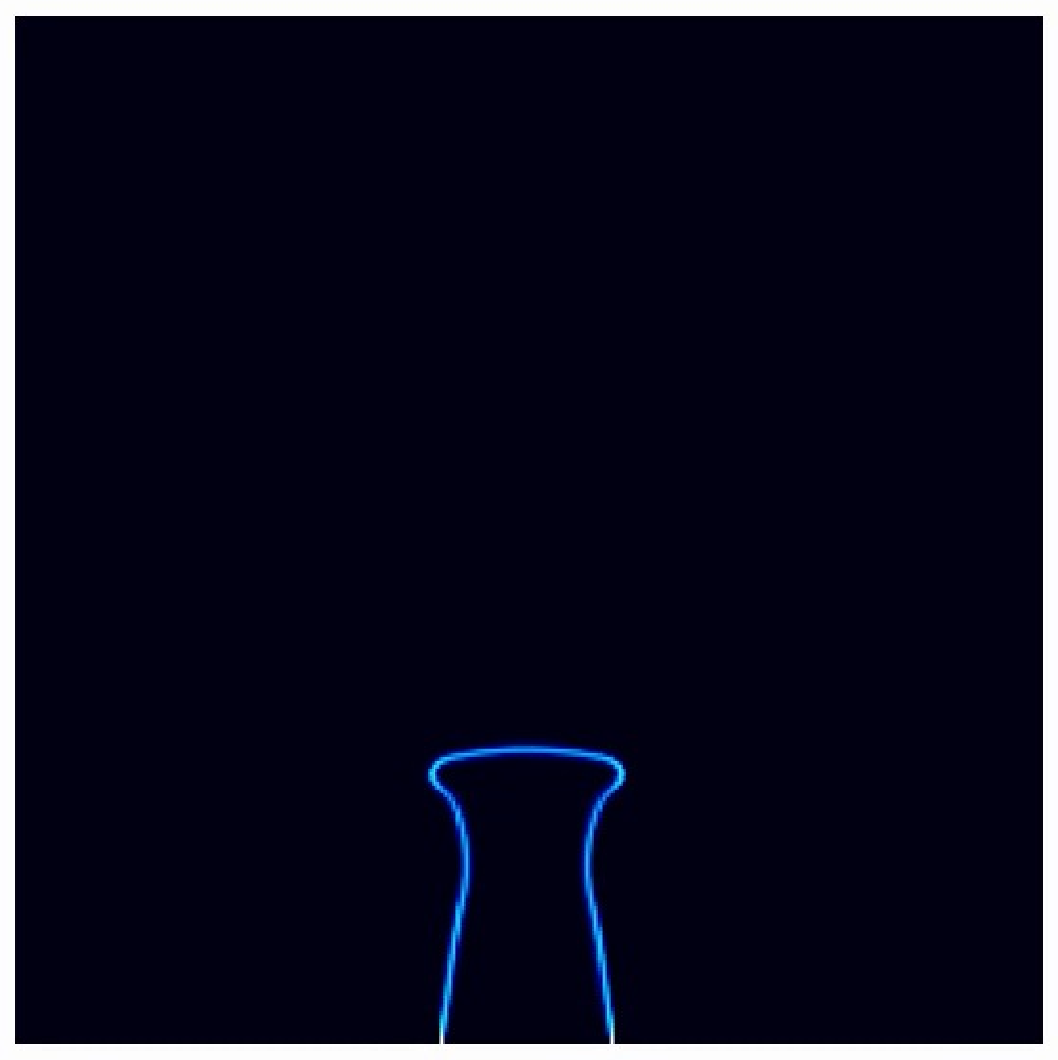
Walls

BC:

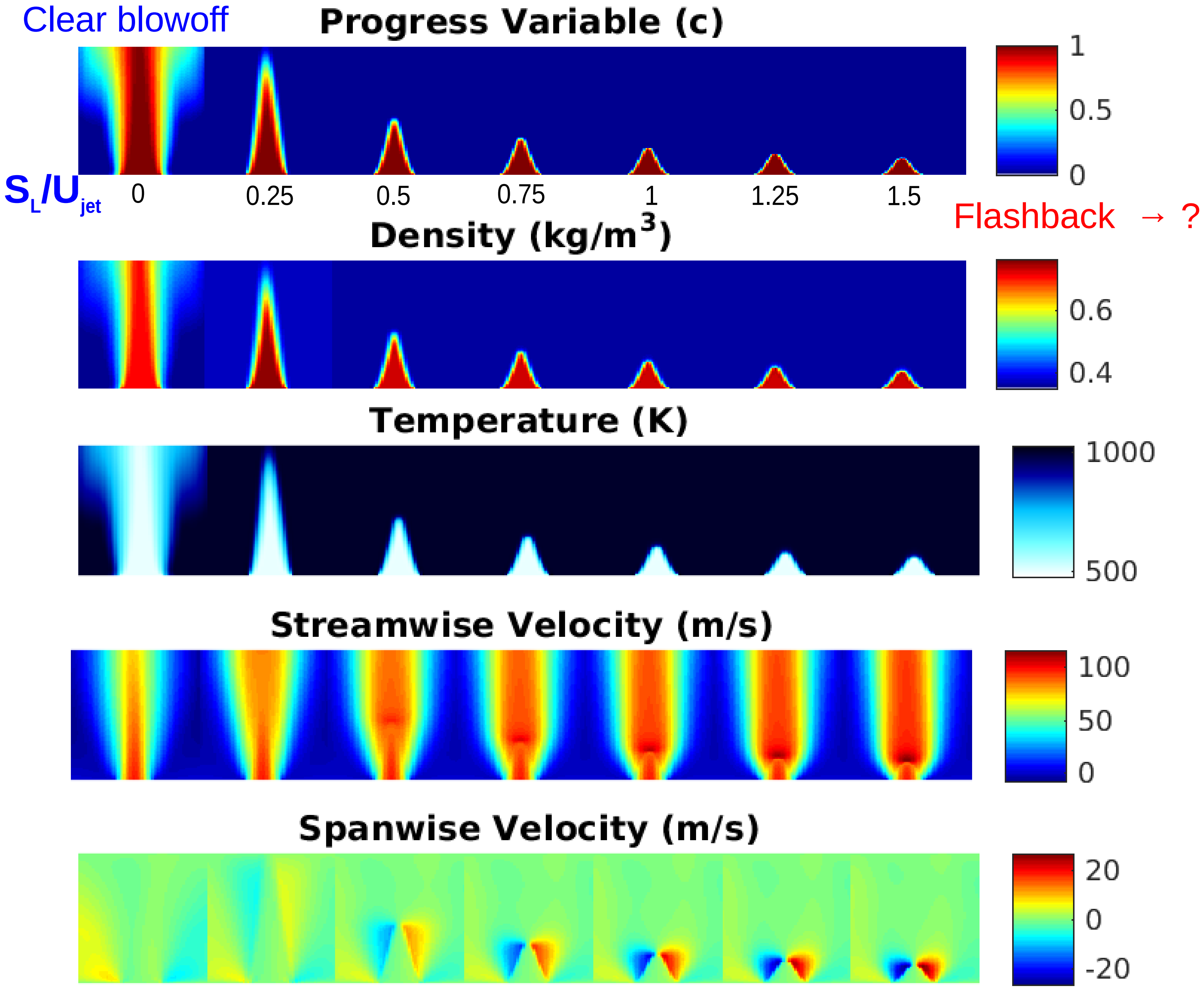
- U,V → no-slip
- p and T → zero gradient
- c → zero gradient

Computational domain

Bunsen Flame – This Case is With Top-Hat Velocity Profile Instead of Parabolic (S_L/U_{jet}=0.75). High Reynolds number.



Bunsen Flame – Influence of Laminar Flame Speed (S_L/U_{jet})



Clear blowoff

Flashback → ?

Progress Variable (c)

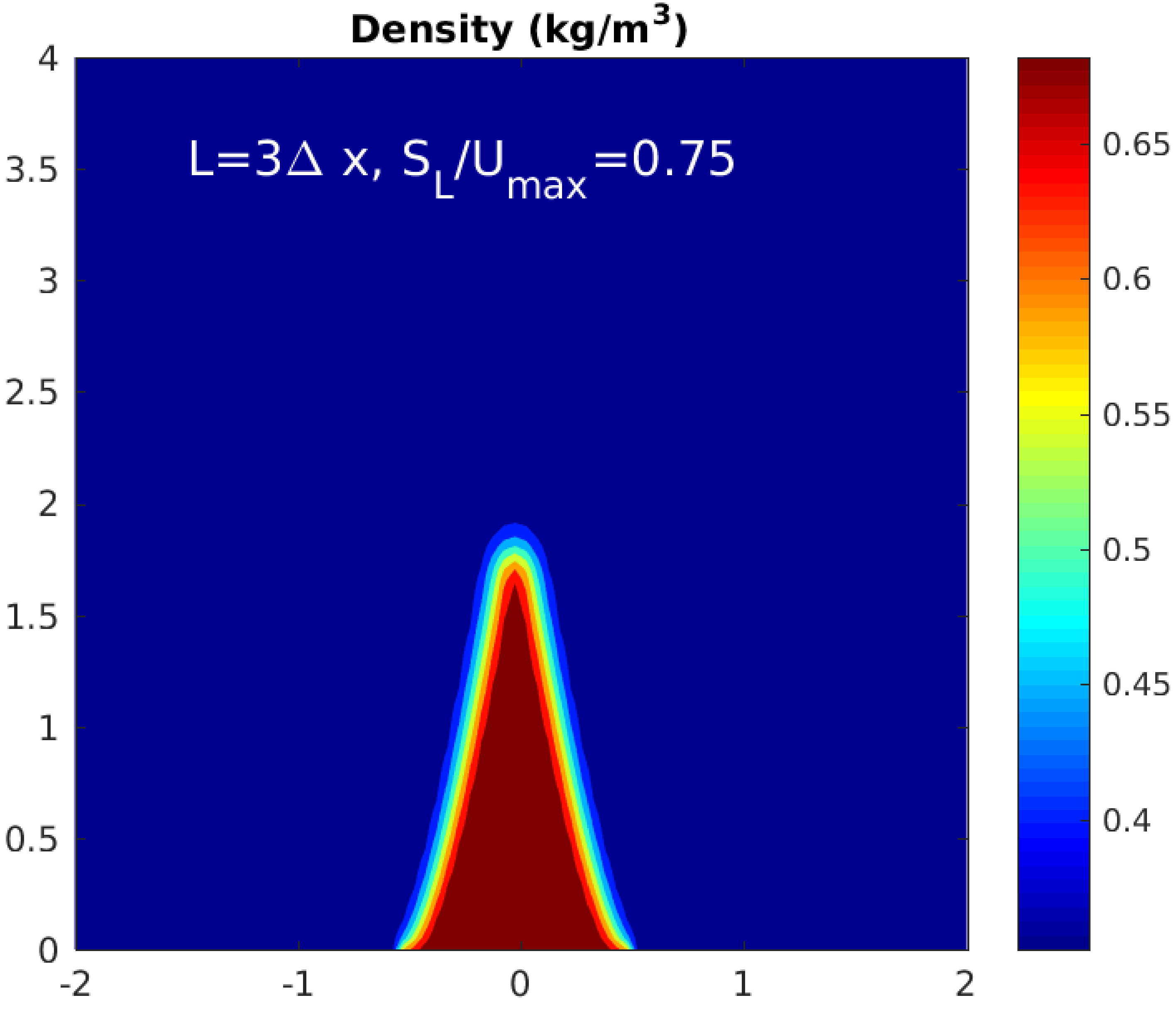
Density (kg/m^3)

Temperature (K)

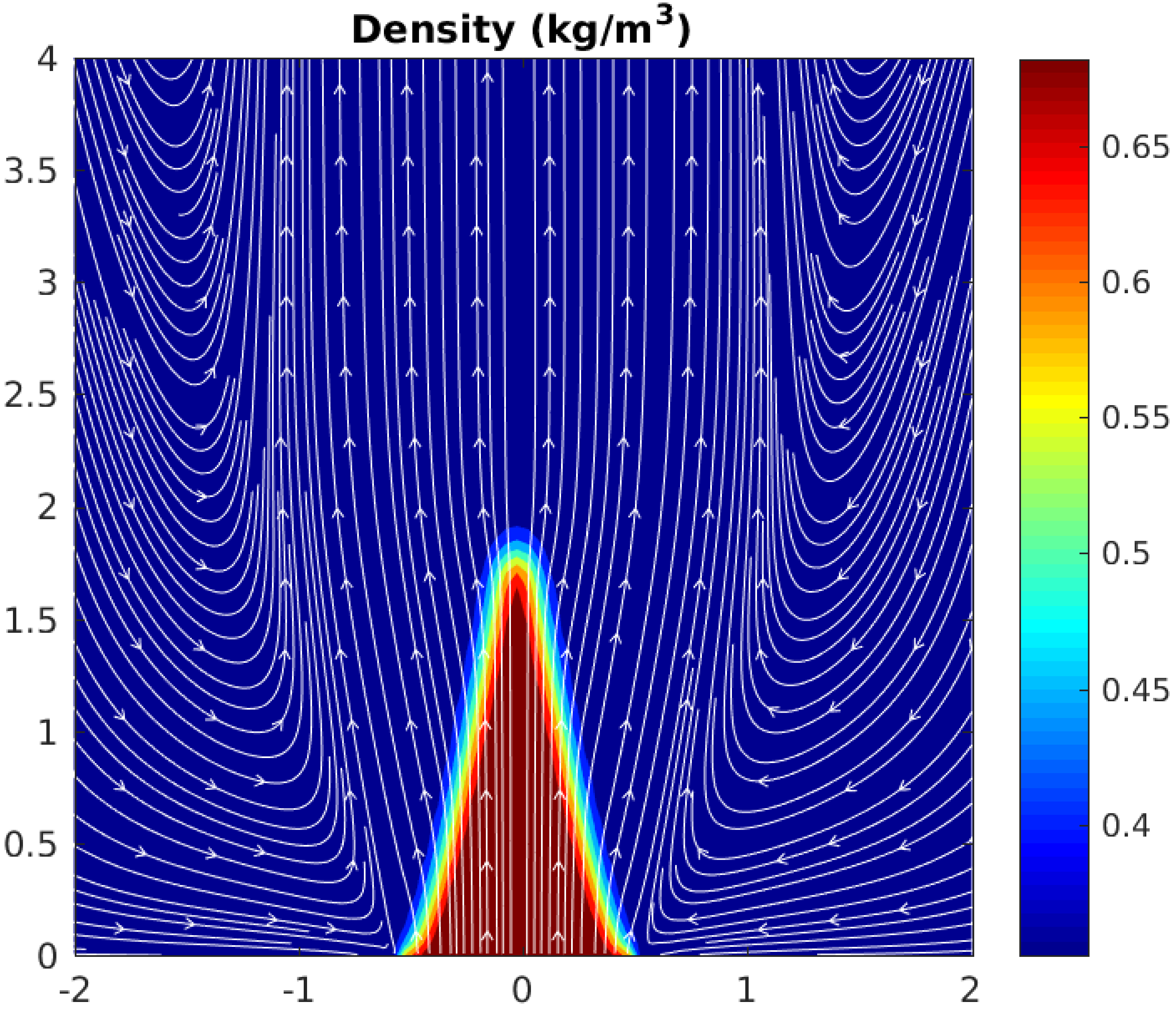
Streamwise Velocity (m/s)

Spanwise Velocity (m/s)

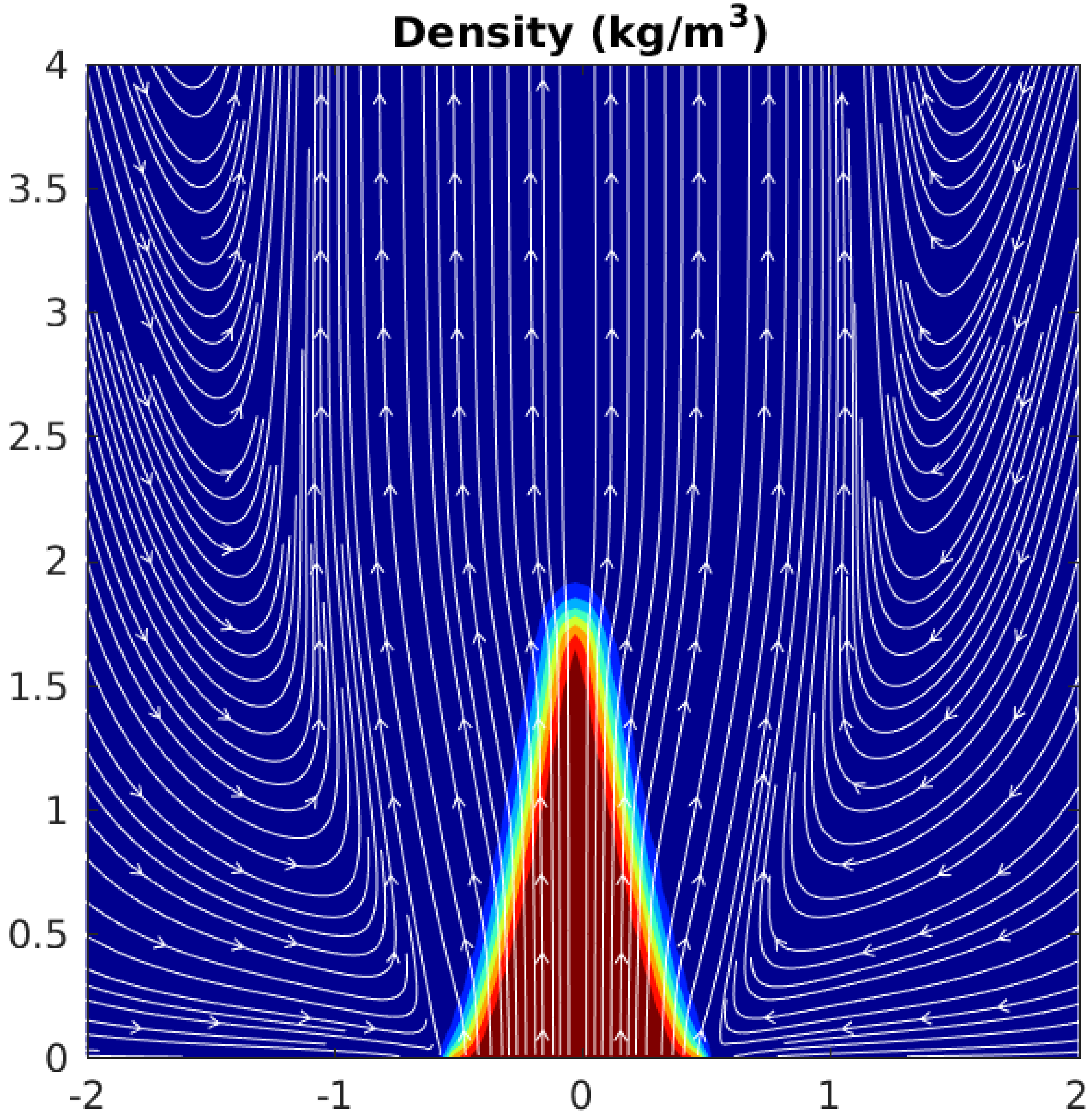
Bunsen Flame – Burnt vs Unburnt Density

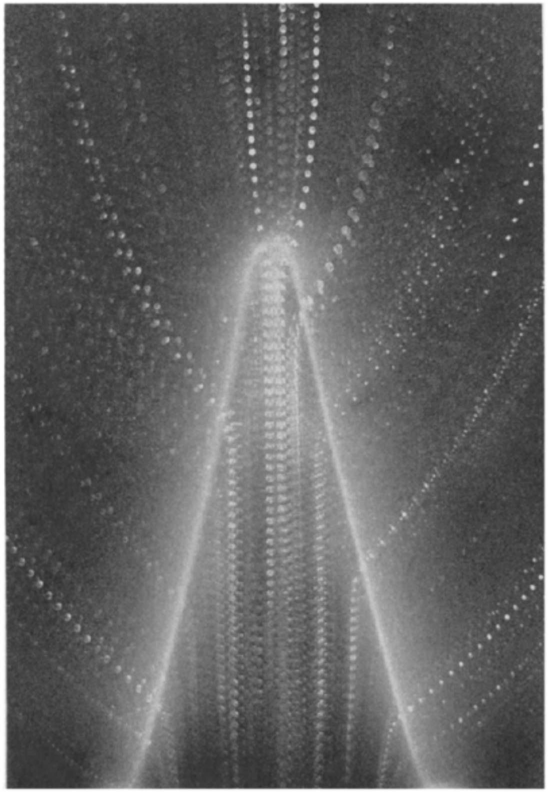


Bunsen Flame – Burnt vs Unburnt Density and Streamlines



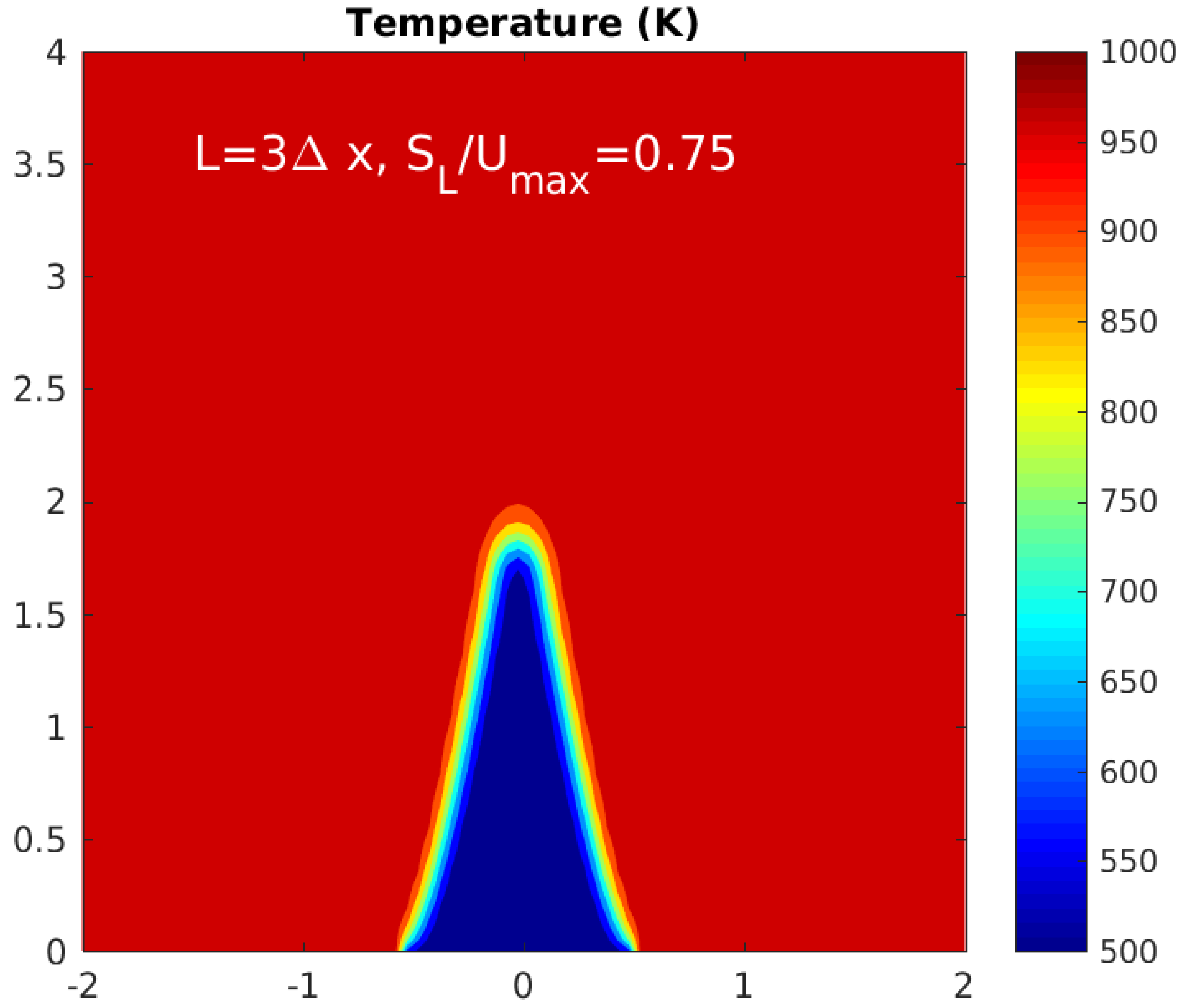
Bunsen Flame – Burnt vs Unburnt Density and Streamlines



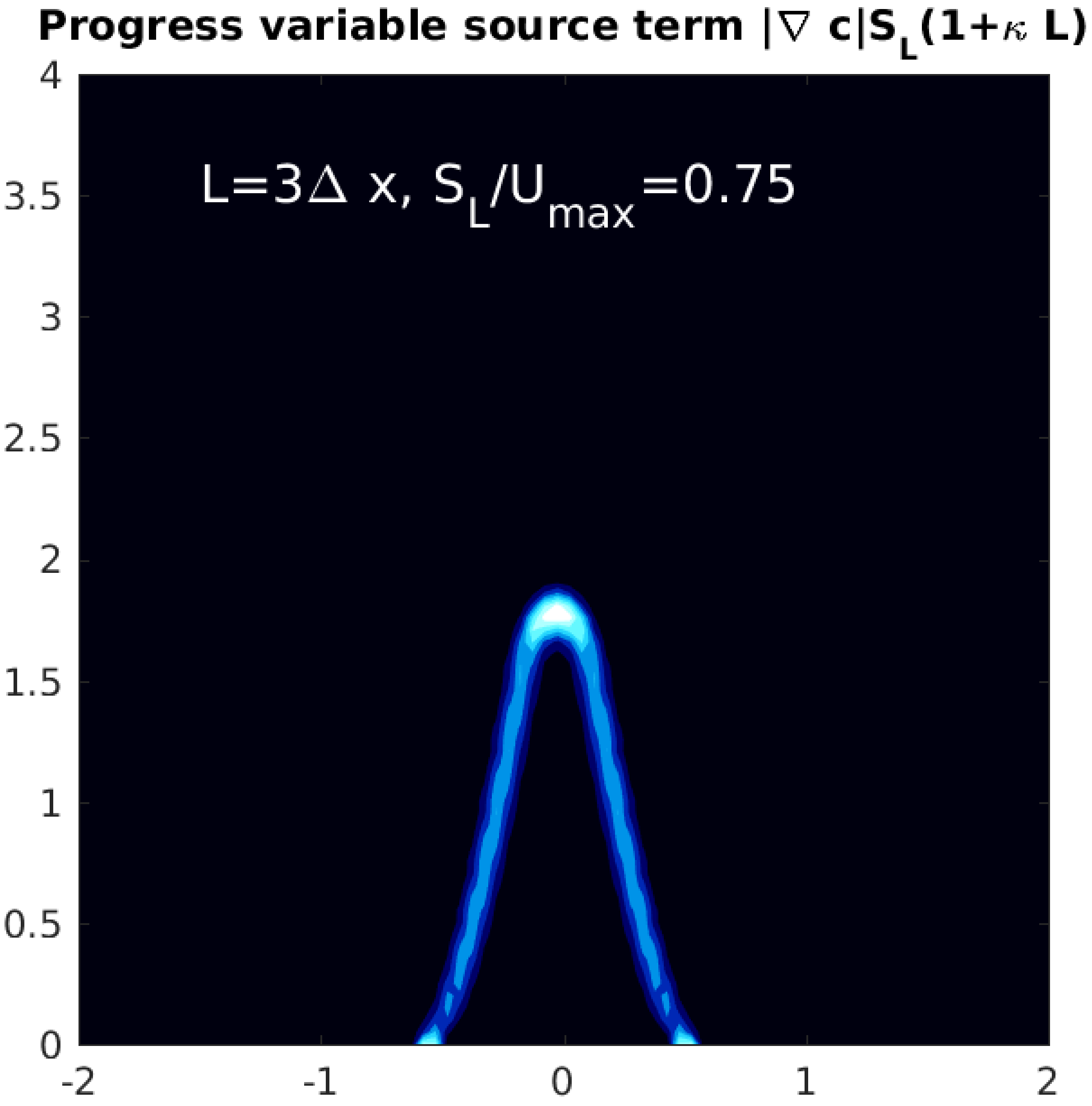


Experiment by Mungal et al. 1990
Symp. Comb.Institute

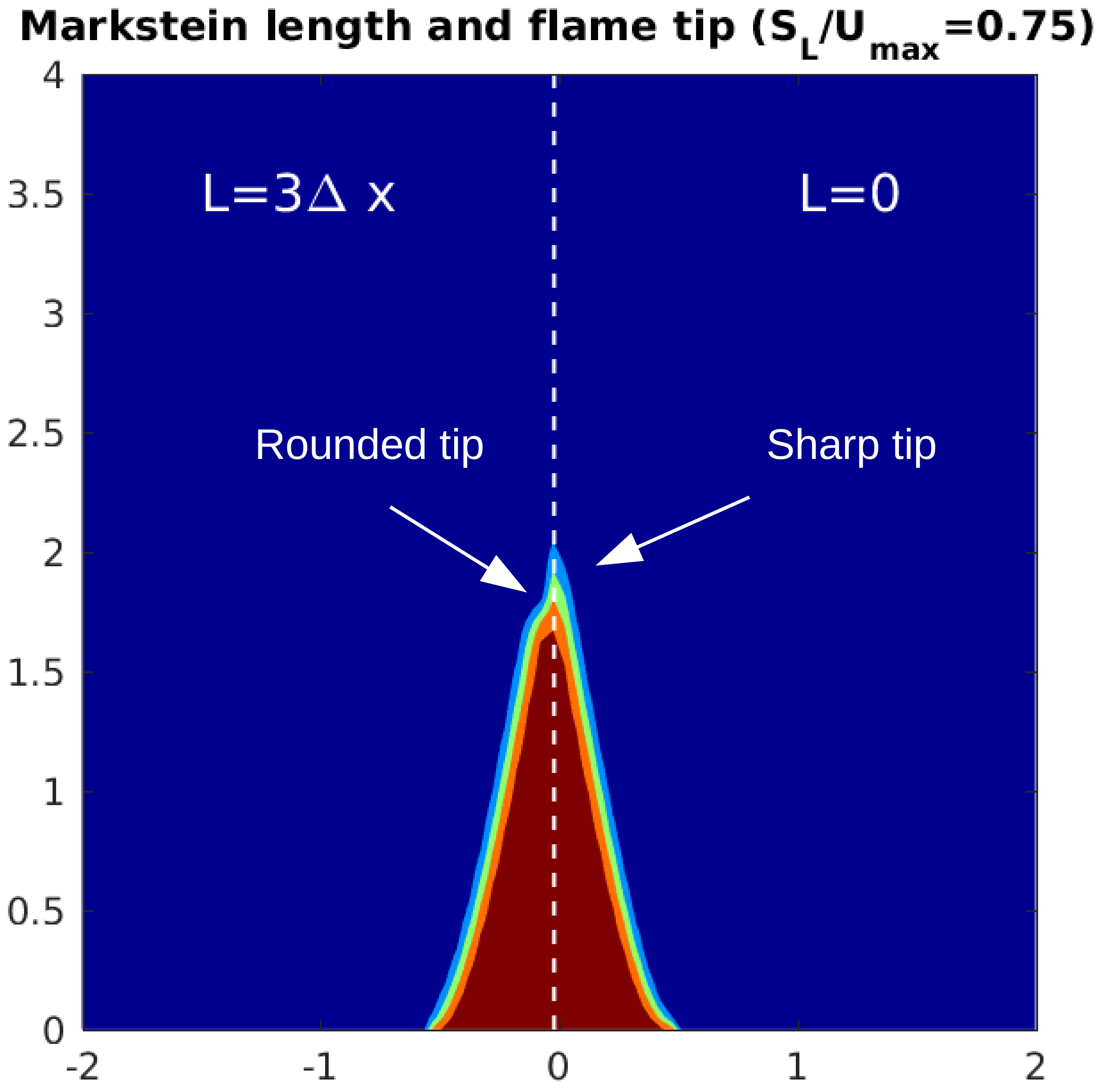
Bunsen Flame – Burnt vs Unburnt Density



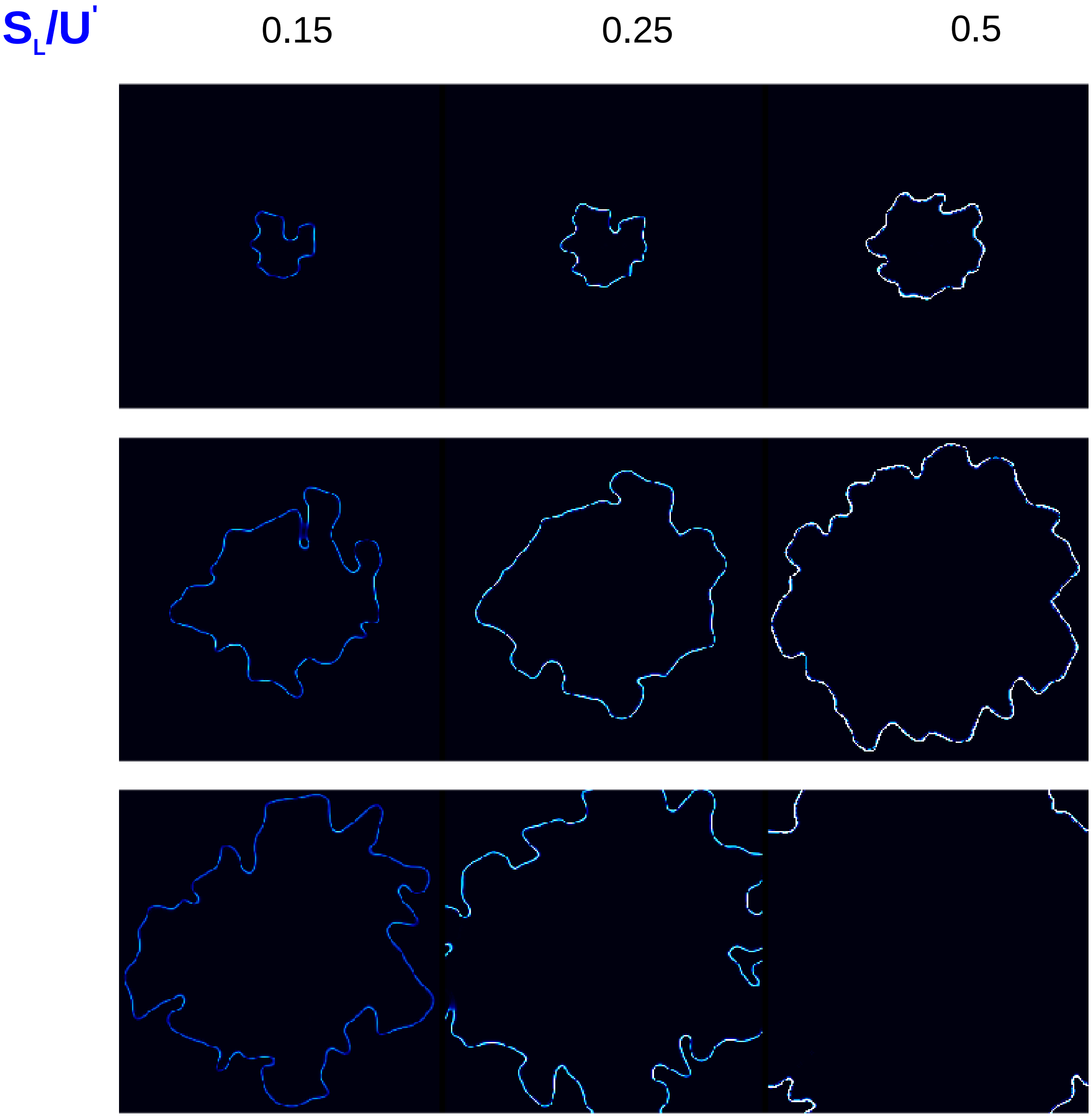
Bunsen Flame – Burnt vs Unburnt Density



Bunsen Flame – Curvature and Markstein Length Effect



Ignition Kernel: U' is the Typical Turbulent Fluctuation “Eddy Amplitude”. We keep here U' constant while changing U'



S_L/U' 0.15 0.25 0.5

→ Reaction rate evolution

$$-S_d \rho_u |\nabla c|$$

→ Note how the curvature term enhances or slows down the flow speed depending on the sign (+/-) of the curvature (see the animations on kernel & Bunsen flame)

Karlovitz number
Damköhler number

Borghi Diagram