# Introduction to Micro-Scale Combustion

Micro spacecraft

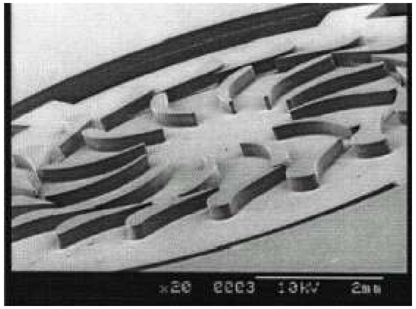
- Primary propulsion and attitude control of micro spacecraft.
- Precise positioning control of spacecraft constellations for interferometry missions.
- Potential gain in thrust-to-weight ratio

$$Thrust \propto P_c A_t \propto L_c^2 \qquad \frac{Thrust}{Weight} \propto L_c^{-1}$$

$$Weight \propto L_c^3$$

- For "Power MEMS" devices, typically in applications where batteries are currently used.

  - high power density



Micro turbine

Pictures are from *http://www.onera.fr/conferences/micropropulsion/*

# Characteristics and Challenges of Micro-Combustion System

- Power-generation devices currently developed are those that aim to generate power in the range of a few watts to milliwatts. The corresponding combustion devices are of the order of one centimeter in size.
- The characteristic length of micro combustiors being developed to date, even in MEMS-sized systems, is sufficiently larger than the molecular mean-free paths of air and other gases flowing through the systems in which the physiochemical behavior of fluids is fundamentally the same as their macro-scale counterparts.
- As combustion volumes are reduced in size, issues of residence time, fluid mixing, thermal management, and wall quenching of gas-phase reactions become increasingly important.
- Surface-induced catalytic reactions is an attractive alternative in micro-systems.

# Thermal-Fluid Issues

- For micro-devices with small characteristic lengths and consequently small Reynolds and Peclet numbers, the flow is primarily laminar, viscous effects and diffusive transport of mass and heat become increasingly important.
- Low Reynolds number makes mixing of reactants a potential problem in micro-systems.
- For diffusion flames, molecular diffusion is the rate-controlling process.
- Since turbulence mixing is weak, species mixing is primarily through diffusion. Based on scaling analysis, the diffusion time and corresponding flame length is given by

$$\tau_{diff} \sim \frac{d_{in}^2}{\mathcal{D}} \qquad L_f \sim U_0 \tau_{diff} \sim \frac{U_0 d_{in}^2}{\mathcal{D}}$$

- Complete and rapid mixing of adjacent laminar streams is desired, as is required for the initiation of a chemical reaction.
- As the device scale is reduced, the increased surface-to-volume ratio results in a large heat loss to the chamber wall. Further, the temperature gradient within the solid wall decreases due to the reduced Biot number.

# Combustion Issues

- For complete combustion, the flow residence time must be larger than the time required for chemical reactions. For non-premixed combustion, extra time and volume are needed for complete mixing.
- Flame quenching occurs if the total power generated inside the combustor is less than the loss to the wall

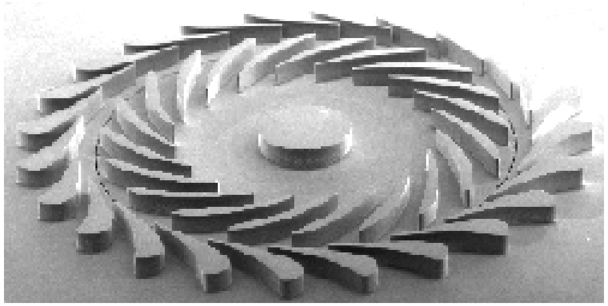
$$\left.\begin{aligned} & W_{tot} < W_{trans} \\ & W_{tot} = \rho_g \Delta H_r U_g \pi D L \sim \rho_g \Delta H_r U_g L^2 \\ & W_{trans} \sim \Pr_g^{1/3} \left( \frac{p_g U_g}{R_g \mu_g} \right)^{1/2} k_f L^{3/2} T_g^{-1/2} (T_g - T_w) \end{aligned}\right\} \quad p_g^{1/2} U_g^{1/2} L^{1/2} < \frac{\Pr_g^{1/3} R_g^{1/2} k_f T_f^{1/2} (T_f - T_w)}{\mu_g^{1/2} \Delta H_r}$$

- A higher chamber pressure and mass flow rate help prevent flames from extinction. An exceedingly high flow velocity, however, may lead to blowoff.

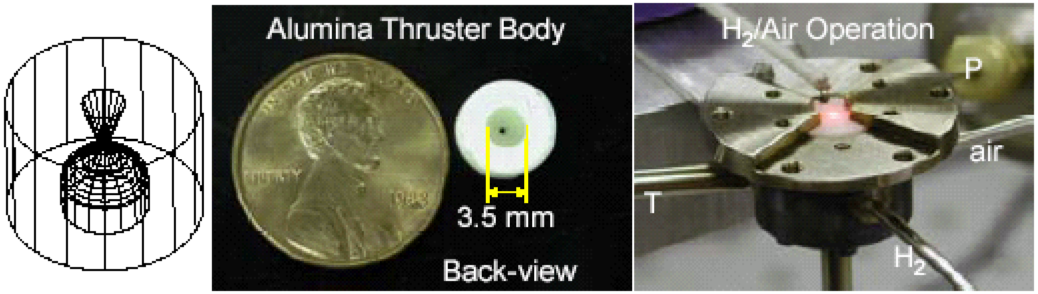
# Development of Micro Power Generation Using Combustion

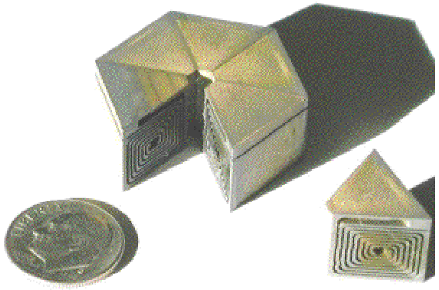
- Micro-scale power generation using combustion:
  - micro-combustors/reactors
  - micro turbines/engines
  - micro-rockets

MEMS-based gas turbine power generator develop at MIT



Meso- and micro- scale combustors developed at Penn State.

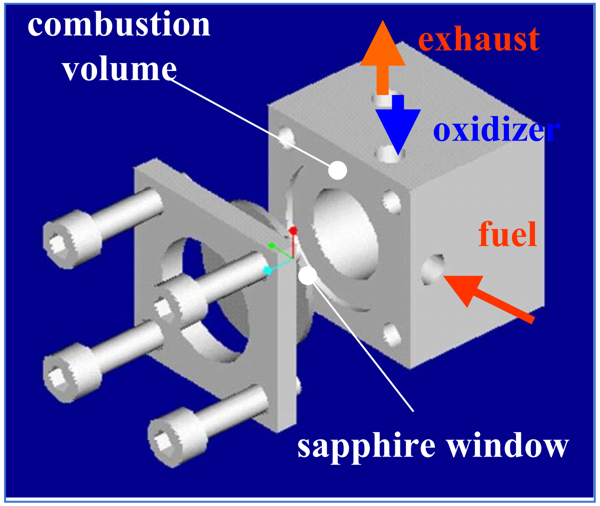


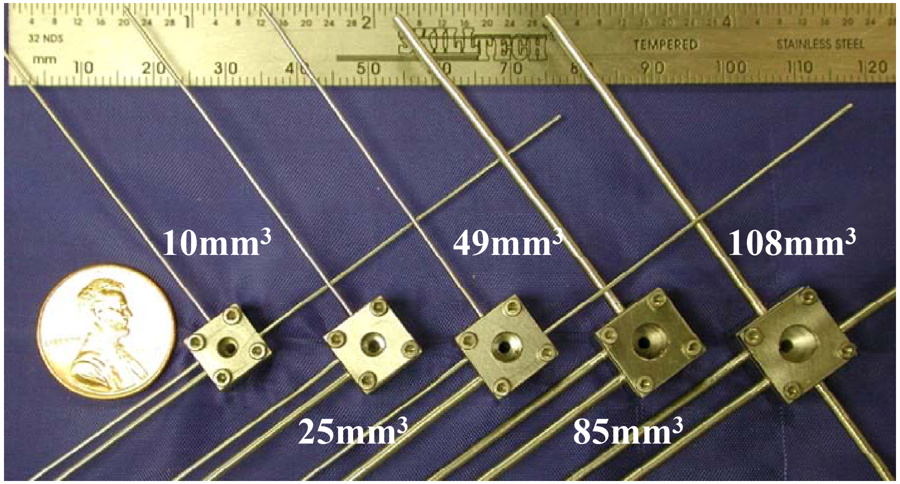


3-D Swiss-roll-type combustor-thermoelectric generator developed at USC

# Whirl Combustor Developed at Penn State

- A scaled down version of a macroscopic whirl combustor (Yetter, Glassman & Gabler, 2000).
- Made of Inconel with electro-discharge machining (EDM).
- Combustor volume ranging from 10 to 108 mm$^3$.
- Fuel injected perpendicularly to the tangentially injected oxidizer, and the flow exits the combustor tangentially.
- Approximate flow residence time on the order of 0.1 to 1 ms for a total mass flow rate at around 0.02 g/s (evaluated at 1500K).





# Theoretical Formulation

### Full conservation equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0$$

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

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \left[ (\rho E + p) u_i \right]}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial (u_i \tau_{ij})}{\partial x_j}$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho Y_k u_j}{\partial x_j} = \dot{\omega}_k - \frac{\partial \rho Y_k U_{k,j}}{\partial x_j}, \qquad k = 1, \ldots, N$$

### *L*-step reaction with *N* species

$$\sum_{k=1}^{N} \nu'_{ki} \chi_k \overset{k_{fi}}{\underset{k_{bi}}{\Leftrightarrow}} \sum_{k=1}^{N} \nu''_{ki} \chi_k \qquad for \quad i = 1, 2, \ldots, L$$

$$k_i(T) = A_i T^b \exp(-E_i / R_u T)$$

$$\dot{\omega}_k = MW_k \sum_{i=1}^{L} (\nu''_{ki} - \nu'_{ki}) \left[ k_{fi} \prod_{k=1}^{N} [\chi_k]^{\nu'_{ki}} - k_{bi} \prod_{k=1}^{N} [\chi_k]^{\nu''_{ki}} \right] \quad for \quad k = 1,\ 2,\ \ldots, N$$

# Numerical Method

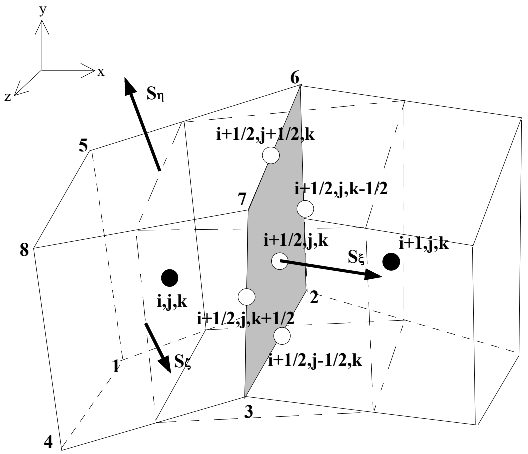
## Preconditioning method (Hsieh et al. 1997)

$$\frac{\partial Q}{\partial t}+\frac{\partial\left(E-E_v\right)}{\partial x}+\frac{\partial\left(F-F_v\right)}{\partial y}+\frac{\partial\left(G-G_v\right)}{\partial z}=H$$

$$\overline{p}=p_0+p_g$$

$$\Gamma\frac{\partial\hat{Q}}{\partial\tau}+\frac{\partial Q}{\partial t}+\frac{\partial(E-E_v)}{\partial x}+\frac{\partial(F-F_v)}{\partial y}+\frac{\partial(G-G_v)}{\partial z}=0$$

$$\hat{Q}=\left[p_g,u,v,w,T,Y_1,Y_2,\ldots,Y_{N-1}\right]^T$$



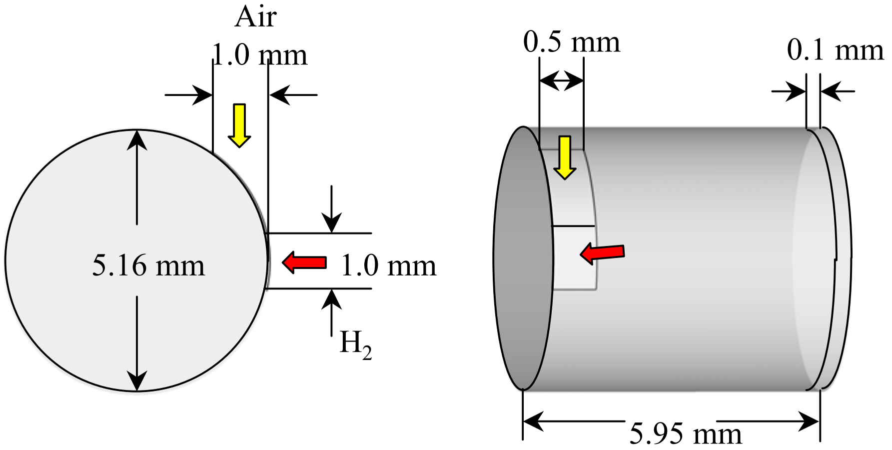
Schematic of three-dimensional adjacent cells

## Finite volume approach

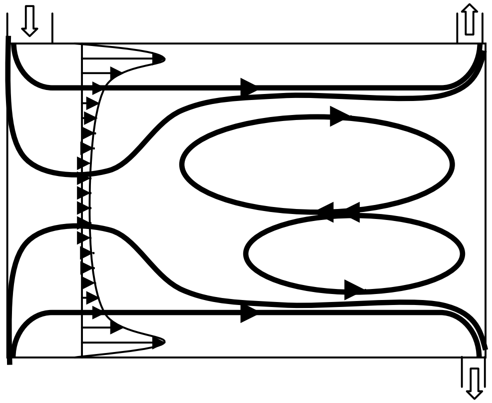
$$\iiint_V\left(\Gamma\frac{\partial\hat{Q}}{\partial\tau}+\frac{\partial Q}{\partial t}\right)dV+\int_{S_\xi}\vec{W}\bullet\vec{n}_\xi dS_\xi+\int_{S_\eta}\vec{W}\bullet\vec{n}_\eta dS_\eta+\int_{S_\zeta}\vec{W}\bullet\vec{n}_\zeta dS_\zeta=\iiint_V \mathrm{H}dV$$

# Behavior of Central Recirculation Zone (1/6)

## Geometry of cylindrical combustor



## Pseudo streamlines



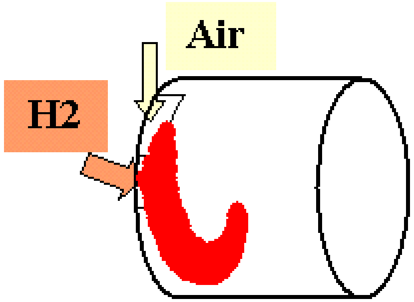
**One-step reversible reaction**

$$2H_2 + O_2 \Leftrightarrow 2H_2O$$

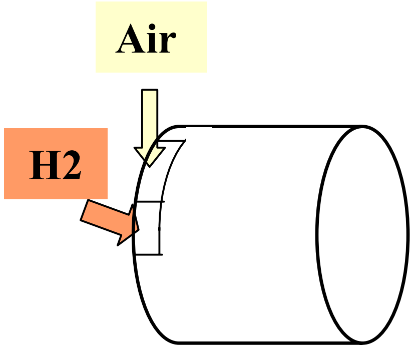
$$\frac{d[c_{H_2}]}{dt} = -2\left[k_f[c_{H_2}]^2[c_{O_2}] - k_b[c_{H_2O}]^2\right]$$

$$k_f = 1.102\times10^{19}\cdot\exp(-8025/T)$$

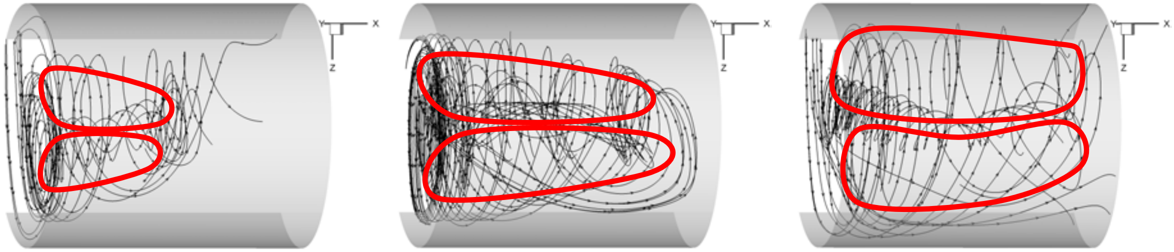
## Basic flame structure



# Behavior of Central Recirculation Zone (2/6)

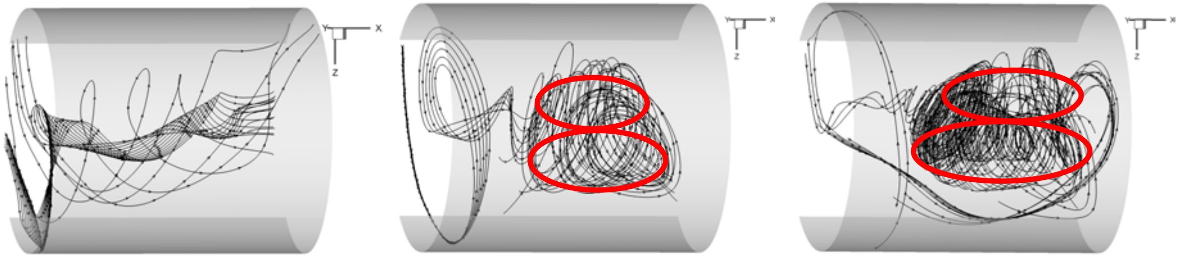


slip upstream end



$U_{in,air} = 20m/s$ $U_{in,air} = 40m/s$ $U_{in,air} = 80m/s$

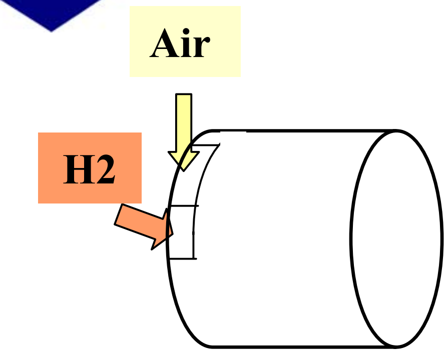
non-slip upstream end



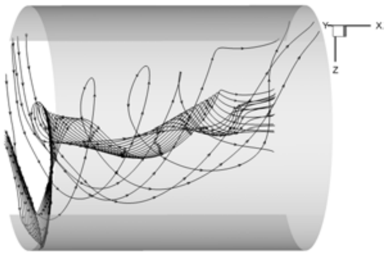
$U_{in,air} = 20m/s$ $U_{in,air} = 40m/s$ $U_{in,air} = 80m/s$

- generation of recirculation zone is caused by centrifugal effect.
- viscous effect at head end reduces the size of flow recirculation.

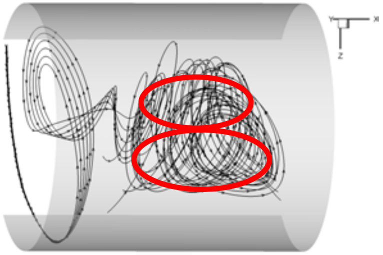
# Behavior of Central Recirculation Zone (3/6)



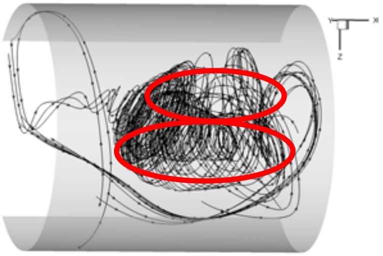
$P_0 = 1atm$



$U_{in,air} = 20m/s$

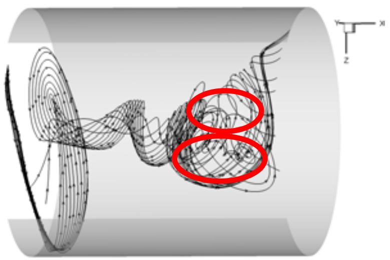


$U_{in,air} = 40m/s$

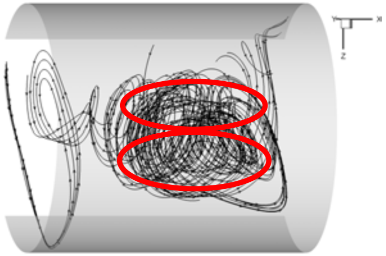


$U_{in,air} = 80m/s$

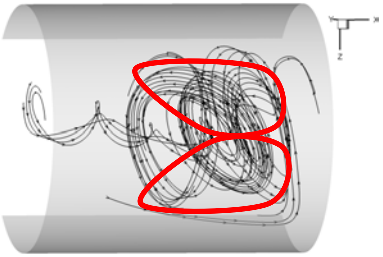
$P_0 = 2atm$



$U_{in,air} = 20m/s$



$U_{in,air} = 40m/s$

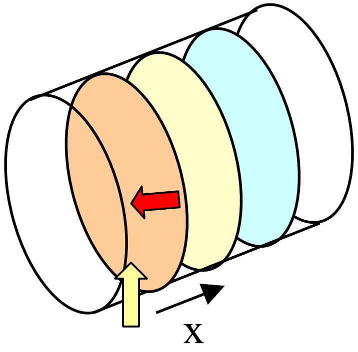


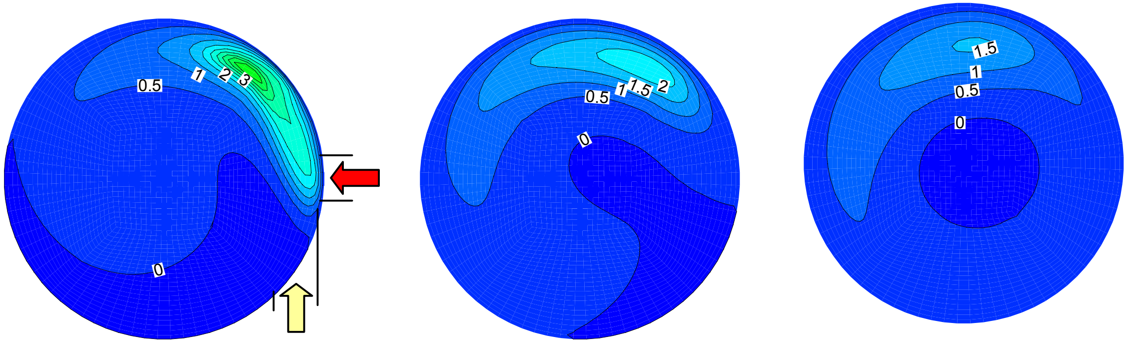
$U_{in,air} = 80m/s$

- Both higher injection velocity and chamber pressure facilitate generation of central recirculation zone.

# Behavior of Central Recirculation Zone (4/6)

Mass flux $\rho v_x$

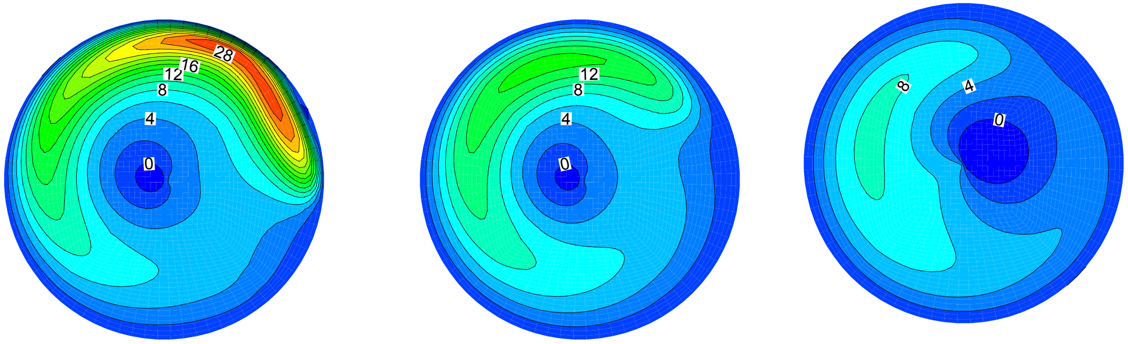




x=0.001mm x=0.003mm x=0.005mm

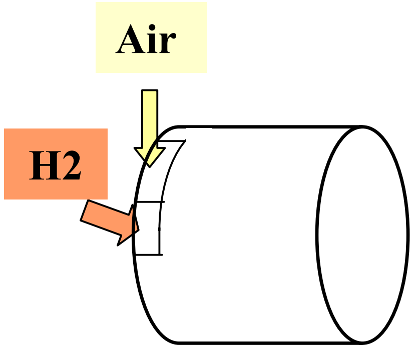
- Fluid is transported downstream mainly in outer region.
- Tangential velocity is much higher in outer region.

Tangential velocity $v_\theta$

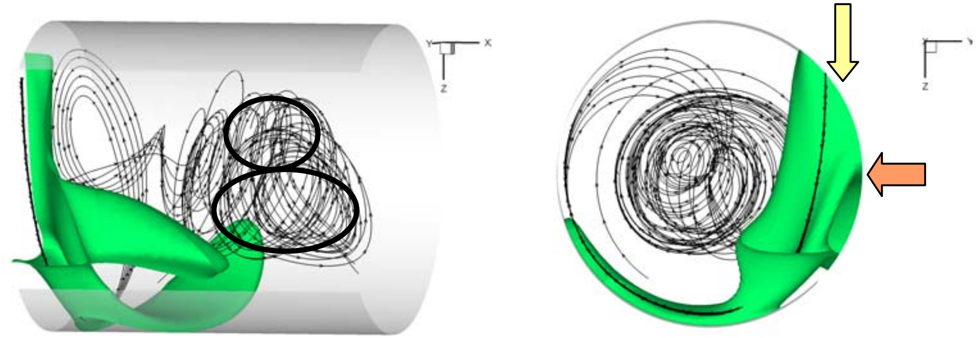


x=0.001mm x=0.003mm x=0.005mm

# Behavior of Central Recirculation Zone (5/6)

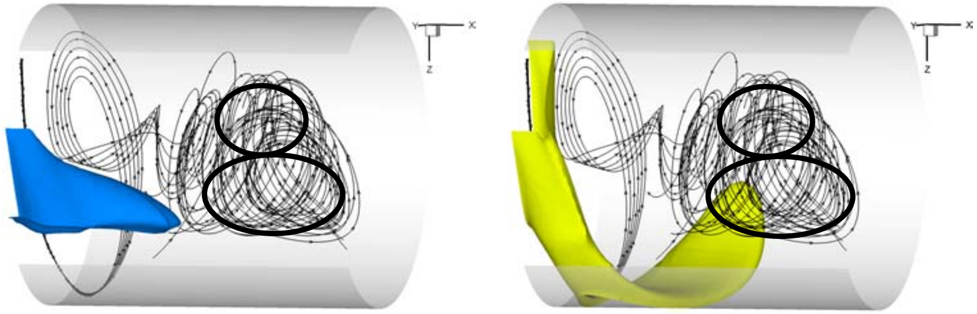


- Flame structure is determined by the injection directions of fuel and air.
- Flame front is located where the fuel and oxidizer meet in stoichiometric proportions.



$T = 1300K$

Iso-surface of temperature

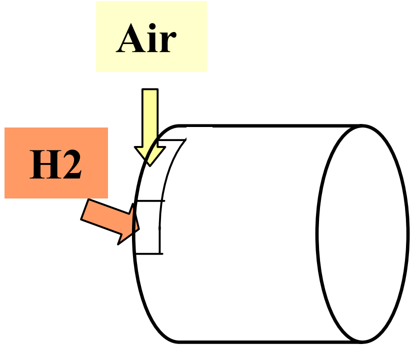


$Y_{H_2} = 0.2$

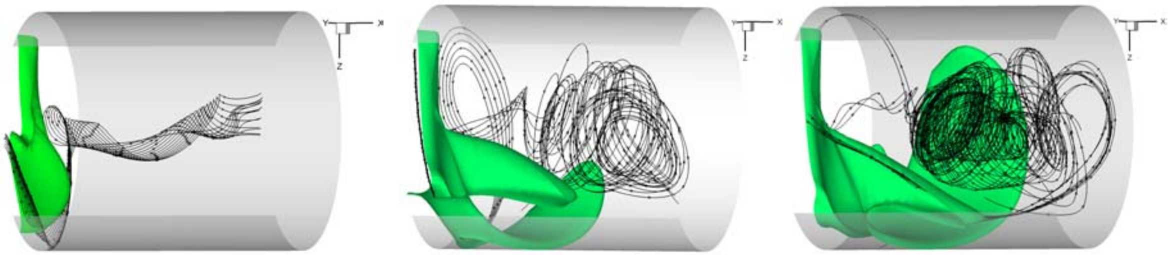
$Y_{O_2} = 0.2$

Iso-surface of mass fraction

# Behavior of Central Recirculation Zone (6/6)



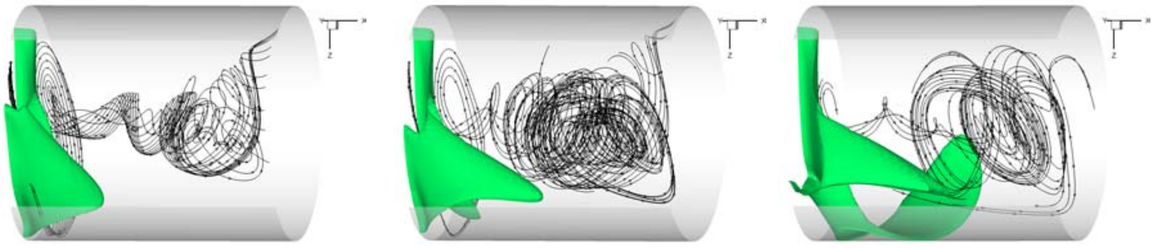
$P_0 = 1atm$



$U_{in,air} = 20m/s$ $U_{in,air} = 40m/s$ $U_{in,air} = 80m/s$

- The flame length increases with increasing injection velocity.
- The flame length decreases with increasing chamber pressure.

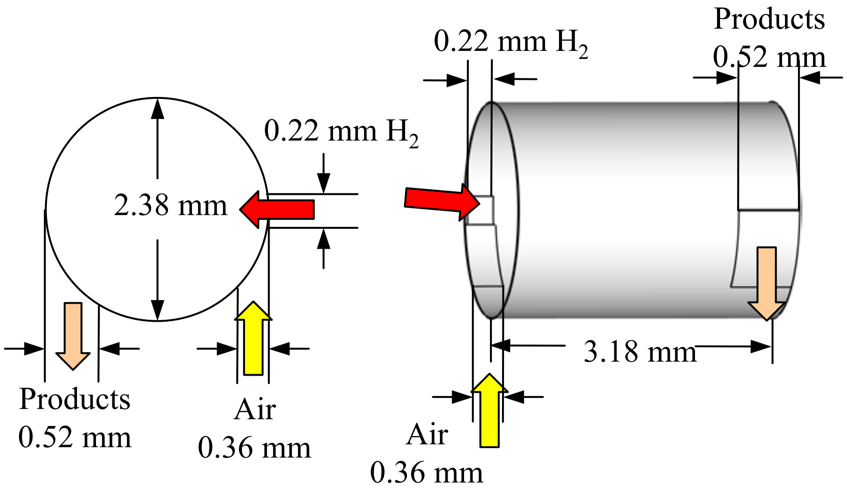
$P_0 = 2atm$



$U_{in,air} = 20m/s$ $U_{in,air} = 40m/s$ $U_{in,air} = 80m/s$

# Combustion in Whirl Combustor (1/4)

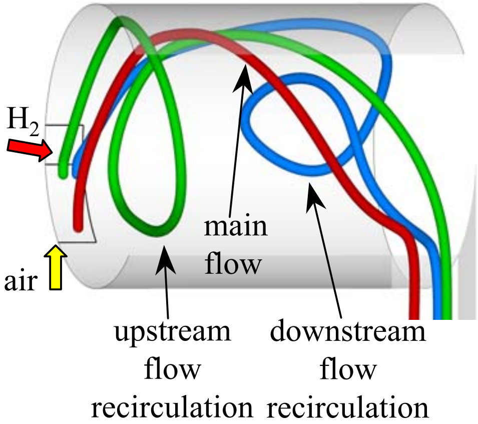
## Geometry of cylindrical combustor



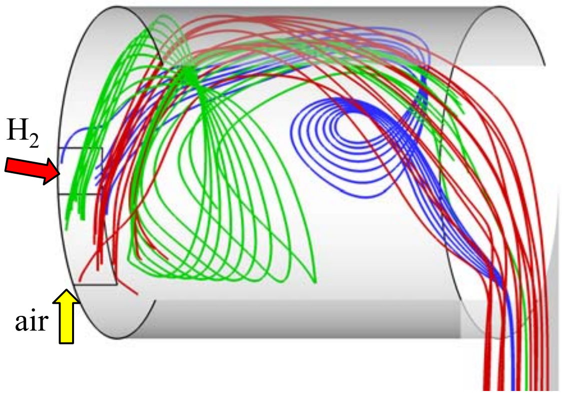
- Combustion products are exhausted through a tangential square port.
- $U_{in,air}$ = 100 m/s
- $P_c$ = 1atm, $T_w$ = 800 K
- $\Phi$ = 1.0

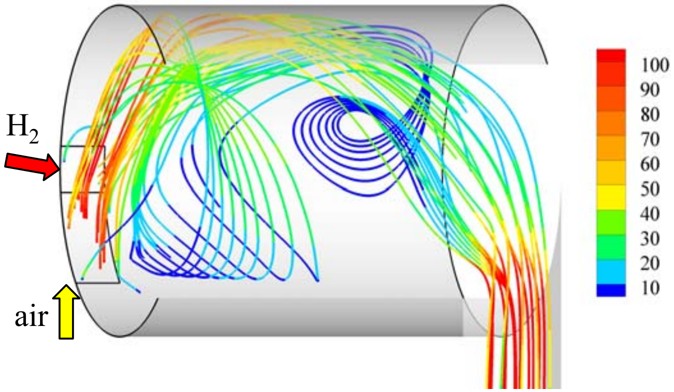
- The flow injected into the combustor is divided into three parts: main flow, upstream and downstream recirculating flows.

## Basic flow structure

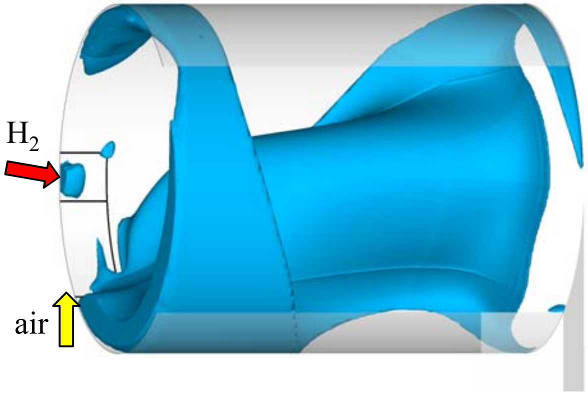


# Combustion in Whirl Combustor (2/4)


3-D flow evolution

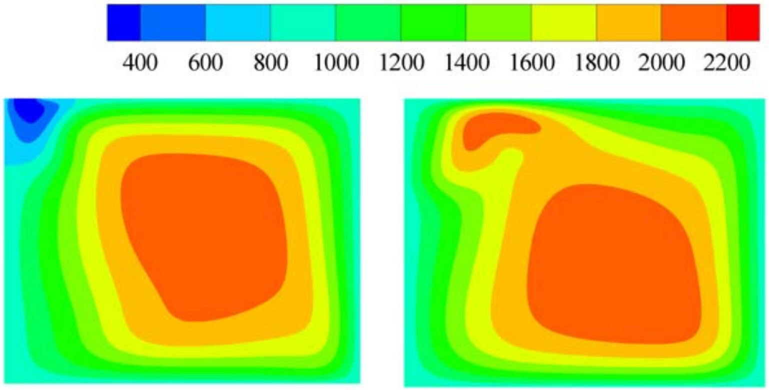

3-D flow traces with velocity magnitude

- The small flow velocity in the recirculation region helps stabilize the flame in the upstream regime.


3-D structure of flow reversal zone

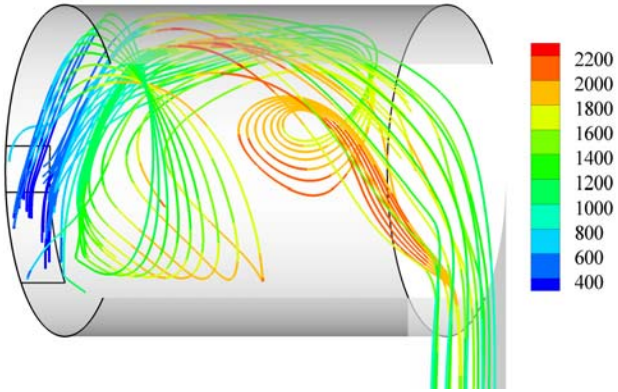
# Combustion in Whirl Combustor (3/4)

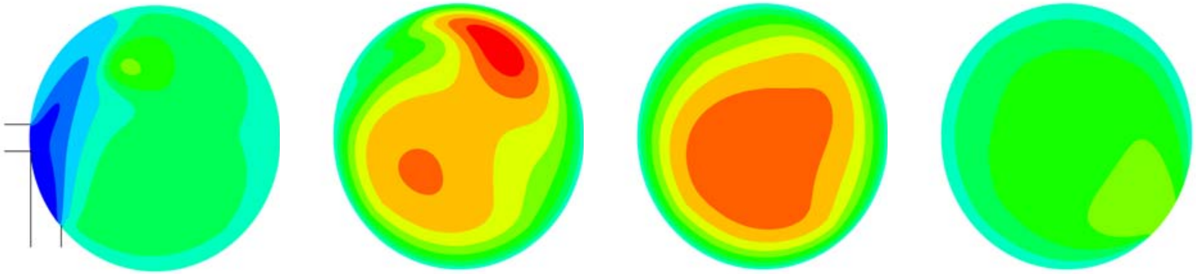
## Distribution of temperature



z = 0 mm

y = 0 mm





x = 0.2 mm

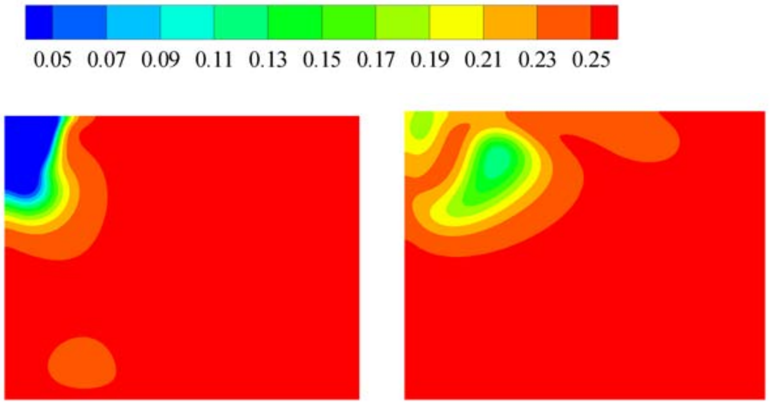
x = 1.0 mm

x = 2.0 mm

x = 3.0 mm

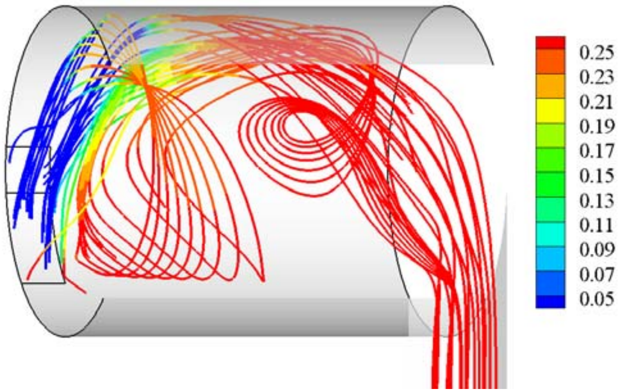
# Combustion in Whirl Combustor (4/4)

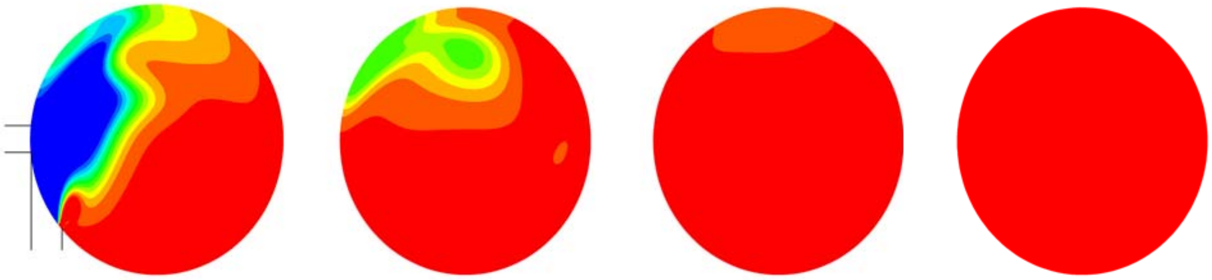
Distribution of water mass fraction



z = 0 mm

y = 0 mm





x = 0.2 mm

x = 1.0 mm

x = 2.0 mm

x = 3.0 mm

- Reactions occur in a limited regime near the head end.