Sıkıştırılabilir (ve Tepkimeli) Akışların HAD Yöntemleri ile Analizi Üzerine

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EURO

TÜBİTAK ULAKBİM

TRUBA Turkish Science e-Infrastructure

HPC HIGH PERFORMANCE COMPUTING

Amaçlar / Sorunlar

Türbülansın, kararlı, sıkıştırılabilir akışların hesaplama yapılmasına uygun boyutta çözüm ağları üzerinde, sonuçta akış fiziğinin öngörülmesine imkan veren benzetimlerinin yapılması.

Sıkıştırılabilir akışların benzetimi için kullanılan lineer olmayan, hiperbolik davranışa sahip denklem setleri:

- Akış değişiminin zamanla hesaplanması sırasında her adımda artan Fourier mode ları: türbülans.

- Çözümde oluşan keskin süreksizlikler: şok veya alev.

RANS / LES /DNS

- **RANS :** modeling all the scales, simulating the average field.
  Low order upwind schemes, complex physical model
  Stationary calculation, 2D or possibly axisymmetric
- **LES :** modeling the small scales, simulating large scales
  Higher order centered schemes, 3D unsteady calculation
  Simple enough (cost) sub-grid models
- **DNS :** nothing is modeled, all the scales are simulated
  Centered higher order schemes, 3D unsteady calculation
  No turbulence model, but precise molecular transport models
- **MILES :** nothing is modelled, no sub-grid models
  No model for turbulence but upwind schemes

Denklemler

Mass conservation : $$\frac{\partial \rho}{\partial t} + (\rho u_j)_{,j} = 0$$

Momentum equation : $$\frac{\partial \rho u_i}{\partial t} + (\rho u_i u_j + p\delta_{ij})_{,j} = \tau_{ij,j}$$

1^{er} Energy equation : $$\frac{\partial \rho E}{\partial t} + [(\rho E + p)\, u_j]_{,j} = (u_i \tau_{ij})_{,j} - \dot{q}_{j,j}$$

Species equation : $$\frac{\partial \rho Y_\alpha}{\partial t} + (\rho u_j Y_\alpha)_{,j} = -J_{\alpha j,j} + \dot{\omega}_\alpha$$

Ideal gas equation : $$p = \sum_{\alpha=1}^{N_{sp}} \rho_\alpha r_\alpha T = \rho \mathcal{R} T \sum_{\alpha=1}^{N_{sp}} \frac{Y_\alpha}{W_\alpha}$$

Hesaplamada Türbülans Nasıl Oluşur ?

- En basit hiperbolik davranışlı denklem (burgers denklemi)

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \vartheta \frac{\partial^2 u}{\partial x^2}$$

başlangıç koşulları: *u(x, t=0) = u°(x)*

- Zaman integrasyonu

$$\begin{aligned} u(x, t+\Delta t) &= u(x,t) + \Delta t \frac{\partial u}{\partial t} + \cdots \\ &= u(x,t) + \Delta t \left(-u\frac{\partial u}{\partial x} + \vartheta \frac{\partial^2 u}{\partial x^2} \right) \end{aligned}$$

Hesaplamada Türbülans Nasıl Oluşur ?

- başlangıç koşulu = 1 mode k

$$u^{\circ}(x) = \hat{u}^{\circ}(k)\, e^{-ikt}\ ;\ \frac{\partial u^{\circ}}{\partial x} = j\, k\, \hat{u}^{\circ}(k)\, e^{-ikt}\ ;\ u^{\circ}\frac{\partial u^{\circ}}{\partial x} = j\, k\, \hat{u}^{\circ 2}(k)\, e^{-i2kt}$$

- Zamanla integrasyon

$$u(x, t = \Delta t) = u^{1}(x) = u^{0}(x) + \Delta t\, \left.\frac{\partial u}{\partial t}\right|^{0} + \cdots$$

$$= \textstyle\sum_{m=1}^{2} \hat{u}^{1}(k_m) e^{-ik_m t}$$: 2 modes

$$u(x, t = n\Delta t) = u^{n}(x) = \textstyle\sum_{m=1}^{2} \hat{u}^{1}(k_m) e^{-ik_m t}$$: 2^n modes

Türbülanslı Akisin Hesaplanması Neden Zor ?

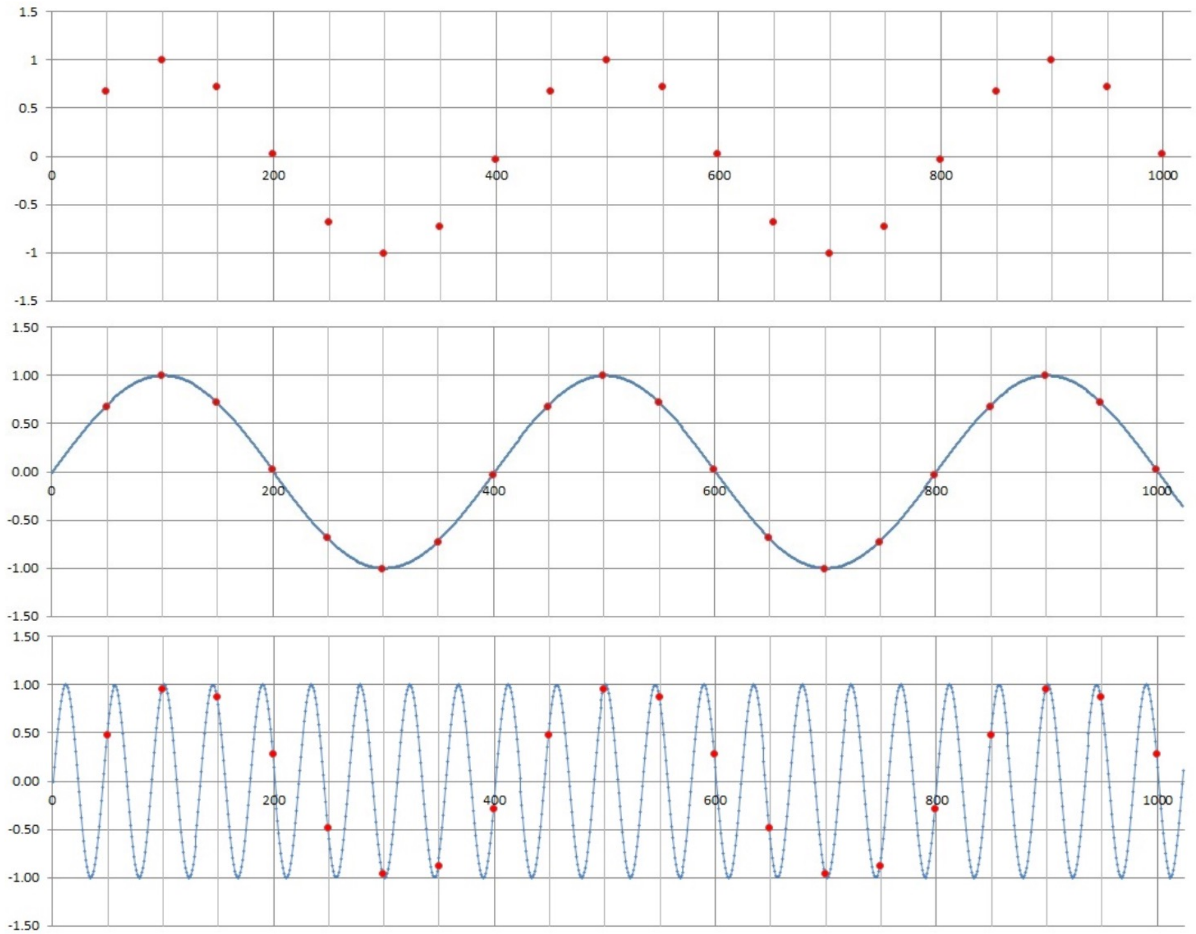
- Uzaysal çözüm ağı : $x_i = i\Delta x \qquad i = 0, \dots, Nx \qquad \Delta x = \frac{L}{N_x}$
- numerik cut-off (Nyquist frequency) :

$$k_c = k_{Nx/2} = \frac{Nx}{2}\frac{2\pi}{L} = \frac{\pi}{\Delta x}$$

aliasing + backscatering = instable calculation

Türbülanslı Akışın Hesaplanması Neden Zor ?

Signal period: 1/f = 400
Sampling rate: f = 2500



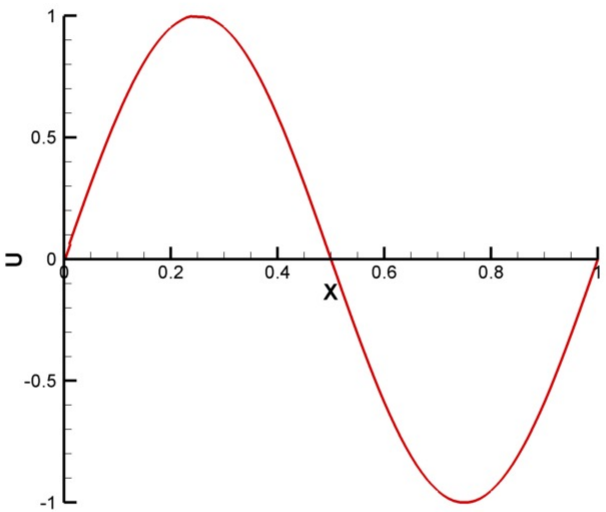
aliasing + backscatering = instable calculation

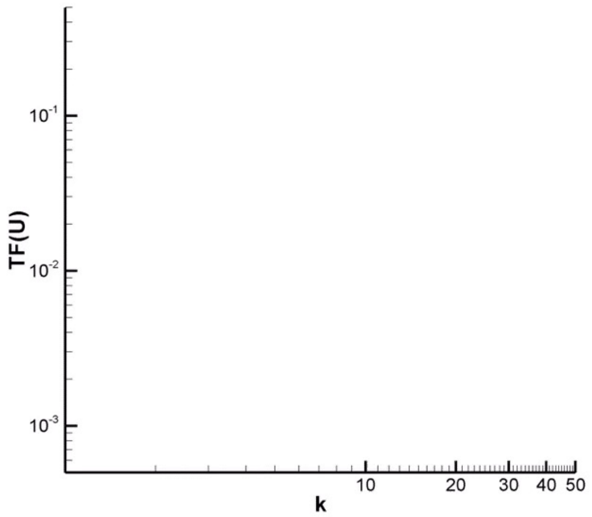
Şoklar Nasıl Oluşur?

- ‘Characteristic ’ lerin kesişimi: sonlu zamanda şok oluşumu:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$$

Burgers equation (non viscous) with upwinding: $\frac{\partial u}{\partial x} \approx \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x)$



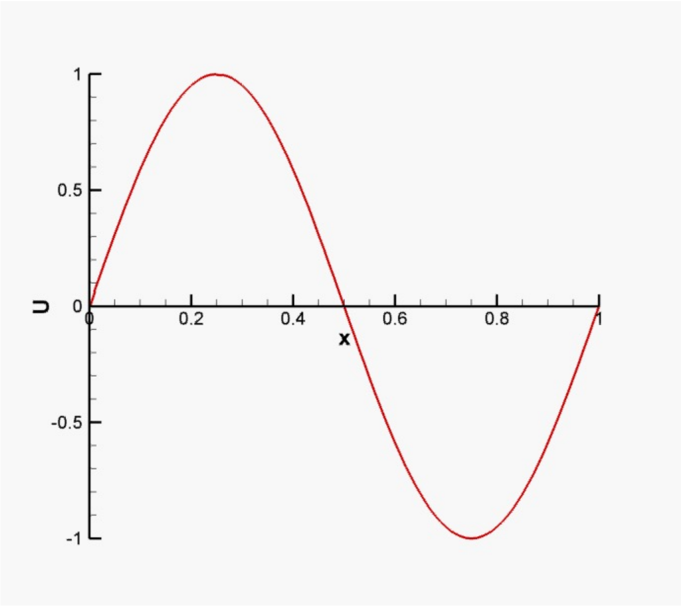


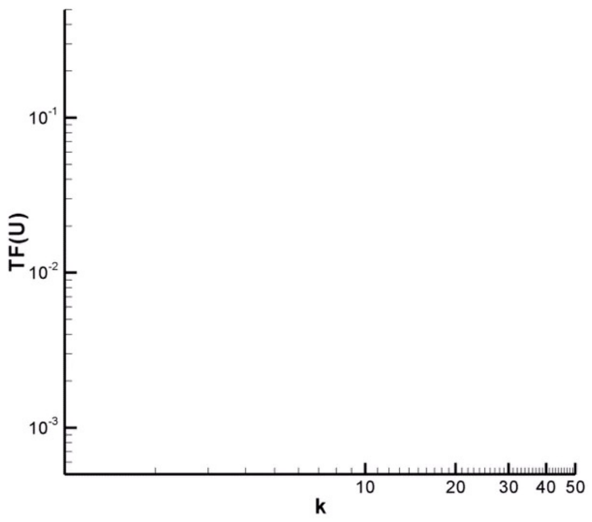
Viskosite Ne İşe Yarar ?

- Non-viscous Burgers equation (ν = 0) : no physical viscosity,

- Spatial centered discretization : no numerical viscosity

$$\frac{\partial u}{\partial x} \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x^2)$$

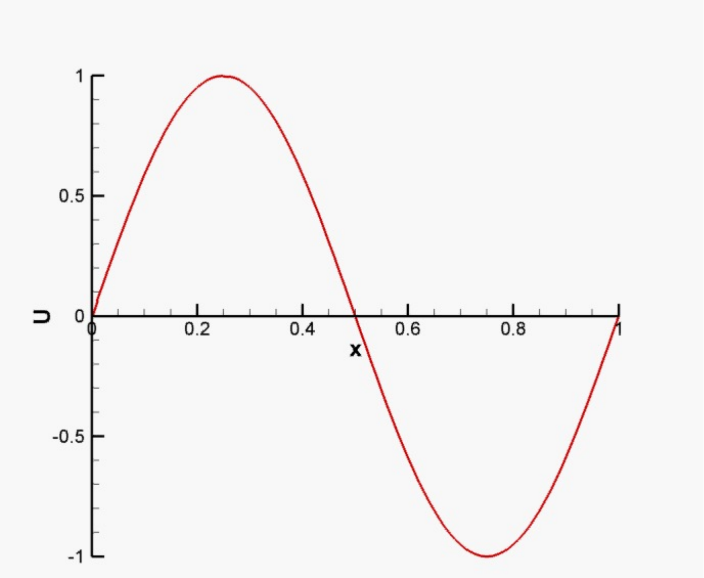


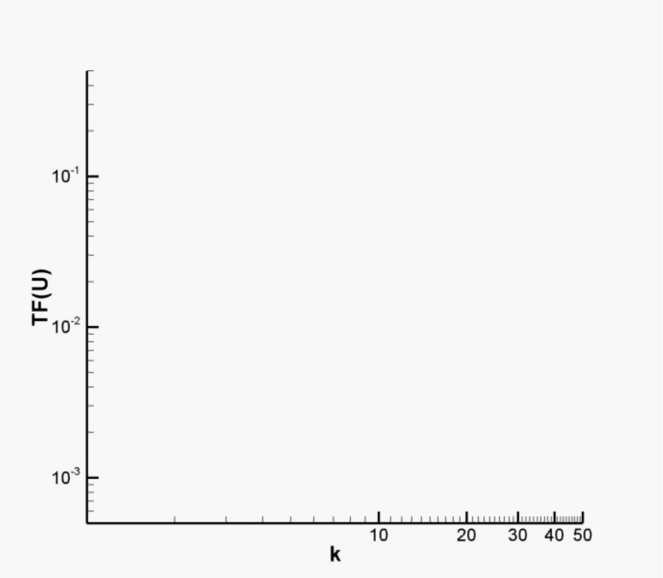


Fiziksel Vizkosite

- Non-viscous Burgers equation (ν = 0.001) : no physical viscosity,
- Spatial centered discretization : no numerical viscosity

$$\frac{\partial u}{\partial x} \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x^2)$$



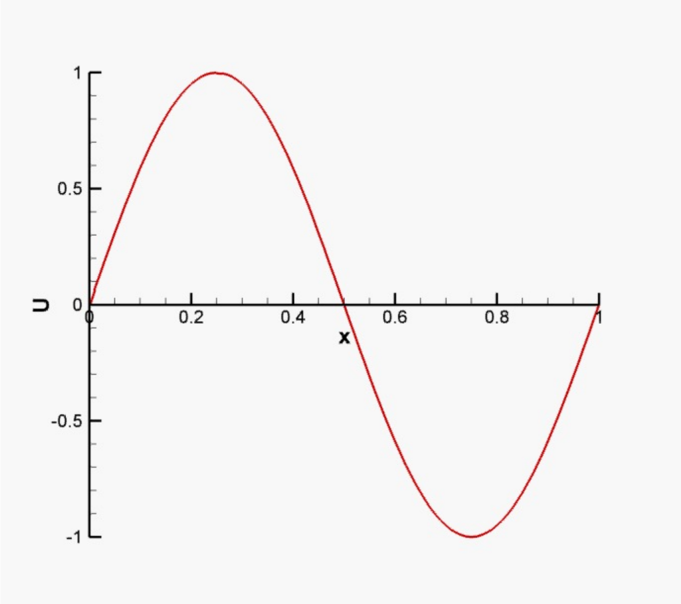


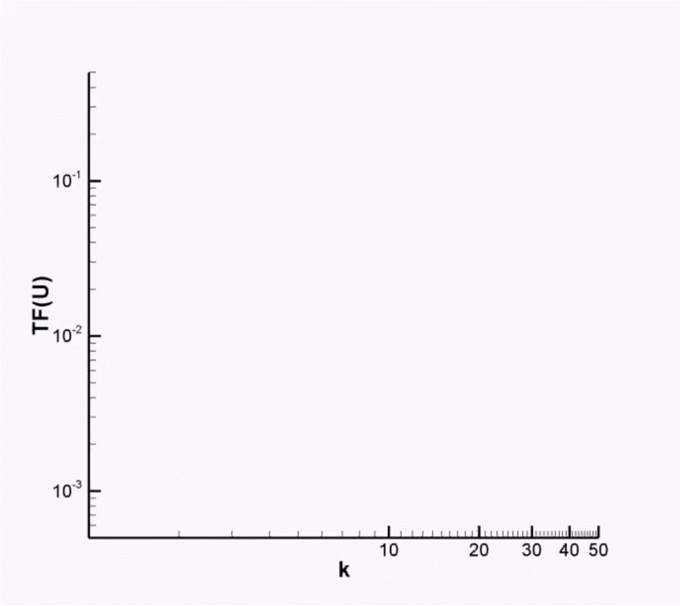
Fiziksel Vizkosite

- Non-viscous Burgers equation (ν = 0.01) : no physical viscosity,

- Spatial centered discretization : no numerical viscosity

$$\frac{\partial u}{\partial x} \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x^2)$$



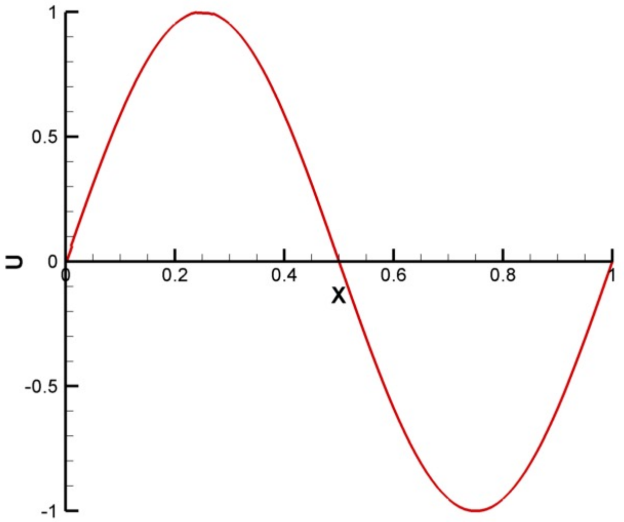


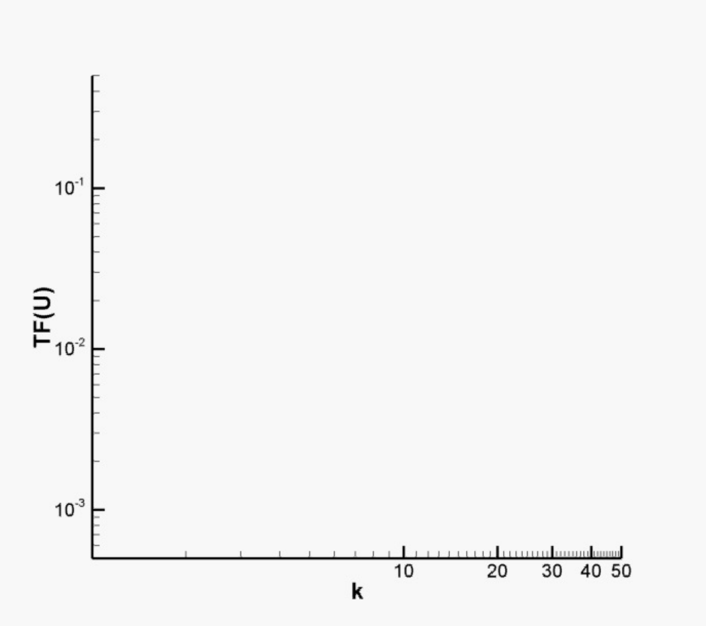
Hesaplama Vizkositesi ?

- Non-viscous Burgers equation (ν = 0) : no physical viscosity,

- Spatial upwind discretization : numerical viscosity

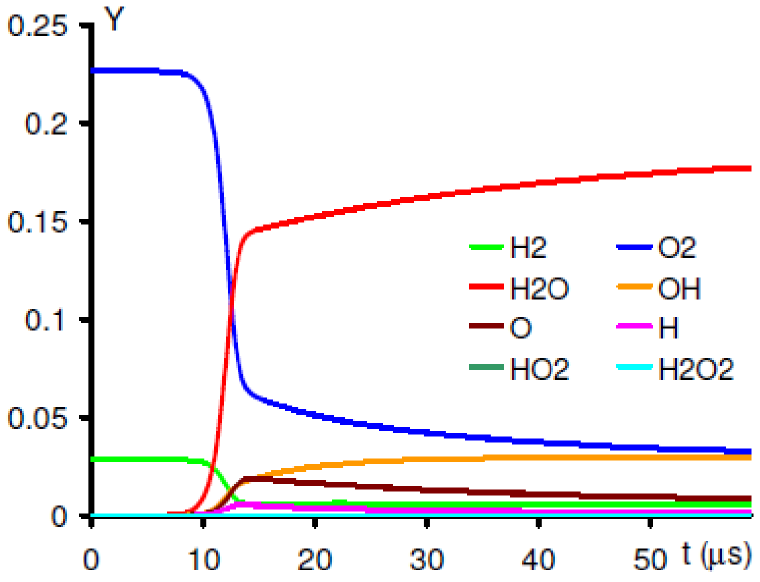
$$\frac{\partial u}{\partial x} \approx \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x^2)$$



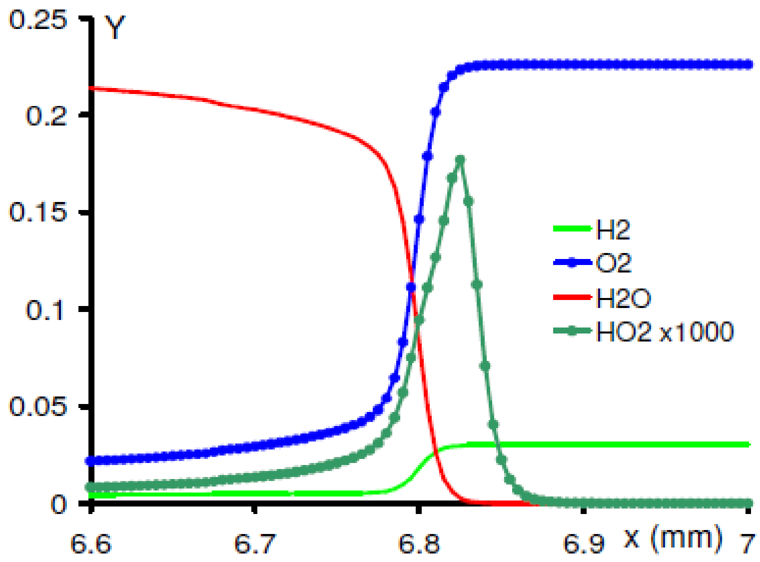


sharp discontinuities due to chemical reaction

- stiffness of the chemical source terms : flame
  - very thin flame front
  - characteristic time of the chemistry is at the order of 1 μs or less



Autoignition of stoichiometric H_2/O_2 stœmixture at 1500 K.



Structure of laminar, premixed flame of stoichiometric air/H_2 stœmixture.

filtreleme !

i.e. box filter :

$$\bar{\varphi}(x) = \frac{1}{\Delta}\int_{x-\Delta/2}^{x+\Delta/2} \varphi(\xi)d\xi$$

$\varphi(x) = \bar{\varphi}(x) + \varphi'(x)$ attention ! $\bar{\bar{\varphi}} \neq \bar{\varphi}$ and $\overline{\varphi'} = 0$

filtering conservative continuity equation :

$$\overline{\frac{\partial\rho}{\partial t} + (\rho u_j)_{,j}} = 0$$

linear filter : $\frac{\partial\bar{\rho}}{\partial t} + \overline{(\rho u_j)_{,j}} = 0$

comutation property : $\frac{\partial\bar{\rho}}{\partial t} + (\overline{\rho u_j})_{,j} = 0$

$\overline{\rho u_i} = \overline{\bar{\rho}\bar{u}_i} + \overline{\bar{\rho}u'_i} + \overline{\rho'\bar{u}_i} + \overline{\rho' u'_i} \neq \bar{\rho}\bar{u}_i$: can not be computed

change of variable (Favre) : $\overline{\rho u_i} = \bar{\rho}\tilde{u}_i$

Denklemler (I)LES

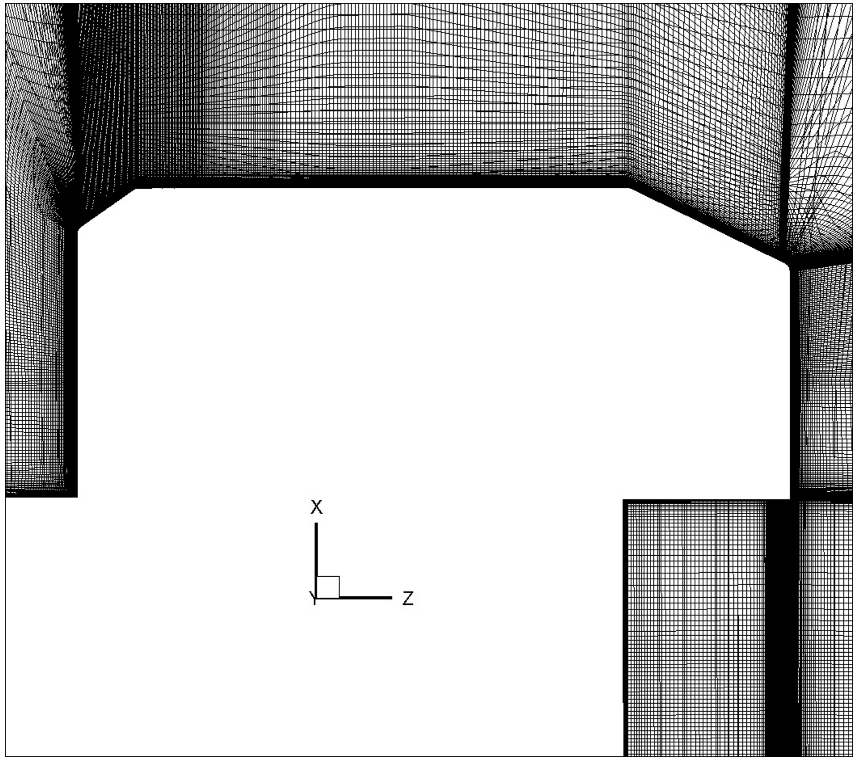
$$\frac{\partial \overline{\rho}}{\partial t} + \left(\overline{\rho}\widetilde{u_j}\right)_{,j} = 0$$

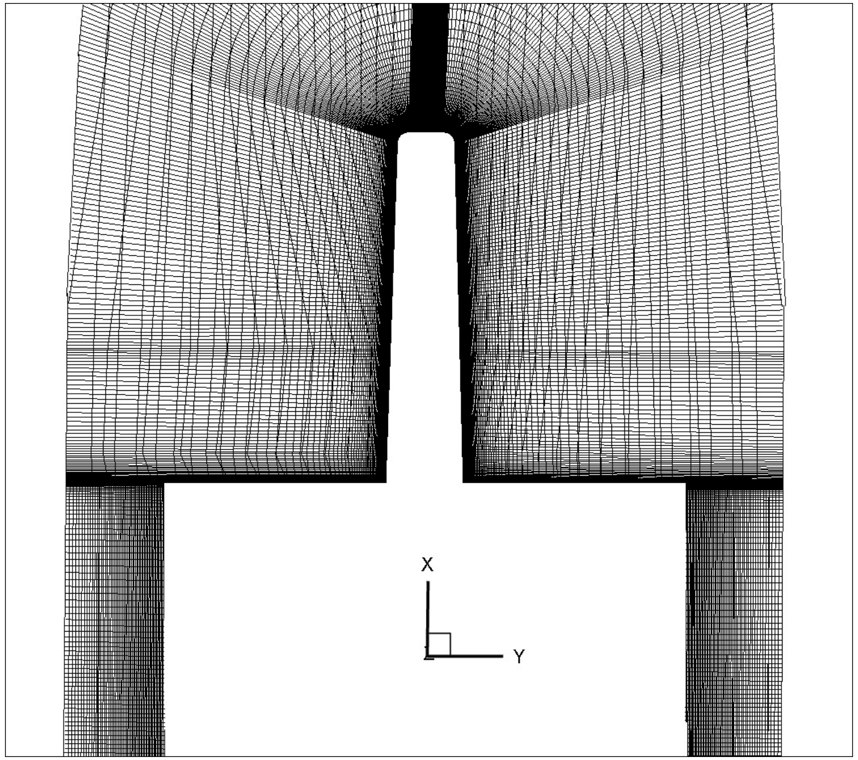
$$\frac{\partial \overline{\rho}\widetilde{u_i}}{\partial t} + \left(\overline{\rho}\widetilde{u_i}\widetilde{u_j} + \overline{p}\delta_{ij}\right)_{,j} = \overline{\tau_{ij}}_{,j} - \underbrace{\tau(\rho u_i u_j)_{,j}}_{\text{sub-grid term}}$$

$$\frac{\partial \overline{\rho}\widetilde{E}}{\partial t} + \left[\left(\overline{\rho}\widetilde{E} + \overline{p}\right)\widetilde{u_j}\right]_{,j} = \left(\overline{u_i\tau_{ij}}\right)_{,j} - \overline{q_j}_{,j} - \underbrace{\tau(\rho E u_j)_{,j}}_{\text{sub-grid term}}$$

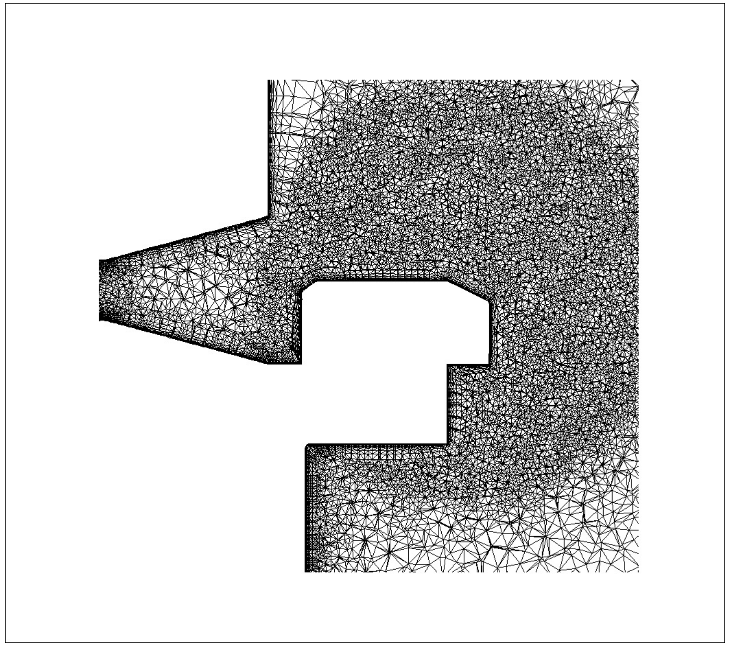
$$\frac{\partial \overline{\rho}\widetilde{Y_\alpha}}{\partial t} + \left(\overline{\rho}\widetilde{Y_\alpha}\widetilde{u_j}\right)_{,j} = -\overline{J_{\alpha j}}_{,j} - \underbrace{\tau(\rho Y_\alpha u_j)_{,j}}_{\text{sub-grid term}}$$

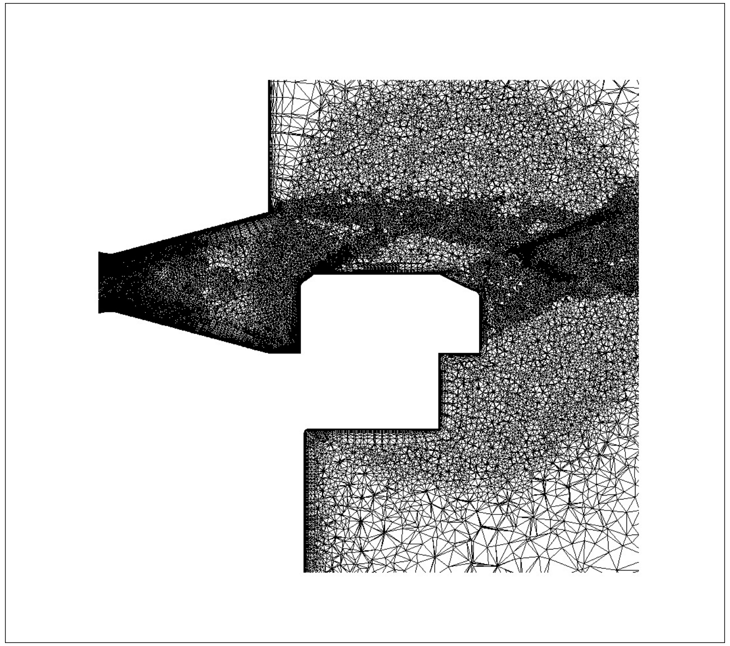
Çözüm Ağı Oluşturma (hexahedral/structured) - RANs Benzetimi



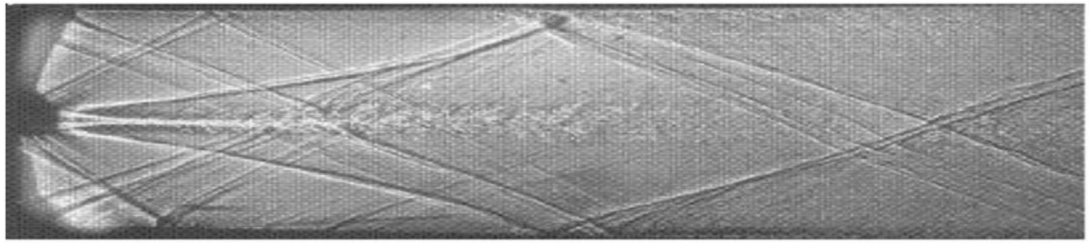


Çözüme Uyarlanan Çözüm Ağı

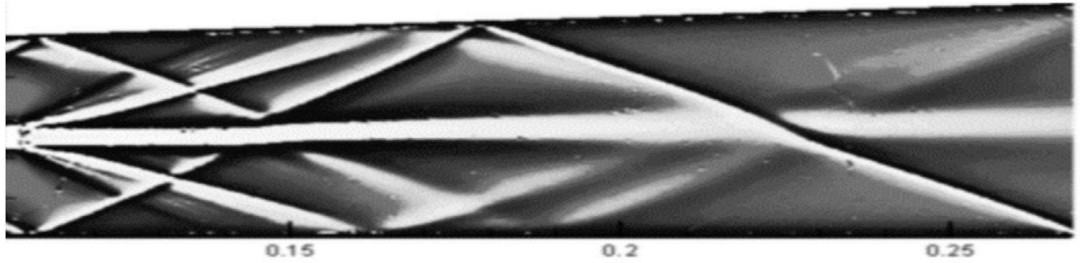




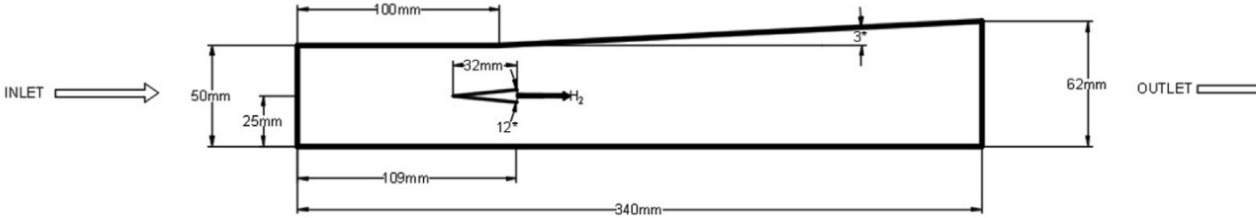
DLR Scramjet Enjeksiyon Degisimi



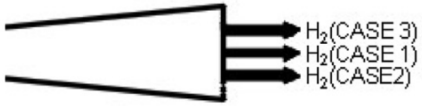
(a)



(b)

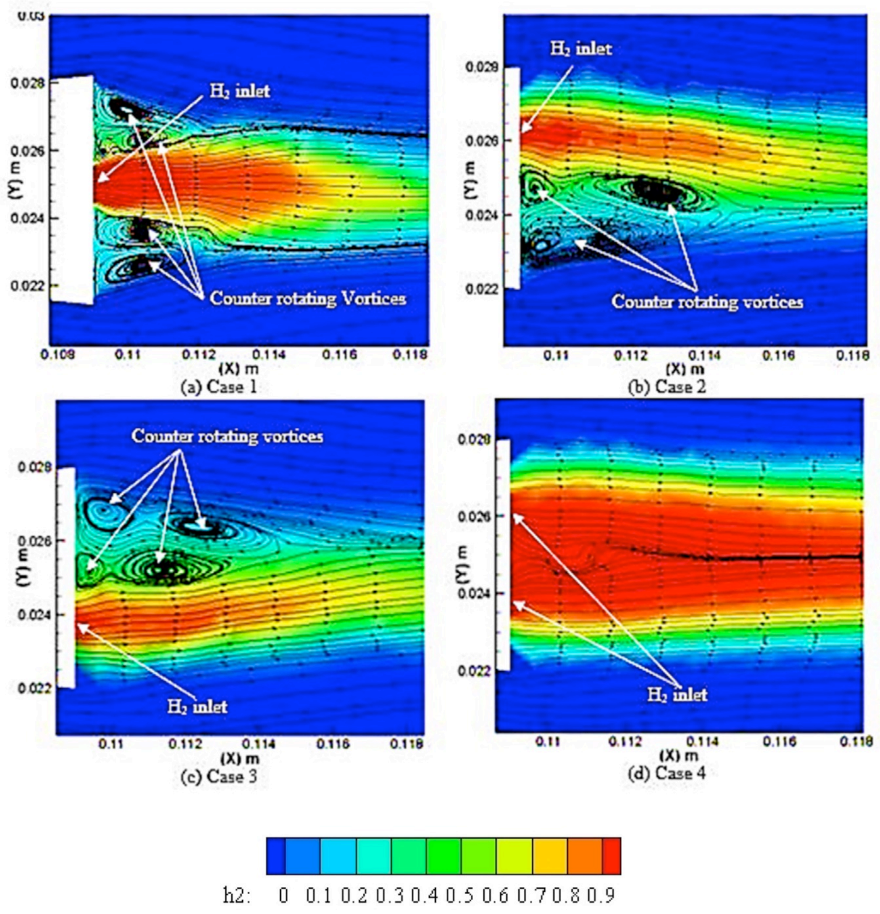


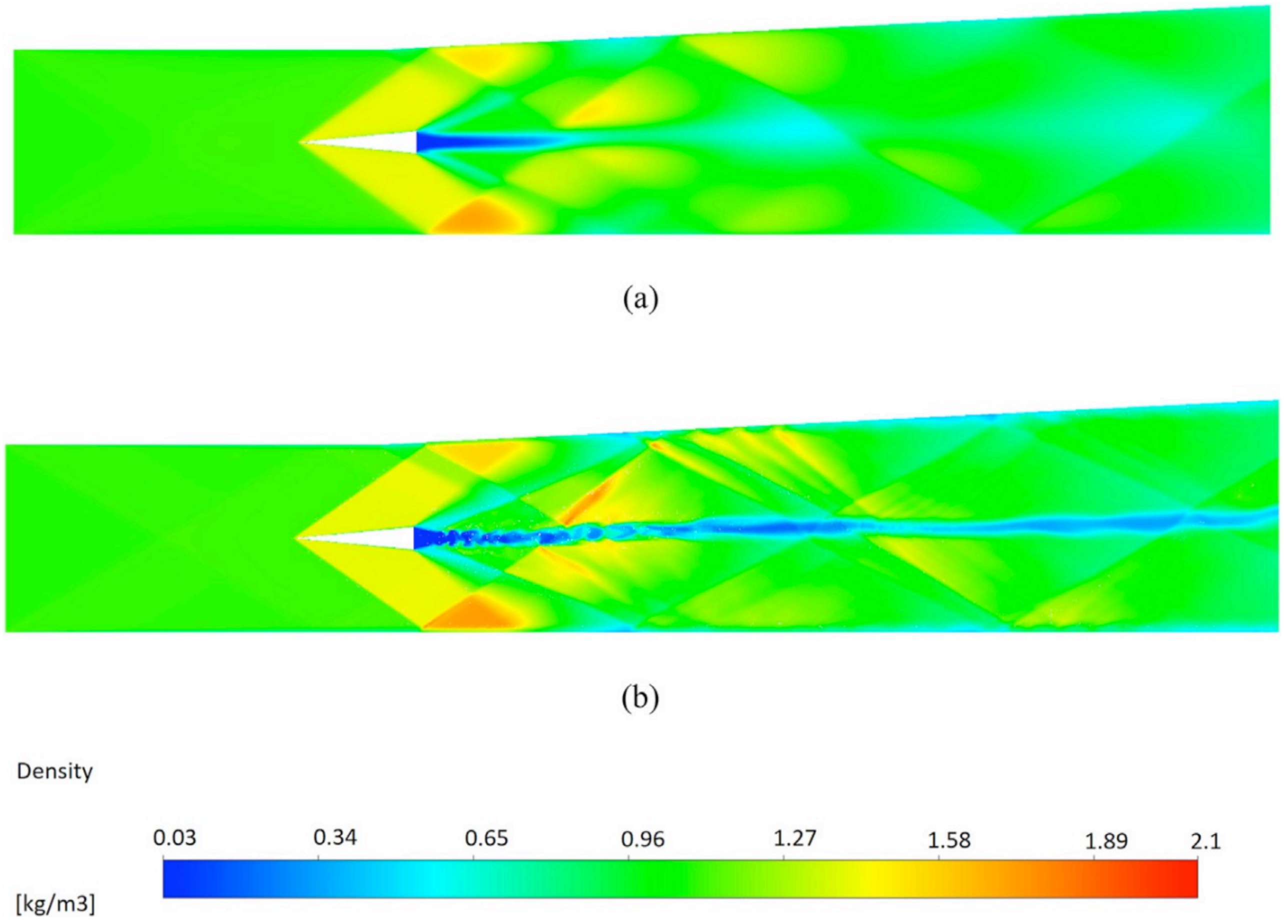
(a)



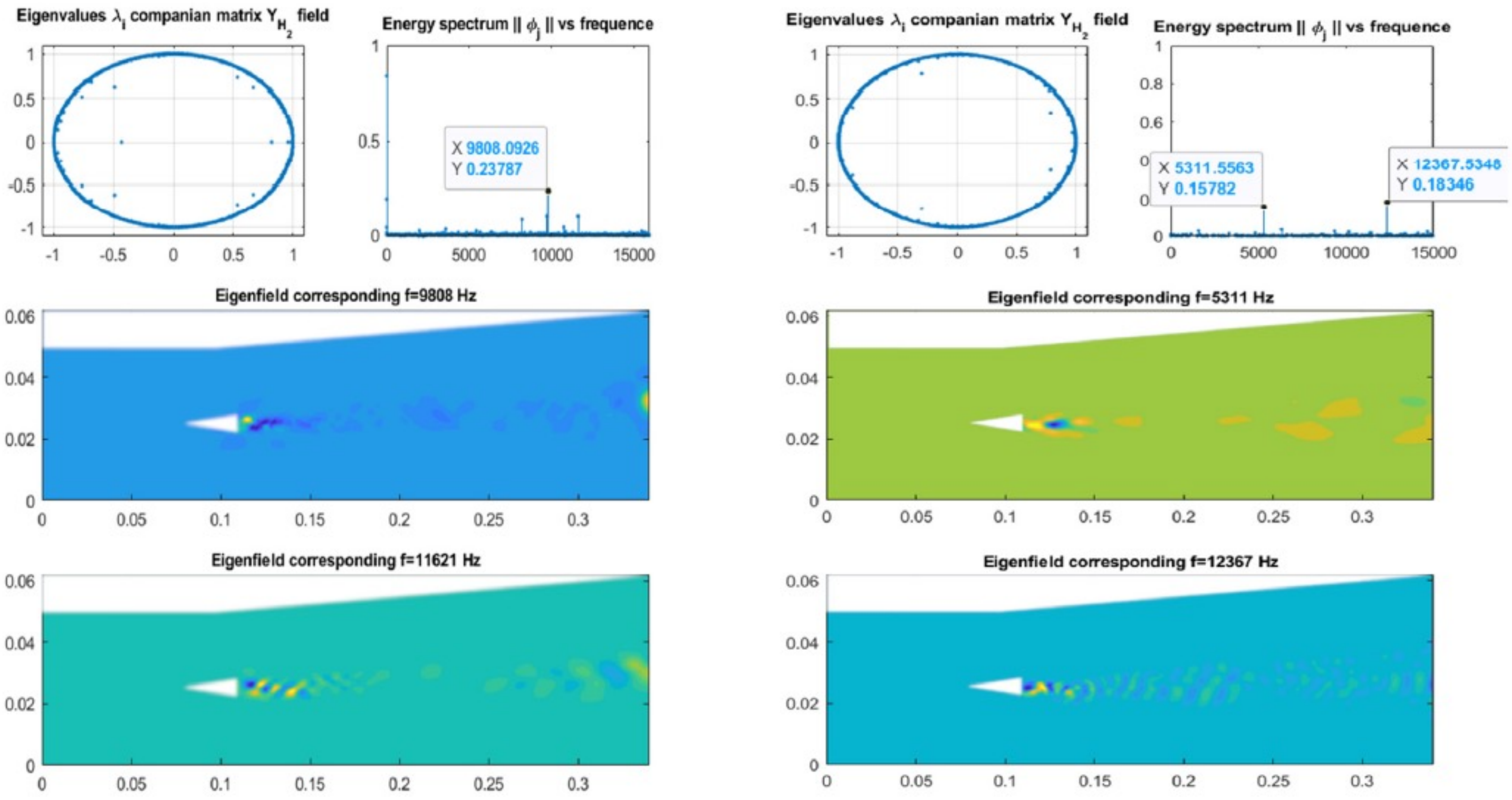
(b)

Sonuçlar


H₂ inlet
Counter rotating Vortices
(X) m
(Y) m
(a) Case 1
H₂ inlet
Counter rotating vortices
(b) Case 2
Counter rotating vortices
H₂ inlet
(c) Case 3
H₂ inlet
(d) Case 4
h2: 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9


(a)
(b)
Density
0.03 0.34 0.65 0.96 1.27 1.58 1.89 2.1
[kg/m3]

Sonuçlar



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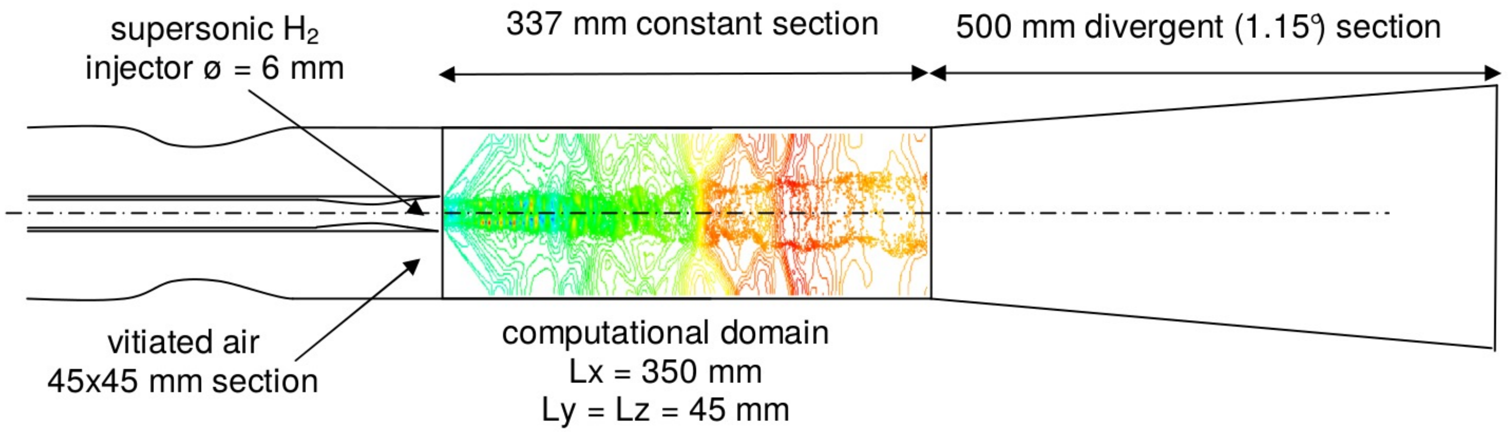
LES Benzetimi (SCRAMJET)

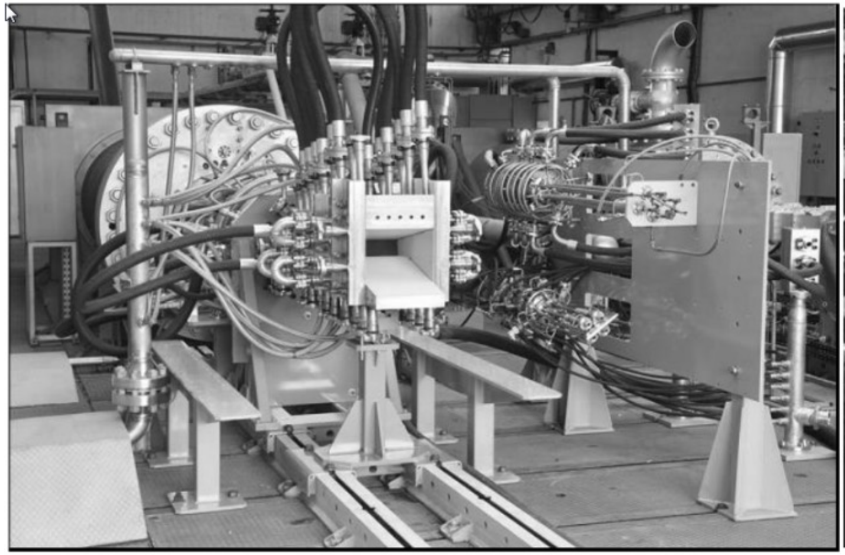


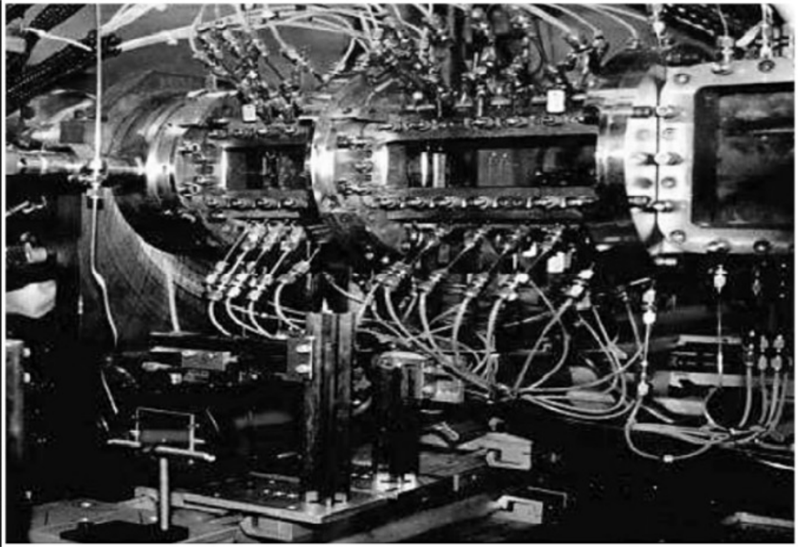
- Modeling the effect of the radical (oxygen atom) contamination for ONERA experimental test facility

Simulations for three different levels of contamination

$Y_O = 0 \,/\, 8.0\ 10^{-5} \,/\, 8.0\ 10^{-3}$

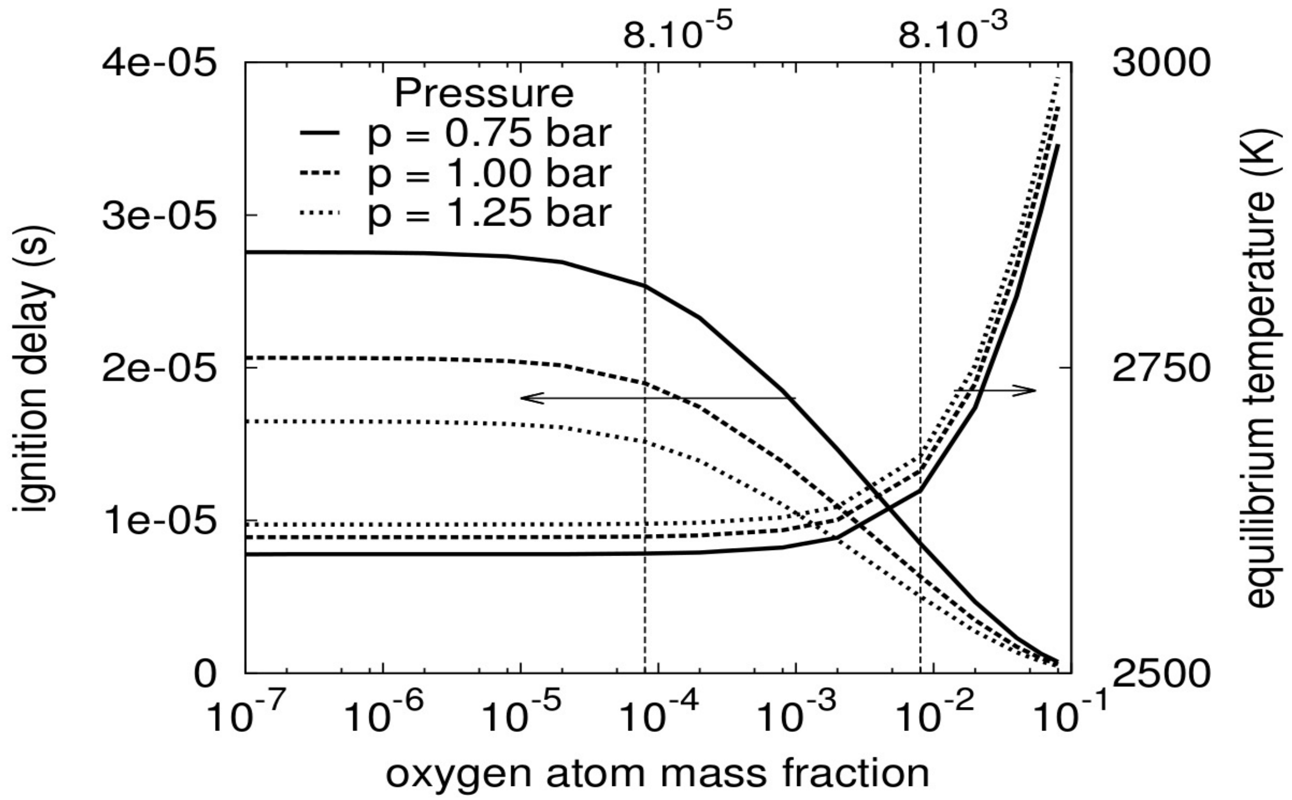
LES Sonuçlar (SCRAMJET)



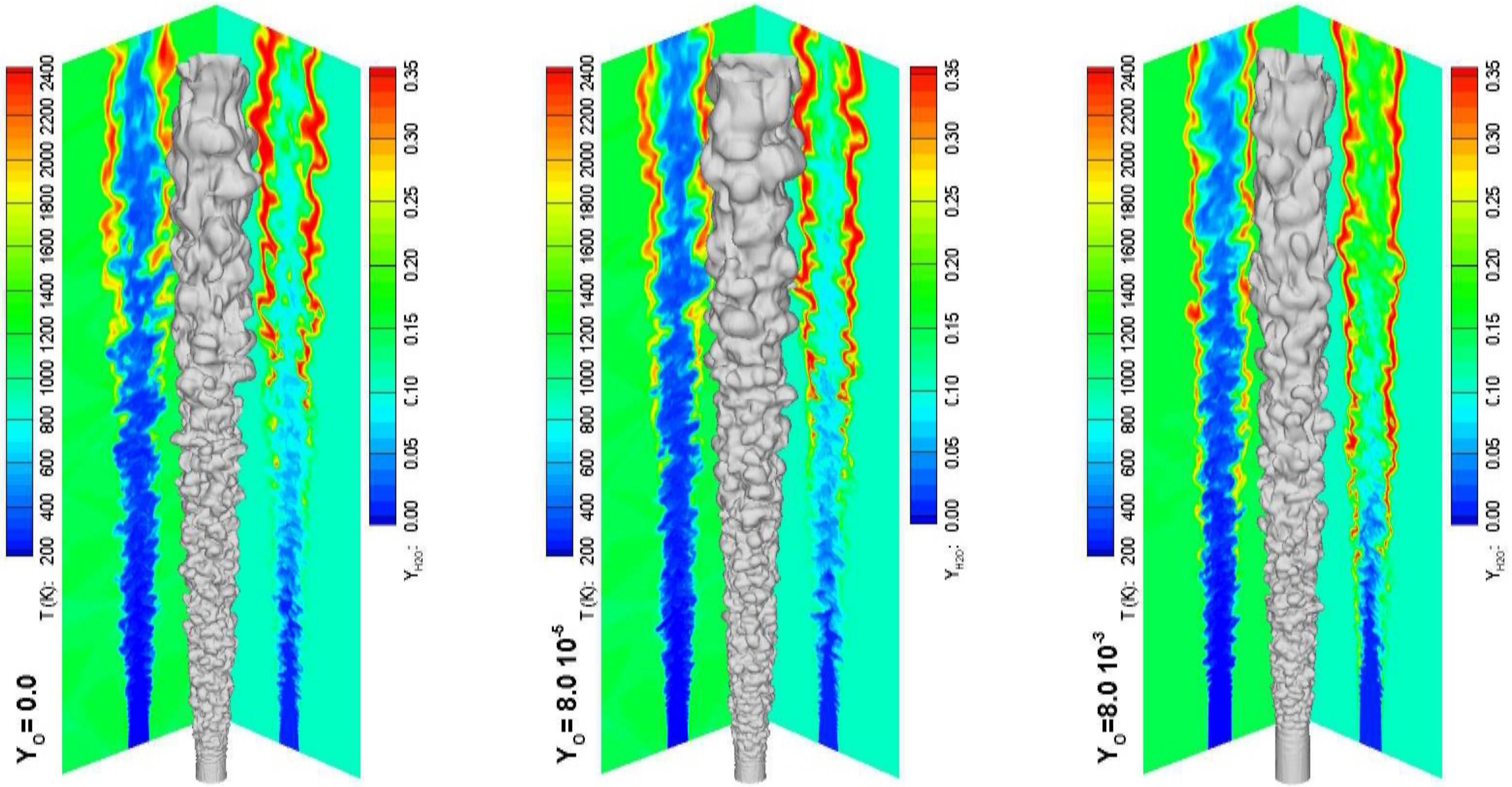


Left: the METHYLE test rig at MBDA Bourges-Subdray,
Right: the LAERTE M=2 combustion chamber at ONERA Palaiseau (Minard & Falempin 2008)

0D Sonuçlar (Fark eden ne??)



Sonuçlar



$Y_O = 0.0$
$Y_O = 8.0\ 10^{-5}$
$Y_O = 8.0\ 10^{-3}$
T(K): 200 400 600 800 1000 1200 1400 1600 1800 2000 2200 2400
Y_{H2O}: 0.00 0.05 0.10 0.15 0.20 0.25 0.30 0.35

• Zaman Birimleri

- the integral time scale "$u^{`2}/\epsilon$" can be computed

$$\tau_t^{-1} = max_{i,j} \frac{1}{2}\left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i}\right)$$

- approximately

$$\tau_t = \left\{\left(\frac{\Delta x}{u'}\right)^2 + \left(\frac{\Delta y}{v'}\right)^2 + \left(\frac{\Delta z}{w'}\right)^2\right\}^{1/2} \qquad (1)$$

- time scale for the finite rate chemistry

$$\frac{d\rho Y_\alpha(t)}{dt} = \dot{\omega}_\alpha(\rho Y_1, \dots, \rho Y_N) \quad ; \quad \alpha = 1, \dots, N = 6$$

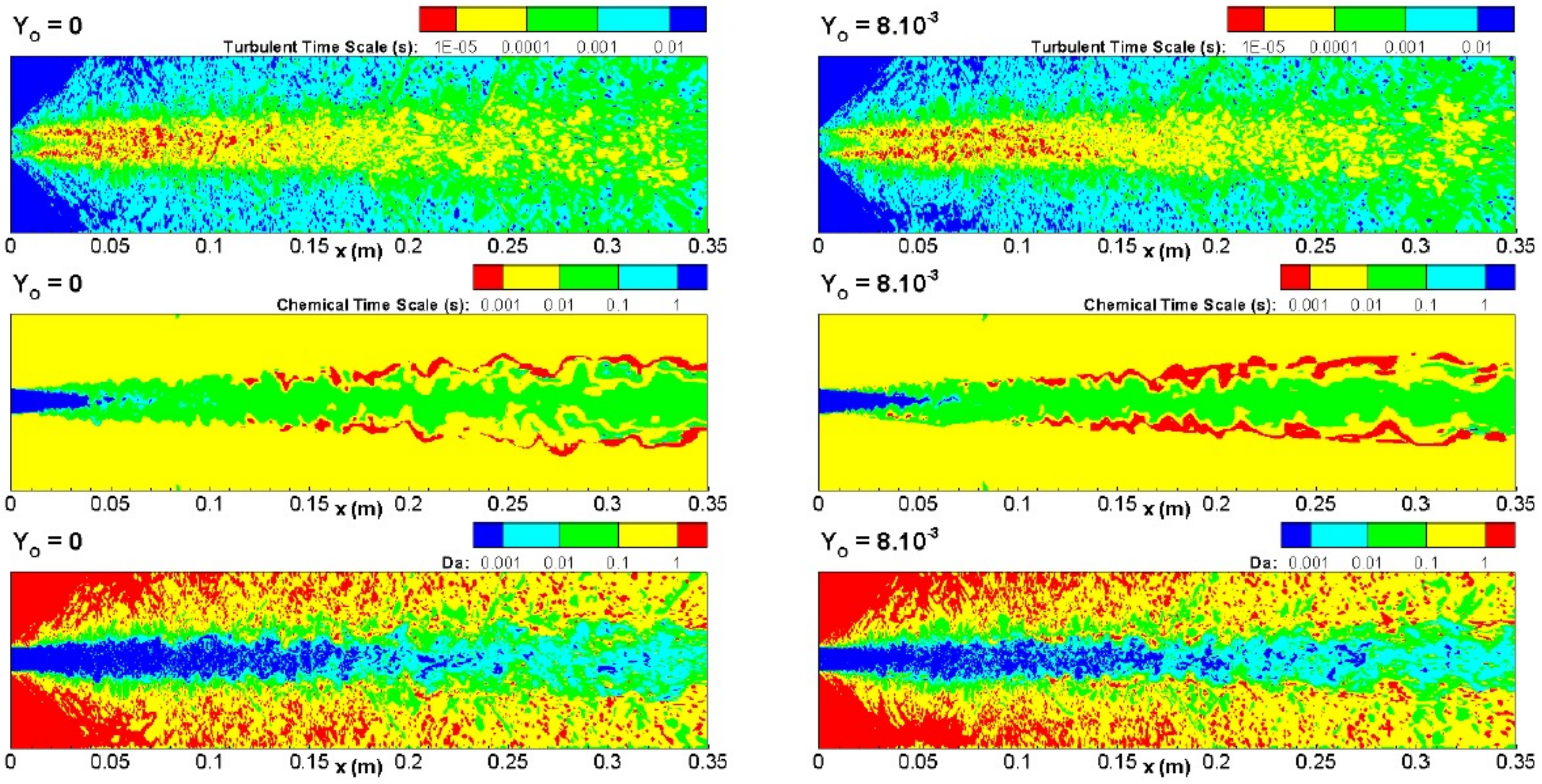
- the steepest charecteristic slope provide shortest chemical time scale

$$J_{\alpha\beta} = \frac{\partial \dot{\omega}_\alpha}{\partial(\rho Y_\beta)} \qquad \tau_c^{-1} = max_\alpha |R(\lambda_\alpha)| \qquad (2)$$

- the relative value of turbulent τ_t and chemical τ_c time scales yields the Damköhler number

Da = τ_t / τ_c

Time Scale Fields



Top: chemical time scale, middle: turbulent time scale, bottom: Damköhler number. Left Y_O=0, right: Y_O=8.10^{-3}.

Natural Convection

- the fluid (gas or liquid) motion without the existence of any external forces
- body forces (i.e. gravity) density gradient temperature variation
  - Buoyant jets
  - Plumes
  - Boundary layer over vertical flat plate
  - **Rayleigh Bénard problem**

$$\nabla \cdot u = 0,$$

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u = -\nabla p + \sqrt{\frac{Pr}{Ra}}\nabla^2 u + Te_z$$

$$\frac{\partial T}{\partial t} + (u \cdot \nabla)T = \frac{1}{\sqrt{\Pr Ra}}\nabla^2 T$$

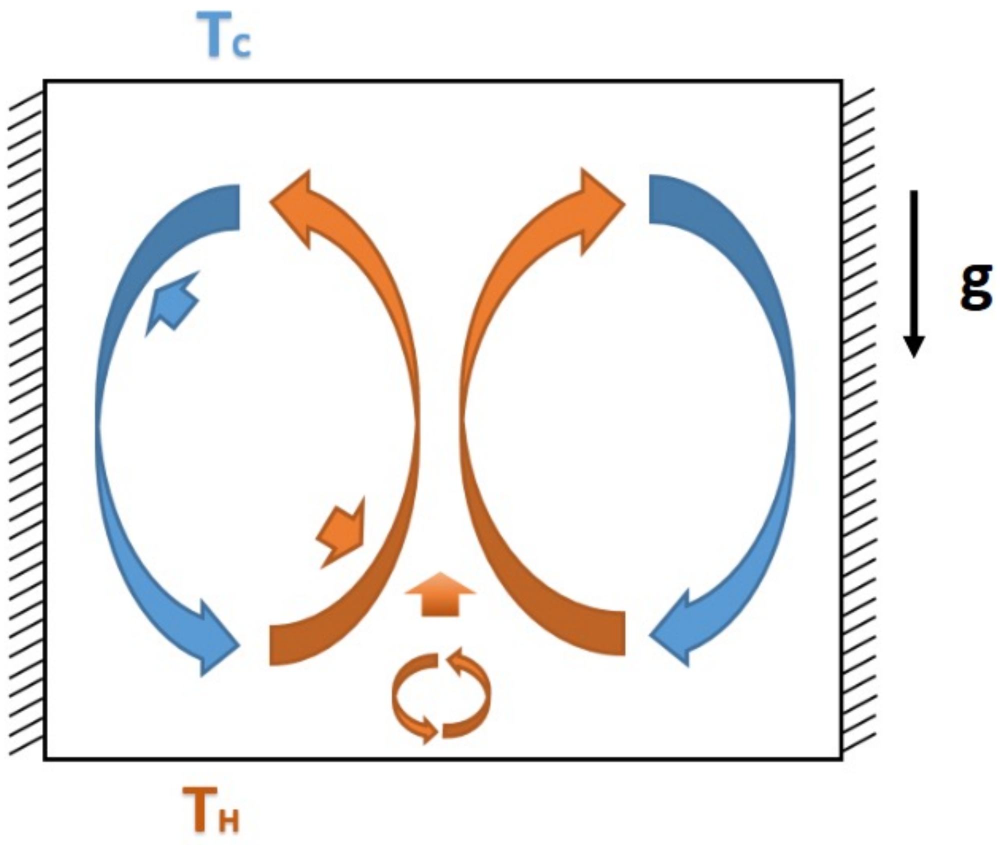
Natural Convection (Test Case Description)

- Density is a function of temperatue only
- 0.35 m x 0.35 m over 351 x 351 nodes
- Second order implicit finite volume simulation using ANSYS Fluent
- Variable thermodynamic properties

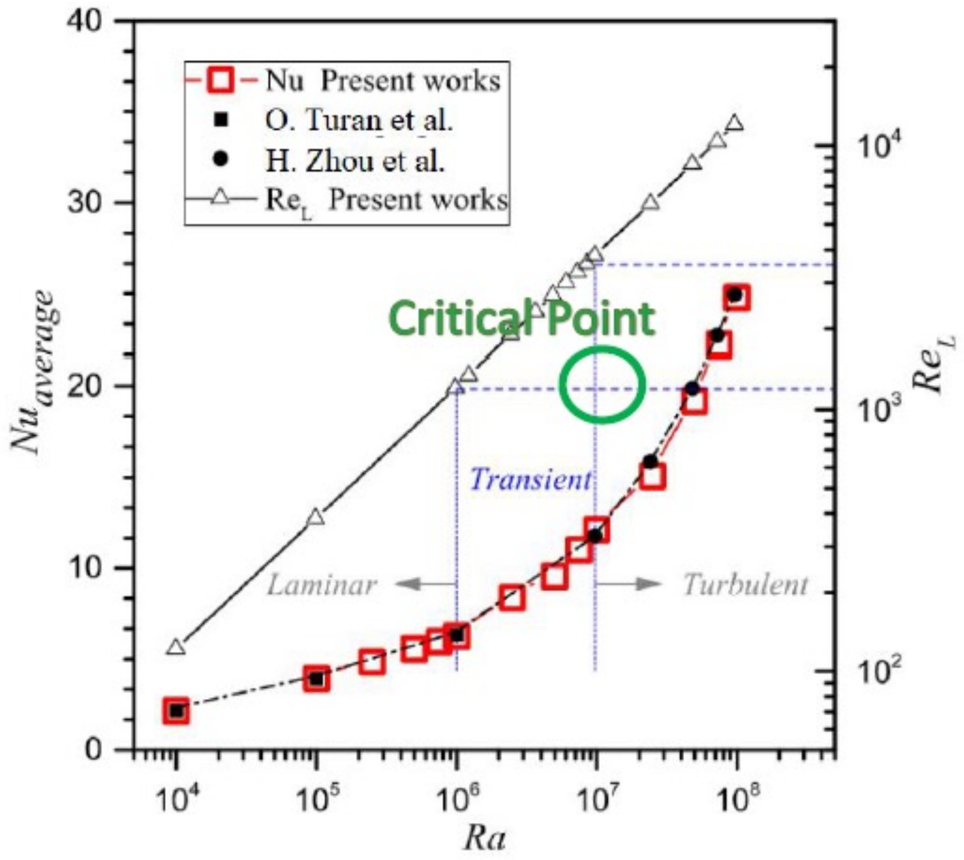
- **Variable / Constant Molecular Transport comparision.**

- Ra = 10e7
- Nu ~ 20

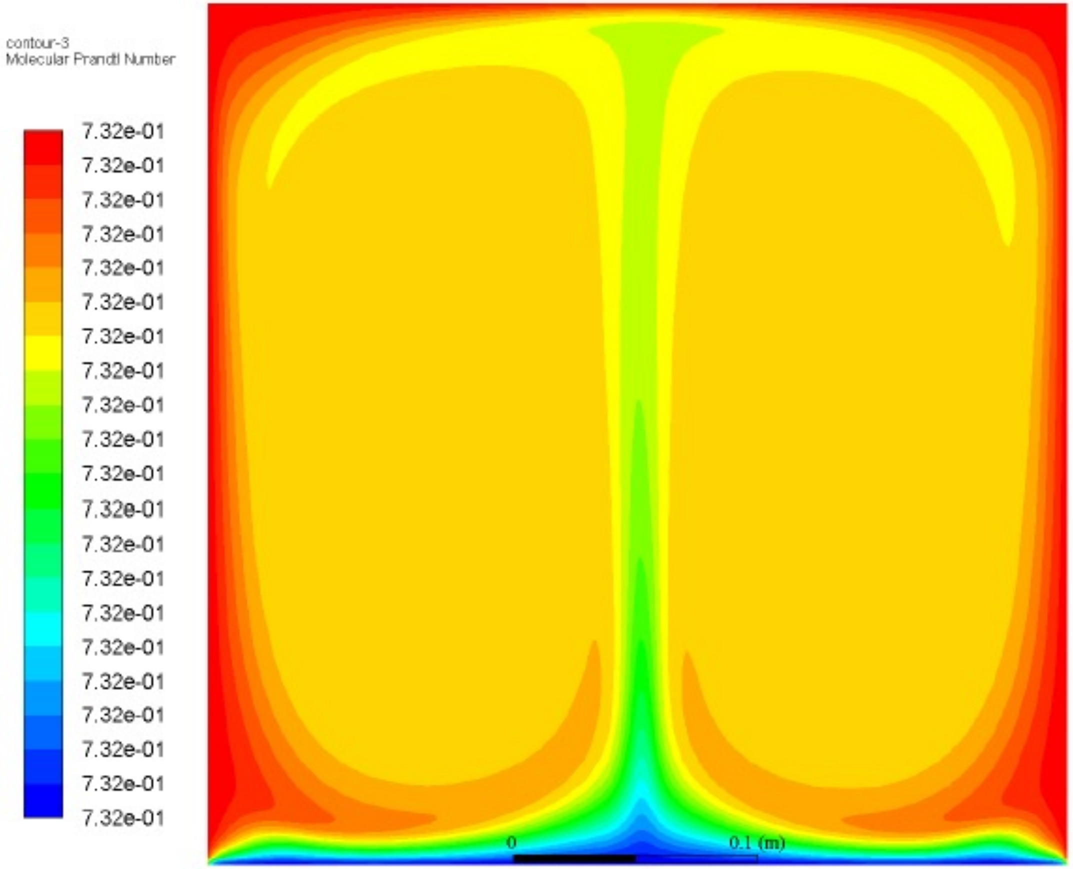
$$\frac{\partial T}{\partial x} = 0$$



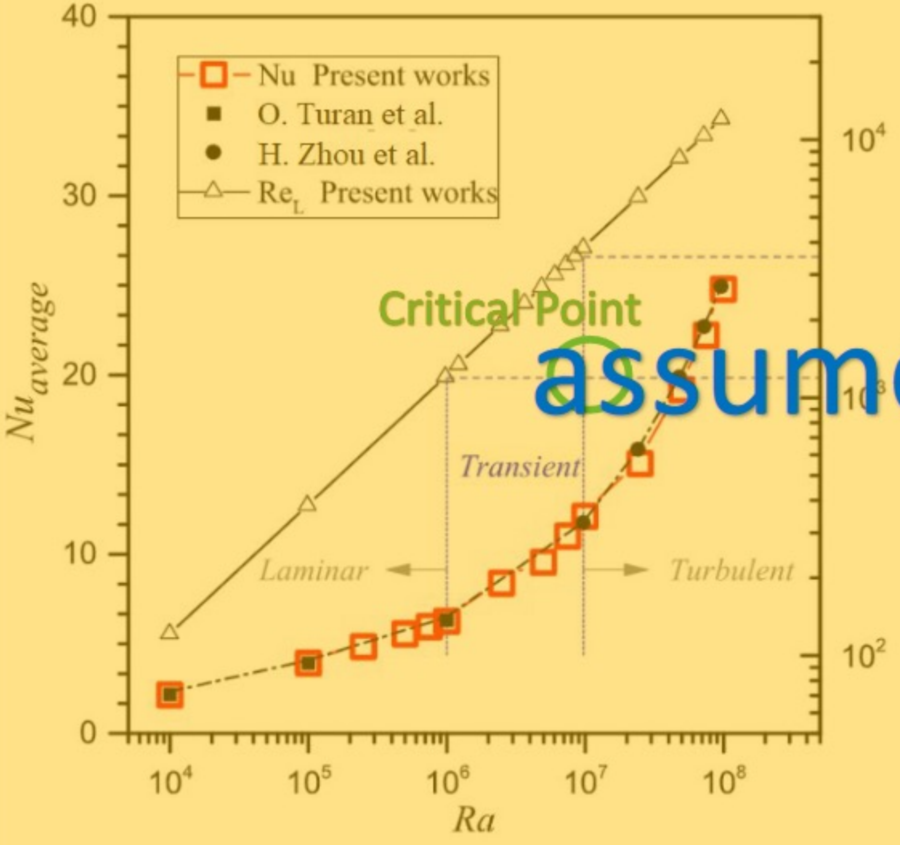
Prandtl Number



J. Zhao et al., International Journal of Heat and Mass Transfer



Prandtl Number



J. Zhao et al., International Journal of Heat and Mass Transfer

$T_c = 17$ C

$T_h = 15$ C

assume Pr constant ?

Temperature Fields

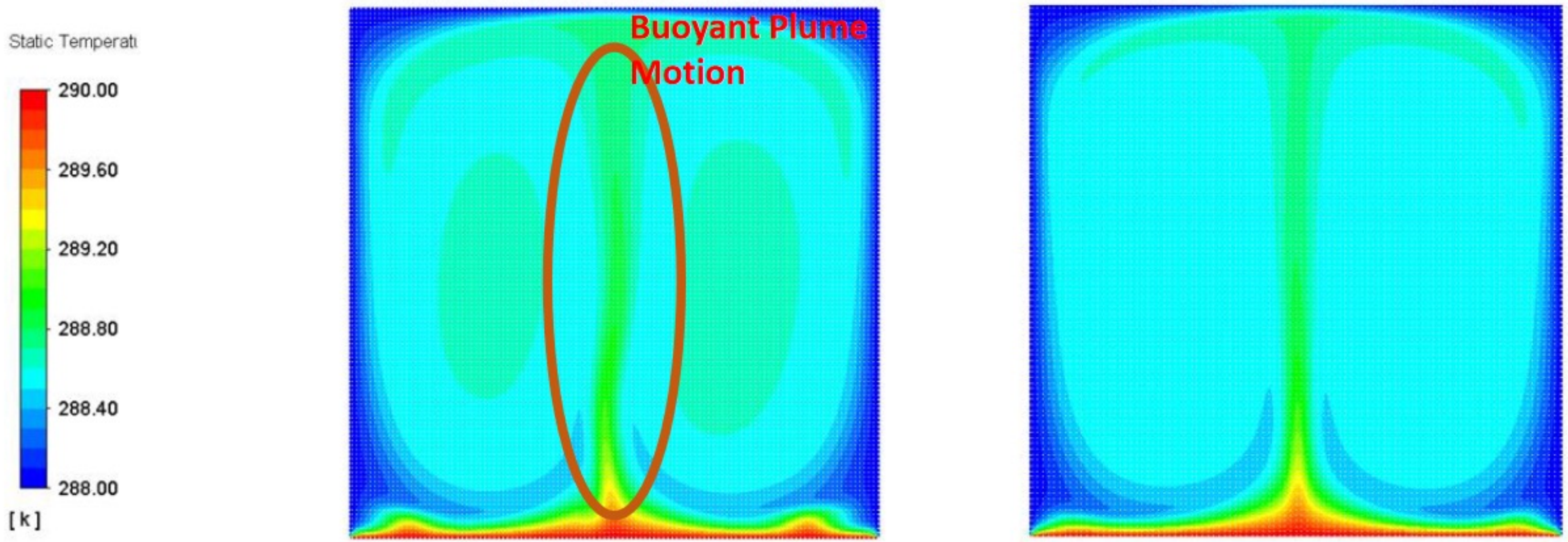
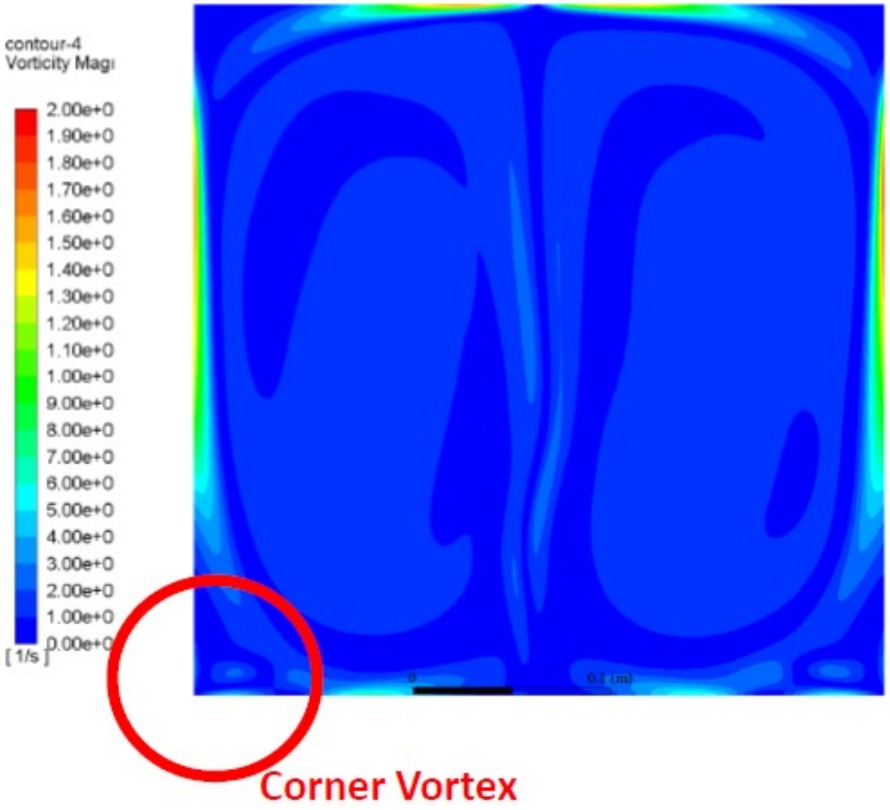
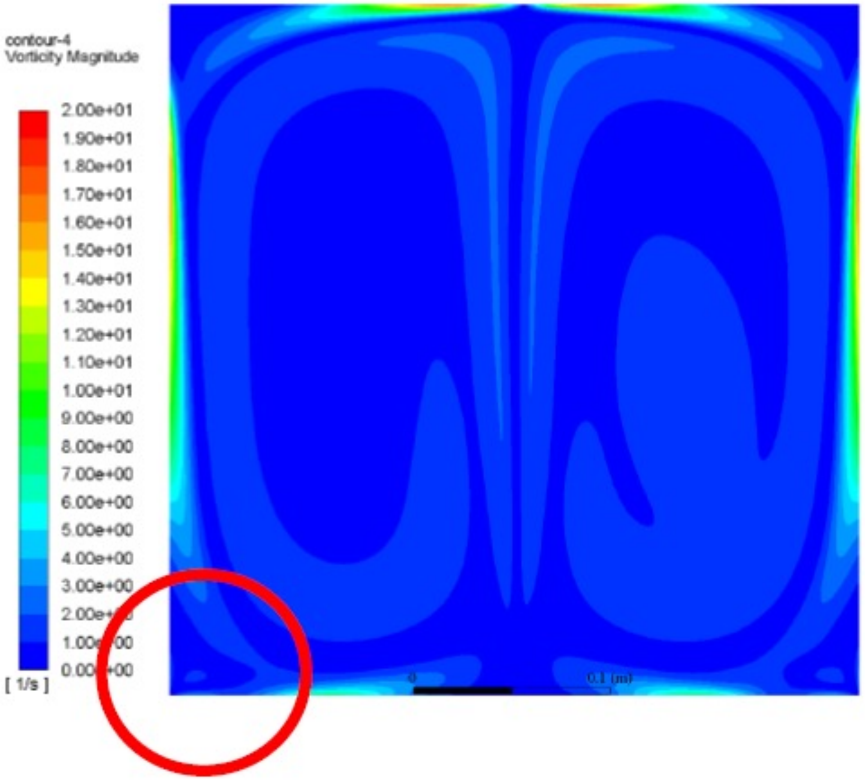


Fig (1) Instantaneous temperature field snapshot at T=600s for constant (left) and variable (right) molecular transport coefficients.

Vorticity Generation





Prototip Akışın Tanımı

- 20 mm x 20 mm physical domain,

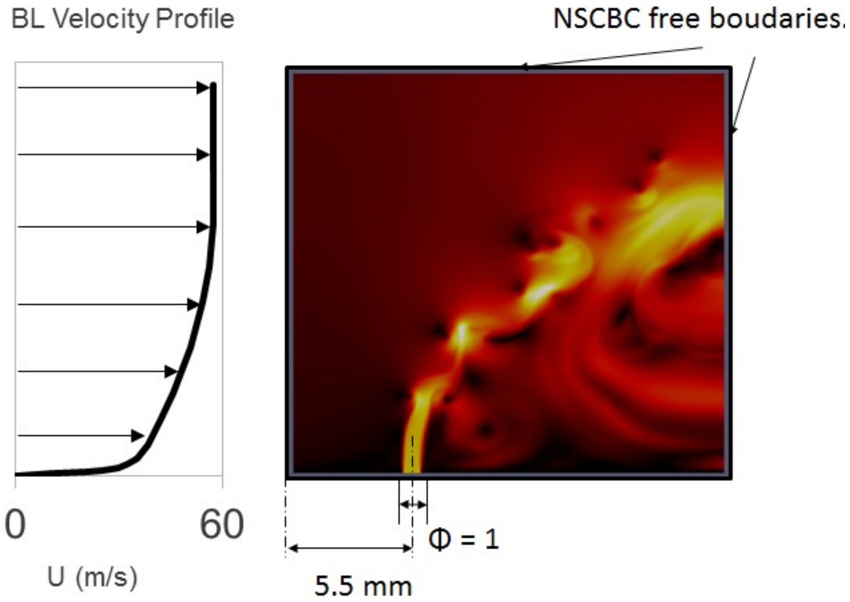
2 ms physical time + 1 ms after ignition

- 400 x 512 numerical domain
- ~1000 proc-hour

Table 1. Cross flow experimental conditions

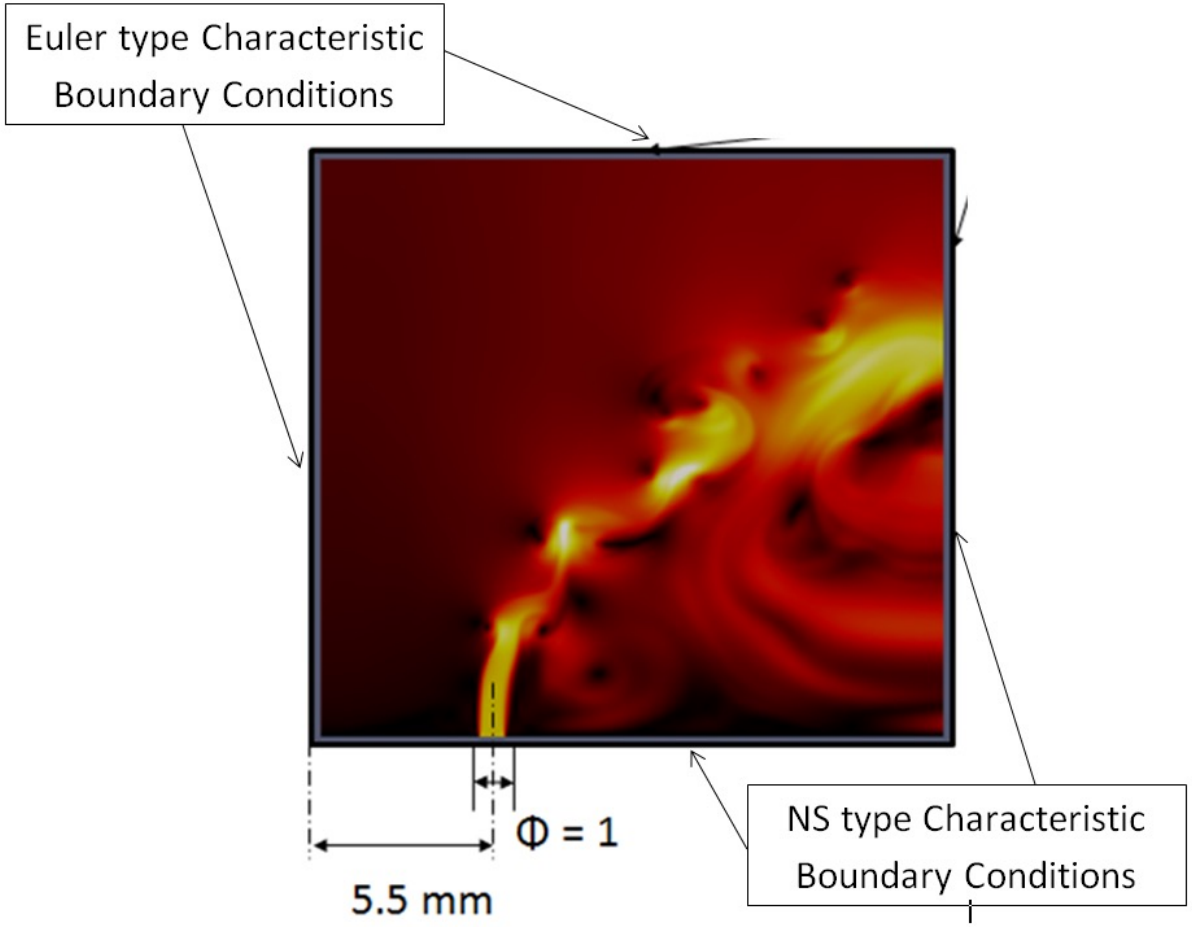
	H_2 /N_2 Jet	cross-flow
U, m/s	254.25	56.5
T_{stat}/T_{tot}, K	420/431	750/751.5
P_{stat}, kPa	102.500	102.500
μ, $kg.m^{-1}.s^{-1}$	$0.1998x10^{-4}$	$0.3394x10^{-4}$
ρ, $kg.m^{-3}$	0.284441	0.4682
Mach	0.3645	0.1

Schematic demonstration

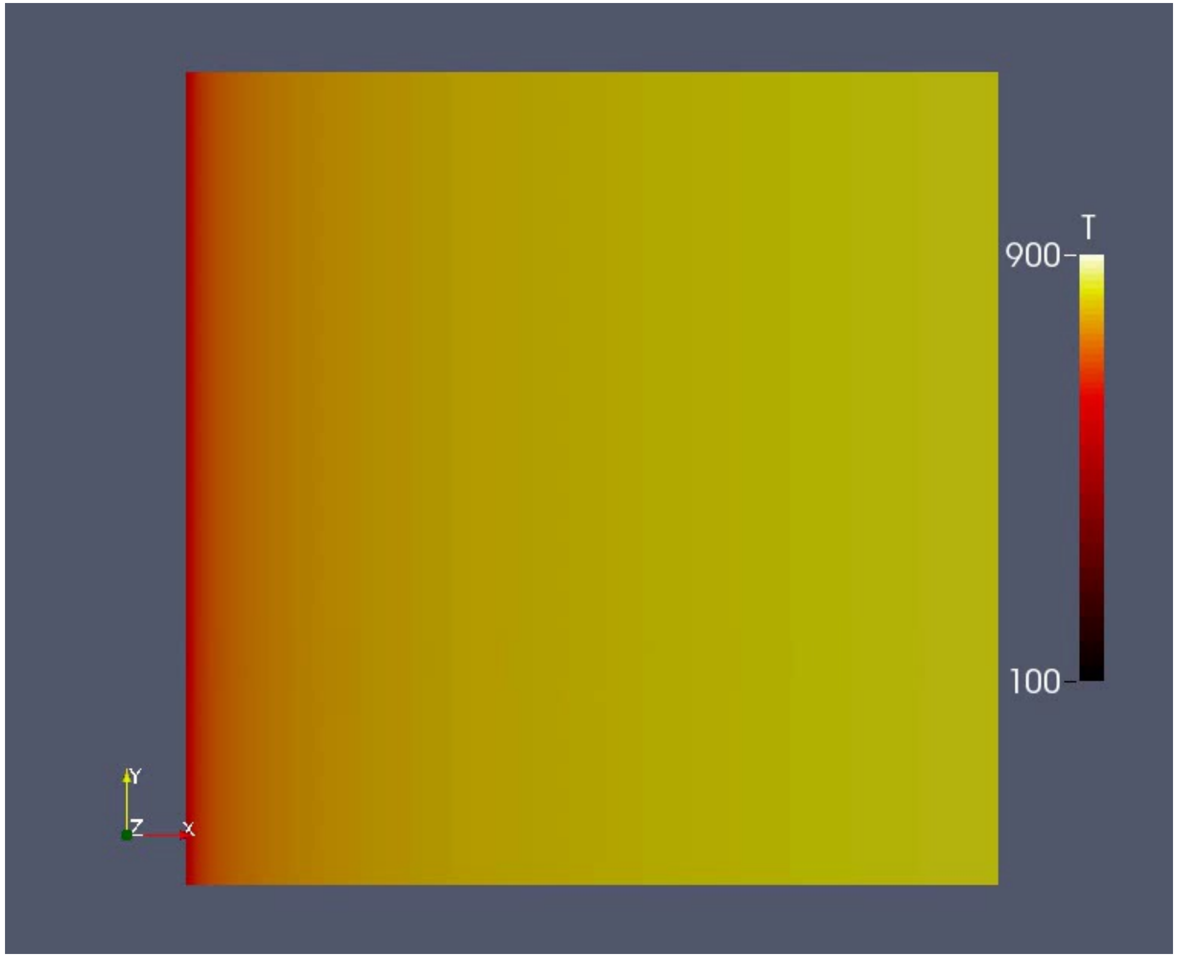


Grout et. al. Journal of Fluid Mechanics, 2012

Yansımasız (NSCBC) Sınır Koşulları



Tepkimesiz Karışım



Yansımasız (NSCBC) Sınır Koşulları (Euler Characteristic)

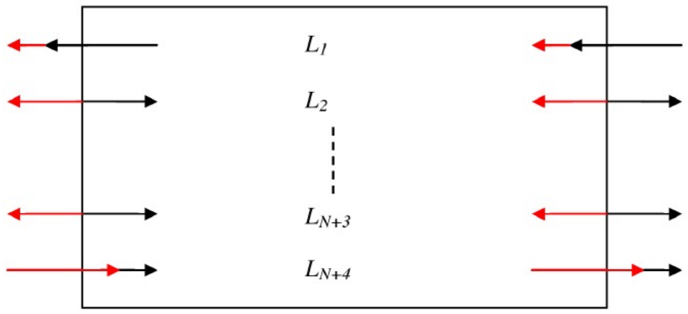
$$\frac{\partial \vec{U}}{\partial t} + [A]\frac{\partial \vec{U}}{\partial x} = \vec{0} \quad where \quad [A]_{ij} = \frac{\vec{F}_i}{\vec{U}}$$

$$\frac{\partial \vec{W}}{\partial t} + \vec{L} = 0$$

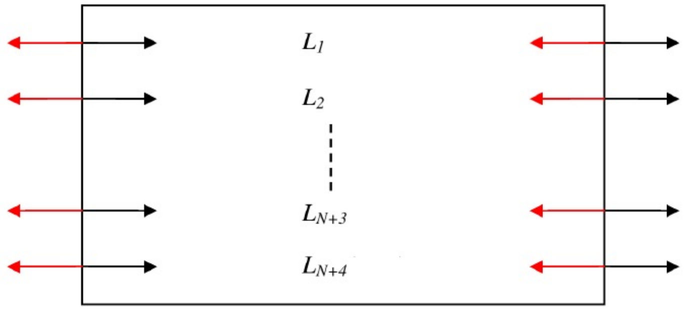
$$\frac{\partial \vec{W}}{\partial x} = [L]\frac{\partial \vec{U}}{\partial x}$$

$$\vec{L} = [\Lambda]\frac{\partial \vec{W}}{\partial t}$$

$$L_i = \lambda^{(i)} \sum_{j=1}^{Nesp+4} l_j^{(i)} \frac{\partial U_j}{\partial x}$$



ECBC subsonic flux directions



ECBC supersonic flux directions

Yansımasız (NSCBC) Sınır Koşulları (Euler Characteristic)

$$L_i = \lambda^{(i)} \sum_{j=1}^{Nesp+4} l_j^{(i)} \frac{\partial U_j}{\partial x}$$

- either set to *zero* : numerical BC
- related to outgoing waves by physical restrictions applied on time derivatives of primitive variables : physical BC

$$[R]\frac{\partial \vec{W}}{\partial t} + [R]\vec{L} = \vec{0}$$

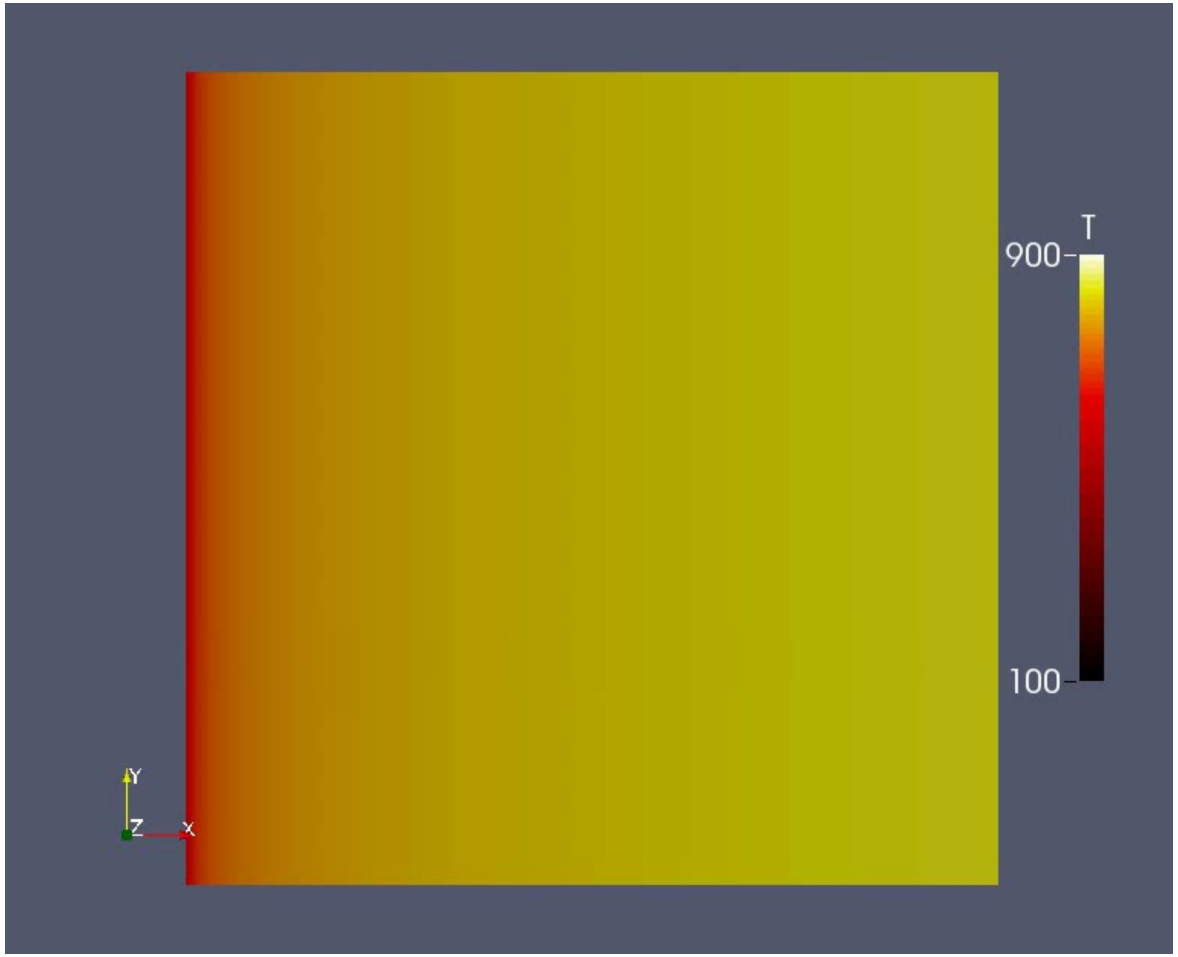
$$\frac{\partial \vec{U}}{\partial t} + \vec{d} = \vec{0} \quad ; \quad \vec{d} = [R]\vec{L}$$

Yansımasız (NSCBC) Sınır Koşulları (NS Tipi)

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{F}}{\partial x} + \frac{\partial \vec{G}}{\partial y} + \frac{\partial \vec{H}}{\partial z} = \vec{V} + \vec{S}$$

Subsonic inflow $u > 0$ at $x = 0$		Subsonic inflow $u < 0$ at $x = l_x$	
Wave velocity	$\mathcal{L}_k^x$ at x = 0	Wave velocity	$\mathcal{L}_k^x$ at x = l_x
$u - c < 0$	$\mathcal{L}_1^x$ computed	$u - c < 0$	$\mathcal{L}_1^x = \beta_1 (u - u_{l_x}) + \mathcal{T}_1^x + V_1^x + S_1^x$
$u > 0$	$\mathcal{L}_2^x = \beta_2 (T - T_0) + \mathcal{T}_2^x + V_2^x + S_2^x$	$u < 0$	$\mathcal{L}_2^x = \beta_2 (T - T_{l_x}) + \mathcal{T}_2^x + V_2^x + S_2^x$
$u > 0$	$\mathcal{L}_3^x = \beta_3 (v - v_0) + \mathcal{T}_3^x + V_3^x + S_3^x$	$u < 0$	$\mathcal{L}_3^x = \beta_3 (v - v_{l_x}) + \mathcal{T}_3^x + V_3^x + S_3^x$
$u > 0$	$\mathcal{L}_4^x = \beta_4 (w - w_0) + \mathcal{T}_4^x + V_4^x + S_4^x$	$u < 0$	$\mathcal{L}_4^x = \beta_4 (w - w_{l_x}) + \mathcal{T}_4^x + V_4^x + S_4^x$
$u + c < 0$	$\mathcal{L}_5^x = \beta_4 (u - u_0) + \mathcal{T}_4^x + V_4^x + S_4^x$	$u + c < 0$	$\mathcal{L}_5^x$ computed
$u > 0$	$\mathcal{L}_{5+i}^x = \beta_{5+i} (Y - Y_{i,0}) + \mathcal{T}_{5+i}^x + V_{5+i}^x + S_{5+i}^x$	$u < 0$	$\mathcal{L}_{5+i}^x = \beta_{5+i} (Y - Y_{i,l_x}) + \mathcal{T}_{5+i}^x + V_{5+i}^x + S_{5+i}^x$

Subsonic outflow $u > 0$ at $x = 0$		Subsonic outflow $u < 0$ at $x = l_x$	
Wave velocity	$\mathcal{L}_k^x$ at x = 0	Wave velocity	$\mathcal{L}_k^x$ at x = l_x
$u - c < 0$	$\mathcal{L}_1^x$ computed	$u - c < 0$	$\mathcal{L}_1^x = \alpha (p - p_\infty) + (1 - a)\, \mathcal{T}_1^x + a\, \mathcal{T}_{exact}^x + V_1^x + S_1^x$
$u < 0$	$\mathcal{L}_2^x$ computed	$u > 0$	$\mathcal{L}_2^x$ computed
$u < 0$	$\mathcal{L}_3^x$ computed	$u > 0$	$\mathcal{L}_3^x$ computed
$u < 0$	$\mathcal{L}_4^x$ computed	$u > 0$	$\mathcal{L}_4^x$ computed
$u + c < 0$	$\mathcal{L}_5^x = \alpha (p - p_\infty) + (1 - a)\, \mathcal{T}_5^x + a\, \mathcal{T}_{exact}^x + V_5^x + S_5^x$	$u + c < 0$	$\mathcal{L}_5^x$ computed
$u < 0$	$\mathcal{L}_{5+i}^x$ computed	$u > 0$	$\mathcal{L}_{5+i}^x$ computed


T
900
100
Y
Z
X