Modeling and simulation of Microfluidics systems

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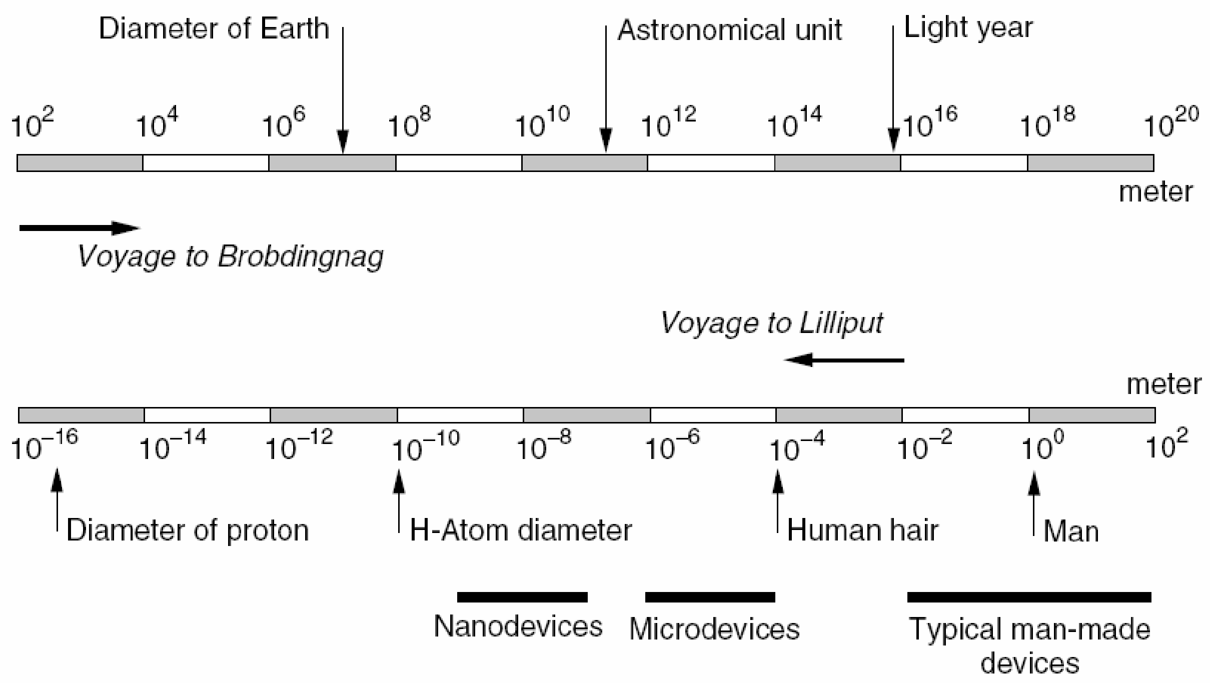


FIGURE 1.1 Scale of things, in meters. Lower scale continues in the upper bar from left to right. One meter is 10^6 microns, 10^9 nanometers, or 10^{10} Angstroms.

- the nature of phenomena changes with reducing sizes. e.g., gravitational force, surface tension effect, magnetic force, etc.

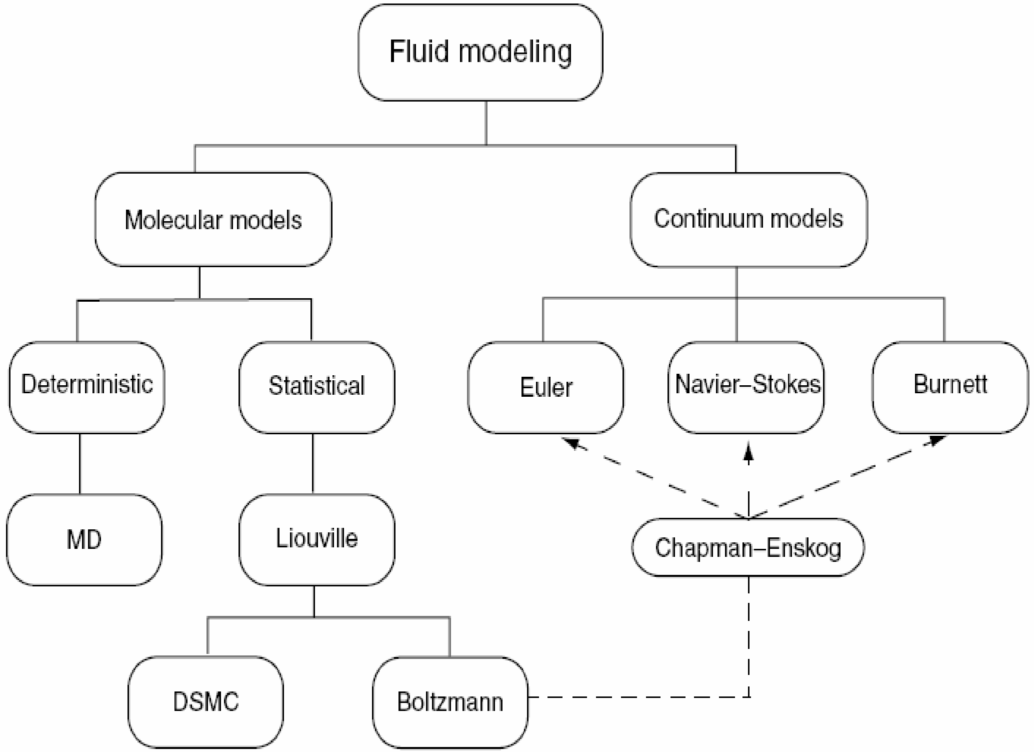


FIGURE 4.1 Molecular and continuum flow models.

$$Kn = \frac{\lambda}{D_h}$$

Knudsen number: D_h is hydraulics diameter and λ is the mean free path of fluid

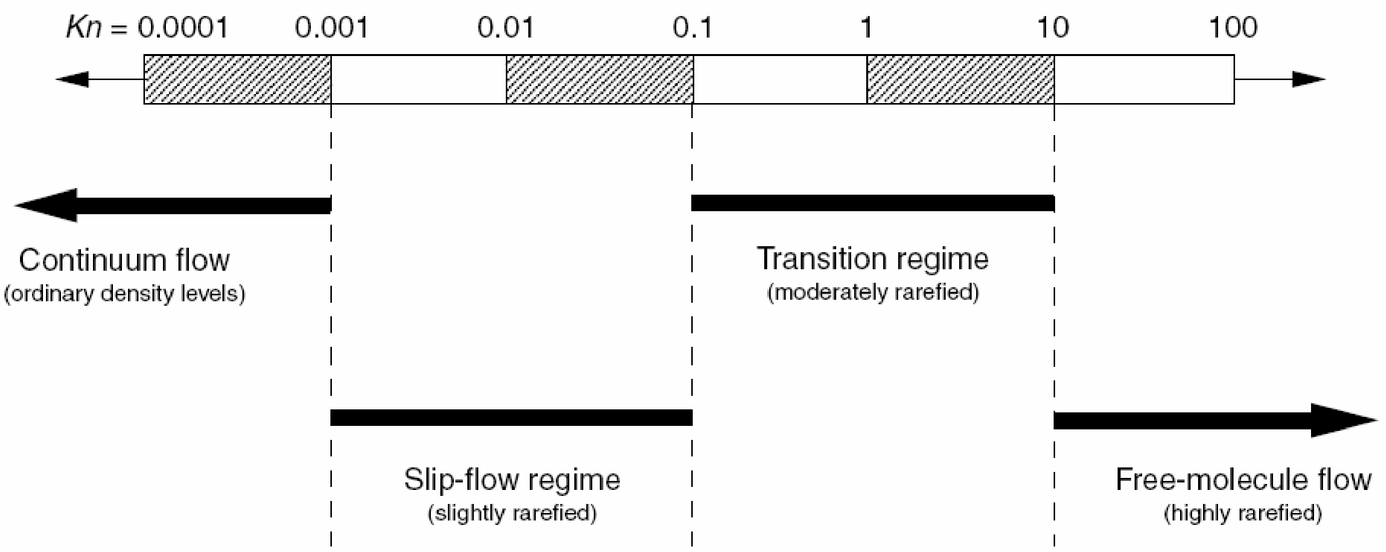
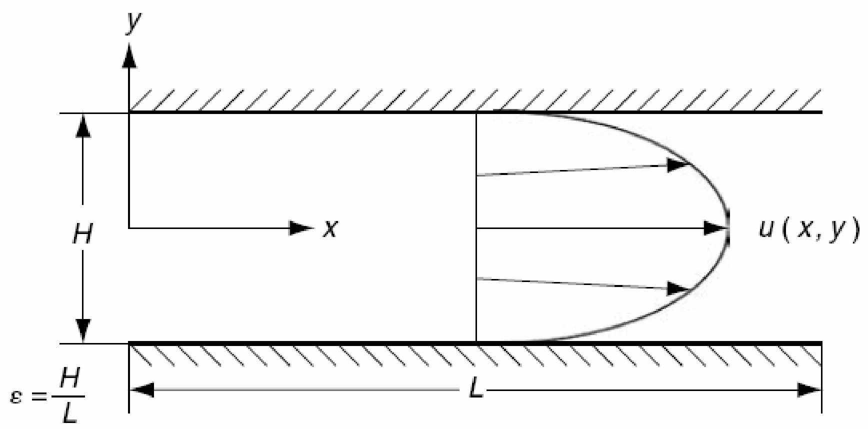


FIGURE 4.2 Knudsen number regimes.

TABLE 8.1 Flow Regimes and Fluid Models

Knudsen Number	Fluid Model
$Kn \to 0$ (continuum, no molecular diffusion)	Euler equations
$Kn \leq 10^{-3}$ (continuum with molecular diffusion)	Navier–Stokes equations with no-slip-boundary conditions
$10^{-3} \leq Kn \leq 10^{-1}$ (continuum–transition)	Navier–Stokes equations with slip-boundary conditions
$10^{-1} \leq Kn \leq 10$ (transition)	Burnett equations with slip-boundary conditions Moment equations Direct Simulation Monte Carlo (DSMC) Boltzmann equation
$Kn > 10$ (free molecular flow)	Collisionless Boltzmann equation DSMC



In a normal size we can assume that near the wall (at wall-fluid interface), velocity of fluid is zero, but due to the small size in microchannel, this assumption is not true.

To reach this fact, researchers suggest the following expression:

$$U = \left(\frac{2-\sigma_V}{\sigma_V}\right) Kn \left.\frac{\partial U}{\partial Y}\right|_{wall} + \frac{3}{2\pi}\frac{(\gamma-1)}{\gamma}\frac{Kn^2 \operatorname{Re}}{Ec}\left.\frac{\partial \theta}{\partial X}\right|_{wall}$$

$$\theta - \theta_{wall} = \left(\frac{2-\sigma_T}{\sigma_T}\right)\left(\frac{2\gamma}{\gamma+1}\right)\frac{1}{\Pr}\left[Kn\left(\left.\frac{\partial \theta}{\partial Y}\right|_{wall}\right) + \frac{Kn^2}{2!}\left(\left.\frac{\partial^2 \theta}{\partial Y^2}\right|_{wall}\right) + \ldots\right]$$

$$U=\left(\frac{2-\sigma_V}{\sigma_V}\right)Kn\left.\frac{\partial U}{\partial Y}\right|_{wall}+\frac{3}{2\pi}\frac{(\gamma-1)}{\gamma}\frac{Kn^2\,\mathrm{Re}}{Ec}\left.\frac{\partial\theta}{\partial X}\right|_{wall}$$

$$U-U_{wall}=Kn\left.\frac{\partial U}{\partial Y}\right|_{wall}$$

$$\theta-\theta_{wall}=\left(\frac{2-\sigma_T}{\sigma_T}\right)\left(\frac{2\gamma}{\gamma+1}\right)\frac{1}{\mathrm{Pr}}\left[Kn\left(\left.\frac{\partial\theta}{\partial Y}\right|_{wall}\right)+\frac{Kn^2}{2!}\left(\left.\frac{\partial^2\theta}{\partial Y^2}\right|_{wall}\right)+\ldots\right]$$

$$\theta-\theta_{wall}=\frac{Kn}{\beta}\left.\frac{\partial\theta}{\partial Y}\right|_{wall}$$

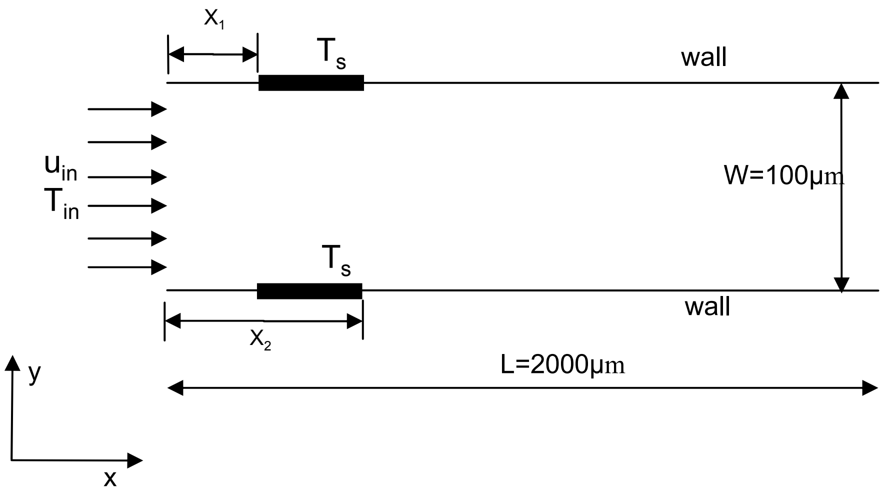
Boundary condition:

Inlet (x=0): $u=u_{in}$, v=0 and $T=T_{in}$

Outlet (x=L): $\frac{\partial \Phi}{\partial x} = 0$

where Φ =u, v, T

but p=0



At wall (y=0, y=W):

u=v=0, $x_1 \le x \le x_2: \quad T = T_s$

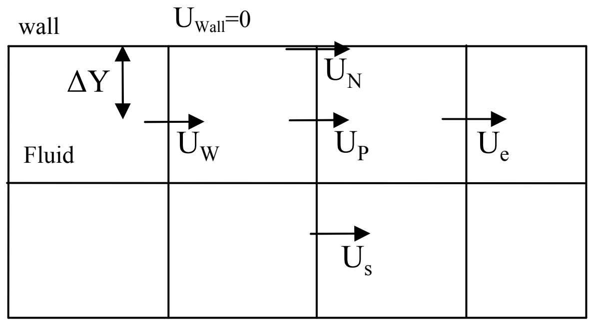
$0 \le x < x_1 \quad and \quad x_2 < x \le L: \quad T = T_0$

also: near the wall $\dot{U} - U_{wall} = Kn \frac{\partial U}{\partial Y}\Big|_{wall}$

$$\theta - \theta_{wall} = \frac{Kn}{\beta} \frac{\partial \theta}{\partial Y}\Big|_{wall} \qquad \beta = \left(\frac{\gamma + 1}{\gamma}\right) \mathrm{Pr}$$

Implementation of of Boundary slip conditions

$$U_N - U_{wall} = Kn \left.\frac{\partial U}{\partial Y}\right|_{wall}$$



$$\frac{\partial U}{\partial Y} = \frac{U_P - U_N}{\Delta Y}$$

$$U_P - U_N = \frac{(U_P - U_{wall})}{\left(1 + \frac{Kn}{\Delta Y}\right)}$$

$$a_N(U_N - U_p) + a_S(U_S - U_p) + a_E(U_E - U_p) + a_W(U_W - U_p) + b = 0$$

$$a_N^*(U_{wall} - U_p) + a_S(U_S - U_p) + a_E(U_E - U_p) + a_W(U_W - U_p) + b = 0$$

$$a_N^* = \frac{a_N}{\left(1 + \frac{Kn}{\Delta Y}\right)}$$

$$a_N^* = \frac{a_N}{\left(1 + \frac{1}{\beta}\frac{Kn}{\Delta Y}\right)}$$

Navier-Stocks Equations

Continuity: $$\frac{\partial u_j}{\partial x_j} = 0$$

Momentum: $$\frac{\partial}{\partial x_j}(\rho u_i u_j) = \frac{\partial}{\partial x_j}\left(\mu(\frac{\partial u_i}{\partial x_j})\right) - \frac{\partial p}{\partial x_i}$$

Energy: $$\frac{\partial}{\partial x_i}\left(\rho c_p u_i T\right) = k \frac{\partial}{\partial x_i}\left(\frac{\partial T}{\partial x_i}\right)$$

Non-dimensional equations

$$X_i = \frac{x_i}{D_h} \quad , \quad U_i = \frac{u_i}{u_{in}} \quad , \quad \theta = \frac{T - T_{in}}{T_{wall} - T_{in}} \quad , \quad P = \frac{p}{\rho u_{in}^2}$$

$D_h = \frac{4A}{S}$, $D_h = \frac{4WH}{2(W+H)}$ and also H >> W So: $D_h = 2W$

$$\Pr = \frac{\mu c_p}{k} \quad , \quad \mathrm{Re} = \frac{\rho u_{in} D_h}{\mu} \quad , \quad Pe = \mathrm{Re}\,\Pr$$

Continuity: $$\frac{\partial U_j}{\partial X_j} = 0$$

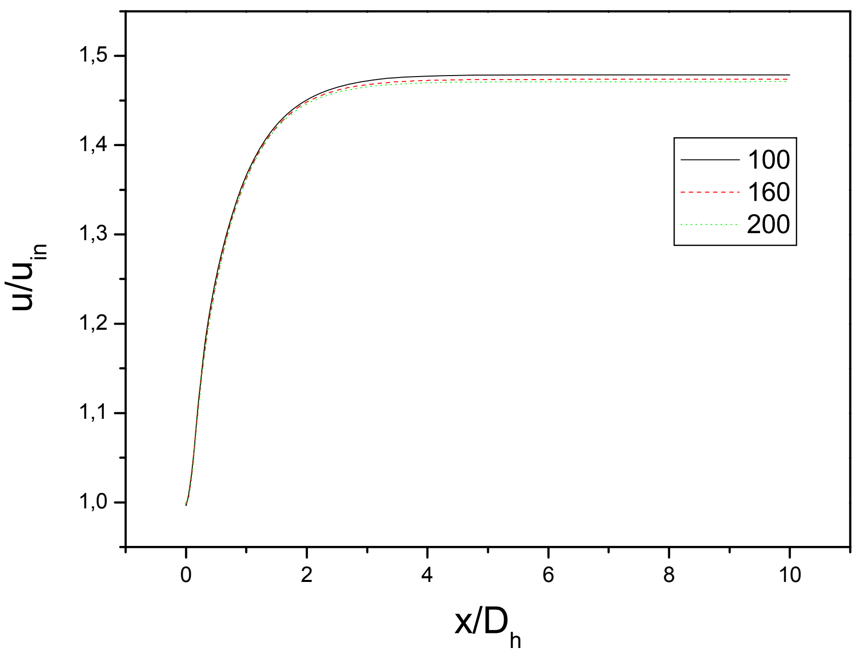
Momentum: $$\frac{\partial}{\partial X_j}(U_i U_j) = \frac{1}{\mathrm{Re}}\left(\frac{\partial^2 U_i}{\partial X_j^2}\right) - \frac{\partial P}{\partial X_i}$$

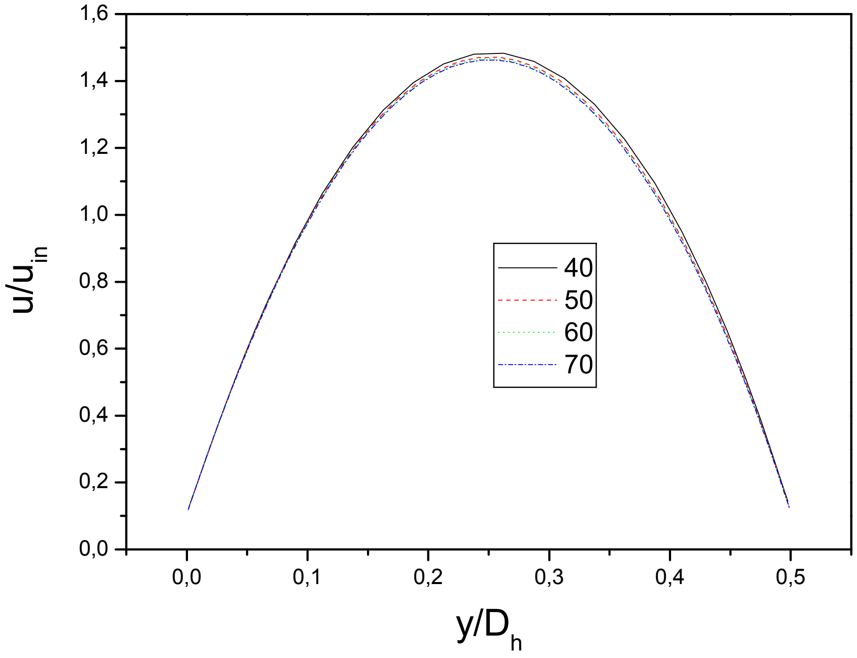
Energy: $$\frac{\partial}{\partial X_i}(U_i \theta) = \frac{1}{Pe}\frac{\partial^2 \theta}{\partial X_i}$$

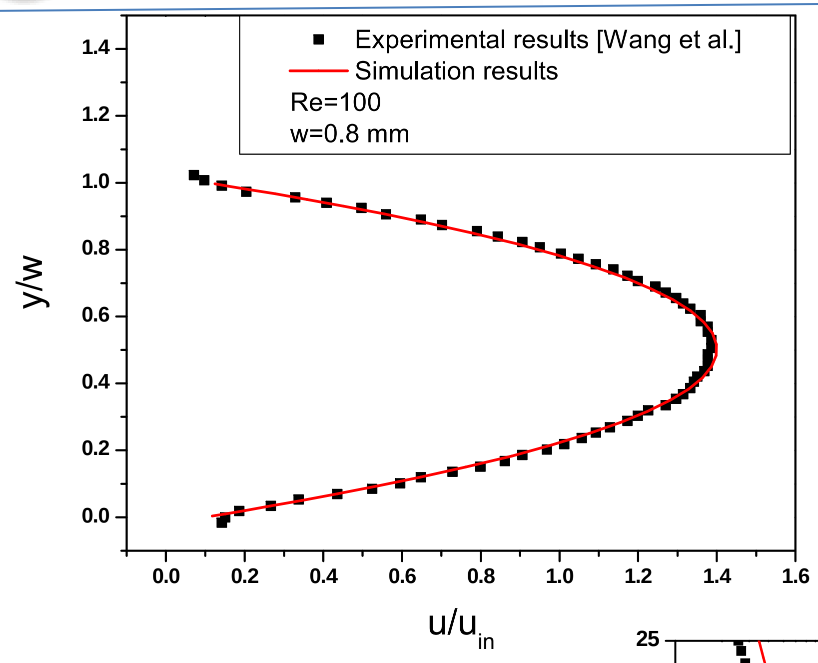
Numerical procedure

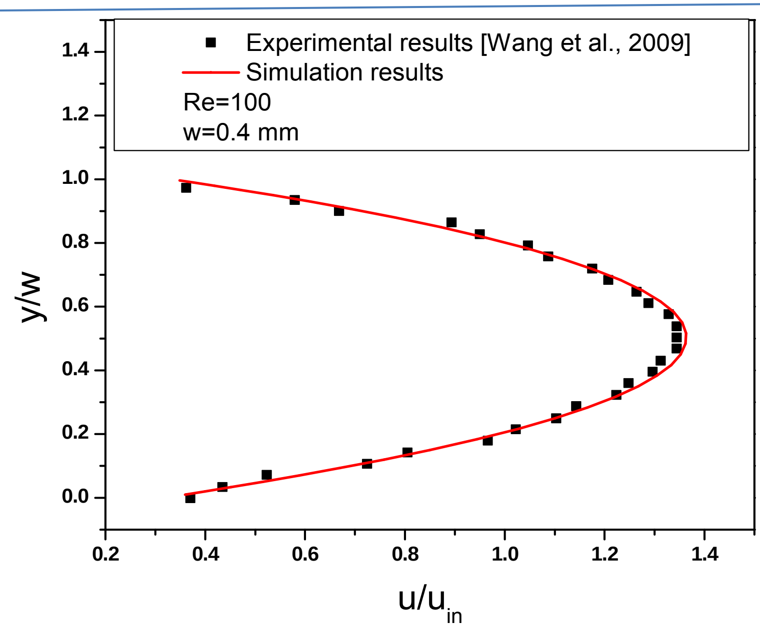
- *Control volume technique*
- *Power law scheme*
- *SIMPLER(Semi-Implicit Method for Pressure-Linked Revised Equations)*
- The discretization grid is non-uniform. It is finer near the tube entrance and near the wall where the velocity and temperature gradient are significant.

Validation and Comparison






Experimental results [Wang et al.]
Simulation results
Re=100
w=0.8 mm
y/w
u/u_in
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6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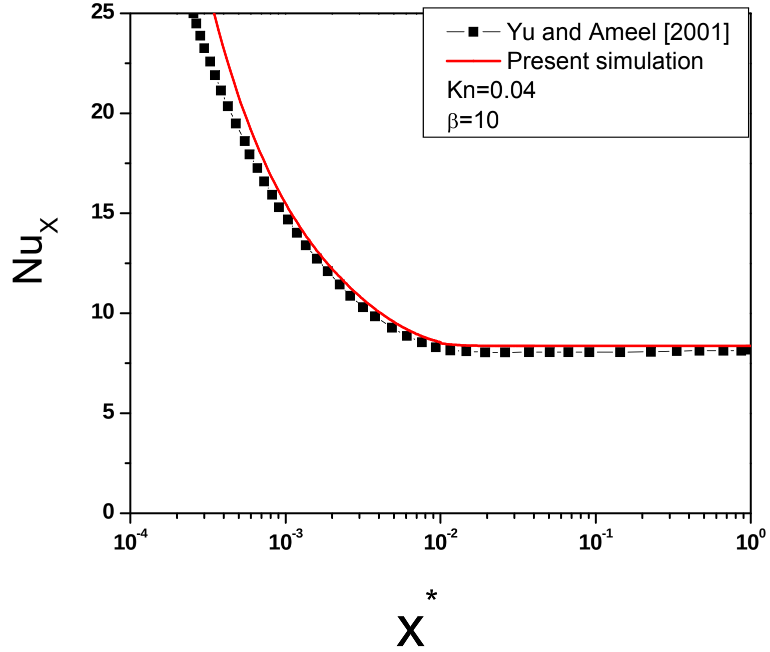
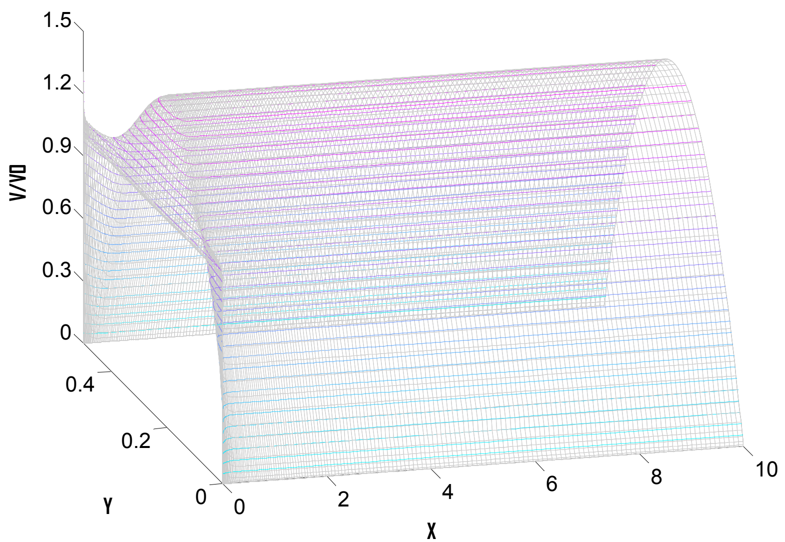
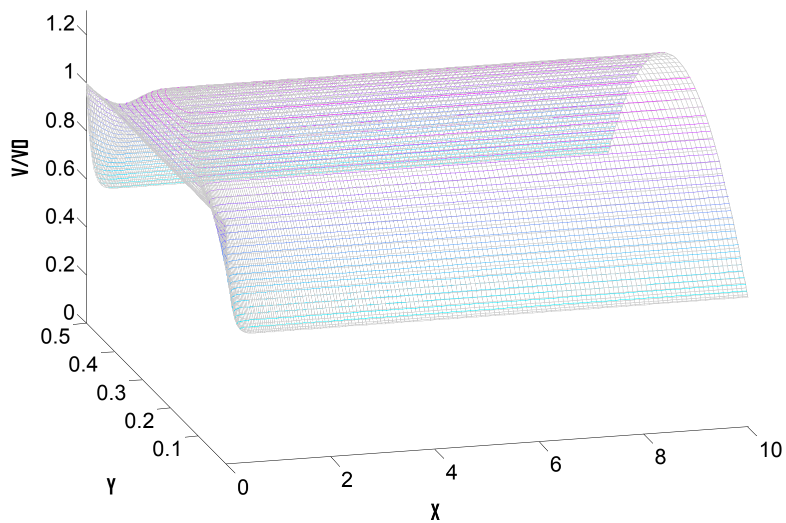

Yu and Ameel [2001]
Present simulation
Kn=0.04
β=10
Nu_X
X*
0
5
10
15
20
25
10^-4
10^-3
10^-2
10^-1
10^0

Contour of the velocity in x direction



Kn=0



Kn=0.1

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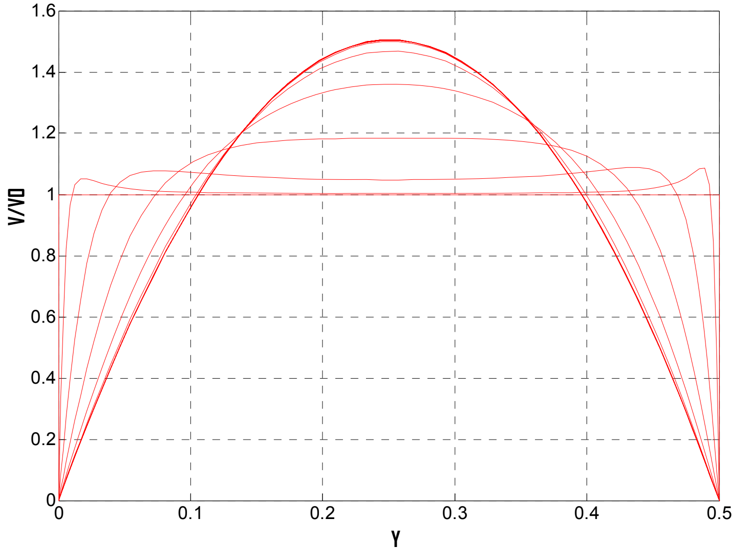
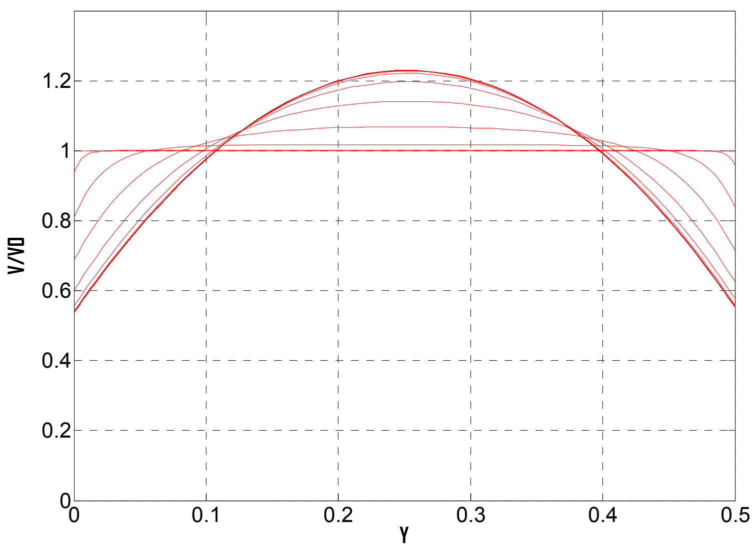


Kn=0



Kn=0.1

Thanks for your consideration