32nd Congress, Venice Italy

Ippen Lecture

Ippen's Analogy and the Development of Hydraulic Models using Boltzmann's Kinetic Theory of Gases

By Mohamed S. Ghidaoui

Department of Civil Engineering,
The Hong Kong University of Science and Technology,
Hong Kong (HKUST).

Kinetic Theory in the 20th and 21st Century

All things are made of atoms--little particles that move around in perpetual motion and gross properties of matter are a manifestations of atomic motion

Temperature, pressure, energy, momentum, density, viscosity, evaporation, surface tension, conduction, diffusion and so on are manifestations of the molecular motion.

Batchelor (1967, page 2, An Introduction to Fluid Dynamics):

The gross properties of solids, liquids and gases are directly related to their molecular structure….

Richard Feynman (1967, chapter 1, page 2, Lectures in Physics):

If, in some cataclysm, all scientific knowledge were to be destroyed, and only one sentence passed on to the next generation of creatures, what statement would contain the most information in the fewest words?

I believe it is the atomic hypothesis...that all things are made of atoms--little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another. In that sentence...there is enormous amount of information about the world, if just a little imagination and thinking are applied.

Kinetic Theory Prior to 20^{th} : Controversial!

- Proponents: **(Democritus Euler & Bernoulli, Maxwell, Boltzmann, Einstein etc.)**

➢ sought to make a hypotheses about the way atoms behave, and see if the assumed behavior can explains macroscopic (observable) properties

- Democritus School(~350 BC)

There exists a void, and in this void the atoms move about always, in motion

- Einstein

Boltzmann is quite magnificent… the question is really about the movement of atoms

- Opponents: **(Aristotle, Mach, Planck, Ostwald, etc)**

➢ unwise to hypothesize upon the existence of things you could not observe, such as molecules, in order to explain why matter behaves the way it does.

➢ research should be restricted to what can be observed and measured, and that theories should be limited to establishing relationships amongst the observed properties only.

- Aristotle School: "Denied the existence of atoms…matter is continuous and looked exactly the same at all scales."

- Mach: At a meeting of the Viennese Academy of Science in (1887), Mach shouted: "I do not believe in atoms!"

Early Efforts in Kinetic Theory

- **Euler & Bernoulli (17th contury):**

  Related pressure to the motion of molecules

- **James Waterston (a Civil Engineer, 18th century)**

  derived the correct relations between pressure, temperature and molecular speed; Derived the equi-energy principle in a mixture of gases; etc.

- Paper submitted Dec. 11th 1845; published 1892!! Long after his death.
- Reviewers: *"nothing but non-sense"; "the whole investigation is confessedly founded on a principle entirely hypothetical….it exhibits many remarkable accordances with facts… [but the assumptions cannot be rigorously justified]*

- Lord Rayleigh: *"The omission to publish it at the time was a misfortune, which probably retarded the subject by ten or fifteen years."*

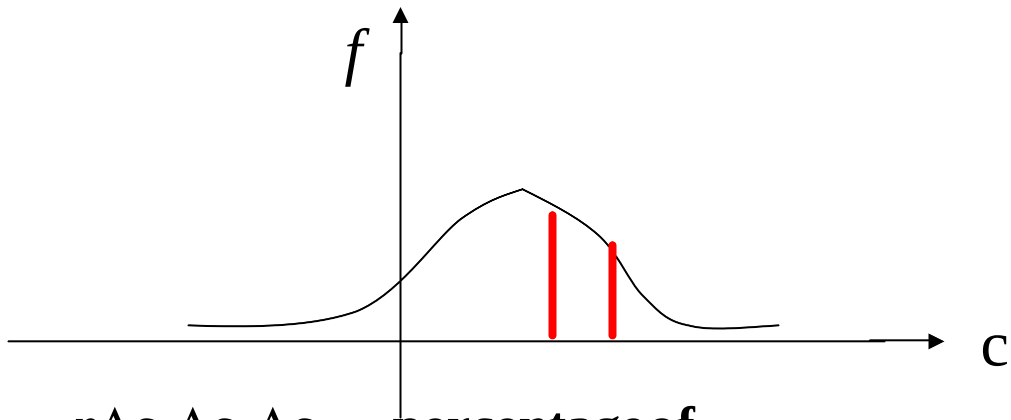
  "a young author who believes himself capable of great things would usually do well to secure the favorable recognition of the scientific world by work whose scope is limited, and whose value is easily judged, before embarking on greater flights"

<u>Equilibrium</u> Kinetic Theory: Maxwell's Probabilistic Approach (~1860)

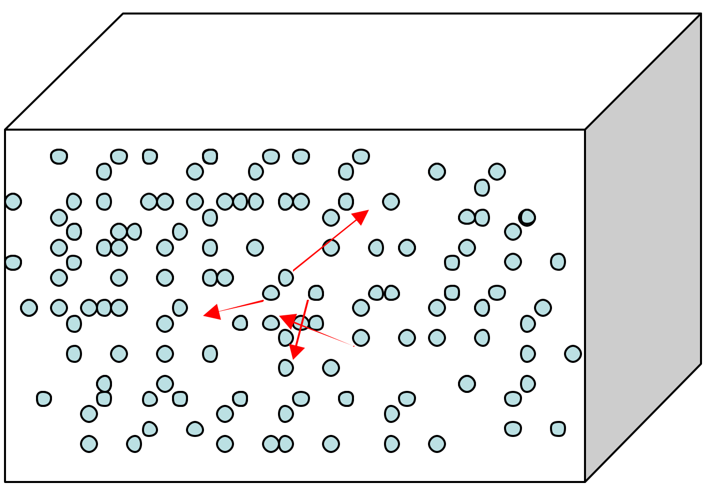
(i) The distribution of velocities in x, y and z are the same; (ii) the distribution depends on the magnitude of particle velocity only

$$p = \left(\frac{m}{2pkT}\right)^{3/2} e^{-\frac{c_x^2 + c_y^2 + c_z^2}{\frac{2kT}{m}}}$$

$$q = rp = r\left(\frac{m}{2pkT}\right)^{3/2} e^{-\frac{c_x^2 + c_y^2 + c_z^2}{\frac{2kT}{m}}}$$



$p\Delta c_x \Delta c_y \Delta c_y$ = **percentage of particles with speeds between c_x and $c_x + ?\, c_x$; c_y and $c_y + ?\, c_y$; c_z and $c_z + ?\, c_z$**

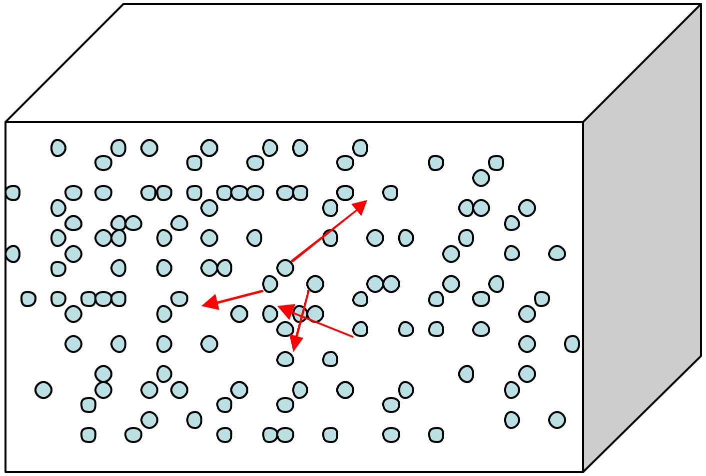


$q\Delta c_x \Delta c_y \Delta c_y \times \forall$ = **Mass of particles in volume ($\forall$) with speeds between c_x and $c_x + ?\, c_x$; c_y and $c_y + ?\, c_y$; c_z and $c_z + ?\, c_z$**

Kinetic Theory and its Relation to Gross Properties

$$\iiint_{R^3} p\,dc_x dc_y dc_z = 1$$

$$\iiint_{R^3} \underbrace{r p}_{q}\,dc_x dc_y dc_z = r$$



Momentum:

$$\iiint_{R^3} c_x q\,dc_x dc_y dc_z = 0; \quad \iiint_{R^3} c_y q\,dc_x dc_y dc_z = 0;$$

$$\iiint_{R^3} c_z q\,dc_x dc_y dc_z = 0;$$

Pressure/Shear:

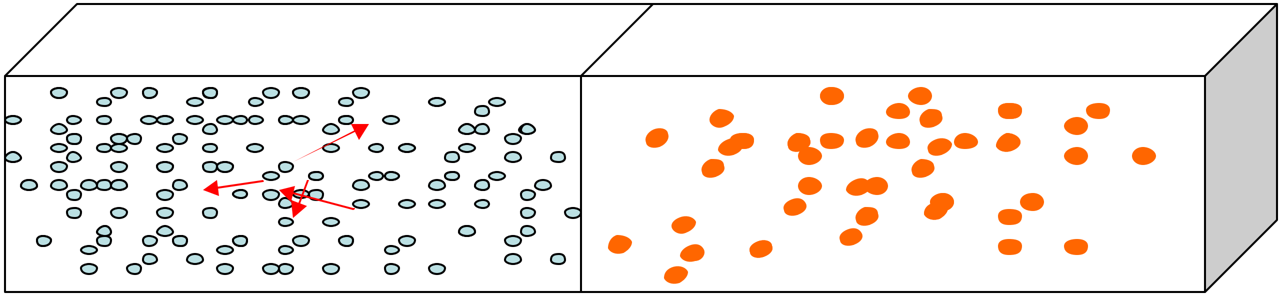
$$p = \iiint_{R^3} \frac{c_x^{\;2} + c_y^{\;2} + c_z^{\;2}}{3} q\,dc_x dc_y dc_z = r\frac{kT}{m} = rRT \qquad t_{xy} = \iiint_{R^3} c_x c_y q\,dc_x dc_y dc_z = 0$$

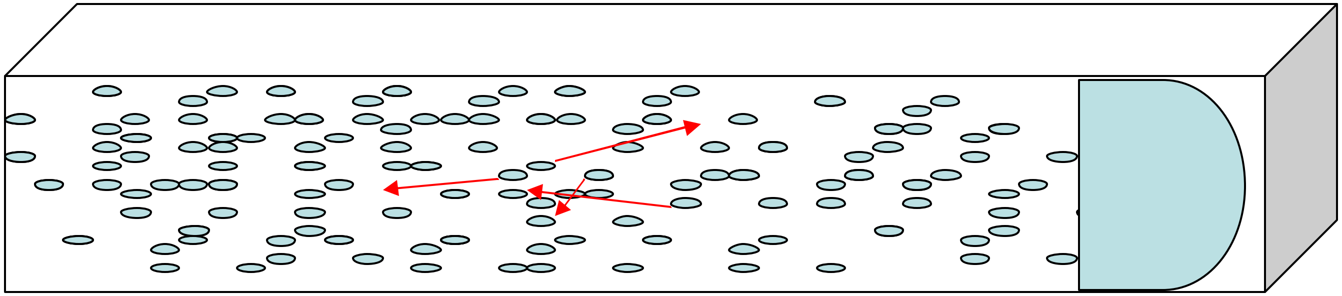
Energy:

$$e = \iiint_{R^3} \frac{c_x^{\;2} + c_y^{\;2} + c_z^{\;2}}{2} q\,dc_x dc_y dc_z = \frac{3}{2} rRT$$

Non-Equilibrium Kinetic Theory: Boltzmann (~1870)

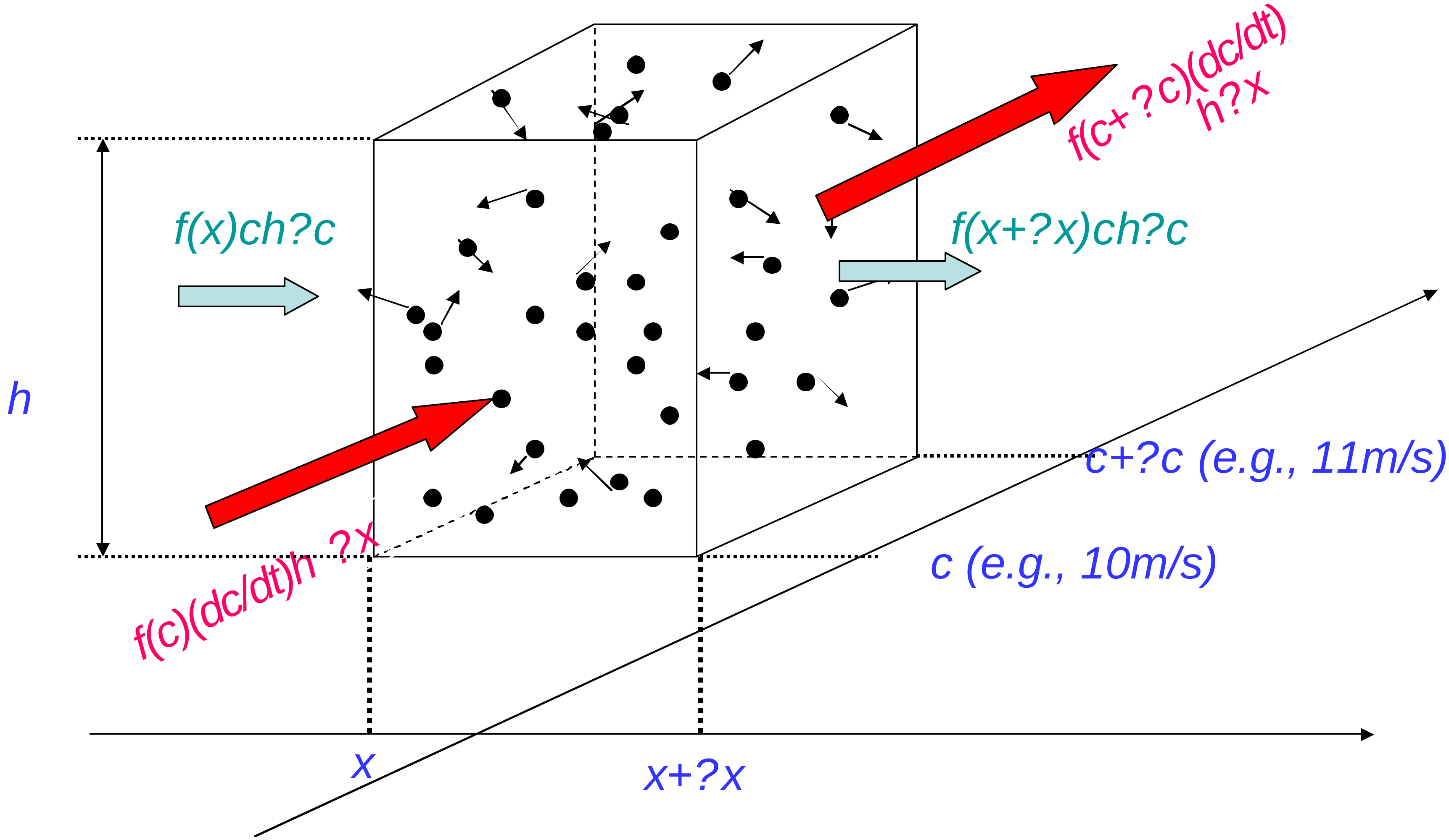
- Some or all macroscopic gradients of properties (pressure, velocity, temperature etc) are non-zero





C.V.: contains particles located between x and x+?x and

possessing speeds between c and x+?c



$$\frac{\partial f}{\partial t} = -c\frac{\partial f}{\partial x} - \frac{dc}{dt}\frac{\partial f}{\partial c} + C(f) = -c\frac{\partial f}{\partial x} - \frac{F}{m}\frac{\partial f}{\partial c} + \frac{q-f}{t}$$

Boltzmann and the NS

$$\frac{\partial f}{\partial t}+c_i\frac{\partial f}{\partial x_i}+\frac{F_i}{m}\frac{\partial f}{\partial c_i}=\frac{q-f}{t}$$

Continuity (Zero-th Moment);

let $\quad d\mathbf{c}=dc_x dc_y dc_z$

$$\iiint\left(\frac{\partial f}{\partial t}+c_i\frac{\partial f}{\partial x_i}+\frac{F_i}{m}\frac{\partial f}{\partial c_i}\right)d\mathbf{c}=\iiint\frac{q-f}{t}d\mathbf{c}$$

:

$$\frac{\partial}{\partial t}\underbrace{\iiint f d\mathbf{c}}_{r}+\frac{\partial}{\partial x_i}\underbrace{\iiint c_i f d\mathbf{c}}_{r u_i}+0=0$$

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

Momentum (First Moment):

$$\iiint c_i\left(\frac{\partial f}{\partial t}+c_j\frac{\partial f}{\partial x_j}+\frac{F_j}{m}\frac{\partial f}{\partial c_j}\right)d\mathbf{c}=\iiint c_i\frac{q-f}{t}d\mathbf{c}$$

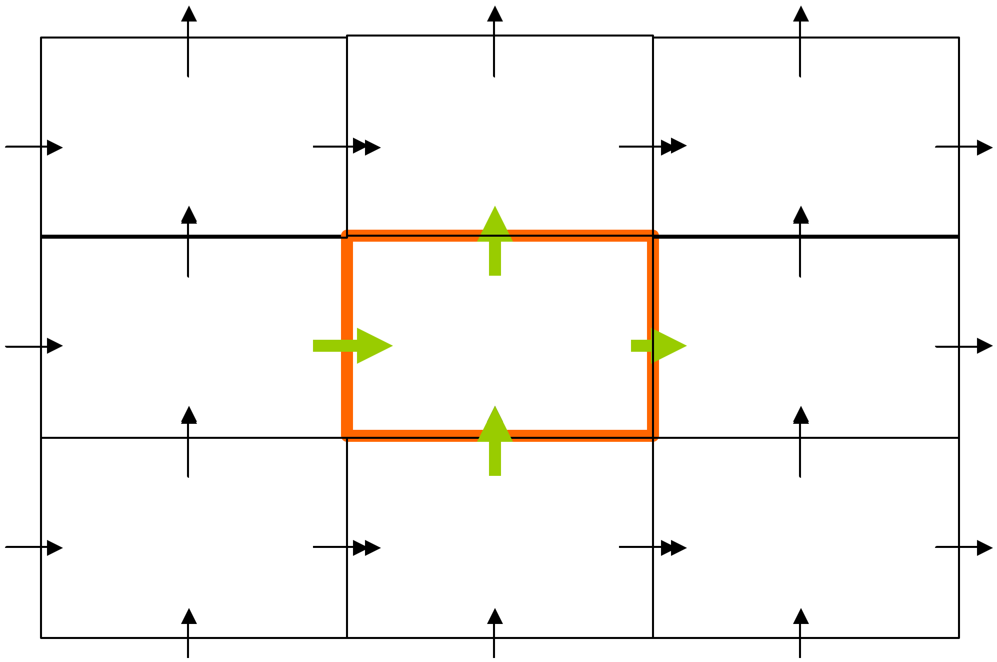
$$\underbrace{\frac{\partial}{\partial t}\iiint c_i f d\mathbf{c}}+\underbrace{\frac{\partial}{\partial x_i}\iiint c_j c_i f d\mathbf{c}}-rF_i=0$$

$$\Rightarrow\overbrace{\frac{\partial r u_i}{\partial t}}+\overbrace{\frac{\partial r u_i u_j}{\partial x_j}+\frac{\partial p}{\partial x_i}-\frac{\partial s_{ij}}{\partial x_j}}-rF_i=0$$

Newtonian viscous stresses are recovered when

$$t=\frac{vr}{p}$$

Boltzmann Based Schemes & the Finite Volume Approach



$$\text{State}(t+\Delta t) - \text{State}(t) = \sum \text{Fluxes during } \Delta t + \sum \text{Sources/sinks during } \Delta t$$

Classical:

- Characteristic Decomposition,
- Waves and diffusion are treated separate,

Boltzmann:

- Particle motion (NO Characteristic Decomposition),
- Flux contains both waves and diffusion (no splitting),

Applications

- Shocks around wings; boundary layers; flow separation etc. (e.g., Aerospace applications).
- Multiphase, multi-components flows
- Flows in complex geometry
- Turbulence
- Problems where the NS are not valid: rarefied gases; very thin shocks; flow in nano and micro-channels

Can the Boltzmann Gas Kinetic model be used for shallow flows? Ippen's analogy!

AF TECHNICAL REPORT No. 5985 May 1950
(Revised Jan. 1951)

STUDIES ON THE VALIDITY OF THE HYDRAULIC

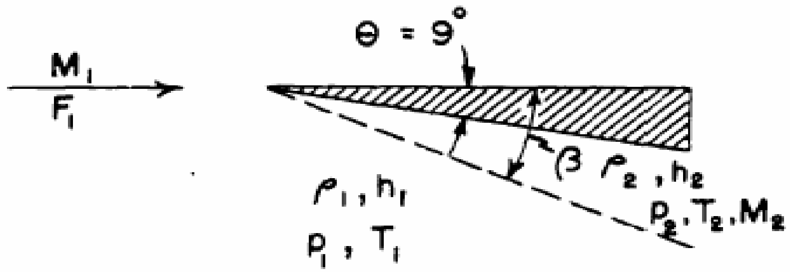
ANALOGY TO SUPERSONIC FLOW

Parts I and II

Summary of Gas-Water Flow Direct Analogy

GAS FLOW	WATER FLOW
Speed of propagation of sound wave $a = \sqrt{\gamma p/\rho}$	Speed of propagation of small gravity wave $c = \sqrt{gh}$
Mach number, $M = \dfrac{V}{\sqrt{\gamma p/\rho}}$	Froude number, $F = \dfrac{V}{\sqrt{gh}}$
Density ratio, ρ_2/ρ_1	Depth ratio, h_2/h_1
Pressure ratio, p_2/p_1	(Depth ratio)^2, $(h_2/h_1)^2$
Temperature ratio, T_2/T_1	Depth ratio, h_2/h_1

Ippen's 1st Modification



Density ratio, ρ_2/ρ_1	Depth ratio, h_2/h_1
Pressure ratio, p_2/p_1	(Depth ratio)^2, $(h_2/h_1)^2$
Temperature ratio, T_2/T_1	Depth ratio, h_2/h_1

Hydraulic theory

$M_1 = 2.50$

Initial Mach No. = 2.5 = Initial Froude No. $\Theta = 9°$

Method of Analysis	Wave Angle β	h_2/h_1	ρ_2/ρ_1	p_2/p_1 Eq(19a)	T_2/T_1 Eq(18)	M_2/M_1 Eq(52b)
Aerodynamic Theory	30°54'	—	1.489	1.759	1.181	0.852
Direct Hydraulic Analogy	32°30'	1.465	1.465 (-1.6%)	2.146 (+22.0%)	1.465 (+24.0%)	0.753 (-11.6%)
First Modification Hyd. Analogy	32°30'	1.465	1.465 (-1.6%)	1.718 (-2.3%)	1.173 (-0.7%)	0.858 (+0.8%)

1. Equate depth ratio to density ratio

2. Calculate from gas theory

Ippen's 2nd Modification

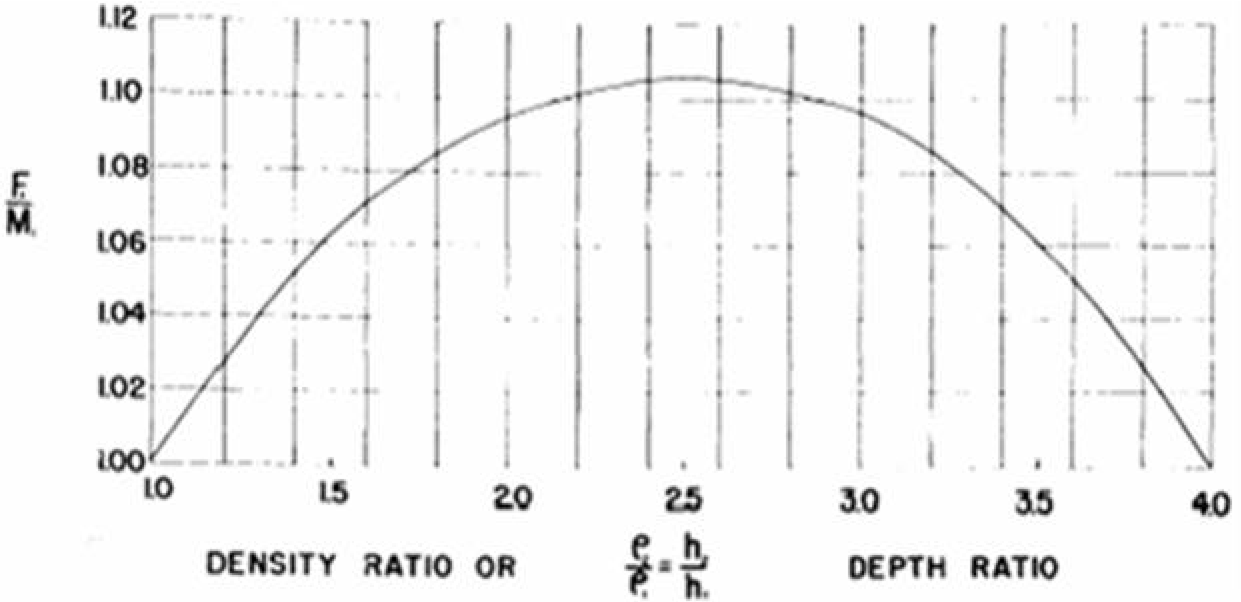
$$\frac{\rho_2}{\rho_1} = \frac{\tan\beta}{\tan(\beta-\theta)} = \frac{h_2}{h_1}$$

$$F_1 \sin\beta_1 = \sqrt{\frac{h_2}{h_1}\cdot\frac{1}{2}\left(1+\frac{h_2}{h_1}\right)} \qquad (34b)$$

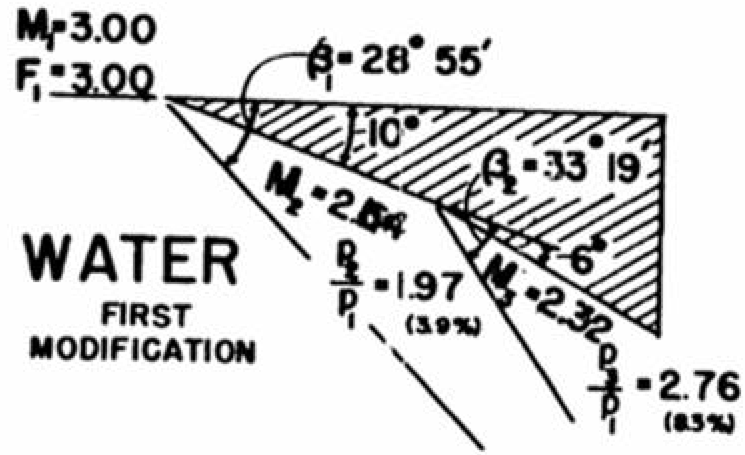
$$M_1 \sin\beta_1 = \sqrt{\frac{\rho_2}{\rho_1}\left(\frac{5}{6-\rho_2/\rho_1}\right)} \qquad (47b)$$

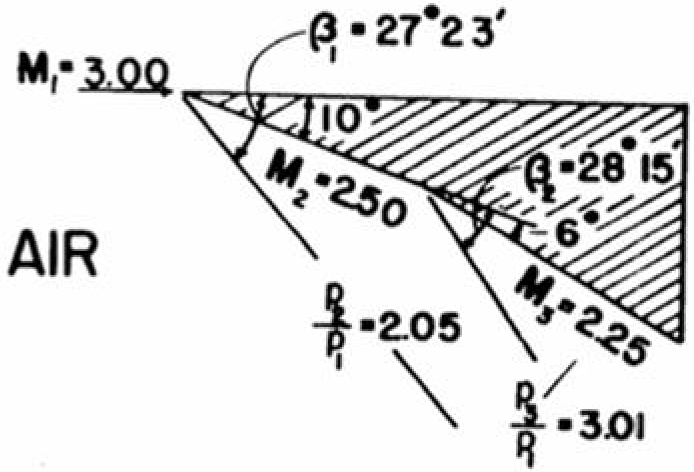
For similar geometry of flow, $h_2/h_1 = \rho_2/\rho_1$. If Eq. (34b) is divided by Eq. (47b):

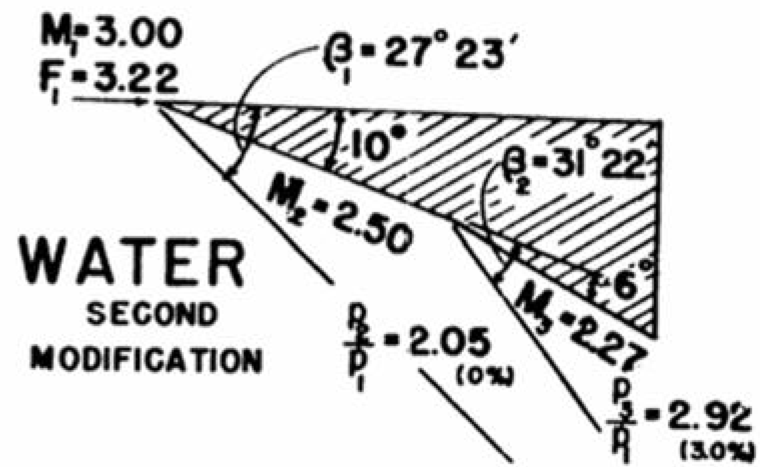
$$\frac{F_1}{M_1} = \sqrt{\frac{(1+\rho_2/\rho_1)(6-\rho_2/\rho_1)}{10}} \qquad (56)$$



note: pressure ratios obtained from water analysis are calculated from eq. (19a) where $\frac{h_2}{h_1} = \frac{\rho_2}{\rho_1}$ and $\gamma = 1.40$
local Mach Numbers are calculated from eq. (52b)

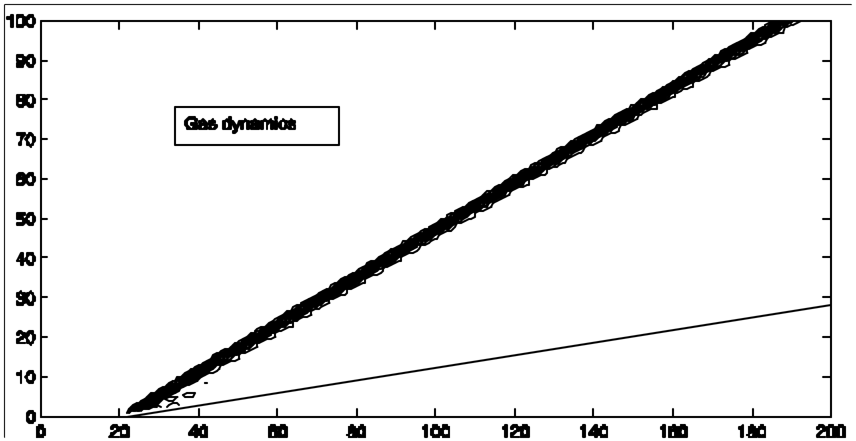


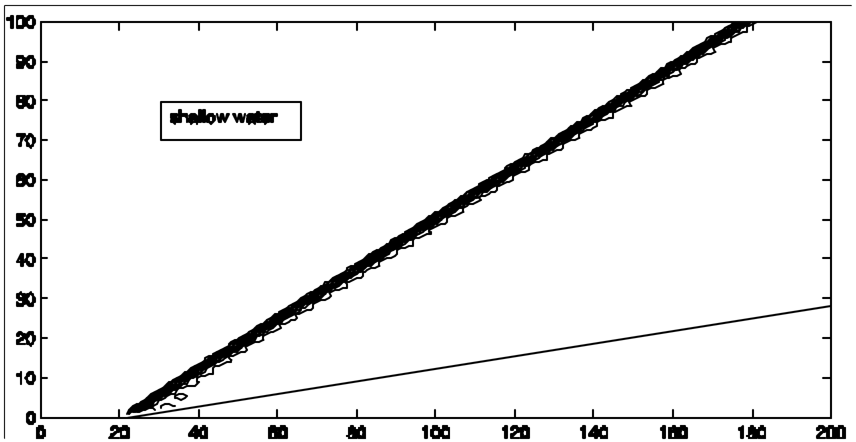




THEORETICAL COMPARISON OF MODIFIED ANALOGY FOR SUCCESSIVE SHOCKS

Ippen's Analogy and Bolzmann Gas model for hydraulics (example 1: M=Fr=2.5)





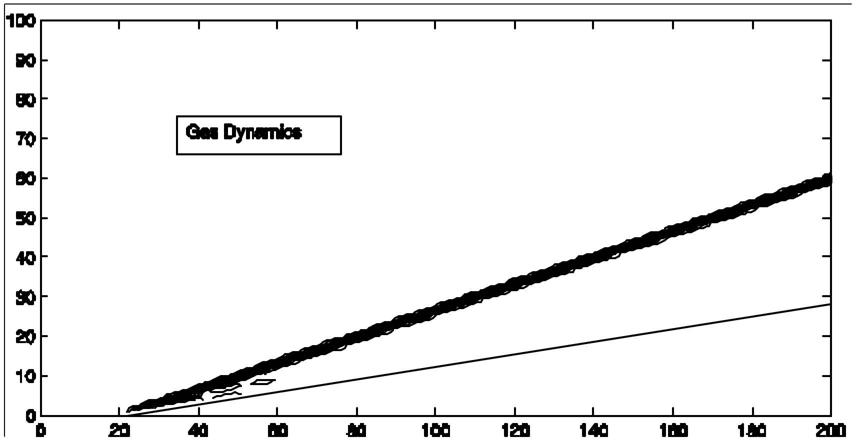
$$\textbf{Boltzmann gas Model:}\ M = 2.5 \Rightarrow \frac{r_2}{r_1} = 1.489;\ b = 30^{\circ}54$$

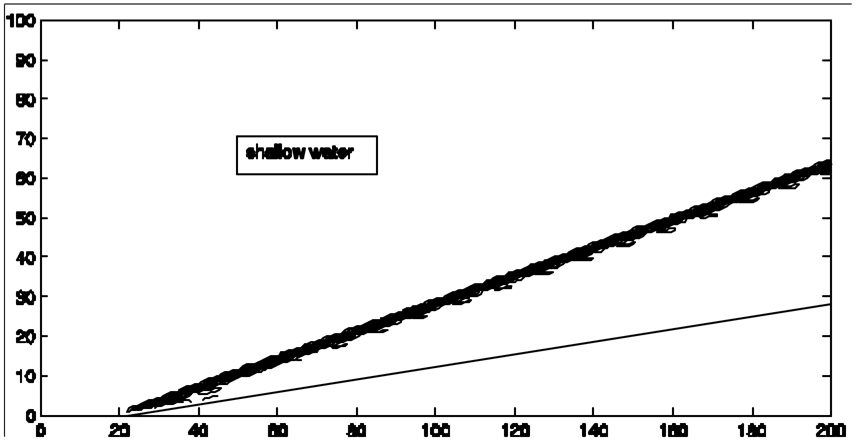
$$\textbf{Hydraulic Theory:}\ F_r = 2.5 \Rightarrow \frac{h_2}{h_1} = 1.465;\ b = 32^{\circ}30$$

Applying Ippen's 2 modifications to Boltzmann Model:

$$\frac{r_2}{r_1} = 1.465 = \frac{h_2}{h_1};\ b_{gas} = 32^{\circ}30 = b_{water};\ \ M = 2.36$$

Ippen's Analogy and Bolzmann Gas model for hydraulics (Example 2: M=Fr=5)





$$\textbf{Boltzmann gas Model}: M = 5 \Rightarrow \frac{r_2}{r_1} = 2.0045;\ b = 18^\circ 36'$$

$$\textbf{Hydraulic Theory}: F_r = 5 \Rightarrow \frac{h_2}{h_1} = 1.911;\ b = 19^\circ 35$$

Applying Ippen's 2 modifications to Boltzmann Model:

$$\frac{r_2}{r_1} = 1.9115 \cong \frac{h_2}{h_1};\ b_{gas} = 19^\circ 35 = b_{water};\ \ M = 4.6$$

Ippen's analogy and the linkage between Boltzmann Gas model and hydraulics

$$q = r\left(\frac{r}{2pp}\right)e^{-\frac{c_x{}^2+c_y{}^2+c_z{}^2}{\frac{2p}{r}}}$$

$$\frac{\partial f}{\partial t} + c_i\frac{\partial f}{\partial x_i} + \frac{F_i}{m}\frac{\partial f}{\partial c_i} = \frac{q-f}{t}$$

$$r \Rightarrow h$$

$$p \Rightarrow \frac{gh^2}{2}$$

$$q = h\left(\frac{h}{2p\frac{gh^2}{2}}\right)e^{-\frac{c_x{}^2+c_y{}^2}{\frac{2\frac{gh^2}{2}}{h}}} = \frac{1}{gp}e^{-\frac{c_x{}^2+c_y{}^2}{gh}}$$

$$\frac{\partial f}{\partial t} + c_i\frac{\partial f}{\partial x_i} + \frac{F_i}{m}\frac{\partial f}{\partial c_i} = \frac{q-f}{t}$$

Continuity (Zero-th Moment)

$$\iiint\left(\frac{\partial f}{\partial t} + c_i\frac{\partial f}{\partial x_i} + \frac{F_i}{m}\frac{\partial f}{\partial c_i}\right)d\mathbf{c} = \iiint\frac{q-f}{t}d\mathbf{c} \qquad \Rightarrow \frac{\partial h}{\partial t} + \frac{\partial hu_i}{\partial x_i} = 0$$

Momentum (First Moment)

$$\iiint c_i\left(\frac{\partial f}{\partial t} + c_j\frac{\partial f}{\partial x_j} + \frac{F_j}{m}\frac{\partial f}{\partial c_j}\right)d\mathbf{c} = \iiint c_i\frac{q-f}{t}d\mathbf{c} \Rightarrow \frac{\partial hu_i}{\partial t} + \frac{\partial hu_iu_j}{\partial x_j} + \frac{\partial gh^2/2}{\partial x_i} - \frac{\partial s_{ij}}{\partial x_j} - rF_i = 0$$

$$t = \frac{vr}{p} \Rightarrow t = \frac{vh}{gh^2/2} = \frac{v}{gh}$$

Does the model handle waves? How well?

Does the model handle viscous/turbulent flows? How well?

Su, Xu, Ghidaoui (1999). ***Journal of Computational Physics***

Ghidaoui, *Deng,* Xu, Gray, (2001). ***International Journal for Numerical Methods in Fluids.***

Deng, Ghidaoui, Gray, Xu (2001). ***Advances In Water Resources.***

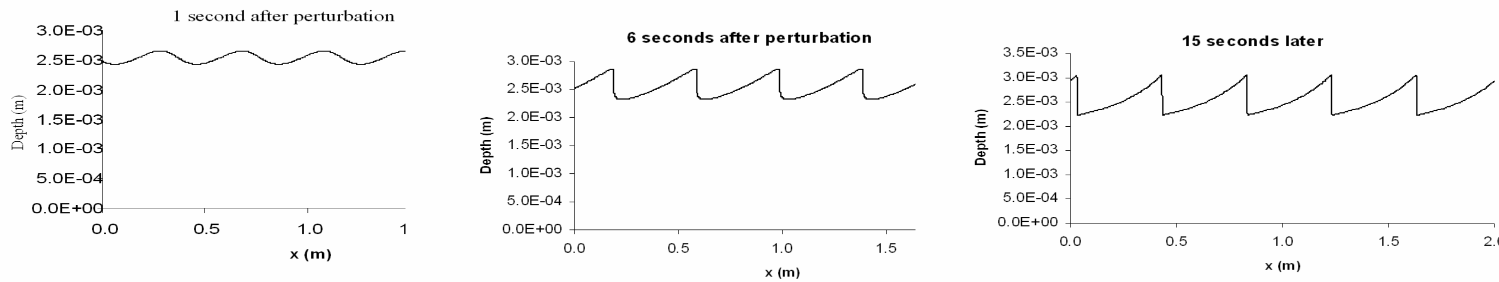
Zhang, Ghidaoui, Gray, *Li,* (2003), ***Advances In Water Resources***.

Ghidaoui, *Li Nanzhou* (2003). ***Journal of Hydroinformatics.***

Liang, Ghidaoui, *Deng*, Gray (2006), ***Journal of Hydraulic Research, IAHR.***

Does the BGK handle waves? How well?

Roll Waves (Fr=2.01)



Tidal Bore in Qiantang River

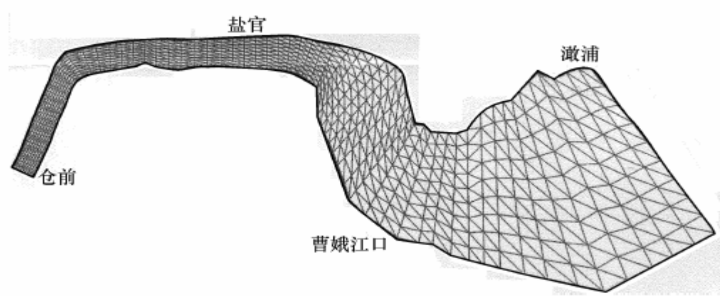
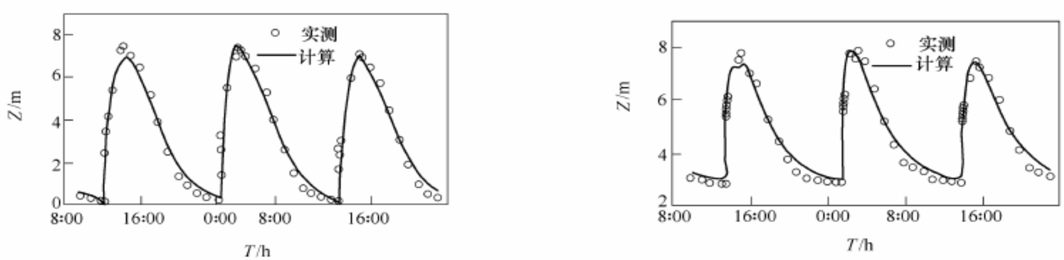
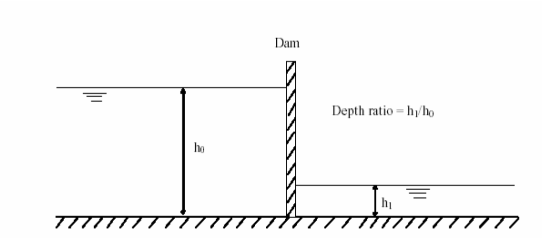
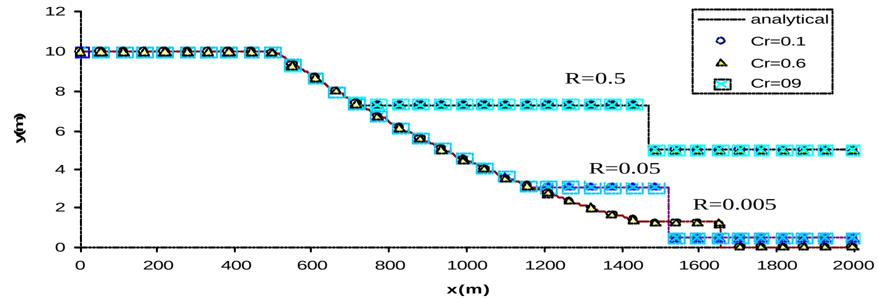


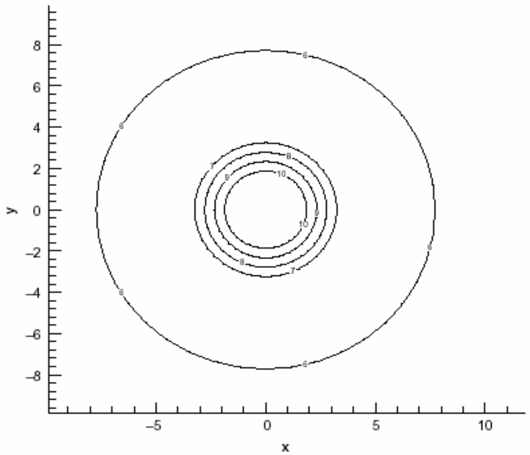
图 4 钱塘江计算网格

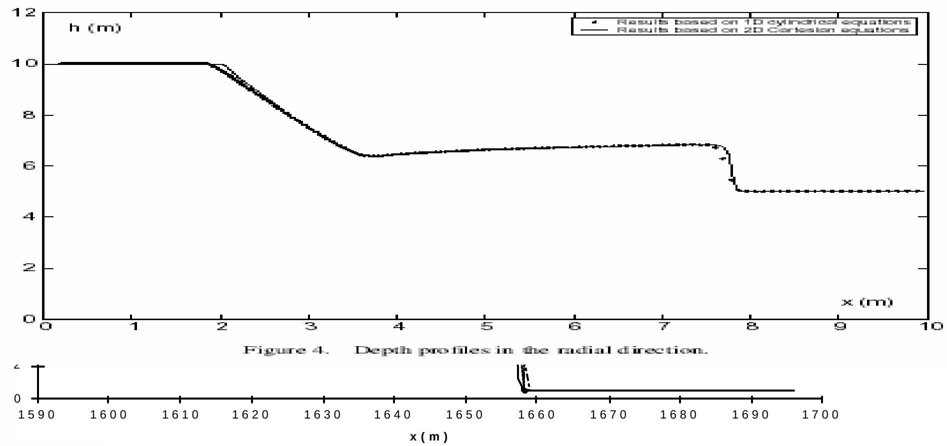


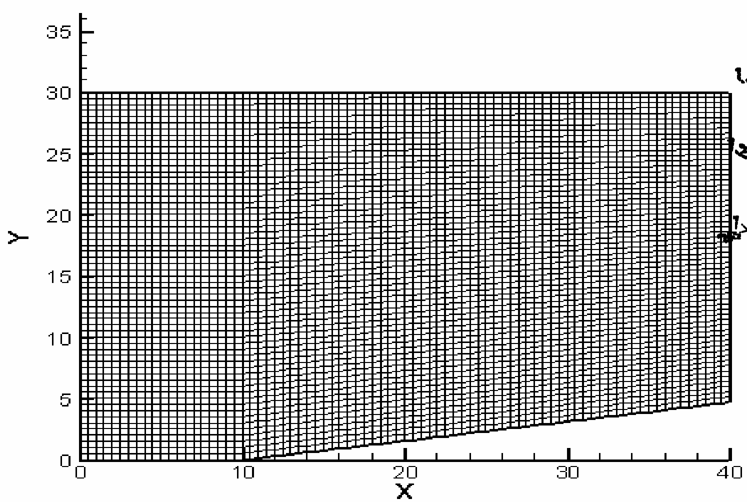
Shock & Expansion Waves

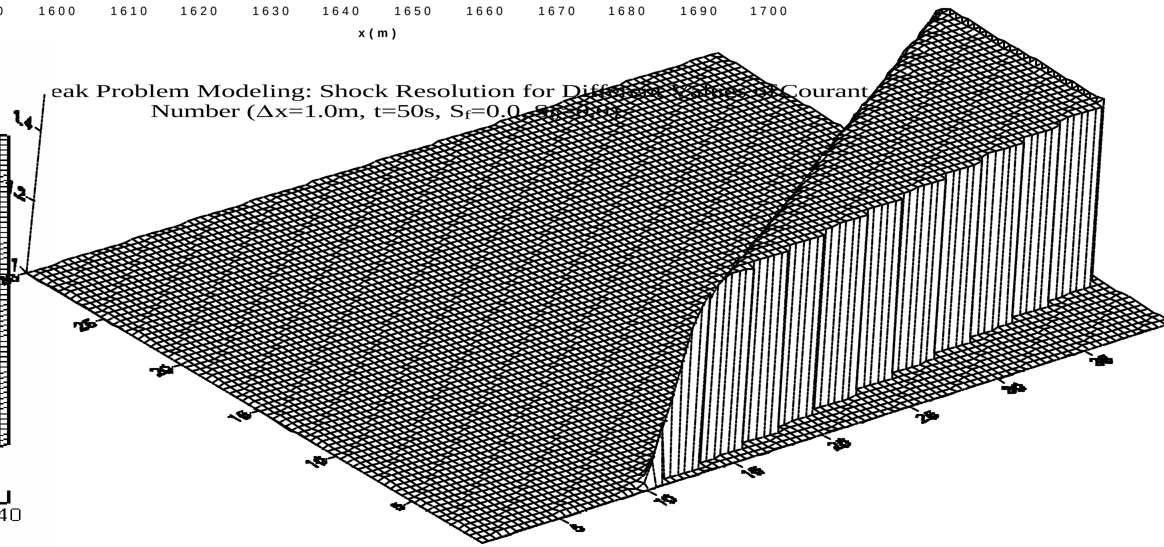


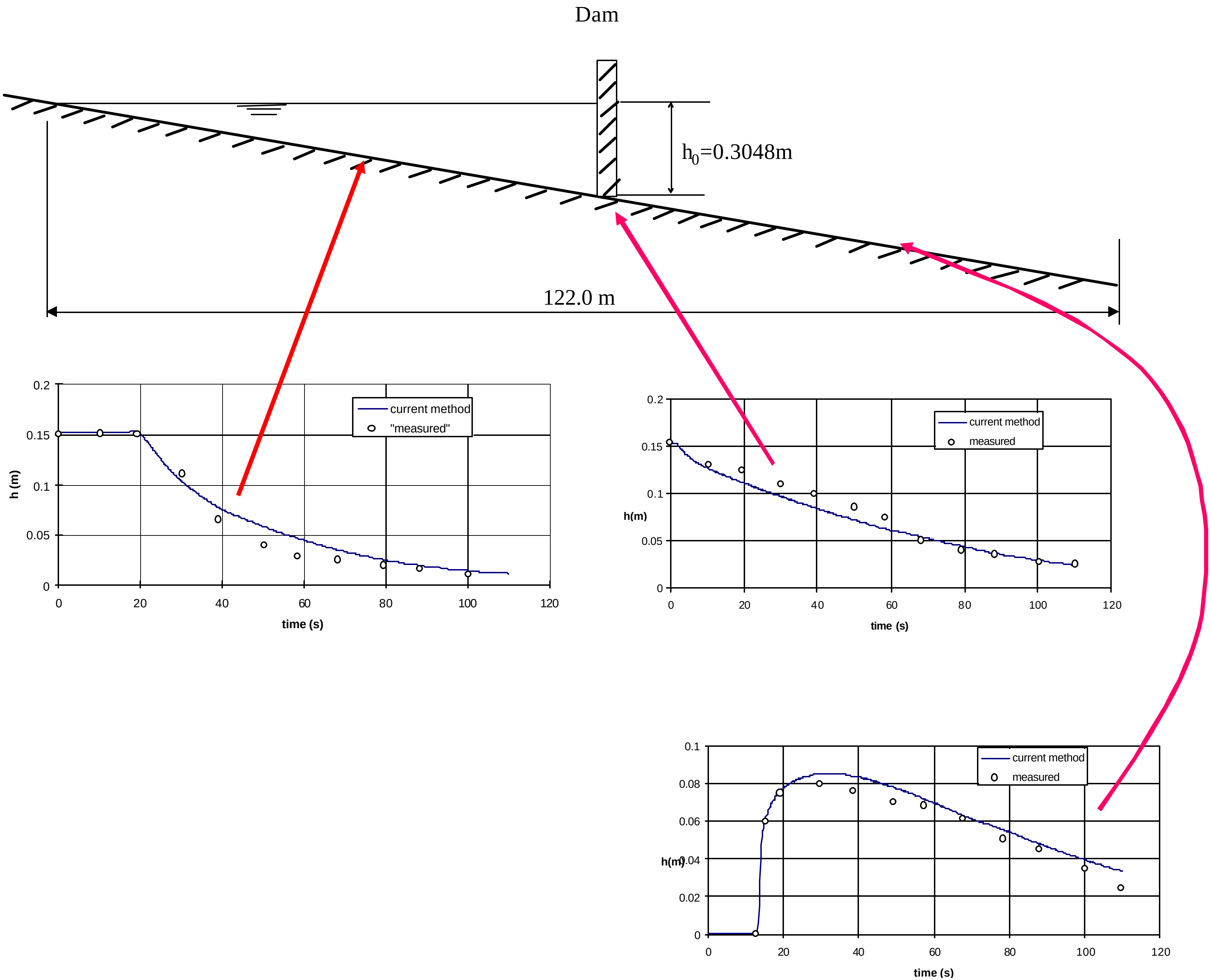






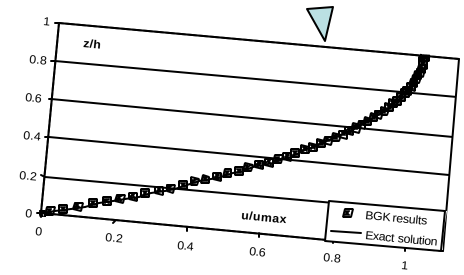


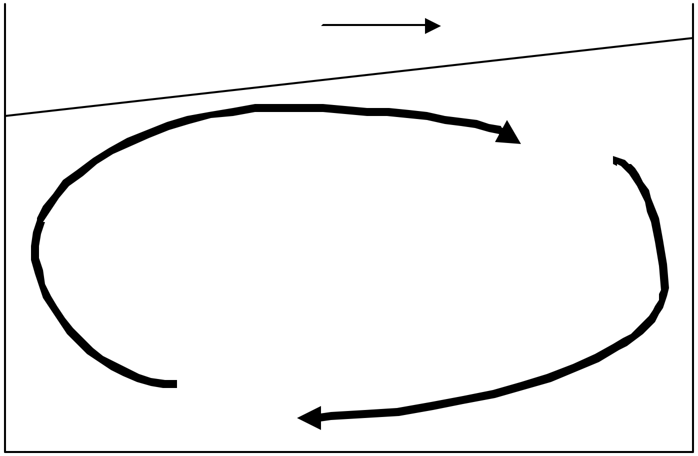


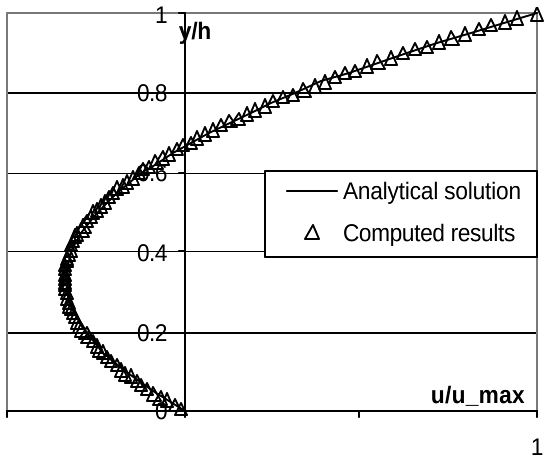


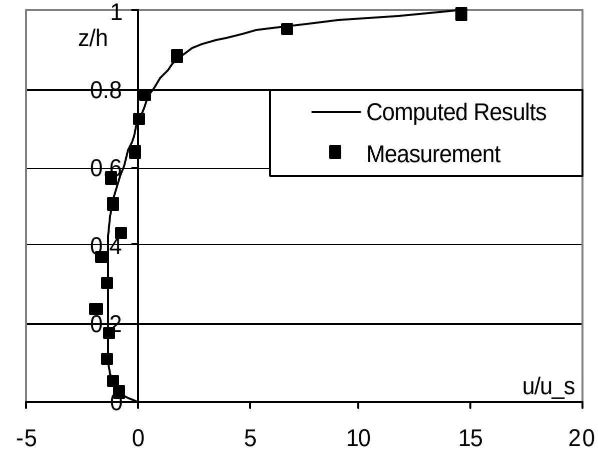
Dam
h0=0.3048m
122.0 m
h (m)
time (s)
current method
"measured"
0
0.05
0.1
0.15
0.2
0
20
40
60
80
100
120
h(m)
time (s)
current method
measured
0
0.05
0.1
0.15
0.2
0
20
40
60
80
100
120
h(m)
time (s)
current method
measured
0
0.02
0.04
0.06
0.08
0.1
0
20
40
60
80
100
120

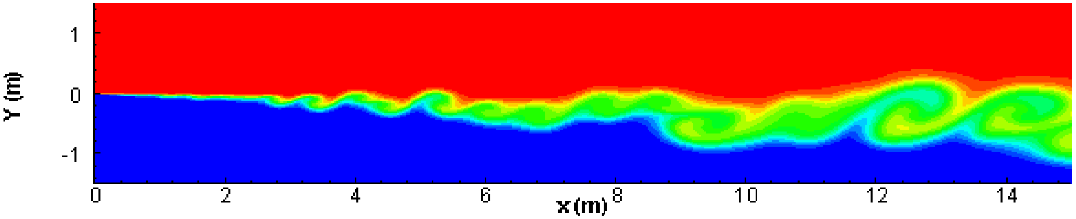
Does the BGK solve viscous/turbulent flows? How well?

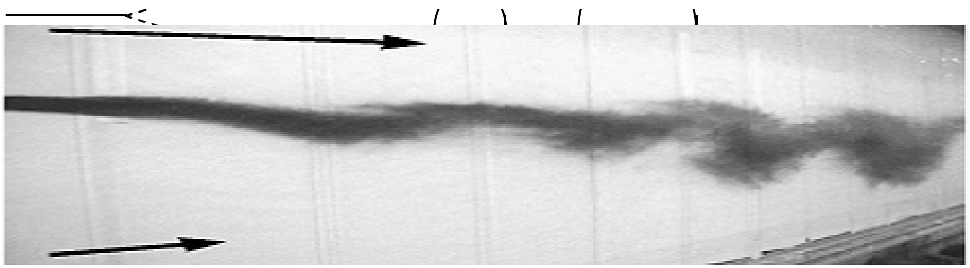




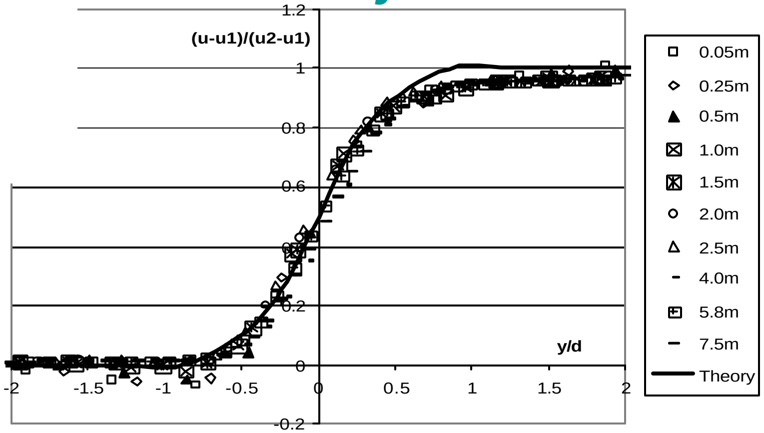


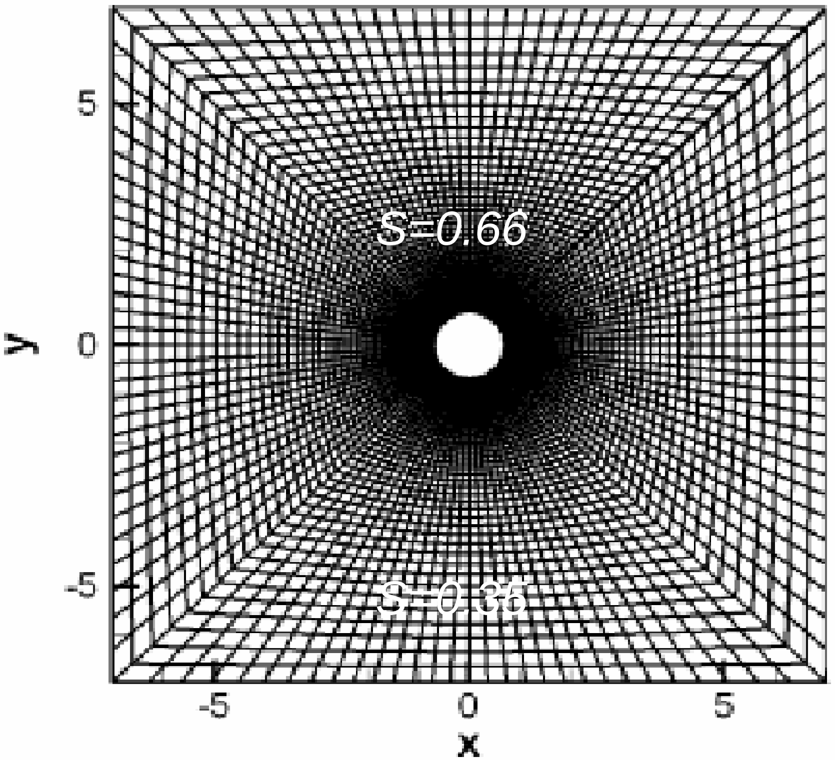


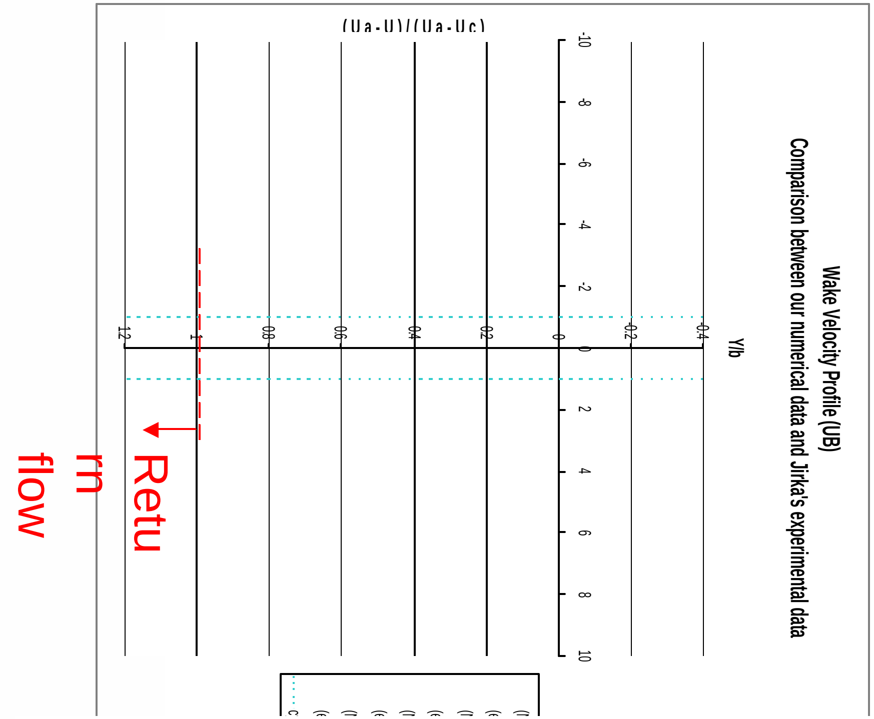


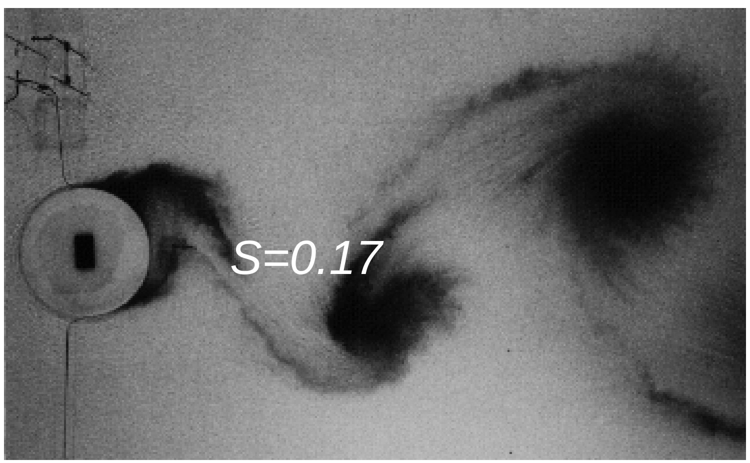


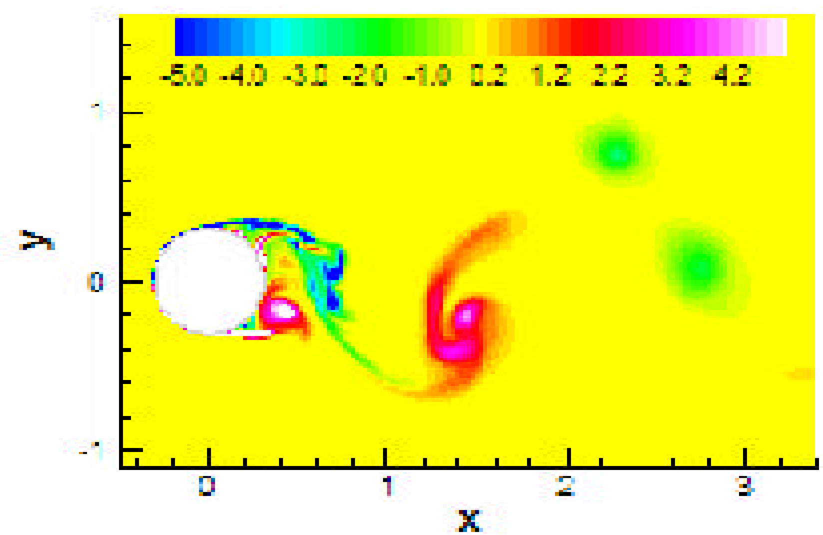
Van Prooijen 2004




S=0.66
S=0.36
y
x


Wake Velocity Profile (UB)
Comparison between our numerical data and Jirka's experimental data
Y/b
Return flow

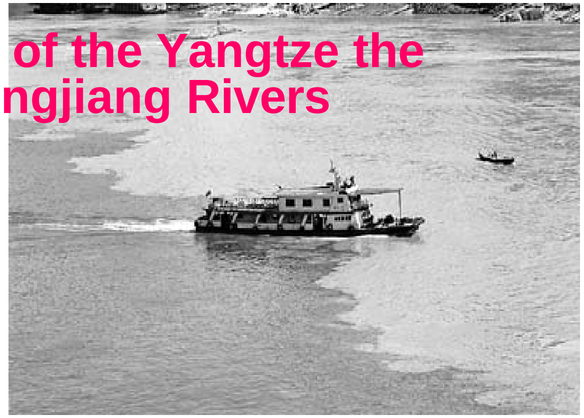

S=0.17


-5.0 -4.0 -3.0 -2.0 -1.0 0.2 1.2 2.2 3.2 4.2
y
x

Large Scale Turbulent Structures in Shallow Flows

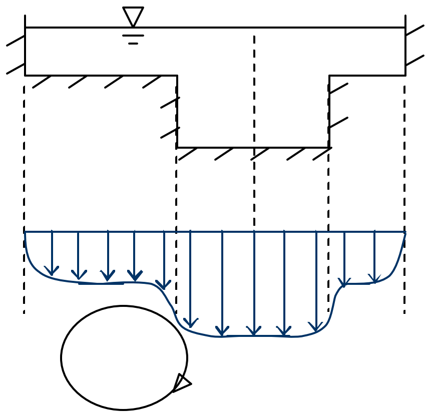
Big Island of Hawaii

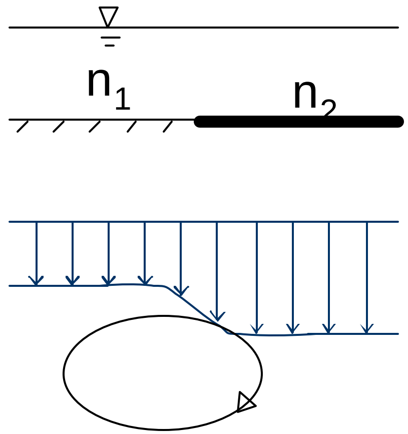
Confluence of the Yangtze the Jialingjiang Rivers

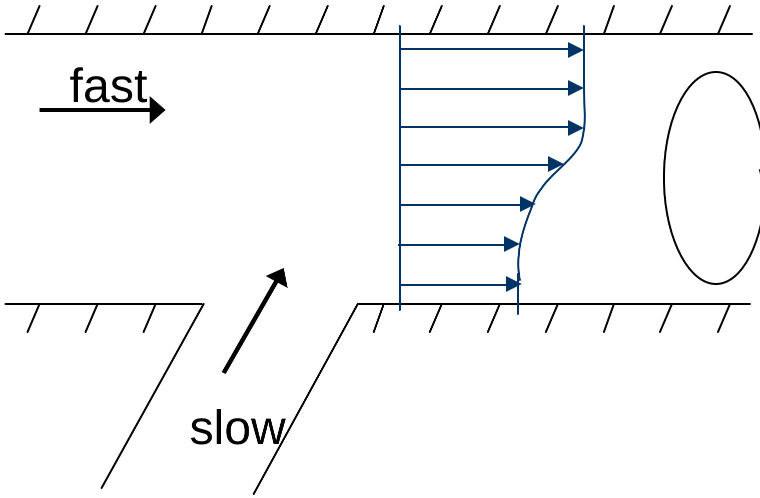


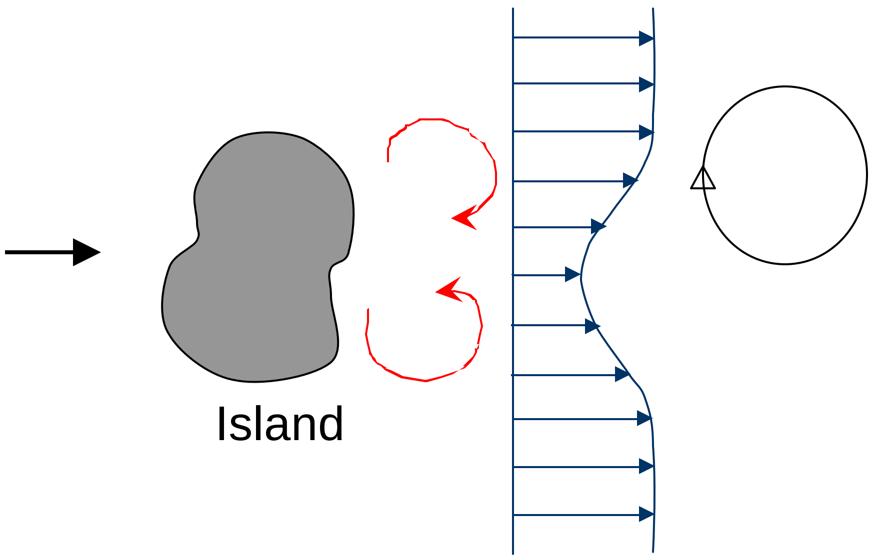
Examples

➢ Flow In Compound and/or Composite Channels



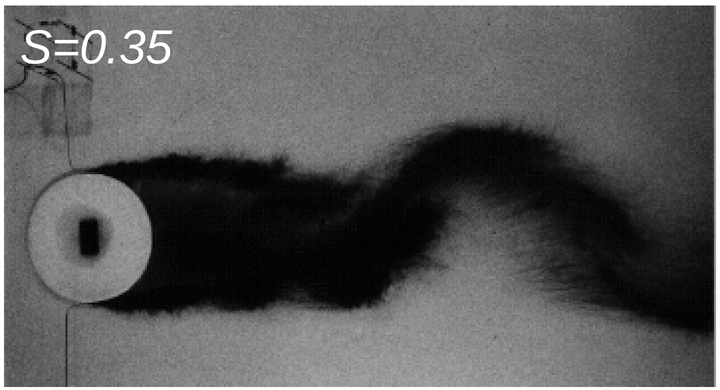




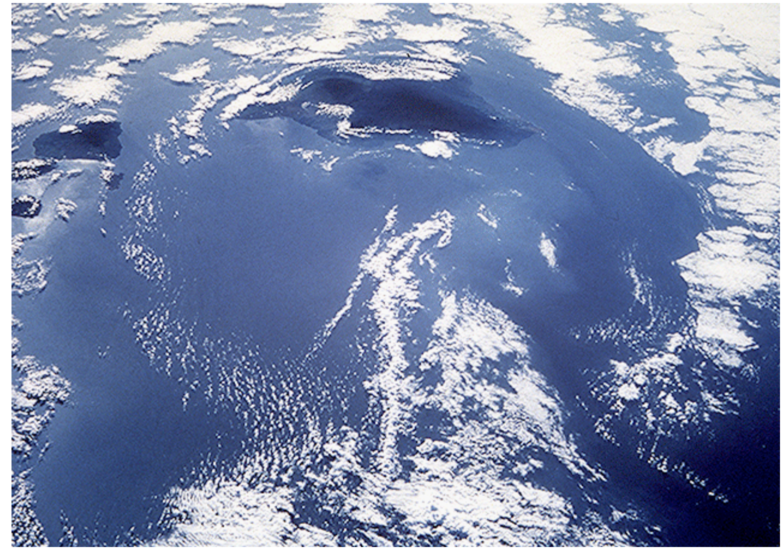


- Controls the mass, momentum and energy transport.
- Traps contaminants (measurements show that concentrations are 5 to 6 times larger than the average);
- The effective resistance is significantly increased

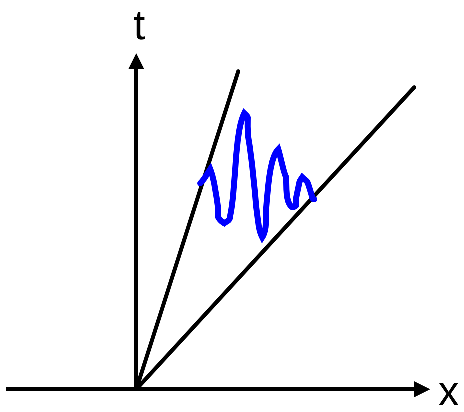
Chen & Jirka (1995)



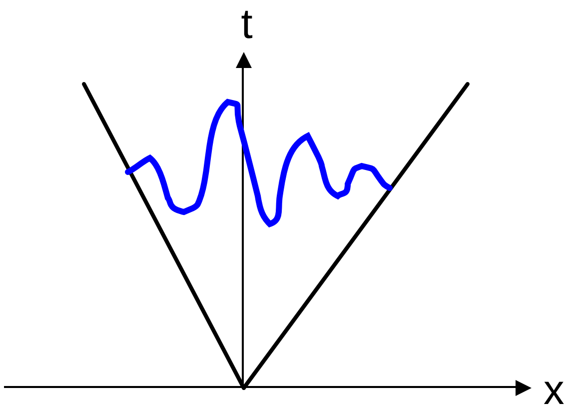
Friction



Source of Vortex Street Oscillations: Absolute or Convective?



Convectively unstable case



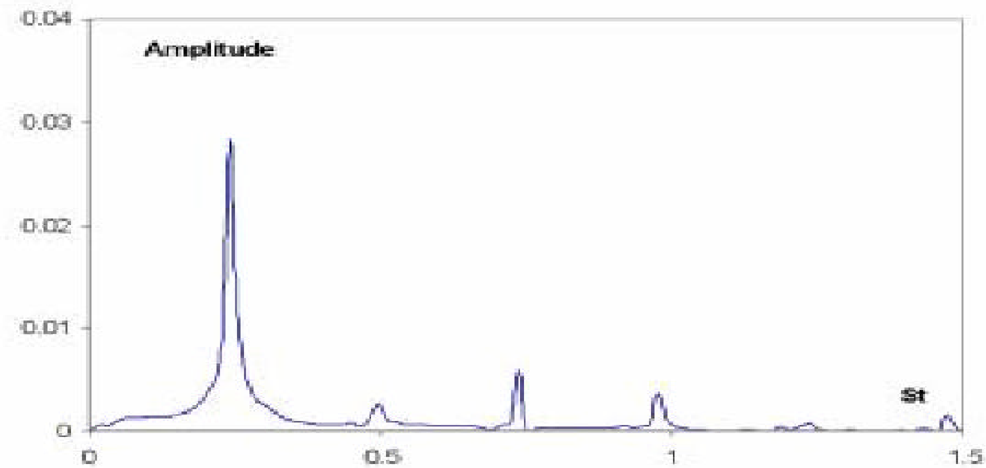
Absolutely unstable case

***Journal of Fluid Mechanics**, 2006 by* Ghidaoui, Kolyshkin, *Chan, Liang,* Xu.

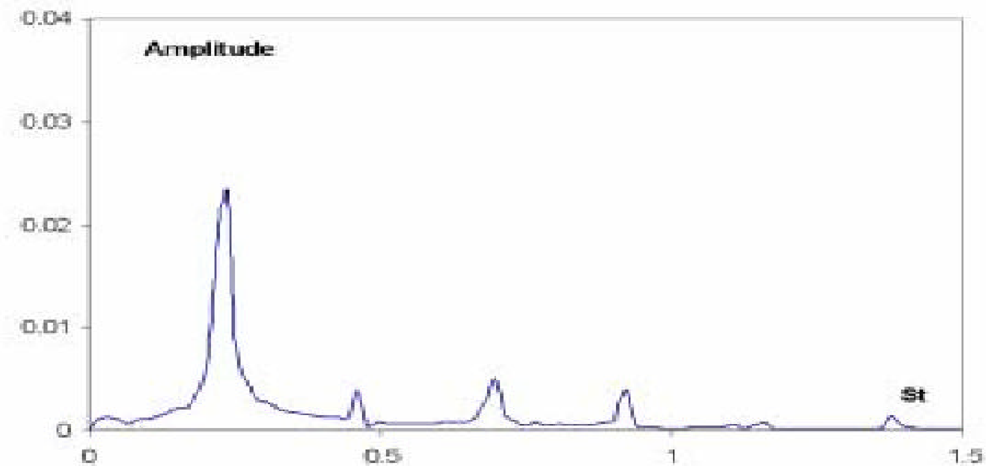
Journal of Fluid Mechanics, 2003, by Kolyshkin, A.A and Ghidaoui, M.S.

Journal of Hydraulic Engineering, 1999, by Ghidaoui, Kolyshkin.

Verification of the Wave-Maker Hypothesis

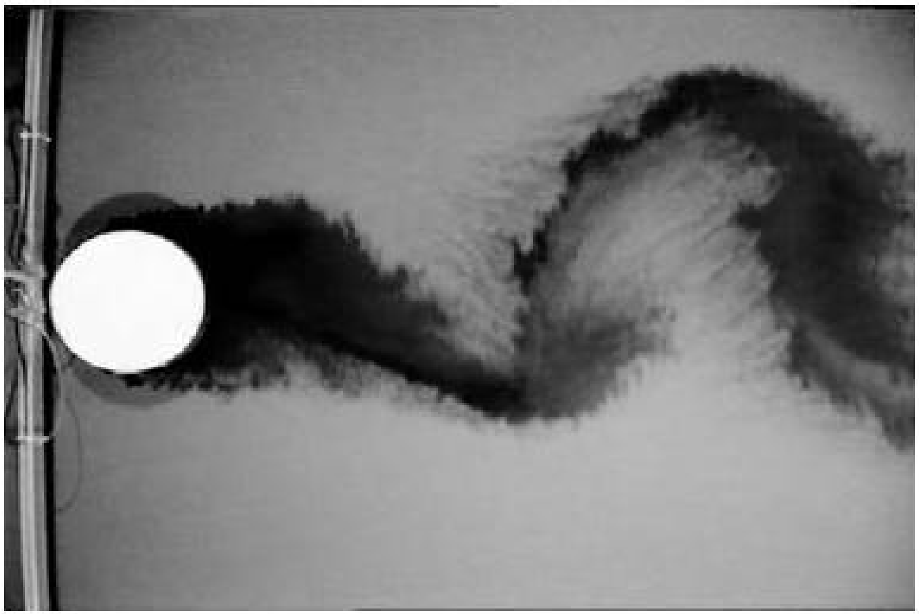


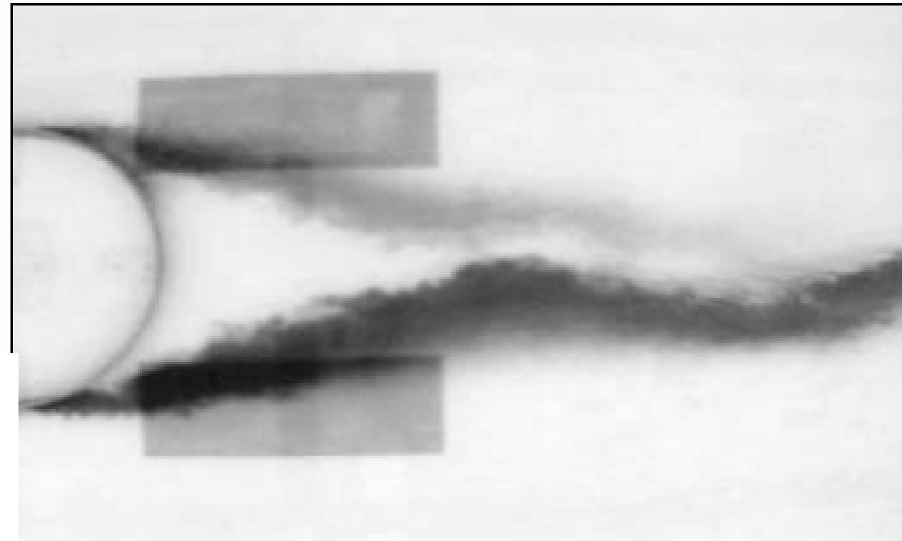
a) without inflow forcing



b) with inflow forcing

Amplitude spectra of longitudinal velocity for $S = 0.16$ at the location $x = 0.7$

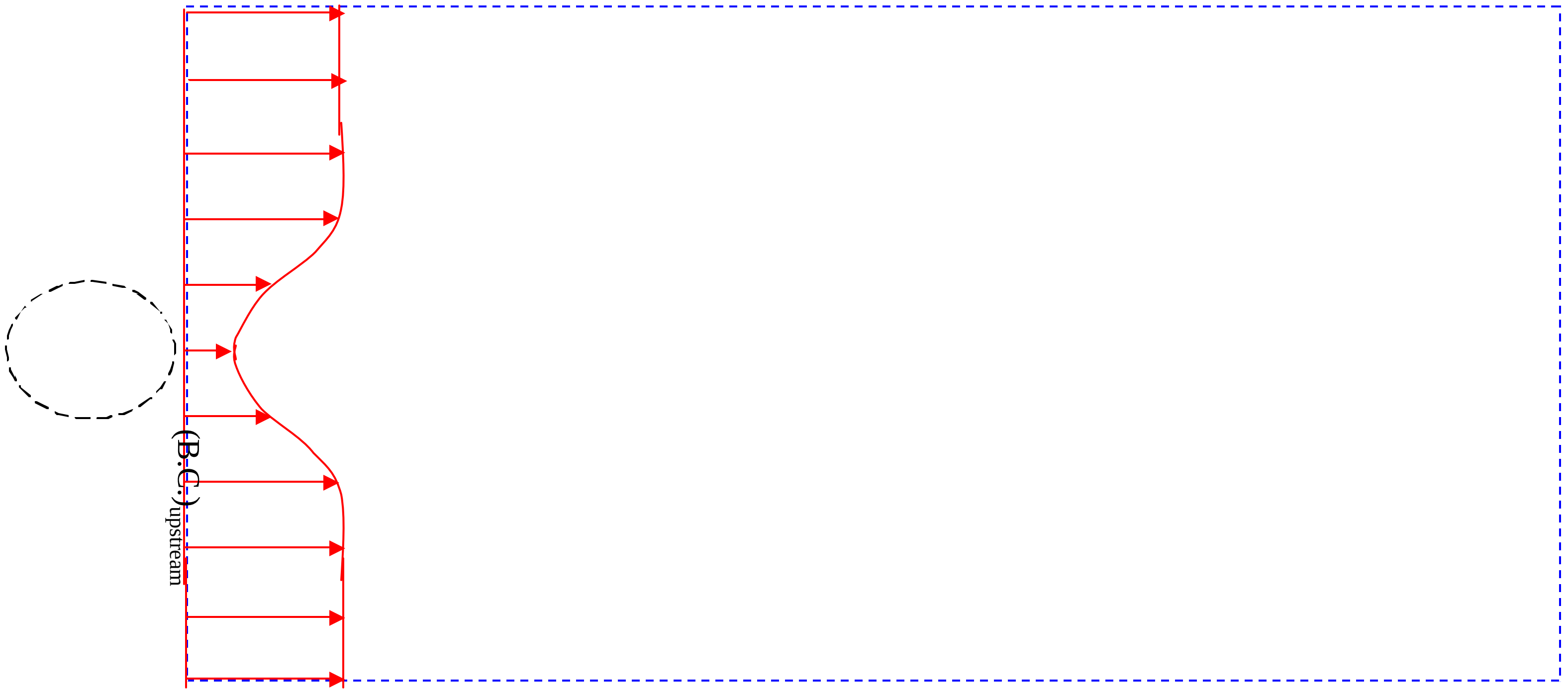




(a) Experiment 2

(b) Experiment 3

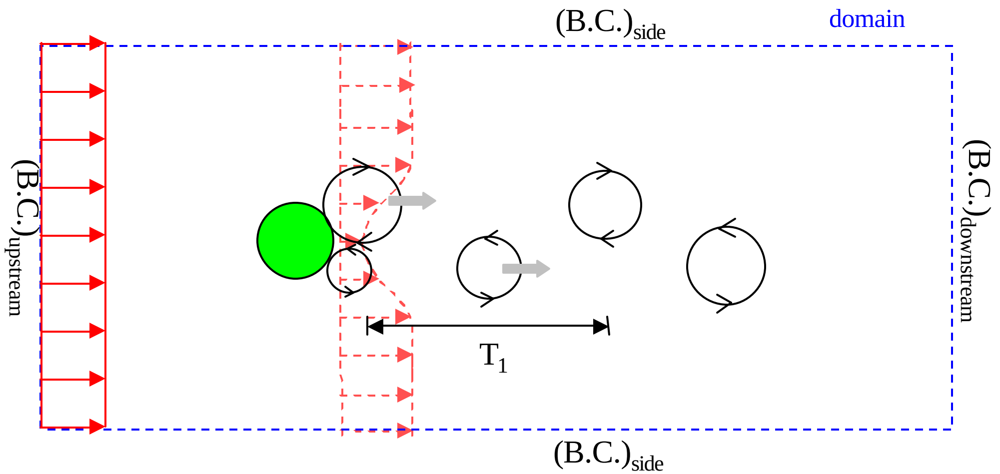
All stability analyses do not explicitly include the Bluff Body! How valid is this approach?



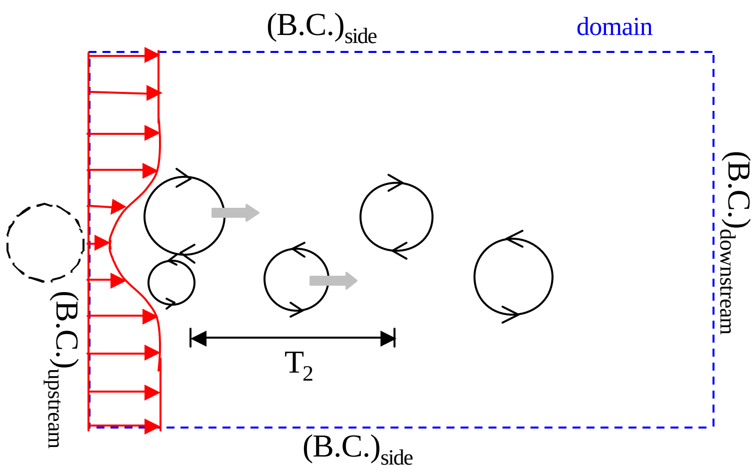
***Physics of Fluids*, 2006, by** *Chan* , Ghidaoui, *Kolyshkin.*

How to test for the validity?

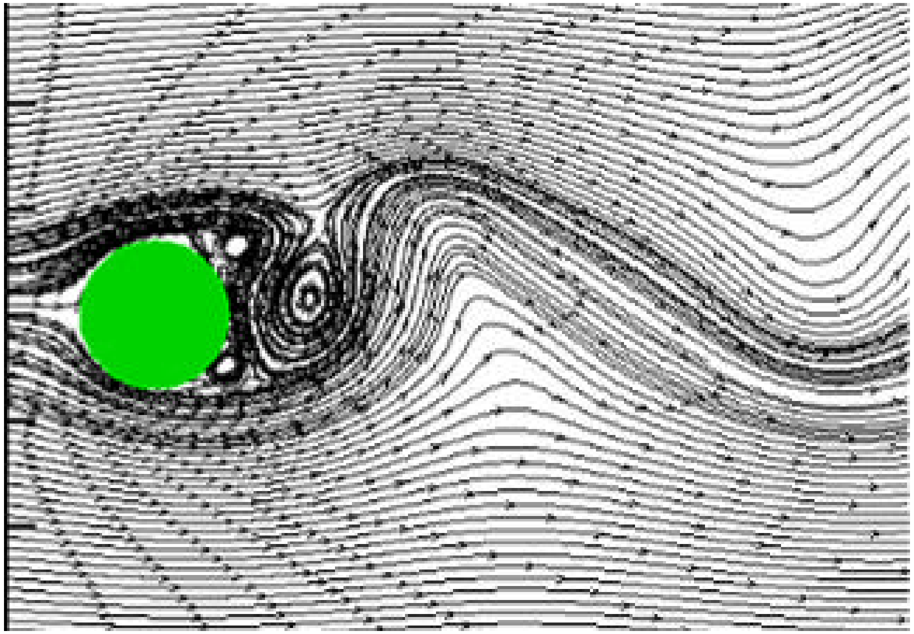
Method 1: With Cylinder



Method 2: No Cylinder

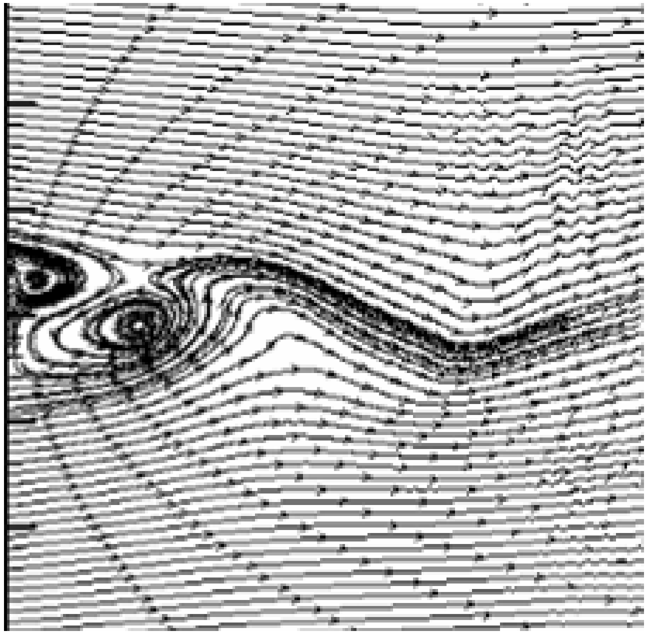


Method 1: With Cylinder



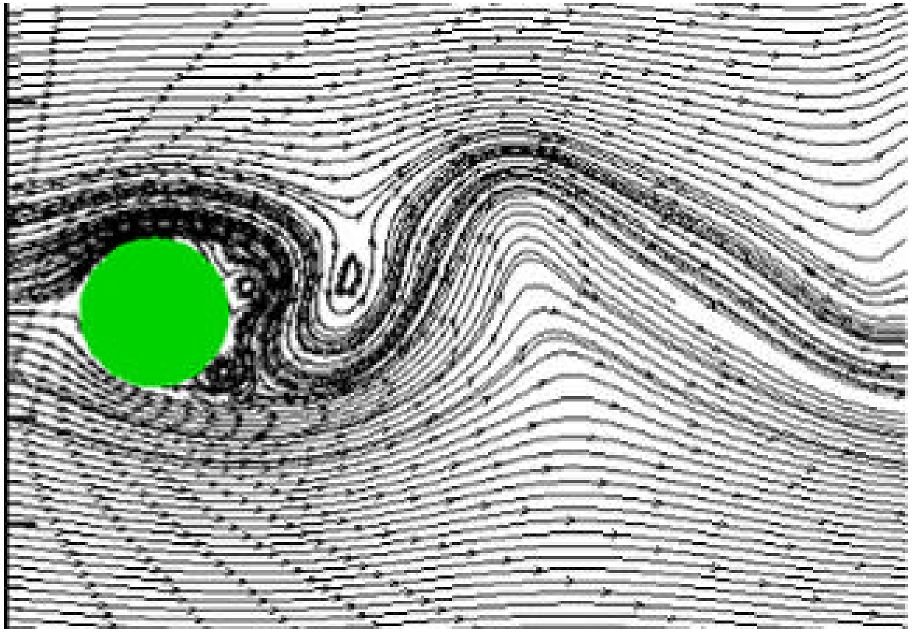
t=T/8=12.19s
T=97.52s

Method 2: No Cylinder



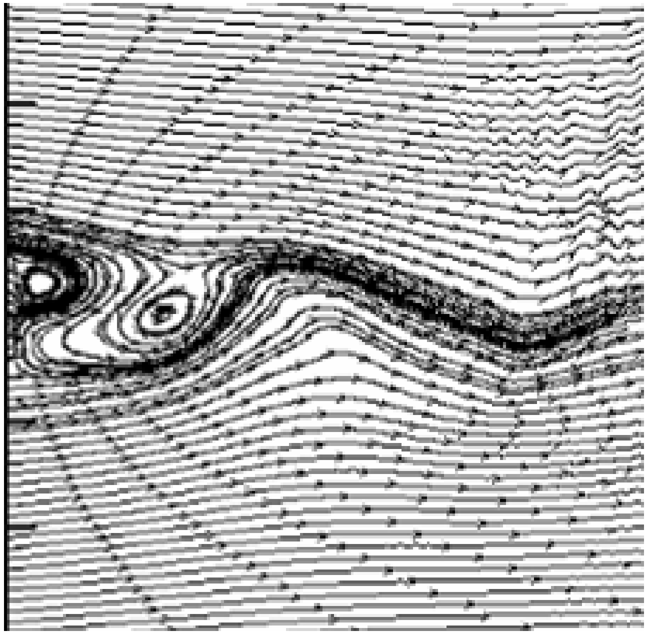
t=T/8=8.4s
T=67.2s

Method 1: With Cylinder



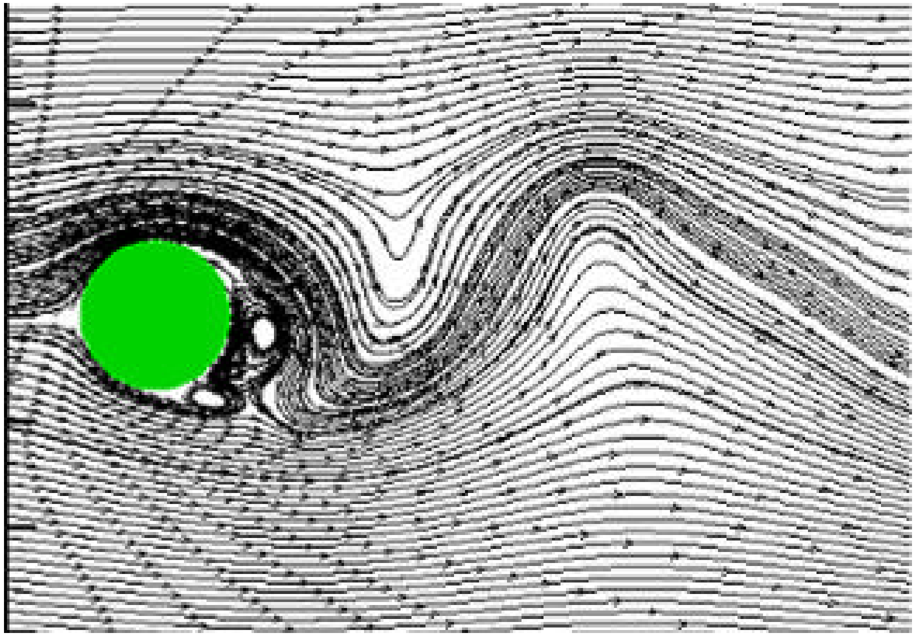
t=T/4=24.38s

Method 2: No Cylinder



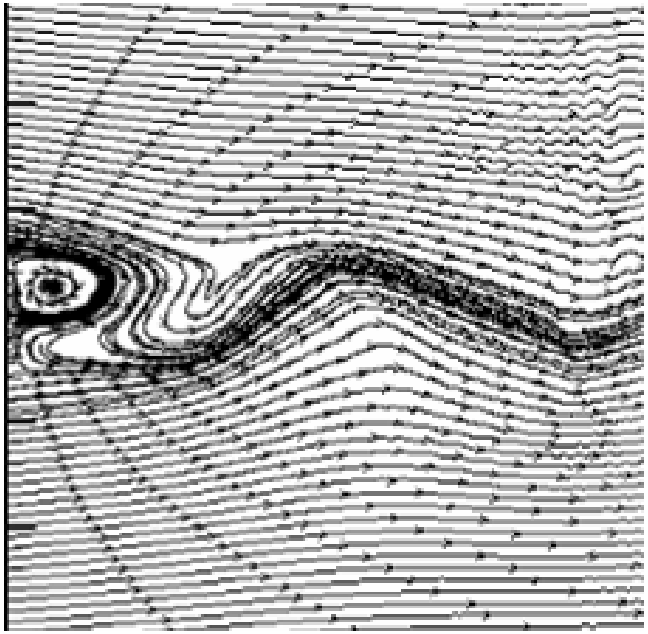
t=T/4=16.8s

Method 1: With Cylinder



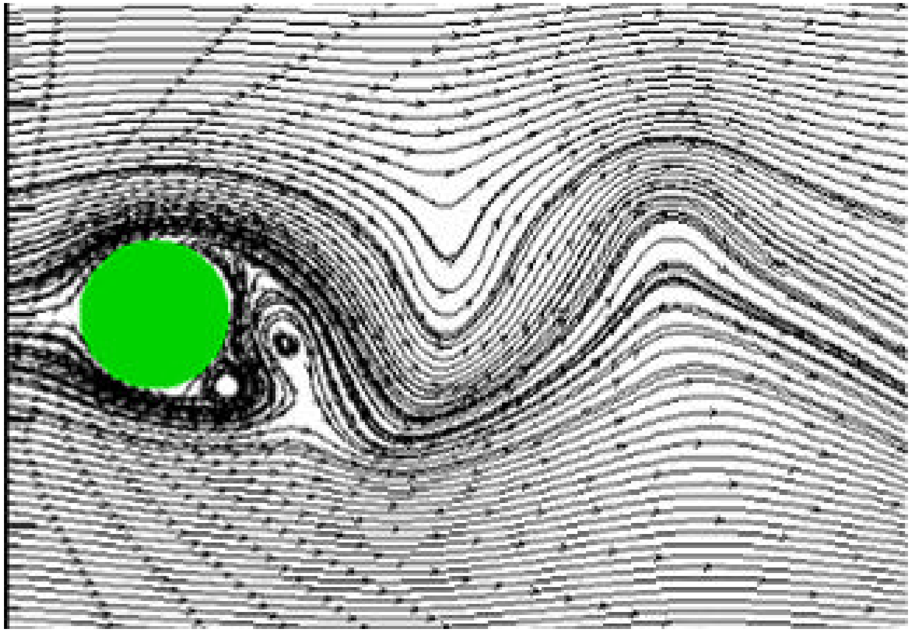
t=3T/8=36.75s

Method 2: No Cylinder



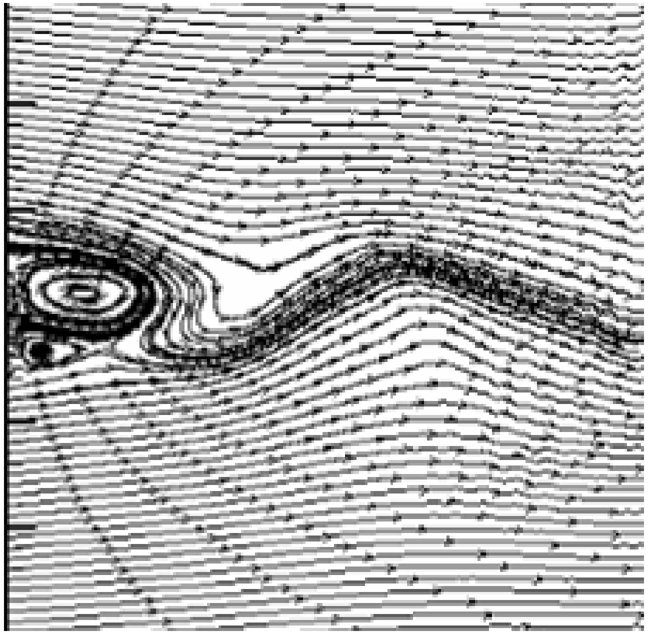
t=3T/8=25.2s

Method 1: With Cylinder



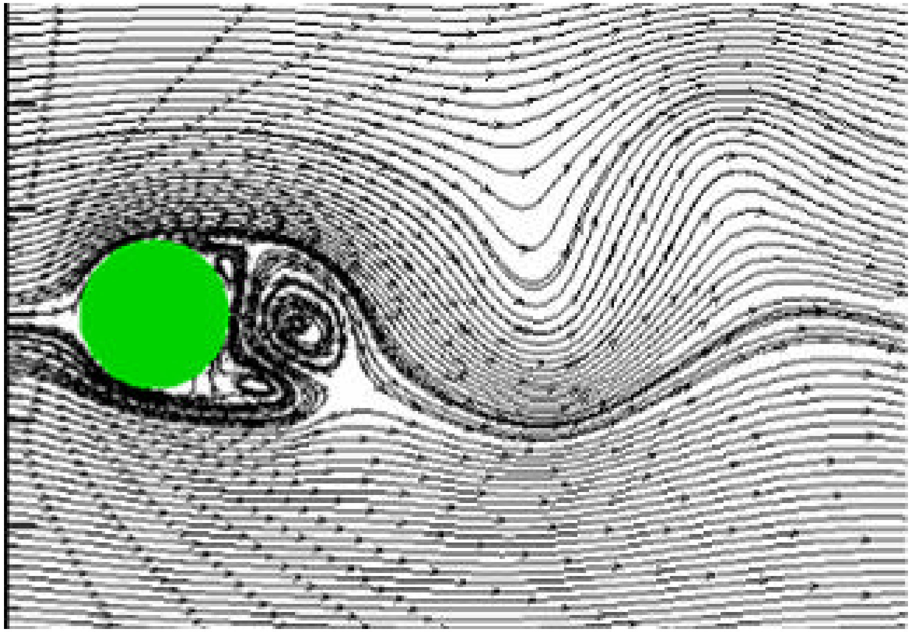
t=T/2=48.76s

Method 2: No Cylinder



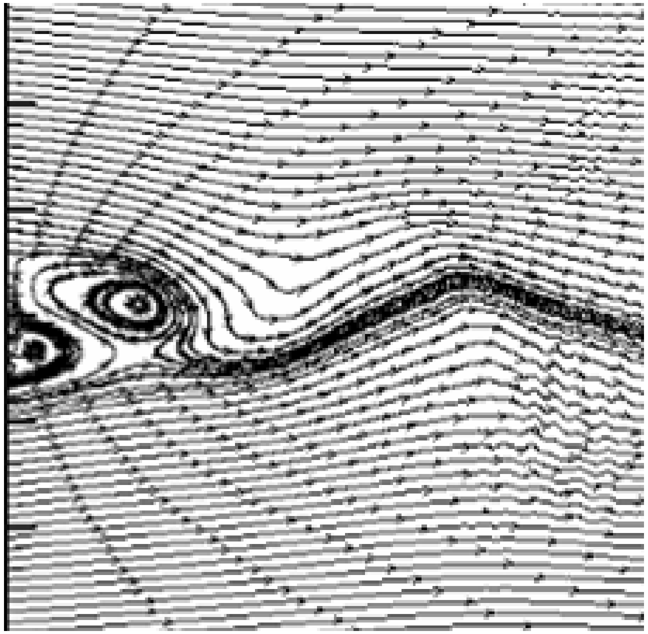
t=T/2=33.6s

Method 1: With Cylinder



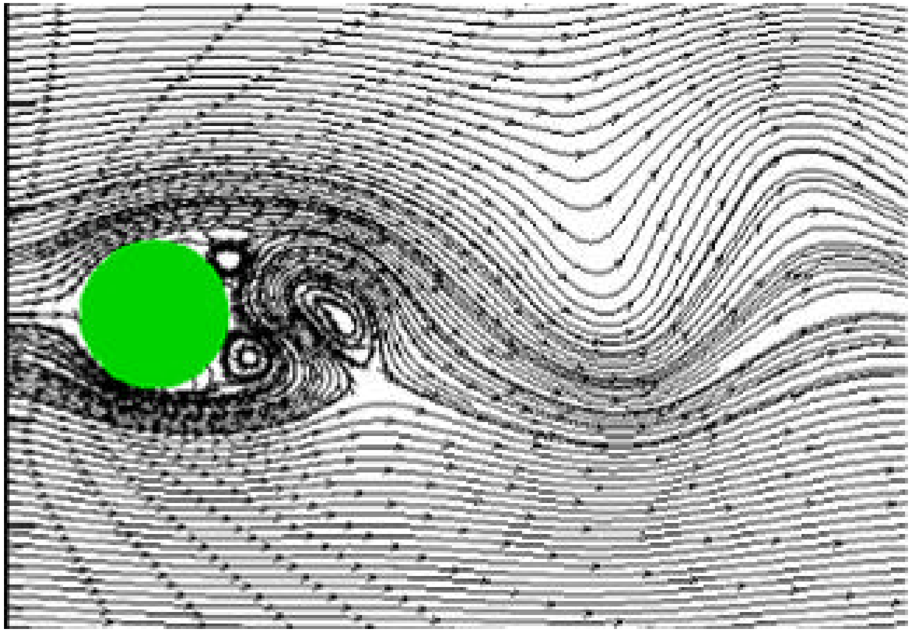
t=5T/8=60.95s

Method 2: No Cylinder



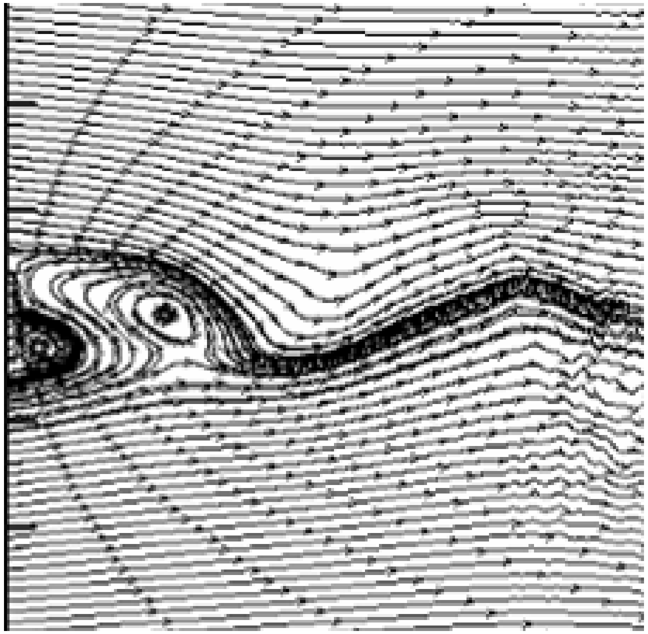
t=5T/8=42.0s

Method 1: With Cylinder



t=3T/4=73.14s

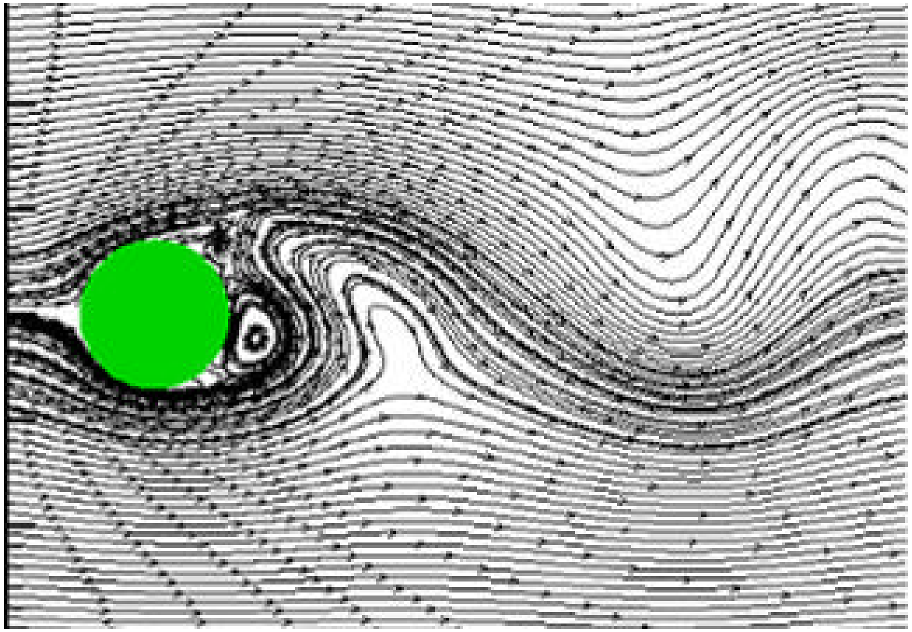
Method 2: No Cylinder



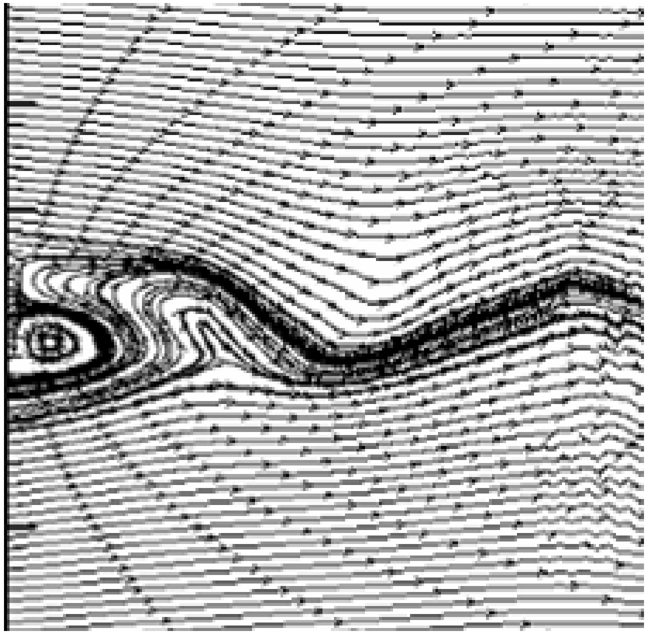
t=3T/4=50.4s

Method 1: With Cylinder

Method 2: No Cylinder

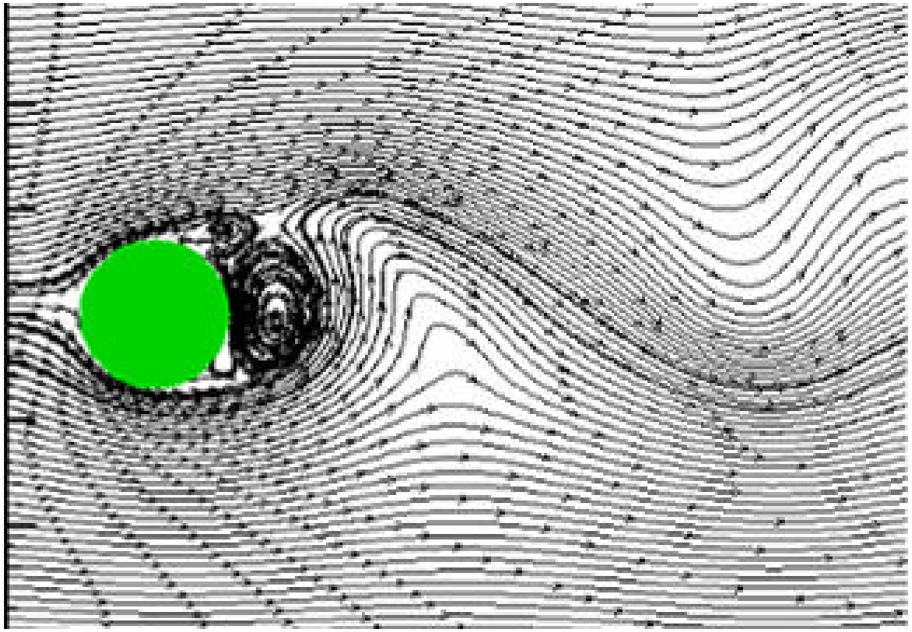


t=7T/8=85.33s



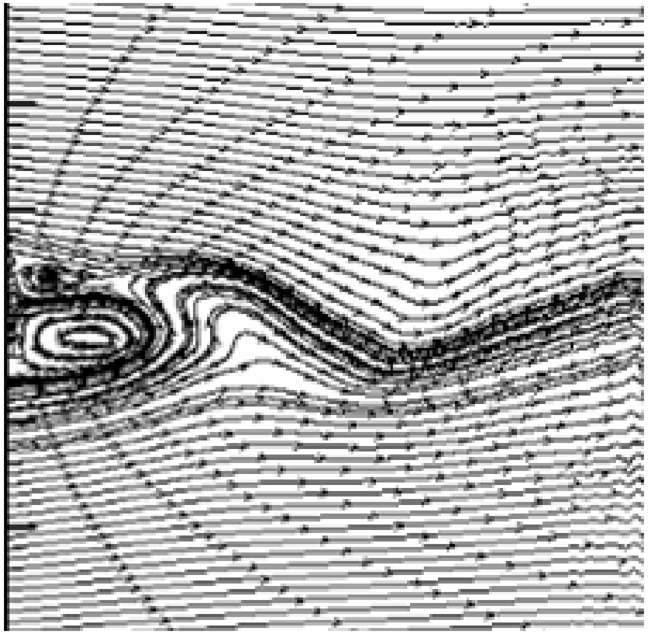
t=7T/8=58.8s

Method 1: With Cylinder

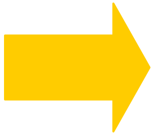


t=T=97.52s

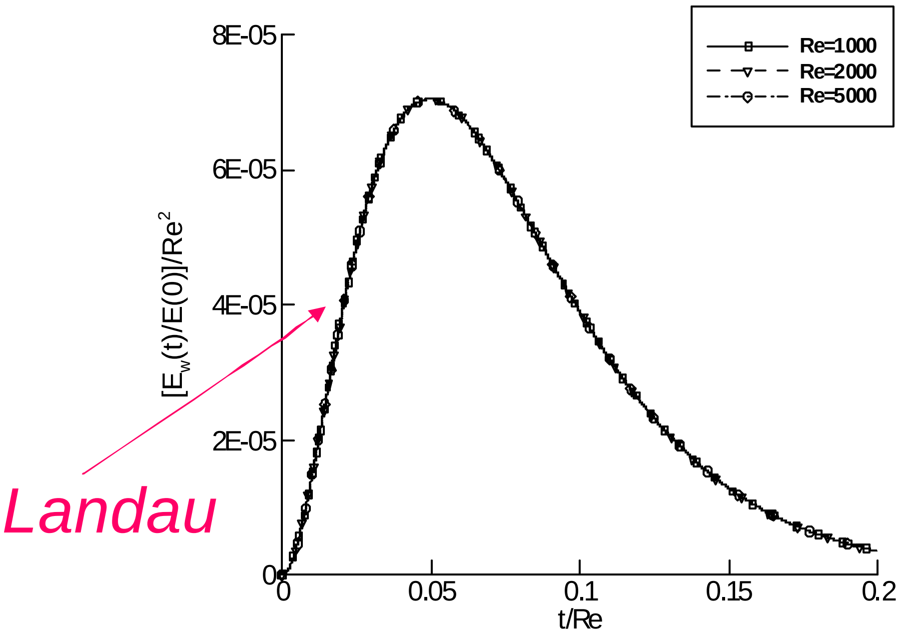
Method 2: No Cylinder

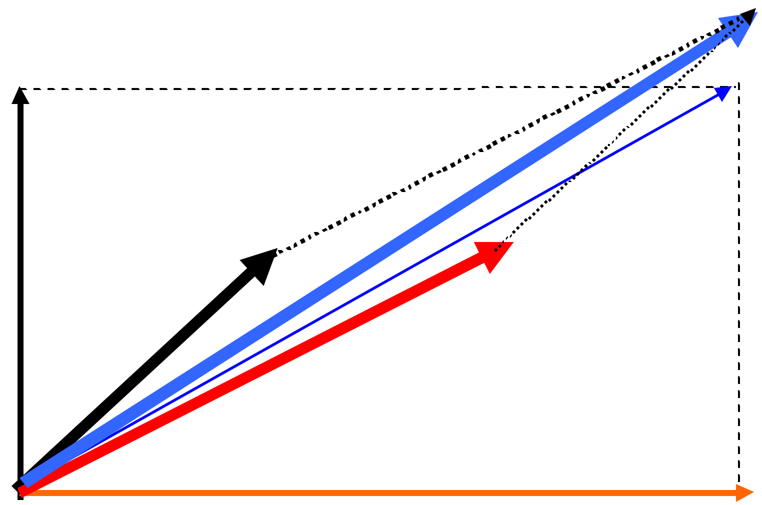


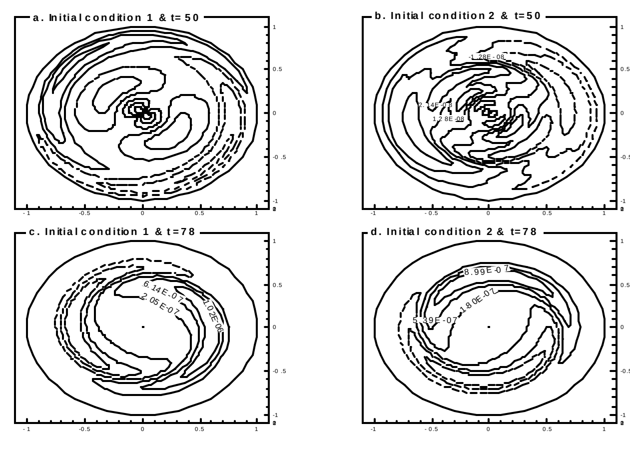
t=T=67.2s



What is the instability mechanism for steadv & unsteady pipe flow?





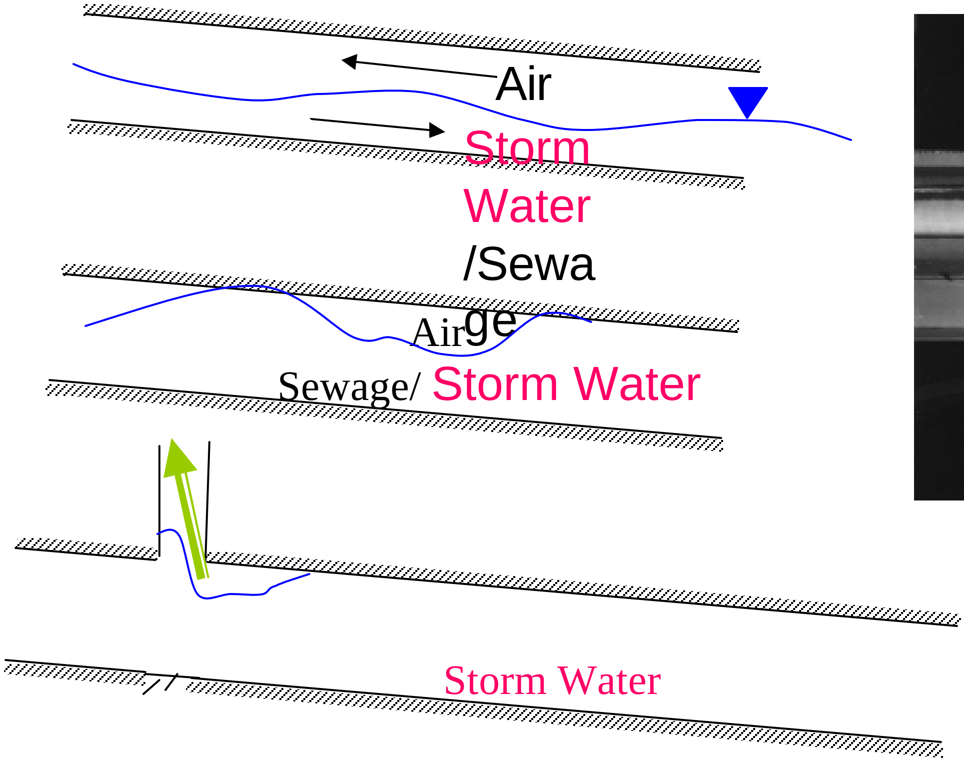


Zhao, Ghidaoui, *Kolyshkin,* (2006). ***Journal of Fluid Mechanics.***

Zhao, Ghidaoui, *Kolyshkin* (2004). ***Journal of Hydraulic Research.***

Ghidaoui, Kolyshkin (2002). ***Journal of Fluid Mechanics.***

Where next? Helmholtz Instability & Sewer Surcharging



Video can be found at http://www.youtube.com/watch?v=4aQySL0sKys

Geysering in Hong Kong; Contact the speaker for a copy of the video

Conclusions

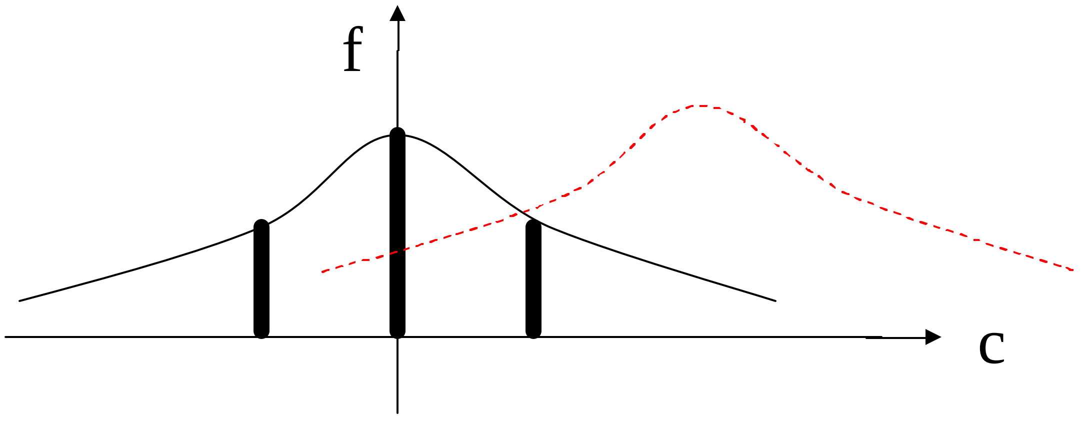
Ippen’s analogy provides a way to link Boltzmann gas kinetic theory to hydraulics

Boltzmann hydraulics model is accurate & efficient tool for surface water problems for it

- Handles complex geometry;
- Handles waves and their interactions;
- Handles turbulent stresses;
- Waves and diffusion do not need splitting.

Other fields:

- Gas dynamics; porous media flow; multiphase flows; etc.



Other Promising applications:

Systems with large numbers of interacting parts (e.g., traffic, Sediment transport; population dynamics; etc)

Turbulence

J. Fluid Mech. (2004), *vol.* 519, *pp.* 301–314.
DOI: 10.1017/S0022112004001211 Printed in the United Kingdom

Expanded analogy between Boltzmann kinetic theory of fluids and turbulence

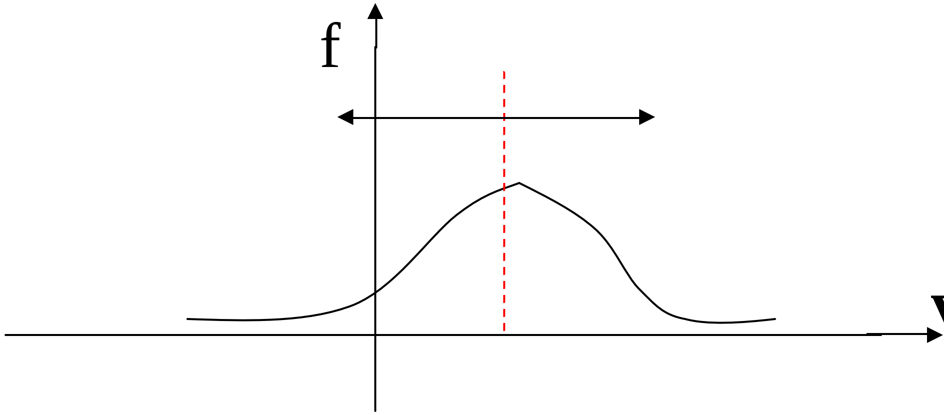
By HUDONG CHEN[1], STEVEN A. ORSZAG[2], ILYA STAROSELSKY[1] AND SAURO SUCCI[3]

[1]EXA Corporation, 3 Burlington Woods Drive, Burlington, MA 01802, USA

[2]Department of Mathematics, Yale University, New Haven, CT 06511, USA

[3]Istituto Applicazioni Calcolo, CNR, viale Policnico 137, 00161 Roma, Italy

Framework



$$\partial_t f + v \cdot \nabla f = C_{turb} \tag{2.1}$$

where the collision term is approximated in so-called BGK form (Bhatnagar, Gross & Krook 1954) as

$$C_{turb} = -\frac{1}{\tau_{turb}}(f - f^{eq}) \tag{2.2}$$

$$\rho = \int \mathrm{d}v\, f,$$

$$\boldsymbol{U} = \langle \boldsymbol{v} \rangle,$$

$$K = \tfrac{1}{2}\langle (\boldsymbol{u}')^2 \rangle \equiv \tfrac{1}{2}\langle (\boldsymbol{v} - \boldsymbol{U})^2 \rangle,$$

$$\sigma_{ij} = \nu_{turb}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right] - \nu_{turb}\frac{\mathrm{D}}{\mathrm{D}t}\left[\tau_{turb}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right]$$
$$- \frac{K^3}{\epsilon^2}\left[C_1 \frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k} + C_2\left(\frac{\partial u_i}{\partial x_k}\frac{\partial u_k}{\partial x_j} + \frac{\partial u_j}{\partial x_k}\frac{\partial u_k}{\partial x_i}\right) + C_3 \frac{\partial u_k}{\partial x_i}\frac{\partial u_k}{\partial x_j}\right]$$