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

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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 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\textsuperscript{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

- **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.

- Democritus School (\textasciitilde 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

- 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 century):**
  
  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”
Equilibrium 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

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

\[
q = \rho p = \rho \left( \frac{m}{2\pi kT} \right)^{3/2} e^{-\frac{c_x^2 + c_y^2 + c_z^2}{2kT/m}}
\]

\[
p \Delta c_x \Delta c_y \Delta c_y = \text{percentage of particles with speeds between } c_x \text{ and } c_x + \Delta c_x; c_y \text{ and } c_y + \Delta c_y; c_z \text{ and } c_z + \Delta c_z
\]

\[
q \Delta c_x \Delta c_y \Delta c_y \times \forall = \text{Mass of particles in volume (}\forall\text{) with speeds between } c_x \text{ and } c_x + \Delta c_x; c_y \text{ and } c_y + \Delta c_y; c_z \text{ and } c_z + \Delta c_z
\]
Kinetic Theory and its Relation to Gross Properties

\[ \iiint_{R^3} p dc_x dc_y dc_z = 1 \]
\[ \iiint_{R^3} \rho p dc_x dc_y dc_z = \rho \]

**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:**
\[ p = \iiint_{R^3} \frac{c_x^2 + c_y^2 + c_z^2}{3} q dc_x dc_y dc_z = \rho \frac{kT}{m} = \rho RT \quad \tau_{xy} = \iiint_{R^3} c_x c_y q dc_x dc_y dc_z = 0 \]

**Energy:**
\[ e = \iiint_{R^3} \frac{c_x^2 + c_y^2 + c_z^2}{2} q dc_x dc_y dc_z = \frac{3}{2} \rho RT \]
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 $x+\Delta x$ and possessing speeds between $c$ and $x+\Delta c$

$$f(x)ch?c f(x+\Delta x)ch?c$$

$$f(c+\Delta c)(dc/dt)h?x$$

$$f(x+\Delta x)ch?c$$

$$f(c)(dc/dt)h?x$$

$$\partial f/\partial t = -c \partial f/\partial x - dc \partial f/\partial c + C(f) = -c \partial f/\partial x - F \partial f/\partial c + q - f/\tau$$
Boltzmann and the NS

\[ \frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + \frac{F_i}{m} \frac{\partial f}{\partial c_i} = \frac{q-f}{\tau} \]

Continuity (Zero-th Moment):

let \( dc = dc_x dc_y dc_z \)

\[ \int \int \int \left( \frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + \frac{F_i}{m} \frac{\partial f}{\partial c_i} \right) dc = \int \int \int \frac{q-f}{\tau} dc \]

\[ \frac{\partial}{\partial t} \int \int \int f dc + \frac{\partial}{\partial x_i} \int \int \int c_i f dc + 0 = 0 \]

\[ \Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \]

Momentum (First Moment):

\[ \int \int \int c_i \left( \frac{\partial f}{\partial t} + c_j \frac{\partial f}{\partial x_j} + \frac{F_j}{m} \frac{\partial f}{\partial c_j} \right) dc = \int \int \int c_i \frac{q-f}{\tau} dc \]

\[ \frac{\partial}{\partial t} \int \int \int c_i f dc + \frac{\partial}{\partial x_i} \int \int \int c_j c_i f dc - \rho F_i = 0 \]

Newtonian viscous stresses are recovered when

\[ \tau = \frac{\nu \rho}{\rho} \]
Boltzmann Based Schemes & the Finite Volume Approach

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!

STUDIES ON THE VALIDITY OF THE HYDRAULIC ANALOGY TO SUPERSOONIC FLOW

Parts I and II
### Summary of Gas-Water Flow Direct Analogy

<table>
<thead>
<tr>
<th>GAS FLOW</th>
<th>WATER FLOW</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speed of propagation of sound</td>
<td>Speed of propagation of small gravity wave</td>
</tr>
<tr>
<td>$a = \sqrt{\gamma p' / \rho}$</td>
<td>$c = \sqrt{gh}$</td>
</tr>
<tr>
<td>Mach number, $M = \frac{V}{\sqrt{\gamma p' / \rho}}$</td>
<td>Froude number, $F = \frac{V}{\sqrt{gh}}$</td>
</tr>
<tr>
<td>Density ratio, $\frac{\rho_2}{\rho_1}$</td>
<td>Depth ratio, $\frac{h_2}{h_1}$</td>
</tr>
<tr>
<td>Pressure ratio, $\frac{p_2}{p_1}$</td>
<td>$(\text{Depth ratio})^2$, $(\frac{h_2}{h_1})^2$</td>
</tr>
<tr>
<td>Temperature ratio, $\frac{T_2}{T_1}$</td>
<td>Depth ratio, $\frac{h_2}{h_1}$</td>
</tr>
</tbody>
</table>
1. Equate depth ratio to density ratio

2. Calculate from gas theory
Ippen’s 2nd Modification

\[ \frac{\rho_i}{\rho_1} = \frac{\tan(\beta)}{\tan(\beta - \theta)} = \frac{h_s}{h_1} \]

\[ F_1 \sin(\beta_1) = \sqrt{\frac{h_s}{h_1}} \cdot \frac{1}{2} \left( 1 + \frac{h_s}{h_1} \right) \quad (34b) \]

\[ M_1 \sin(\beta_1) = \sqrt{\frac{c_1}{c_i}} \left( \frac{5}{6} - \frac{c_2}{c_i} \right) \quad (47b) \]

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

\[ \frac{F_i}{M_i} = \sqrt{\frac{(1+\rho_{2}/\rho_1)(6-\rho_{2}/\rho_1)}{10}} \quad (56) \]
Note: Pressure ratios obtained from water analysis are calculated from eq. (19a) where \( \frac{D_i}{H_i} = \frac{D_1}{H_1} \) and \( \gamma = 1.40 \).

Local Mach Numbers are calculated from eq. (52b).

**Air**

\[ M = 3.00 \]
\[ \beta = 27.23' \]
\[ \frac{D_i}{H_i} = 2.05 \]
\[ \frac{D_1}{H_1} = 3.01 \]

**WATER**

**First Modification**

\[ M = 2.64 \]
\[ \beta = 28.55' \]
\[ \frac{D_i}{H_i} = 1.97 \]
\[ \frac{D_1}{H_1} = 2.76 \]

**Second Modification**

\[ M = 2.32 \]
\[ \beta = 27.23' \]
\[ \frac{D_i}{H_i} = 2.05 \]
\[ \frac{D_1}{H_1} = 2.92 \]

**THEORETICAL COMPARISON OF MODIFIED ANALOGY FOR SUCCESSIVE SHOCKS**
Ippen’s Analogy and Boltzmann Gas model for hydraulics (example 1: \( M=Fr=2.5 \))

**Boltzmann gas Model**: \( M = 2.5 \Rightarrow \frac{\rho_2}{\rho_1} = 1.489; \ \beta = 30°54' \)

**Hydraulic Theory**: \( Fr = 2.5 \Rightarrow \frac{h_2}{h_1} = 1.465; \ \beta = 32°30' \)

**Applying Ippen’s 2 modifications to Boltzmann Model**: 

\[
\frac{\rho_2}{\rho_1} = 1.465 = \frac{h_2}{h_1}; \ \beta_{\text{gas}} = 32°30' = \beta_{\text{water}}; \ \ M = 2.36
\]
Ippen’s Analogy and Boltzmann Gas model for hydraulics (Example 2: $M=Fr=5$)

Boltzmann gas Model: $M = 5 \Rightarrow \frac{\rho_2}{\rho_1} = 2.0045; \beta = 18^\circ 36'$

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

Applying Ippen’s 2 modifications to Boltzmann Model: 
\[
\frac{\rho_2}{\rho_1} = 1.9115 \equiv \frac{h_2}{h_1}; \beta_{gas} = 19^\circ 35 = \beta_{water}; \ M = 4.6
\]
Ippen's analogy and the linkage between Boltzmann Gas model and hydraulics

\[ q = \rho \left( \frac{\rho}{2\pi p} \right) e^{-\frac{c_x^2 + c_y^2 + c_z^2}{2p}} \]

\[ \rho \Rightarrow h \]

\[ p \Rightarrow \frac{gh^2}{2} \]

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

Continuity (Zero-th Moment)

\[ \int c \left( \frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + \frac{F_i}{m} \frac{\partial f}{\partial c_i} \right) \, dc = \int c \left( q - f \right) \, dc \quad \Rightarrow \frac{\partial h}{\partial t} + \frac{\partial hu_i}{\partial x_i} = 0 \]

Momentum (First Moment)

\[ \tau = \frac{\nu p}{gh^2 / 2} = \frac{v}{gh} \]
Does the model handle waves? How well?

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

Su, Xu, Ghidaoui (1999). *Journal of Computational Physics*
Zhang, Ghidaoui, Gray, Li, (2003), *Advances In Water Resources.*
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
Shock & Expansion Waves

1-D Dam-Break Problem Modeling: Shock Resolution for Different Values of Courant Number (Δx=1.0m, t=50s, S_f=0.0, S_0=0.0)

- Analytical solution
- Numerical solutions for different Courant numbers (Cr=0.1, Cr=0.6, Cr=0.9)

Mesh for the Oblique Jump
Dam

$h_0 = 0.3048 \text{ m}$

122.0 m

$h(t)$ graph with time (s) on the x-axis and $h$ (m) on the y-axis.
Does the BGK solve viscous/turbulent flows? How well?

Van Prooijen 2004
Wake Velocity Profile (UB)

Comparison between our numerical data and Jirka's experimental data

\[ \frac{U_a - U_l}{U_a - U_c} \]

\[ \frac{U_a - U_l}{U_a - U_c} \]

Y/b

-10 -8 -6 -4 -2 0 2 4 6 8 10

-0.4 -0.2 0 0.2 0.4 0.6 0.8 1 1.2

\( S = 0.66 \)

\( S = 0.35 \)

\( S = 0.17 \)
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
Source of Vortex Street Oscillations: Absolute or Convective?

Convectively unstable case

Absolutely unstable case


Verification of the Wave-Maker Hypothesis

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

\[ t = \frac{T}{8} = 12.19 \text{s} \]
\[ T = 97.52 \text{s} \]

Method 2: No Cylinder

\[ t = \frac{T}{8} = 8.4 \text{s} \]
\[ T = 67.2 \text{s} \]
Method 1: With Cylinder

Method 2: No Cylinder

$\text{t} = \frac{T}{4} = 24.38\text{s}$

$\text{t} = \frac{T}{4} = 16.8\text{s}$
Method 1: With Cylinder

Method 2: No Cylinder

\[ t = \frac{3T}{8} = 36.75s \]

\[ t = \frac{3T}{8} = 25.2s \]
Method 1: With Cylinder

Method 2: No Cylinder

t=T/2=48.76s

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

\[ t = \frac{3T}{4} = 73.14 \text{s} \]

Method 2: No Cylinder

\[ t = \frac{3T}{4} = 50.4 \text{s} \]
Method 1: With Cylinder

Method 2: No Cylinder

$t = \frac{7T}{8} = 85.33s$

$t = \frac{7T}{8} = 58.8s$
Method 1: With Cylinder

Method 2: No Cylinder

$t=T=97.52s$

$t=T=67.2s$
What is the instability mechanism for steady & unsteady pipe flow?


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**


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**Expanded analogy between Boltzmann kinetic theory of fluids and turbulence**

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\[ \partial_t f + \mathbf{v} \cdot \nabla f = C_{\text{turb}} \]  
where the collision term is approximated in so-called BGK form (Bhatnagar, Gross & Krook 1954) as

\[ C_{\text{turb}} = -\frac{1}{\tau_{\text{turb}}} (f - f^{eq}) \]  

\[ \rho = \int \mathbf{v} f, \]

\[ \mathbf{U} = \langle \mathbf{v} \rangle, \]

\[ K = \frac{1}{2} \langle (\mathbf{u}')^2 \rangle \equiv \frac{1}{2} \langle (\mathbf{v} - \mathbf{U})^2 \rangle, \]

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