Molecular Tagging techniques
Part - 1

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Molecule-based flow diagnostic techniques!? Why!!?

- **Particle-based techniques** (LDV, PIV, PDV and Particle Image Thermometry):
  - The *particle-based* techniques measure the velocity or temperature of *tracer particles*, other than the velocity or temperature of *working fluid* directly.
    - *Flow tracking issues* (particle size, density mismatch, …)
    - *Seeding issues* (particles don’t always go where you need them)
    - *Thermal response of the tracer particles for temperature measurements.*

- **Molecule-based techniques**:
  - *Flow tracking issues* can be solved.
    - *Molecular tracers can usually be dissolved in the working fluids, which move exactly with the same velocity as the local fluid molecules.*
  - *Thermal response* for fluid temperature measurement can be significantly mitigated, and perhaps even eliminated.
    - *The sizes* of the molecular tracers are usually *much smaller* than particle tracers.
  - *Simultaneous measurements of multiple flow parameters.*
    - *In addition to velocity field measurement, simultaneous mapping of scalar parameters such as temperature and concentration of fluid spices can also be achieved easily.*
Molecular Tagging Velocimetry (MTV): General Description

- Whole field, non-intrusive, optical diagnostic technique
- Use special chemical molecules premixed in fluid flows as long lifetime tracers
- A pulsed laser is used to "tag" small regions of interest
- Tagged regions are imaged twice with pre-set time delay
- The displacement vectors of the tagged regions provide the estimate of the velocity vectors of the fluid flow.
- Line (1-d), Grid (2-d), Stereoscopic (3-d) MTV
- Flow visualization and quantitative measurements
- Scalar field measurements, simultaneous velocity/scalar field measurements
## Comparison between MTV and PIV

<table>
<thead>
<tr>
<th></th>
<th>PIV</th>
<th>MTV</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Tracer</strong></td>
<td>particles (~μm)</td>
<td>molecules (~nm)</td>
</tr>
<tr>
<td><strong>Image photon source</strong></td>
<td>scattering light</td>
<td>emission (fluorescence/phosphorescence)</td>
</tr>
<tr>
<td><strong>Laser source</strong></td>
<td>conventional laser</td>
<td>UV laser</td>
</tr>
<tr>
<td><strong>signal intensity</strong></td>
<td>strong</td>
<td>weak</td>
</tr>
</tbody>
</table>

### Advantage of MTV
- Flows are hard to seed by particles
  - boundary layers or vortex cores
- Particles may change flows
  - micro-flows
- Particles do not follow flows
  - high speed flows, shock waves
- Particles may change the physics of phenomena
  - solidification
- Simultaneous vector/scalar distribution measurements.

### Disadvantage of MTV
- Less light compared to PIV
  - Emission rather than scattering
  - May require intensified cameras
- Chemicals
- Photon Source
  - UV and/or deep UV
  - High Energy
  - Some require multiple photon sources
- Equipment Cost
Components of Molecular Tagging Visualization / Velocimetry

- **Long Lifetime Molecular Tracers**
  The tracer photophysics dictates the type and number of lasers needed

- **Tagging Methods**
  - Single-line, Multi-line
  - Grid, Laser sheet

- **Detection**
  - Standard CCD Cameras
  - Gated Image-Intensified Cameras
  - Dual Detector for Increased Accuracy
  - Multi-Camera for Stereo MTV

- **Processing**
  - Line Center Methods
  - Direct Spatial Correlation

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**Liquid Phase**
- Photochromic Molecules (*Hummel, Falco*)
- Caged Laser Dyes (*Lempert*)
- Phosphorescent Supramolecules

**Gas Phase**
- Vibrationally Excited O₂ (*Miles*)
- Ozone (O₃) (*Pitz*)
- OH (dissociation of H₂O) (*Boedeker, Pitz*)
- NO (dissociation of Tert-butyl nitrite) (*Grünefeld*)
- NO (air photolysis) (*Sijtsema et al.*)
- Ionic Strontium Fluorescence (*Rubinsztein-Dunlop et al.*)
- Phosphorescent Molecules (Biacetyl, Acetone, etc.)
Long Lifetime Phosphorescent Molecular Tracers for Liquids

- Lifetime decreases in the presence of a quencher

\[
\tau = \frac{\tau_0}{1 + K_q [Q] \tau_0}
\]

Lifetime without quencher

- Design molecular complexes with small quenching rate \( K_q \)

- Minimize quencher concentration \([Q]\)

Emission from the phosphorescent triplex 1-BrNp • Gβ-CD • ROH ;

(A) without alcohol, (B) with alcohol.
Molecular Tagging Velocimetry (MTV) technique
(line-typed tagging for one-component velocity measurement)

- Tagged lines are imaged twice with known time delay
- Intensity profile for each row -> line center locations
- Difference between the line centers gives displacement
- Velocity = displacement / delay time

Flow visualization of the vortex shedding from the trailing edge of an oscillating airfoil (Bohl et al. 2002)
Molecular Tagging Velocimetry (MTV)  
(Grid-typed tagging for two-component velocity measurement)

- Create a 2-D grids with multiple laser beams.
- Take two images with known time delay.
- Find the displacement vectors of the grids through an image processing procedure.
- Local velocity = displacement/time delay.

First image  
(right after the laser pulse)

Second image  
(imaged 3.5 ms later)

The velocity field derived using a spatial correlation procedure (Bohl et al. 2002)
Planar MTV (two-component measurements)

Tagged regions imaged right after the laser pulse
Tagged regions imaged 8 ms later
The velocity field derived using a spatial correlation procedure

Results taken from (Bohl et al. 2001)
Image Processing for Planar MTV

- Create a 2-D contrast field
- Select a region in the first image (green)
- Search in the second image for the matching pattern (red)
- Pattern is matched via direct correlation technique

Results taken from (Bohl et al. 2001)
Stereoscopic Molecular Tagging Velocimetry (velocity three-component measurements)

- Use 2 cameras viewing from different perspectives.
- Each camera is processed using a planar MTV technique.
- Information from the two cameras is combined to reconstruction three components of velocity vectors.

Results taken from (Bohl et al. 2001)
Applications: Unsteady Flow Separation on Airfoils

- Airfoils moving to high angles of attack undergo dynamic stall, characterized by large excursions in lift and pitching moment.

Boundary layer resolved vorticity measurements have revealed the flow physics at the onset of the separation process, and its spatial and temporal scales.

NACA-0012 airfoil pitching to high angle of attack, hydrogen-bubble visualization.
Quantitative MTV Measurements

Using the grid tagging method, the in-plane velocity components and the vorticity field are mapped. Data below are for $k = 11.5$.

Strong concentrated vortices are formed immediately at the trailing edge. Instantaneous streamlines are highly curved near the trailing edge. Note the location and sign of the vortices formed at the trailing edge.  

(Bohl et al. 2004)
Applications: MTV Measurements in a Motored IC Engine

Optically accessible Ford 4-valve, 4.6L engine

Imaged plane at late compression, 270 CAD

Two instantaneous realizations showing the large cycle-to-cycle variability of the flow field.

Goh, Koochesfahani & Schock (2001)
Applications: Uni-Directional Solidification of Optically Transparent Binary Alloy Analog, NH$_4$Cl

- Uni-directional solidification provides increased resistance to creep rupture and thermal fatigue in the final solidified ingot.
- Solutal and thermal forces produce imperfections in the final solidified ingot in the form of solute-rich channels.

(Lum et al. 2004)
• Velocity vector of plume (79 min into the solidification process)
• Maximum magnitude of velocity is ~7mm/s within the plume

*(Lum et al. 2004)*