Laser Diagnostics in Turbulent Combustion Research

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Lecture 4 – Velocimetry Techniques
Overview and Outline of Lecture

Goal: Providing a Background for Velocimetry in Turbulent Reacting Flows

- Define needs and goals of velocity measurements
- Survey of existing approaches
- Challenges with reacting flow measurements
- Why PIV has become the *de facto* measurement
As we briefly discussed in the last lecture, the flame will interact with the flow turbulence.

Flow turbulence can interact and displace, wrinkle, or extinguish a local flame segment.

These interactions can change flame propagation rates, rates of reaction, rate of heat release, species formation (i.e., NOx and CO), etc.

Thus, we are quite concerned with turbulence-flame interactions or so-called “turbulence-chemistry interactions.”

In this manner, experimentalists target measurements of velocity and its derivatives.

In addition, velocity measurements provide critical boundary conditions for modelers (for simulating the “actual” experiment).
Velocity Measurements - Background

Velocity, $\vec{V}(x, y, z, t)$, is a time-dependent vector with three scalar components (denoted $u$, $v$, $w$)

$$\vec{V} = u\hat{i} + v\hat{j} + w\hat{k} \quad (51)$$

The velocity gradient is described by a 2nd-order tensor:

$$\nabla \vec{V} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) = \begin{pmatrix}
\frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\
\frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\
\frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z}
\end{pmatrix} \quad (52)$$
Vorticity describes the angular motion of the fluid (relative to some local fluid particle’s center of mass).

Vortices (perhaps “eddies” in turbulent flows) and their interactions with flames are quite important.

Vortex stretching (lengthening of vortices) is central to the description of the turbulence energy cascade. Fluid elements are stretched and folded in a non-linear manner which gives rise to the structural topology.

Vorticity is defined as \( \vec{\omega} = \nabla \times \vec{V} \) such that

\[
\vec{\omega} = (\omega_x, \omega_y, \omega_z) = \left( \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z}, \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}, \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right)
\]

Vorticity measurements can also become important in the context of the vorticity transport equation or in the context of enstropy, \( \vec{\omega} \cdot \vec{\omega} \) and its transport equation (measurements can assess certain models of terms).
Vorticity - Importance

DNS study – flame significantly attenuates small-scale turbulence

Products

Reactants

Flow

Bobbitt et al, POF, 2016
Before moving to turbulence, consider a simple interaction of a vortex with a counterflow flame:

Flame extinction (CH PLIF) due to vortex interaction (PIV)

Outwardly rotating eddies create flame wrinkle

The flame attenuates the vorticity

Flame-generated vorticity is formed downstream of flame wrinkle

Steinberg et al, Exp. Fluids, 2008
The interaction between turbulent structures and flame fronts leads to “straining” of the flame.

It can be shown (just a little math) that the strain exerted on a flame does not involve vorticity, but is directly related to the fluid strain rate tensor.

That is, vortices can “wrinkle” the flame, but the fluid strain rate can generate additional flame surface area (both processes act in combination – fluid strain rate generates flame surface area; vortical structures redistribute the flame front into increasingly wrinkled structures).

The strain rate tensor is defined as

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = \left[ \begin{array}{ccc}
\frac{\partial u}{\partial x} & \frac{1}{2} \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) & \frac{1}{2} \left( \frac{\partial w}{\partial z} + \frac{\partial u}{\partial x} \right) \\
\frac{1}{2} \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) & \frac{\partial v}{\partial y} & \frac{1}{2} \left( \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right) \\
\frac{1}{2} \left( \frac{\partial w}{\partial z} + \frac{\partial u}{\partial x} \right) & \frac{1}{2} \left( \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right) & \frac{\partial w}{\partial z}
\end{array} \right]
\]
In reacting flows, the interaction between vorticity and strain rate is a primary mechanism for inter-scale energy transfer via vortex stretching.

Strain rate fluctuations affect heat release and scalar dissipation rate; the latter can be considered a controlling parameter in turbulent non-premixed flame modeling.

Instantaneous strain rates greatly exceed extinction strain rates from steady, laminar flames.

Flame chemistry does not respond to high-frequency strain rate field.

Donbar et al, CNF, 2001
Turbulence-scalar interactions are heavily influenced by the alignment of the principal strain rates and the scalar gradients.

Heat release generates additional effects (dilatation; increases in diffusivity and viscosity; decrease in density) that affect the strain rate field and scalar gradient production.

Coriton and Frank, PCI, 2017
Velocity measurements can be divided into three basic categories: (i) kinematic, (ii) dynamic, and (iii) physical (some overlap with one another).

- **Kinematic** – a specific volume (perhaps very small) of the fluid stream is “marked” and the motion of this marked volume is monitored and recorded. For example, tracer methods (solid, liquids, gas).

- **Dynamic** – An interaction between the flow and measuring probe is monitored. This interaction gives information about the velocity. This interaction can be hydrodynamic, thermodynamic, or magnetohydrodynamic. For example, pitot probe (velocity is function of stagnation pressure ahead of probe).

- **Physical** – Natural or artificially organized processes in the flow whose characteristics depend on velocity are monitored. For example, hot wire (dependence of convective heat transfer on velocity).
You are probably familiar with a **pitot tube** for wind tunnel applications, etc. Simple device to measure stagnation pressure (pitot-static probe also measures static pressure).

It is a small tube with one open and one closed end. The open end faces the flow (as shown below). The other end connects to a pressure recorder.

Bernoulli’s equation is used to approximate the local fluid speed

\[ V = C \left[ \frac{2(P_3 - P_4)}{\rho} \right]^{1/2} = C \left[ \frac{2(P_o - P_\infty)}{\rho} \right]^{1/2} \]

Can be used in incompressible or compressible flow.

Generally not recommended for turbulent flows, but can be used if the tube is smaller than integral scale (and other calibrations).

Only provides mean data and a single point.

Can be used in high-temperature flows with cooling, but not flame temperatures.
You may be familiar with hot wire anemometry for velocity measurements. This is the “backbone” of classical turbulence research.

High-frequency response – enables time-resolved measurements at a point or series of points – produce turbulence spectra!

The hot-wire anemometer (HWA) is based on the dependence of the sensor heat transfer on fluid velocity, temperature, and composition.

The sensor is a thin metal wire (see figure) with a high electrical resistance ($R_w$) such as tungsten, platinum, rhodium, or iridium.

The wire temperature ($T_w$) needs to be substantially higher than the gas temperature ($T_w > T_g$).

The HWA can operate under constant current conditions ($I_w = \text{constant}$) or constant temperature conditions ($T_w = \text{constant}$).

[Diagram of a hot wire anemometer with labels for $u$, $v$, $w$, $\beta$, $\gamma$, and $\delta$.]
A thermal balance can be written as

\[ Q_J = Q_{\text{conv}} + Q_{\text{other}} \]

where \( Q_J = I_2 R_w \) is the Joule heating of the wire, \( Q_{\text{conv}} \) is the heat removed by forced convection (due to the flow) and \( Q_{\text{other}} \) represents the heat losses due to free convection, radiation, and changes in heat capacity of the sensor due to turbulent fluctuations. \( Q_{\text{other}} \) typically is ignored.

The forced convection depends on the heat transfer coefficient which is a function of the flow velocity. Using proper calibration, the output voltage \((E)\) and the flow velocity are related via

\[ \frac{E^2 R_w}{(R_c + R_w)} = (A + B U^n)(T_w - T_g) \]

where \( R_c \) is the resistance connected to the bridge in series with the sensor and A and B are constants determined by the properties of the gas.
Calibrations are carried out in flows of known properties to relate the velocity to the output voltage. Therefore, \( E = \text{fcn}(U) \) and \( S_u = \partial E/\partial U \), which is the derivative of the calibration dependence on the mean velocity \( U \).

Therefore, fluctuations in voltage \((e')\) and velocity \((u')\) values are related via \( e' = u'S_u \) and RMS values are related via \( e'_{\text{RMS}} = S_u u'_{\text{RMS}} \).

With multiple wires that are tilted (X-wire probes), the transverse velocity components are measured. However, the output voltage (for single tilted wire) is dependent on two velocity components.

For example, \((e'_1 + e'_2)^{1/2} = 2(u'^2)^{1/2}S_u\); \((e'_1 - e'_2)^{1/2} = 2(v'^2)^{1/2}S_v\); and \(e'_1'_{\text{RMS}} + e'_2'_{\text{RMS}} = 4S_u S_v <u'v'>\).

By solving the set of three equations and three unknowns, \( u'_{\text{RMS}}, v'_{\text{RMS}}, \) and \(<u'v'>\) are determined.
…so what about reacting flows???

First, you need a material that can withstand flame temperatures.

Most common materials oxidize at high temperatures and form nasty oxides.

However, the biggest problems is that since the hot wire is sensitive to heat transfer, it is very difficult to separate out the velocity and temperature fluctuations!

For non-isothermal flows, the output voltage is simultaneous affected by temperature and velocity fluctuations.

Let’s go back to the single wire. If we introduce the sensitivity coefficient $S_{\text{temp}} = \partial E / \partial T$ associated with $e'_{\text{RMS}} = S_{\text{temp}} T'_{\text{RMS}}$, then we can write:

$$e'_{\text{RMS}} = S_u u'_{\text{RMS}} + S_{\text{temp}} T'_{\text{RMS}} - 2S_{\text{temp}} S_u <u'T'>$$

In order to determine the three turbulence quantities, detailed calibrations are needed and the results are determined by least squares method.
Laser Doppler Velocimetry

One of the oldest laser diagnostic approaches; first introduced in 1964

Overview:  
(i) involves seeding flow with particles  
(ii) illumination of laser light  
(iii) scattered radiation from particles is Doppler shifted  
(iv) measure Doppler shift and infer velocity

Benefits:  
(i) Non-intrusive  
(ii) Used in hostile environments (combustion is no problem)  
(iii) Most accurate velocimetry approach  
(iv) Calibration free  
(v) High data acquisition rates  
(vi) Good spatial resolution

Limitations:  
(i) Complicated and expensive equipment  
(ii) Does require flow seeding with particles  
(iii) Single-point measurement  
(iv) Difficult to acquire measurements near surfaces
LDV operates on the concept of the Doppler effect. We are familiar with this idea in the context of sound; that is, the change in pitch (high to low) as an object moves away from us. This effect also is observed with light.

First, we must note that the particles move relative to both (i) stationary light source and (ii) stationary observer.

Thus, there are two Doppler shifts of the scattered light: (i) relative to illumination and (ii) relative to stationary observer.
Can we directly measure the Doppler shift?

Measure laser frequency and the observed frequency? The Doppler shift is approximately 1 GHz, but the laser frequency is approximately $10^{14}$ Hz (small number from large number → high uncertainty)

To improve measurement, the principle of heterodyning is used – we will now describe the “two-beam approach”

An incident laser beam is split into two components of equal intensity.

The two beams intersect at probe volume.

Particles that pass through the measurement volume scatter light from both beams.

Laser Doppler Velocimetry

- Laser
- BS
- Mirror
- Lens
- Particle
- Detector

\[ \alpha_1 = +\theta/2 \quad \alpha_2 = -\theta/2 \]

\[ \beta_1 = +\theta \quad \beta_2 = -\theta \]
The scattering from both beams contain a Doppler shift, but each is different because orientation to the detector is different ($\alpha$ and $\beta$ are different)

The frequencies of the two scattered beams will be $f + \Delta f_1$ and $f + \Delta f_2$

Since $\Delta f << f$ the scattered light waves are nearly the same frequency

When waves of equal amplitude and almost equal frequency are superimposed, there is a modulation of the signal or a “beat”. The beat frequency is $\frac{1}{2}$ of the difference between the two original frequencies

The signal recorded on the detector has a signal with a beat frequency of $|\Delta f_1 - \Delta f_2|/2$, which is the desired Doppler frequency
The Doppler frequencies for each beam can be computed as

$$\left| \frac{\Delta f_1 - \Delta f_2}{2} \right| = \frac{2V}{\lambda} \sin \theta$$

where $V$ is $\vec{V} \cos \alpha$, which is the velocity component orthogonal to the bisector of the two beams.
Laser Doppler Velocimetry

- One additional way to interpret the signal collected on the detector...

- Since the two beams are from the same laser source, they are mutually coherent and thus the scattering from one beam is coherent with the scattering from the other beam.

- Crossing the two beams will generate an interference pattern. The interference pattern are alternating zones of constructive and destructive interference (bright and dark).
The fringe spacing is

\[ d_f = \frac{\lambda}{2 \sin \theta} \quad (57) \]

As particles cross the interference patterns, the recorded intensity is modulated based on their interaction with the alternating light and dark regions.

A particle with velocity component perpendicular to the fringes crosses at a rate of

\[ f = \frac{V}{d_f} = \frac{2V \sin \theta}{\lambda} \]

Laser Doppler Velocimetry
Laser Doppler Velocimetry

- Two get more than one velocity component, you need 2 or 3 laser systems and corresponding number of detectors (system can get complex)
- However, measurement is still at a single point in space...
- Field measurements are highly desired and thus over the past 30 years there has been substantial efforts in planar measurements ("imaging") and more recently in volumetric measurements

http://www.newvistaresearch.com
Majority of measurements are used for single-point information (but can be time resolved!) Excellent for turbulence statistics!

By translating measurements, the mean and RMS fields can be determined

Schneider et al., CNF, 2003

Weigand et al., CNF, 2005
Summary of LDV

- LDV uses a continuous wavelength laser focused to a small probe volume in space. It is a “0D” measurement
- LDV takes advantage of the Doppler effect to measure velocity
- LDV is very accurate; most accurate measurement for turbulence statistics
- LDV can be used in a flame; seed particles must survive flame conditions
- Measurements can be performed at high sampling rates; can deduce single-point spectra
- Multiple velocity components can be measured simultaneously – need multiple wavelengths (i.e., 488 nm and 514 nm of Ar\(^+\); 532 nm Nd:YAG; 632 He-Ne)
- A major “step” is signal processing during collection (not discussed here!). This is critical to properly deduce velocity and to avoid several biases.
Currently, there are three primary “field techniques” for velocity measurements; that is, velocimetry approaches that give velocity measurements at several simultaneous spatial points (I’ll include 1D – 3D):

(i) Planar Doppler Velocimetry (PDV)
(ii) Molecular Tagging Velocimetry (MTV)
(iii) Particle Imaging Velocimetry (PIV) – next lecture
(iv) Optical Flow – “new”; discussed in a few lectures

http://www.metrolaserinc.com/technologies/planar-doppler-velocimetry/
http://www.psp-tsp.com
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MTV(HTV)

Ribarov, 2004
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Lecture 5 – Particle Imaging Velocimetry: Part 1 – Basics and Operating Principles
Overview and Outline of Lecture

Goal: Providing a Background for Particle Imaging Velocimetry (PIV)

- Overview of PIV
- Instrumentation and General Approach
- Tracer Particles – Proper Tracking and Light Scattering
- Introduction to Extensions beyond Planar PIV
Particle Imaging Velocimetry

... a bit of history

- Long history of determining motion from change of particles, debris, smoke, etc. in “photographs”
- Quantitative velocity data from particle streak photos (1930)
- Laser speckle velocimetry – Young’s fringes (1977)
- First paper on “PIV” – Adrian (1984)
- First commercial system – TSI (1988)
Value of PIV

Conventional methods (HWA, LDV)
- Single-point measurement!
- Must transverse measurement (time consuming)
- Primarily statistics
- Limited spatial gradients (if any)

PIV
- Whole field method
- Instantaneous flow field and structural topology
- Large domain of spatial gradients
Principle of PIV Measurement

- Flow is seeded with tracer particles
- Illuminated by two successive laser pulses separated by $\Delta t$
- Double exposure of particle field provides 2D displacement of particles
- Images are analyzed over a series of grids (interrogation windows) throughout measurement plane
- Interrogation windows need to be large enough for sufficient number of particle images, but small enough such that velocity is uniform within window
- Displacement (typically) is computed through cross correlation
- Not too many things change when operating in reacting flows as opposed to non-reacting flows, although there are some challenges as discussed below

https://www.dantecdynamics.com/measurement-principles-of-piv
Summary of PIV Measurement

- Laser source
- Light sheet optics
- Camera
- Tracer particles

Measurement settings ($\Delta t$)
- Software/correlation
- Post-processing

https://www.dantecdynamics.com/measurement-principles-of-piv
Light Source, Optics, and Camera

- Dual cavity Nd:YAG laser
- Light sheet optics
- Measurement volume
- CCD camera

Frame 1: $t = t_0$
Frame 2: $t = t_0 + \Delta t$
Divide image pair into interrogation windows
Select small sub-region: quasi-uniform particle motion
Compute displacement of particles and velocity vectors
Repeat!!!
PIV Laser

- Nd:YAG is most common solid-state laser for PIV
- Frequency-doubled output is at 532 nm
- Can generate short-duration laser pulses (5-10 ns) that “freezes” flow
- Typical operation is at 10-30 Hz
- Dual cavity configuration allows short time intervals ($\Delta t$) between laser pulses
The optical setup for planar (or stereoscopic) PIV is fairly straightforward.

I’ll talk specifically about tomographic PIV later.

The Nd:YAG output (two spatially overlapping beams, but offset in time by $\Delta t$) needs to be formed into a laser sheet(s) to illuminate the measurement domain and scatter light from particles.

The light sheets are formed by a combination of spherical and cylindrical lenses. Concave cylindrical lens expands beam in one direction, while convex spherical lens focuses expanding beam to a thin waist. The order of the spherical and cylindrical lenses can be changed based on a particular setup.

A common setup is a “diverging” sheet.
Light Source and Optics

Upper view

Side view

Laser sheet thickness

Laser sheet height (H)

\[ L = f_1 + f_2 = f_1 - |f_2| \]

\[ \frac{H}{d} = \frac{|f_1|}{|f_2|} \]

Thin laser sheet – better spatial resolution, but out-of-plane particle movement

Thick laser sheet – poorer spatial resolution and decrease in S/N, but fewer lost particles
Camera

What do we need in a PIV camera?

- Record multiple images (at least 2) in consecutive frames [thought question – what would 3 or more give you?]

- High dynamic range and spatial resolution (large number of small pixels) [the spatial resolution of modern CCD arrays is at least two orders of magnitude lower than photographic film!]

- Low noise; high sensitivity

Single frame/ multi-exposure

Multi-frame/ multi-exposure

Ambiguity in the direction of the flow
Camera gating

Laser pulsing

Inter-pulse separation (Δt)

Why so long?

Where can this be a problem?

A common method for acquiring multiple exposures on multiple frames with a single camera is referred to as frame straddling.
Camera

CCD Camera: Frame straddling technique

Transfer time: → pixel to frame storage area: **500 ns**
→ frame storage area to PC: **33 ms**

1000 pixels
For an optically homogeneous fluid, motion cannot be observed directly.

- Tracers must be added to fluid; serve as scattering sites for the laser light.
- The fluid motion is represented as a particle displacement field; that is, the velocity is inferred (velocity is measured indirectly).
- There is error between actual fluid velocity and inferred velocity from particle displacement.

Particles

What do we assume about the tracer particles in PIV?

- Particles follow fluid motion and do not alter fluid motion
- Tracers are distributed homogeneously (needed to obtain an unbiased estimate of the displacement field)
- Uniform displacement within interrogation window


\[ \bar{D}(\bar{X}; t', t'') \approx \int_{t'}^{t''} \bar{u}[\bar{X}(t), t] dt \]
Particles

*Why do we assume uniform displacement of particles?

- **Physical** – non-uniform displacement leads to internal gradients within the interrogation window. With gradients, derived velocity would not be characteristic of all (or any) of the velocity inside of the interrogation window.

- **Processing** – displacements inside of interrogation window are determined using spatial correlation (more on this later).

  Spatial correlation is an estimate of the two-point ensemble correlation. Spatial correlation and the two-point ensemble correlation are identical for a statistically stationary, ergodic process. This is the case under the assumption that the displacement field is uniform within the interrogation window.
Particles

- Tracer should be small enough to follow flow, BUT large enough to effectively scatter light.
- The tracing ability and the dispersion of the particles depends on the aerodynamic characteristics of the particles AND the continuum medium.
- The visibility (light scattering) depends on the scattering characteristics of the particles.

Light scattering is characterized by the scattering cross section, $C_s$.

$C_s$ is defined as the ratio of the total scattered power, $P_s$ to the incident laser intensity, $I_0$

\[
C_s = \frac{P_s}{I_0}
\]  

(refractive index $n = 1.6$).
Light Scattering of Particles

\[ \Delta \text{Scattering cross section} \]

<table>
<thead>
<tr>
<th>Diameter ( d_p )</th>
<th>Scattering cross section ( C_s )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecule</td>
<td>( C_s \propto \left( \frac{d_p}{\lambda} \right)^6 ) ( \approx 10^{-33} \text{m}^2 )</td>
</tr>
<tr>
<td>1( \mu \text{m} )</td>
<td>( C_s \propto \left( \frac{d_p}{\lambda} \right)^4 ) ( \approx 10^{-12} \text{m}^2 )</td>
</tr>
<tr>
<td>10( \mu \text{m} )</td>
<td>( C_s \propto \left( \frac{d_p}{\lambda} \right)^2 ) ( \approx 10^{-9} \text{m}^2 )</td>
</tr>
</tbody>
</table>
Light Scattering of Particles

The Lorenz-Mie solution to Maxwell’s equations describes scattering of an E-M plane wave by a homogeneous sphere.

“Mie scattering” is more broadly used to describe the situation where the size of the scattering particles is $O(\lambda)$ [if $d_p << \lambda$, the Rayleigh scattering approximation is valid].

Light Scattering by an oil particle in air when refractive index $n \sim 1.4$.

1µm diameter

10µm diameter
Particle Tracking Characteristics

- Tracer particles are a critical consideration for both LDV and PIV.
- Again, the choice of particles is always dictated by a compromise between flow tracking and scattering efficiency.
- Tracking depends on: (1) particle shape – assumed spherical, so particle diameter, $d_p$, (2) particle density, $\rho_p$, (3) fluid density, $\rho_f$, and (4) fluid viscosity, $\mu$ or $\nu$.
- We will start with Newton’s law governing the motion of a single particle:
  \[ m_p \ddot{a} = \sum_i F_i \]  \[ \rho_p \frac{\pi d_p^3}{6} \frac{d\vec{v}_p}{dt} = \sum_i \vec{F}_i \]

- Let’s also define the fluid mass taken up by the particle:
  \[ m_f = \rho_f \frac{\pi d_p^3}{6} \]
Particle Tracking Characteristics

We need to include “all” forces experienced by the particle

\[ m_p \frac{d\vec{v}_p}{dt} = 3\pi \mu d_p (\vec{u} - \vec{v}_p) + \frac{1}{2} m_f \left[ \frac{d\vec{u}}{dt} - \frac{d\vec{v}_p}{dt} \right] + \frac{m_f}{\rho_f} \nabla p - m_p \left( 1 - \frac{\rho_f}{\rho_p} \right) \vec{g} \]  

(61)

- LHS is the acceleration of the particle
- RHS: (1) viscous drag according to Stokes Law
- (2) Resistance of an inviscid fluid to the acceleration of the sphere (“added mass”) – potential flow theory
- (3) Acceleration of particle leads to a pressure gradient in vicinity of particle. This is the force due to the pressure gradient
- (4) \( \rho_f \neq \rho_p \), so there are buoyancy effects

We have neglected (i) non-linear drag (only needed for high-speed flows), (ii) Basset history effects – resistance cause by unsteadiness in flow field.
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Particle Tracking Characteristics

\[ m_p \frac{d\vec{v}_p}{dt} = 3\pi \mu d_p \left( \vec{u} - \vec{v}_p \right) + \frac{1}{2} m_f \left[ \frac{d\vec{u}}{dt} - \frac{d\vec{v}_p}{dt} \right] + \frac{m_f}{\rho_f} \nabla p - m_p \left( 1 - \frac{\rho_f}{\rho_p} \right) \vec{g} \]

- Inertia
- Viscous drag
- Added mass
- Pressure gradient
- Buoyancy

Some of these terms can be neglected if the particle Reynolds number is small (\( Re_p < 1 \); Stokes flow)

\[ Re_p = \frac{\rho_f V d_p}{\mu} = \frac{V d_p}{\nu} \]  \( \text{(62)} \)

Example: consider a 1-µm particle in air with fluid velocity of 10 m/s

\[ Re_p = (10 \text{ m/s}) \times (1 \times 10^{-6} \text{ m}) / (1.5 \times 10^{-5} \text{ m}^2/\text{s}) = 0.67 \]

Even for cases where \( Re_p > 1 \), we can still assume Stokes linear drag

Stokes’ drag law gives a conservative estimate of tracking ability; actual drag tends to be higher
Particle Tracking Characteristics

- We will only consider viscous drag
  \[ m_p \frac{d\mathbf{v}_p}{dt} = 3\pi\mu d_p (\mathbf{u} - \mathbf{v}_p) \]

- We will define \( v_p \) as the magnitude of \( \mathbf{v}_p \) and \( U \) as the magnitude of \( \mathbf{u} \)

- How does a particle respond to a step change in velocity?
  \[ \frac{d\mathbf{v}_p}{dt} = \frac{3\pi\mu d_p}{m_p} (\mathbf{u} - \mathbf{v}_p) \]
  \[ \frac{dv_p}{dt} = \frac{18\mu}{\rho_p d_p^2} (U - v_p) \quad \text{In one dimension} \]
  \[ \frac{dv_p}{dt} = \frac{1}{\tau_p} (U - v_p); \quad \tau_p = \frac{\rho_p d_p^2}{18\mu}; \quad \tau_p = \text{characteristic particle time} \]

- Integrate…
  \[ v_p = U + C_1 e^{(-t/\tau_p)} \]
Apply initial conditions (ICs)

\[ u = \begin{cases} 
0 & \text{for } t < 0 \\
U & \text{for } t \geq 0 
\end{cases} \]

\[ v_p = \begin{cases} 
0 & \text{for } t = 0 \\
\text{fcn}(U) & \text{for } t \geq 0 
\end{cases} \]

Substitution of \( v_p = 0 \) at \( t = 0 \) yields \( C_l = -U \) and

\[ \frac{v_p}{U} = 1 - e^{(-t/\tau_p)} \quad (63) \]

The particle response time should be evaluated against a relative fluid mechanic time scale

Stokes number, \( St \), is the ratio of the particle response time to a characteristic fluid mechanic time scale

\[ St = \frac{\tau_p}{\tau_f} \quad (64) \]
Particle Tracking Characteristics

- Stokes number, $St$, is the ratio of the particle response time to a characteristic fluid mechanic time scale
  \[ St = \frac{\tau_p}{\tau_f} \]  
  (65)

- $St$ determines the degree of coupling between particle and fluid

- $St \rightarrow 0$ the particles behave like tracers

- $St \rightarrow \infty$ the particles are completely unresponsive to the fluid flow.

- A common value of $\tau_f$ is the Kolmogorov time scale, which is the turnover time for the smallest turbulent eddies, $\tau_f = \tau_k$

- A common recommendation is that particles, which exhibit $St < 0.1$, sufficiently track the fluid mechanics
An alternative method was proposed by Melling (1997)

Assuming \( \rho_p >> \rho_f \), Eq. (61) can be written as

\[
m_p \frac{d\vec{v}_p}{dt} = -C(\vec{v}_p - \vec{u})
\]

where \( C \) is a characteristic frequency of the particle motion, which from the previous analysis is

\[
C = \tau_p^{-1} = \frac{18\mu}{\rho_p d_p^2}
\]

Under the conditions of homogeneous, stationary turbulence with particles smaller than the smallest length scales of turbulence; \( \rho_p >> \rho_f \), and using utilizing energy spectrum for fully developed pipe flow

\[
\frac{\bar{u}_p^2}{\bar{u}_f^2} = \frac{1}{(1 + \omega_c / C)}; \quad f_c = \frac{\omega_c}{2\pi}
\]

(66)

where \( \omega_c \) is the angular frequency of turbulence and \( f_c \) is the turbulence frequency of interest.
A criterion for acceptable flow tracking must be chosen.

Using $\frac{\overline{u_p^2}}{\overline{u_f^2}} = 0.95$ as a criteria, then the response of a particle of any size can be determined.

Example 1: consider a 1-µm glass bead in air

$$C = 18 \times (1.5 \times 10^{-5} m^2/s) \times (2000 \text{ kg/m}^3)^{-1} \times ((1 \times 10^{-6} m)^2)^{-1} = 1.35 \times 10^5 \text{ Hz} \rightarrow$$

$$\omega_c = 7105 \text{ Hz} \rightarrow f_c = 1130 \text{ Hz}$$

The particle can effectively follow a fluid time scale of ~ 1 ms.

If the particle diameter is 0.5 µm then $f_c = 5.4 \times 10^5 \text{ Hz}$, such that the particle can follow a fluid time scale of 100 µs.

(Melling, 1997)
Dimensionality

- Traditional **planar PIV** is often referred to as 2D2C (two-dimensional measurement and two components, \(u, v\))
yield: \(2/3 u_i; 4/9 \partial u_i/\partial x; 4/9 S_{ij}; 1/3 \omega_i\)

- **Stereoscopic PIV** uses two cameras arranged in a stereo configuration to measure all 3 velocity components, \(u, v, w\)
yield: \(3/3 u_i; 5/9 \partial u_i/\partial x; 4/9 S_{ij}; 1/3 \omega_i\)

- **Tomographic PIV** uses 3 or more cameras to measure velocities in a “thin volume”
yield: \(3/3 u_i; 9/9 \partial u_i/\partial x; 9/9 S_{ij}; 3/3 \omega_i\)

- If planar and stereoscopic PIV are performed at high sampling rates, Taylor’s hypothesis (TH) can be applied to yield additional terms (with the normal caveats to where TH can be applied)

\[
\frac{\partial w}{\partial t} = - \langle u \rangle \frac{\partial w}{\partial x}
\]

Increasing complexity and cost

(Scarano, 2013)
Stereoscopic PIV uses two cameras (+ laser sheet) to record two distinct off-axis views of the same region of interest.

Scheimpflug condition should be satisfied (The lens plane, the object plane, and the image plane for each cameras has to intersect in a common line.)

https://velocimetry.net/stereo_principles.htm
Tomographic PIV was first introduced by Elsinga et al in 2005.

“Tomo PIV” uses three or more cameras (+laser slab) to record multiple distinct off-axis views of the same region of interest.

Scheimpflug condition should be satisfied for all cameras.

3D volumetric reconstruction of the particle fields is required.

Processing details are discussed in next lecture.

(Elsinga, 2005)
Laser Diagnostics in Turbulent Combustion Research

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Lecture 6 – Particle Imaging Velocimetry: Part 2 – Analysis, Examples, and Limitations
Overview and Outline of Lecture

Goal: Describe Data Analysis and Measurement Limitations for Particle Imaging Velocimetry (PIV)

- Effects of Experimental Parameter Variation
- Cross Correlation Analysis
- PIV Design Rules
- Extensions to Stereoscopic and Tomographic PIV
- Limitations to PIV
- Challenges in Reacting Flows
Quick definition of terminology:

“Particle field image” or “ensemble of particle images”

“Particle image”
Particle Seed Density

How dense should seeding be?

We will define two terms: (i) source density \( N_s \) and the image density \( N_I \).

Source density:

\[
N_s = \frac{C \Delta z_0 \pi}{m^2} \frac{d_i^2}{4}
\]

The particle image diameter is defined as

\[
d_i = \left( m^2 d_p^2 + d_{blur}^2 \right)^{1/2}
\]

\[
d_{blur,diff} = 2.44(1+m) \lambda FN
\]

The source density \( N_s \) represents what “type” of image that is recorded:

- \( N_s < 1 \) – individual particle image
- \( N_s > 1 \) – speckle pattern
The image density is defined as

$$N_I = \frac{C \Delta z_0}{m^2} D_i^2$$  \hspace{1cm} (69)

- $C$: tracer concentration [m$^{-3}$]
- $\Delta z_0$: light-sheet thickness [m]
- $m$: image magnification [-]
- $D_i$: interrogation-spot diameter [m]

The image density represents the mean number of particles in an interrogation window.

For PIV, $N_I > 10-15$ (for 16 x 16 pixels this is 0.05 ppp). We will discuss this in a moment.
Particle Seed Density

How dense should the seeding be?

\[ N_I = \frac{C\Delta z^o}{m^2} D_i^2 \]

Low image density \( N_I = O(1) \) \implies \text{Particle tracking velocimetry}

Fluid motion is determined by “tracking” a pattern of particles

If \( N_I \) is low, the distance between the particles is greater than the particle displacement

Can evaluate displacement of individual particles

Information from image is low
**Particle Seed Density**

- How dense should the seeding be?

\[ N_I = \frac{C \Delta z^2}{m^2} D_i^2 \]

- High image density \( N_I \gg 1 \)  \( \Rightarrow \) **Particle imaging velocimetry**

- As \( N_I \) increases the particle displacement is greater than the spacing between the particles
- Particles cannot be matched unambiguously
- Need a statistical approach for “pattern matching”
- Information from image is higher

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Particle Seed Density

- When the image density is high \((N_I >> 1)\), the particle images cannot be matched by proximity.

- Can use correlation analysis

- Consider a single particle - If you determine the distance histogram of all possible matches, all have equal probability, BUT only one is correct

- If you do this for all particles, only matching particle pairs will “add up”, whereas random uncorrelated pairs will not.

- A sharp peak appears, which is the displacement histogram of entire particle image pattern
Correlation for Estimating Particle Motion

First, the image intensities are separated into:

\[ I = \bar{I} + I' \quad \text{or} \quad I' = I - \bar{I} \]

where \( \bar{I} \) is the mean intensity of an interrogation window and \( I' \) is the intensity fluctuation.

The correlation coefficient is computed as

\[
R(i, j) = \frac{\sum_{k=1}^{B_x} \sum_{l=1}^{B_y} (I_a(k,l) - \bar{I}_a)(I_b(k+i,l+j) - \bar{I}_b)}{\left(\sum_{k=1}^{B_x} \sum_{l=1}^{B_y} (I_a(k,l) - \bar{I}_a)^2\sum_{k=1}^{B_x} \sum_{l=1}^{B_y} (I_b(k+i,l+j) - \bar{I}_b)^2\right)^{1/2}}
\]  \hspace{1cm} (70)

\[
\bar{I}_a = \frac{1}{B_x B_y} \sum_{k=1}^{B_x} \sum_{l=1}^{B_y} I_a(k,l)
\]

In this definition, \( a \) and \( b \) represent two different images; \( (k,l) \) represent the \( k^{th} \) and \( l^{th} \) pixel; \( B_x \) and \( B_y \) are the total number of pixels in the x and y directions of the interrogation window.
Correlation for Estimating Particle Motion

- Why compute the correlation of the intensity fluctuation?
- The correlation coefficient can be separated into three different terms

\[ R(i, j) = R_C(i, j) + R_F(i, j) + R_D(i, j) \]

- \( R_C \) -- mean background correlation
- \( R_F \) -- correlation between mean intensity and intensity fluctuations (noise and particles)
- \( R_D \) -- correlation of image fluctuations (particles and particles)

- When mean intensity is substracted, \( R_C = R_F = 0 \)
Correlation for Estimating Particle Motion

- Shift window with respect to the first (typically 16x16 or 32x32 pixels) and calculate “match” (correlation coefficient)

\[
R(i,j) = \frac{\sum_{k=1}^{B_x} \sum_{l=1}^{B_y} (I_a(k,l) - \bar{I}_a)(I_b(k+i,l+j) - \bar{I}_b)}{\left[ \sum_{k=1}^{B_x} \sum_{l=1}^{B_y} (I_a(k,l) - \bar{I}_a)^2 \sum_{k=1}^{B_x} \sum_{l=1}^{B_y} (I_b(k+i,l+j) - \bar{I}_b)^2 \right]^{1/2}}
\]

- Repeat to find best estimate...

Bad match:
sum of product of intensities low

Good match:
sum of product of intensities high
Correlation for Estimating Particle Motion

- Select an interrogation window (pattern) in 1\textsuperscript{st} image, P1
- Select a domain in 2\textsuperscript{nd} image where the pattern matching between the 1\textsuperscript{st} and 2\textsuperscript{nd} image is to be performed (P1 vs P2)
- Compare P1 to ALL P2s in the domain – the two patterns with maximum similarity are identical
- Displacement between two centers of the two patterns is the average velocity of the interrogation window
- The evaluation of similarity is the cross correlation coefficient.
- This is SLOW – method needs \((NM)^2\) computation time, where N and M are the width and height of the patterns.
- This has to be repeated for all IW’s in all images – too SLOW!!!
Correlation for Estimating Particle Motion

- Computation via FFT – reduces the computation time
- For each interrogation window, do the following:

\[
R(i,j) = \text{FFT}^{-1} \left[ F(s,t) \cdot G^*(s,t) \right]
\]

\[
(\Delta x, \Delta y) \rightarrow (u,v)
\]
Influence of \( N_I \)

\[
N_I = \frac{C \Delta z_0}{m^2} D_i^2
\]

- \( C \): tracer concentration [m\(^{-3}\)]
- \( \Delta z_0 \): light-sheet thickness [m]
- \( m \): image magnification [-]
- \( D_i \): interrogation-spot diameter [m]

\( N_I = 5 \) \hspace{1cm} \( N_I = 10 \) \hspace{1cm} \( N_I = 25 \)

- More particles: better signal-to-noise ratio
- Unambiguous detection of peak from noise: \( N_I = 10 \) (average), minimum of 4 per area in 95% of areas (number of tracer particles is a Poisson distribution)
- PTV: 1 particle used for velocity estimate; error \( e \)
- PIV: error \( \sim e/\sqrt{N_I} \)

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Influence of In-plane Displacement

\[ \Delta X / D_I = 0.00 \]
\[ F_I = 1.00 \]
\[ \begin{array}{cccc}
0.28 & 0.56 & 0.36 & 0.85 \\
0.56 & 0.36 & 0.16 & \\
\end{array} \]

\[ R_D \sim N_I F_I \Rightarrow F_I(\Delta X, \Delta Y) = \left( 1 - \frac{\Delta X}{D_I} \right) \left( 1 - \frac{\Delta Y}{D_I} \right) \]

Recommendation: X,Y-Displacement < \( \frac{1}{4} \) interrogation window
Influence of Out-of-Plane Displacement

\[
\frac{\Delta Z}{\Delta z_0} = 0.00
\]
\[
F_O = 1.00
\]

\[
\frac{\Delta Z}{\Delta z_0} = 0.25
\]
\[
F_O = 0.75
\]
\[
\frac{\Delta Z}{\Delta z_0} = 0.50
\]
\[
F_O = 0.50
\]
\[
\frac{\Delta Z}{\Delta z_0} = 0.75
\]
\[
F_O = 0.25
\]

\[
R_D \sim N_I F_I F_O \Rightarrow F_O (\Delta z) = 1 - \frac{|\Delta z|}{\Delta z_0}
\]

Recommendation: Z-Displacement < ¼ of light sheet thickness (\(\Delta z_0\))
PIV “Design Rules”

- image density \( N_I > 10 \)
- in-plane motion \( |\Delta X| < \frac{1}{4} D_I \)
- out-of-plane motion \( |\Delta z| < \frac{1}{4} Dz_0 \)
- spatial gradients \( m|\Delta u|\Delta t < d_i \)

Obtained by Keane & Adrian (1992) using synthetic data

* It should be noted that these “rules” are actually guidelines and they are more applicable for traditional PIV w/o consideration for multi-pass algorithms and/or overlapping/deforming interrogation windows
Uncertainty and Dynamic Range

The following analysis follows from Adrian (1997) assuming diffraction-limited imaging and Gaussian noise:

Uncertainty of velocity component \( u_i \) is

\[
\sigma_{u_i} = \frac{\sigma_{\Delta x}}{\Delta t}
\]  \hspace{1cm} (71)

\( \sigma_{\Delta x} \) is the uncertainty of the particle displacement in the fluid (object) plane; related to uncertainty in the image plane (\( \sigma_{\Delta x} \)) via:

\[
\sigma_{\Delta x} = \frac{\sigma_{\Delta x}}{m}
\]  \hspace{1cm} (72)

Adrian suggests that \( \sigma_{\Delta x} = c_\tau d_\tau \), where \( c_\tau \) is a constant particular to a given PIV algorithm characterizing the ability to determine the displacement between images (typically 1 – 10%) and \( d_\tau \) is the recorded image diameter:

\[
d_\tau^2 = d_i^2 + d_r^2
\]  \hspace{1cm} (73)

*R. J. Adrian, "Dynamic ranges of velocity and spatial resolution of particle image velocimetry," Measurement Science and Technology, vol. 8, no. 12, p. 1393, 1997:
Uncertainty and Dynamic Range

\[ d_t^2 = d_i^2 + d_r^2; \quad d_i \text{ is the diameter of the optical image and } d_r \text{is the resolution of the camera} \]

The optical image diameter is given by

\[ d_i = \left( m^2 d_p^2 + d_{\text{blur,diff}}^2 \right)^{1/2} \quad (68) \]

\[ d_{\text{blur,diff}} = 2.44(1 + m)\lambda FN \quad (38) \]

Thus, the uncertainty can be written as

\[ \sigma_{u_i} = \frac{c_t \sqrt{m^2 d_p^2 + d_{\text{blur,diff}}^2 + d_r^2}}{\Delta t} \quad (74) \]

*R. J. Adrian, "Dynamic ranges of velocity and spatial resolution of particle image velocimetry," Measurement Science and Technology, vol. 8, no. 12, p. 1393, 1997:
From these expressions the measurement dynamic range can be estimated.

Assume that the uncertainty of the velocity measurement is the smallest resolvable velocity fluctuation (fluctuations below this are below noise floor).

The dynamic velocity range (DVR) is defined as the ratio of the largest possible velocity \( u_{\text{max}} \) to the velocity uncertainty

\[
DVR = \frac{u_{\text{max}}}{\sigma_u} = \frac{\Delta x_{p,\text{Max}}/\Delta t_{\text{PIV}}}{c_\tau d_\tau/\Delta t_{\text{PIV}}}
\]  

(75)

The maximum particle displacement \( \Delta x_{p,\text{Max}} \) is estimated as 1/4th of the largest interrogation window per the “design rules” discussed above.

*R. J. Adrian, "Dynamic ranges of velocity and spatial resolution of particle image velocimetry," Measurement Science and Technology, vol. 8, no. 12, p. 1393, 1997:
Dimensionality

Traditional **planar PIV** is often referred to as 2D2C (two-dimensional measurement and two components, u, v) yield: $\frac{2}{3} u_i; \frac{4}{9} \frac{\partial u_i}{\partial x_i}; \frac{4}{9} S_{ij}; \frac{1}{3} \omega_i$

**Stereoscopic PIV** uses two cameras arranged in a stereo configuration to measure all 3 velocity components, u, v, w yield: $\frac{3}{3} u_i; \frac{5}{9} \frac{\partial u_i}{\partial x_i}; \frac{4}{9} S_{ij}; \frac{1}{3} \omega_i$

**Tomographic PIV** uses 3 or more cameras to measure velocities in a “thin volume” yield: $\frac{3}{3} u_i; \frac{9}{9} \frac{\partial u_i}{\partial x_i}; \frac{9}{9} S_{ij}; \frac{3}{3} \omega_i$

If planar and stereoscopic PIV are performed at high sampling rates, Taylor’s hypothesis (TH) can be applied to yield additional terms (with the normal caveats to where TH can be applied)

\[ \frac{\partial w}{\partial t} = -<u> \frac{\partial w}{\partial x} \]

(Scarano, 2013)
Stereoscopic PIV

- Scheimpflug condition should be satisfied (The lens plane, object plane and, the image plane for each cameras has to intersect in a common line)

- This leads to a strong perspective distortion

- This is corrected using “mapping functions” (typically 2nd order) which is a matrix that transforms the pixel coordinate system into a real world coordinate system

- Stereo PIV requires a model of how objects in space are mapped onto the sensor (planar projection model)

- Model parameters come from calibration (i.e., calibration targets are needed)

- Field-of-view (stereo evaluation) is available only where covered by both cameras (each image is a trapezoidal region)

(Prasad, 2000)

https://velocimetry.net/stereo_principles.htm
Stereoscopic PIV – Procedure/Algorithm

- “Left” and “Right” camera images recorded simultaneously
- Conventional PIV processing is performed on each image – produces two, 2D (2C) vector maps, one as seen from “left” and one as seen from “right.”
- Using the camera model (including calibration parameters), the points in the interrogation grid are mapped from object plane onto the “left” and “right” image planes (camera sensor)
- 2D vector maps are re-sampled in new, common (i.e., bilinear interpolation)
- The “left” and “right” results are combined – generates one 2D (3C) vector map
- How? With a 2D displacement as seen from both the “left” and “right” camera views, but at the same points in physical space, the true 3D displacement is estimated (3 unknowns; 4 equations) using least squares methodology (its just trigonometry)
Planar projection model of stereoscopic PIV is replaced with a more general 3D measurement domain description.

Laser sheet is replaced with a “slab”. Thickness typically is ¼ of width of FOV, but can vary (one needs more laser energy!)

Particle images need to be in focus – requires relatively large depth-of-field.

3D representation of the particle field is reconstructed from a small number of projections. Commonly done using multiplicative algebraic reconstruction technique or MART.

Calibrations (relating object and image planes) are similar to those in stereoscopic PIV, but are obtained at several depths and the precision requirements is much stricter!

With a reconstructed pair of particle volumes, 3D cross correlation is performed to obtain motion.
PIV Limitations

While PIV has been a significant tool in fluid mechanics research, the technique has some inherent limitations:

- Non-dense estimate of the velocity field – one velocity vector per interrogation window. Spatial resolution of velocity measurement is more than one order-of-magnitude less than that of detector.
- Spatial resolution limitations cause problems in turbulent flows with strong gradients (i.e., gradients exist within interrogation window).
- Local large gradients can lead to unequal particle displacements. This leads to multiple correlation peaks – bias error.
- Calculated vector may not represent the local flow.
While PIV has been a significant tool in fluid mechanics research, the technique has some inherent limitations:

- Accuracy of velocity gradients and gradient quantities are affected by spatial resolution.
- PIV velocity field can be considered as a low-pass filtered representation of the true velocity field.
- Derivative quantities can be underestimated.

2D DNS data
Challenges in Reacting Flows

- A big challenge in combustion environments is particle seeding.
- Tracer particles must survive and not chemically react.
- Ceramics (TiO$_2$, SiO$_2$, etc.) are suited for this.
- Ceramic particles tend to cluster to larger sizes – ability to follow flow may diminish.
- Because of density gradients, uniform seeding can be a challenge.

Non-reacting turbulent jet  
Turbulent non-premixed jet flame
Challenges in Reacting Flows

Because of density gradients, uniform seeding can be a challenge.

Premixed flame
https://en.wikipedia.org/wiki/Particle_image_velocimetry

- Additional issues include flame luminosity (discussed earlier) and thermophoretic forces.
- Thermophoresis describes particle movement due to a thermal gradient (high to low temperature). This is usually minor in turbulent flames.
Challenges in Reacting Flows

Thermophoresis describes particle movement due to a thermal gradient (high to low temperature). This is usually minor in turbulent flames.
Examples of PIV in Turbulent Flames
Laser Diagnostics in Turbulent Combustion Research

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Lecture 7 – Emerging and Alternative Velocimetry Approaches

BONUS LECTURE

Turbulence and Combustion Research Laboratory
Overview and Outline of Lecture

Goal: Introduce Recent High-Resolution Velocimetry Approaches

- The “Push” for Higher Resolution
- “Shake-the-box” approach (non-reacting)
- Optical Flow Methods
Laser Diagnostics in Turbulent Combustion Research

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Lecture 8 – Basic Spectroscopy

Turbulence and Combustion Research Laboratory
Goal: Provide an Overview of the Fundamentals of Spectroscopy

- Brief Description of Energy Levels
- Spectroscopy Fundamentals
- Discussion of Rotational, Vibrational, and Electronic Transitions
- Preparation for Laser-Induced Fluorescence
An Introduction to the Interaction of Light and Matter

- **Spectroscopy:** Science which uses absorption/emission of electromagnetic radiation to deduce atomic/molecular properties.

- A large number of “combustion diagnostics” are spectroscopic based.

- **Quantum Mechanics (QM):** we will accept QM rules such as (1) Quantized (discrete) energy levels and (2) “allowed transitions”

- **Molecules** have **electronic, vibrational, and rotational** energy

- We describe the energy of a diatomic molecule as the sum of electronic, vibrational, and rotational energies

\[ E_{\text{int}} = E_e + E_{\text{vib}} + E_{\text{rot}} \]

- Molecules can only rotate and vibrate at discrete frequencies (energies)
Energy Levels

\[ E_{\text{int}} = E_e + E_{\text{vib}} + E_{\text{rot}} \]

Potential energy curve for 1 electronic state

Transition between electronic states
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\[ E_{\text{int}} = E_e + E_{\text{vib}} + E_{\text{rot}} \]

Energy Levels

Vibrational energy states give fine structure to the electronic states

\[ \nu = 0 \text{ is lowest vibrational freq.; } \nu > 0 \text{ corresponds to higher vibration freq.} \]

Transition between vibrational energy levels
\[ E_{\text{int}} = E_e + E_{\text{vib}} + E_{\text{rot}} \]

Rotational energy states give fine structure to the vibrational bands.

\( J = 0 \) is lowest rotational energy state; \( J > 0 \) correspond to higher rotational energies.

Energy between rotational energy levels.
Line positions are determined from difference between energy levels

Energy levels are discrete; spectra are discrete (optically allowed in certain cases)

An example: OH absorption

\[(3,0) \quad (2,0) \quad (1,0) \quad (0,0)\]

\[T = 2000 \text{ K}\]
Energy Levels and Spectra

- Line positions are determined from difference between energy levels.
- Energy levels are discrete; spectra are discrete (optically allowed in certain cases).
- **An example: OH absorption**

![Diagram showing energy levels and spectra with labels: (3,0), (2,0), (1,0), (0,0).]

**T = 2000 K**

---

Mavrodineanu and Boiteux, 1965
Line positions are determined from difference between energy levels.

Energy levels are discrete; spectra are discrete (optically allowed in certain cases).

An example: OH absorption

T = 2000 K

Mavrodineanu and Boiteux, 1965
Energy Levels and Spectra

T = 2000 K

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Let’s start with our representation of the energy states for the valence electron of a diatomic molecule.

Vibrational energy is quantized; at one vibrational level, two nuclei oscillate within a potential well (small \( r \rightarrow \) repel; large \( r \rightarrow \) attract).

Vibrational energy characterized by the vibrational quantum numbers:
- \( \nu'' \) = lower state (X-state)
- \( \nu' \) = excited state (A-state)

Molecule also rotates; rotational energy is quantized as well.

Rotational energy characterized by the rotational quantum numbers:
- \( J'' \) = lower state (X-state)
- \( J' \) = excited state (A-state)

\( \Delta E \) can be related to optical frequency.
Structure of a Molecule

We can separate out the nuclear (vibration, rotation) from the electronic solutions to Schrödinger’s equation (due to Born-Oppenheimer approximation).

We can solve for rotational and vibrational states of the nuclei with reasonable accuracy.

We can start with vibration and rotational separately, but then need to consider their effects on one another.

Finally, we can discuss electron interactions with the nuclei.
Nuclear Solution

We introduce the Schrödinger equation for a diatomic molecule:

\[
\left[ -\frac{\hbar^2}{2\mu} \nabla^2 - \frac{\hbar^2}{2m_e} \sum_{i=1}^{N} \nabla_i^2 + \hat{\mathcal{V}} \right] \Psi = E \Psi; \quad \Psi = \Psi(\vec{r}, \vec{R}) \tag{69}
\]

where \( \hbar = h/2\pi; \ \mu = (m_1m_2)/(m_1+m_2); \ m_e = \) electronic mass, \( N = \) number of electrons, \( \hat{\mathcal{V}} \) represents various potential interactions, \( \vec{r} \) is a position vector, and \( \vec{R} \) is the nuclear coordinate (spacing between nuclei)

Applying the B-O approximation

\[
\Psi(\vec{r}, \vec{R}) = \psi_{\text{elec}}(\vec{r}, \vec{R})\psi_N(\vec{R}) \tag{70}
\]

and substituting into Eq. (69) yields

\[
\left[ -\frac{\hbar^2}{2\mu} \nabla^2 + E_{\text{elec}}(\vec{R}) \right] \psi_N(\vec{R}) = E\psi_N(\vec{R}) \tag{71}
\]

where Eq. (71) is the nuclear Schrödinger equation, \( \psi_N(\vec{R}) \) is the nuclear wavefunction, \( E_{\text{elec}}(\vec{R}) \) is the electric potential distribution, which is an eigenvalue of the electronic Schrödinger equation, and the nuclear solution only is dependent on \( \vec{R} \)
The nuclear Schrödinger equation is further separable such that vibration and rotation can be examined separately, i.e.,

$$\psi_N(\vec{R}) = \psi_{\text{trans}}(\vec{R}_{\text{COM}})\psi_{\text{int}}(\vec{R}, \theta, \phi)$$  \hspace{1cm} (72)

$$E = E_{\text{trans}} + E_{\text{int}}$$  \hspace{1cm} (73)

$$\psi_{\text{int}}(\vec{R}, \theta, \phi) = \psi_{\text{vib}}(\vec{R})\psi_{\text{rot}}(\theta, \phi)$$  \hspace{1cm} (74)

$$E_{\text{int}} = E_{\text{elec}} + E_{\text{vib}} + E_{\text{rot}}$$  \hspace{1cm} (75)

For vibration, an eigenvalue equation of the Hamiltonian for the relative motion between two nuclei (for zero angular momentum) can be written as

$$\left[ -\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right] \psi_{\text{vib}}(r) = E_{\text{vib}}\psi_{\text{vib}}(r)$$  \hspace{1cm} (76)

A key to solving this is choosing the potential function $V(r)$, i.e., modeling the potential well of the molecule.
Molecular Vibration

A common approach is to perform a Taylor expansion of the potential function around its equilibrium position $r = r_e$:

$$V(r) = -V_o + \frac{1}{2} \frac{\partial^2 V}{\partial r^2} (r - r_e)^2 + ...$$  \hspace{1cm} (77)

which is just $V(r_e) + 1/2kx^2$, where $k$ is a force constant at the minimum of the potential well and $x = (r - r_e)$. Substitution into Eq. (76) yields the equation for a 1D harmonic oscillator Hamiltonian.

The eigenvalue solution for the vibrational energy for a harmonic oscillator is

$$E_{vib} = (\nu + 1/2)\hbar\omega_e$$  \hspace{1cm} (78)

where $\omega_e$ is the vibrational angular frequency written as $\omega_e = (k/\mu)^{1/2}$

The harmonic oscillator is a convenient approximation for diatomic molecules, but breaks down in terms of application of selection rules and leads to increasing error for excited states $\nu' > 1$.
Molecular Vibration

A more accurate description of the vibrational energies is given by the use of the anharmonic oscillator, also called the Morse potential

\[ V(r) = -D_e \left( 1 - e^{-\sqrt{k_e/2D_e}(r-r_e)} \right)^2 \] (79)

where \( D_e \) is the well depth of the potential.

The eigenvalue solution or the vibrational energy using the Morse potential is

\[ E_{\text{vib}} = \hbar c \left[ \nu_e (\nu + 1/2) - \nu_e x_e (\nu + 1/2)^2 \right] \] (80)

where \( \nu_e \) and \( \nu_e x_e \) are constants and \( \nu_e \) is a wavenumber.

A comparison of the potential energy diagram using both the harmonic oscillator and Morse potentials is shown.

The Morse potential displays uneven spacing between energy levels, which decreases as the energy approaches the dissociation energy.

Such anharmonicity allows for “overtones.”
Molecular Rotation

For rotation we will use what is referred to as a “rigid rotor model”. For this model, the separation between masses (two atoms) is considered fixed. Why?

The bond length ($l$) connecting the two masses is much greater than $\Delta l$ due to vibration in the bond.

The bond ($l = R_1 + R_2$) rotates around the COM with a frequency of $\omega_{rot}$ in rad/sec.

Let’s start with a bit of classical mechanics:

\[
M_1 R_1 = M_2 R_2 \quad \text{(81)}
\]

\[
R_1 = \frac{M_2}{M_1 + M_2} l; \quad R_2 = \frac{M_1}{M_1 + M_2} l; \quad \text{(82)}
\]

The total kinetic energy in the system is

\[
T = \frac{M_1 v_1^2}{2} + \frac{M_2 v_2^2}{2} = \frac{M_1 R_1^2}{2} + \frac{M_2 R_2^2}{2} \omega \quad \text{(83)}
\]
Molecular Rotation

- The moment of inertia \( I = M_1R_1^2 + M_2R_2^2 \) can be substituted into Eq. (83) to simplify the expression for the kinetic energy

\[
T = \frac{I\omega^2}{2}
\]  

(84)

- The moment of inertia is further reduced (using Eq. 82)

\[
I = \mu l^2
\]

(85)

where \( \mu \) is the reduced mass defined previously.

- Finally, we can define the angular momentum \( L = I\omega \), which when combined with Eq. (84) yields an expression for the moment of inertia

\[
T = \frac{L^2}{2I} \quad \text{or} \quad L^2 = 2IT
\]

(86)

- Ok, back to the Schrödinger equation (but in cylindrical coordinates) with zero potential energy (no resistance to rotation)

\[
-\frac{\hbar^2}{2\mu l^2} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2}{\partial \phi^2} \right] Y(\theta, \phi) = EY(\theta, \phi)
\]

(87)
**Molecular Rotation**

- Define an angular momentum operator, \( \hat{L} = 2I\hat{T} = 2I\hat{H} \) with
  \[
  \hat{L} = -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2}{\partial \phi^2} \right]
  \]  
  \( (\text{88}) \)

- ...and the Schrödinger equation is now
  \[
  -\frac{\hbar^2}{2I} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2}{\partial \phi^2} \right] Y(\theta, \phi) = EY(\theta, \phi)
  \]  
  \( (\text{89}) \)

- The equation is solved using separation of variables (and a lot of work) and yields
  \[
  E_{\text{rot}} = \frac{\hbar^2}{2I} J(J+1) = B_e J(J+1)
  \]  
  \( (\text{90}) \)

  where \( J \) is the nuclear angular momentum quantum number. It is related to the rotational quantum number, but we do have to account for interactions with the electronic transition.

- Now are all transitions allowed? No – there are so-called “selection rules”

- For purely rotational transitions (i.e., microwave region), \( \Delta J = \pm 1 \); if there is an electronic transition (i.e., \( X \rightarrow A \)), \( \Delta J = 0, \pm 1 \)
Molecular Rotation

Let’s consider the selection rules in the context of absorption. When a molecule is irradiated with photons, it MAY absorb the photons and undergo an energy transition. The energy of the transition must match the energy of the incident photons, given by \( E = hf \).

The energy difference for a diatomic molecule has to obey the selection rule, so

\[
\Delta E = E_{J+1} - E_J = B_e (J + 1)(J + 2) - B_e (J)(J + 1) = 2B_e (J + 1)
\]

(91)

\[
f = \frac{2B_e (J + 1)}{h}; \quad \nu = \frac{2B_e (J + 1)}{hc}
\]

The vibrational transitions also have selection rules. For the pure harmonic oscillator, \( \Delta \nu = \pm 1 \); for the anharmonic oscillator, \( \Delta \nu = \pm 2 \) is allowed, leading to overtones.

As molecules are excited to higher rotational energies they spin faster. This increases the centrifugal force pushing outward on molecule and increases the average bond length, thus “distorting” the spacing between rotational levels. The correction for centrifugal distortion is cast as

\[
E_{\text{rot}} = B_e J(J + 1) + D e J^2 (J + 1)^2
\]

(92)
So far we have considered vibrational and rotational motion separately. However, we now consider the fact that rotational transitions are on the order of 1 cm\(^{-1}\), while vibrational transitions are on the order of 1000 cm\(^{-1}\). In this manner, rotational levels can be superimposed within vibrational levels (as you have seen on the potential energy curves).

Due to this structure, there will be interactions between the molecule’s vibration and rotational motion.

For rotational motion, our rigid rotor assumption stated that the bond length between two atoms in a diatomic is fixed. However, our anharmonic vibrational model (Morse potential) shows that the distance between vibrational energy levels and the bond length decrease as higher vibrational levels are accessed.

Recall, there was relationship between the rotational constant and the bond length:

\[ B_e = \frac{\hbar^2}{2I} = \frac{\hbar^2}{2\mu l^2} \]  

(93)
Ro-Vibrational Interactions

The rotational constant also can be written in spectroscopic units:

\[ \tilde{B}_e = \frac{B_e}{hc} = \frac{h}{8\pi^2 c \mu l^2} \]  \hspace{1cm} (94)

Since the rotational constant is a function of bond length, then it is dependent on the vibrational level:

\[ \tilde{B}_v = \tilde{B}_e - \tilde{\alpha}(v + \frac{1}{2}) \]  \hspace{1cm} (95)

where \( \tilde{\alpha} \) is an anharmonicity correction factor

The spacing between rotational levels decreases at higher vibrational levels and leads to unequal spacing between rotational levels in the ro-vibrational spectra.
Combining all aforementioned factors, the energy of a ro-vibrational state is

$$\tilde{E}(\nu, J) = (\nu + 1/2)\nu_e - (\nu + 1/2)^2\nu_e x_e + \tilde{B}_e J(J + 1) - \tilde{D}_e J^2 (J + 1)^2 - \tilde{\alpha}(\nu + \frac{1}{2})J(J + 1)$$

harmonic oscillator  anharmonicity  rigid rotor  centrifugal distortion  rovibrational coupling

(96)

We can now predict the ro-vibrational spectra (in a single electronic state) using Eq. (96) and selection rules!!! This would correspond to IR spectra.

- For the R-branch ($\Delta J = +1$), find $\nu = \tilde{E}(1, J + 1) - \tilde{E}(0, J)$
- For the P-branch ($\Delta J = -1$), find $\nu = \tilde{E}(1, J - 1) - \tilde{E}(0, J)$

There can also be rotational-vibrational transitions during an electronic transition. The energy distribution function changes between electronic transitions and complicates everything!

Compare the structure of an IR and UV spectrum of nitric oxide (NO)

So, the next step is to examine electronic states and the coupling between the electronic and nuclear modes.
Molecular electronic transitions are induced by UV/visible light ($\Delta E_{\text{elec}} \gg \Delta E_{\text{vib}} \gg \Delta E_{\text{rot}}$).

Difficult to calculate electronic states – there are *ab initio* solutions. Levels typically are measured with spectroscopy. Lowest energy level is assumed to be the X-state. Electronically excited states are labeled as A, B, C, …

The spectroscopic constants are different for each electronic transition. Certain rules governing electronic transitions exist, but they are different for each molecule (difficult to generalize).

Examining a set of potential curves again, we see that each potential well has a different shape. This means that each transitions has a different electronic potential distribution function, $E_{\text{elec}}(\vec{R})$ and thus different vibrational dependent rotational constants.

There are many electrons! We have to account for their cumulative behavior. The math behind it is well beyond the scope of this lecture. We just want to examine “how” they couple.
Electronic States

- In addition to the rotational and vibrational energy, we now need to include the energy of the electrons and in particular, the angular momentum of the electrons (recall we talked about the angular momentum of the molecule about an axis perpendicular to the bond).

- The orbital angular momentum around the internuclear axis also is called $\vec{L}$ (with quantum number $L$) and the component of $\vec{L}$ along the internuclear axis is $\vec{\Lambda}$. $\vec{\Lambda}$ controls how the electronic and nuclear modes couple. $\vec{\Lambda}$ has two potential directions (lambda doubling) and can lead to “degeneracy” or “splitting”.

- We have to include the contributions of “electron spin” ($\vec{S}$) and determine the total electronic orbital + spin angular momentum. “Spin” is an additional angular momentum effect (electrons don’t actually spin) that accounts for some extra splitting of the lines.

- The component of the spin along the internuclear axis is called $\vec{\Sigma}$ and the total the total electronic orbital + spin angular momentum (along z axis) is $\vec{\Omega} = |\vec{\Lambda} + \vec{\Sigma}|$. 

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Now, when the electronic orbit couples to the internuclear axis, it changes the rotational contributions to the observed spectrum.

These are categorized as “Hund’s” coupling cases. For diatomics, we generally only care about cases ‘a’ and ‘b’.

**Hund’s case a:** Weak interaction between electronic angular momentum and nuclear rotation; that is the interaction between \( \vec{L} \) (nuclear) and \( \vec{\Omega} \) is weak.

The total angular momentum is \( \vec{j} = \vec{L} + \vec{\Omega} \).

The quantum number is \( J = L + \Omega \) and the rotational energy is written as:

\[
\tilde{E}_{rot} = \tilde{B}_v J(J+1) - \tilde{B}_v \Omega^2
\]

\[\text{(97)}\]
Hund’s case b: spin and electronic orbital angular momentum do not couple

Spin couples to $\vec{L}$ (nuclear)

This leads to a new total angular momentum $\vec{N} = \vec{L}$ (nuclear) + $\vec{\Lambda}$

The total rotation is $\vec{J} = \vec{N} + \vec{S}$

Hund’s case B is common in flame-generated radicals

The rotational energy formula is molecule-specific, although they look similar to what we have seen before
Hund’s case b example: OH

For example, OH (A-state) is a Hund’s case b molecule

Recall, the formulations are different for each electronic transition!

The rotational energies are spin split such that the total rotational energy can be written as $\tilde{E}_{rot} = \tilde{E}_{rot,1} + \tilde{E}_{rot,2}$ (again this is molecule specific)

For the excited state ($A^2\Sigma^+$): $J = N \pm \frac{1}{2}$ ($S = \frac{1}{2}$)

- For $N+\frac{1}{2}$:
  $$\tilde{E}_{rot,1} = \tilde{B}_v N(N + 1) - \tilde{D}_e N^2 (N + 1)^2 + \gamma_v N$$

- For $N - \frac{1}{2}$:
  $$\tilde{E}_{rot,2} = \tilde{B}_v N(N + 1) - \tilde{D}_e N^2 (N + 1)^2 - \gamma_v (N + 1)$$

where $\gamma_v$ is a spin splitting constant (although spin splitting is weak)

For the ground state ($X^2\Pi$):

- For $N+\frac{1}{2}$:
  $$\tilde{E}_{rot,1} = \tilde{B}_v \left\{ (N+1)^2 - \Lambda^2 - \frac{1}{2} \left[ 4(N+1)^2 + Y_v (Y_v - 4) \Lambda^2 \right]^{1/2} \right\} - \tilde{D}_e [N(N+1)]^2$$

- For $N - \frac{1}{2}$:
  $$\tilde{E}_{rot,2} = \tilde{B}_v \left\{ N^2 - \Lambda^2 - \frac{1}{2} \left[ 4N^2 + Y_v (Y_v - 4) \Lambda^2 \right]^{1/2} \right\} - \tilde{D}_e [N(N+1)]^2$$

$$Y_v = \frac{A}{\tilde{B}_v}$$
Electronic States

- **Selection rules**: $\Delta J = \pm 1$, $\Delta J = 0$ for $J > 0$; $\Delta J = \pm 2$ for weak “satellite” transitions, called O and S (much weaker than P, R, Q)

  $\Delta \nu$ is free from restrictions; $\Delta \Lambda = 0, \pm 1$; $\Delta S = 0$

  - Hund’s case a: $\Delta \Sigma = 0$; $\Delta \Omega = 0$;
  - Hund’s case b: $\Delta N = 0, \pm 1$

What we can see is that the situation is becoming exceedingly complex as compared to our “nuclear” ro-vibrational excitation

- The vibrational energy is

  $$\tilde{E}_{vib} = (\nu + 1/2)\nu_e - (\nu + 1/2)^2 \nu_x e - (\nu + 1/2)^2 \nu_y e$$

  which is identical to the case of pure ro-vibrational excitation (IR), except that we include an additional higher-order anharmonicity correction

- Finally, once we have all of the “term energies” we can determine calculate the spectra using selection rules:

  $$\nu = (\tilde{E}'_{elec} - \tilde{E}''_{elec}) + (\tilde{E}'_{vib} - \tilde{E}''_{vib}) + (\tilde{E}'_{rot} - \tilde{E}''_{rot})$$
When reading a paper on OH LIF, what does the $R_1(6)$ line of the $(1,0)$ vibrational band of the $A^2\Sigma^+ \leftarrow X^2\Pi$ mean?

- An electronic state can be described by $\beta^{(2S+1)}\eta^\alpha$
  
- “$\beta$” represents the valence electron level (i.e., $X$ for ground state and $A, B, C$ for the first, second, and third excited electron states, respectively)

- $(2S+1)$ is the multiplicity, which describes the possible number of orientations of the total spin relative to the total orbital angular momentum. States with multiplicity of 1, 2, 3, are called singlets, doublets, triplets, etc.

- “$\eta$” is the designation for the value of the orbital angular momentum $\Lambda$ ($\Sigma, \Pi, \Delta, \ldots$ for $\Lambda = 0, 1, 2, \ldots$)

- “$\alpha$” denotes the parity, where it is “+” for symmetric wavefunctions and “-” for asymmetric wavefunctions or is neglected if a state has no net parity (i.e., lambda doubled configuration with different parities)

- The arrow indicates the direction in which the transitions goes (lower energy level to the right)

- Vibrational band notation is written as $(v', v'')$
Spectroscopic Notation

Rotational notation is complex

A rotational line can be described by $\beta_{\eta,\alpha}(J'' \text{ or } N'')$

- "\(\beta\)" represents the branch which is S, R, Q, P, O for \(\Delta J = +2, +1, 0, -1, -2\)
- "\(\eta\)" is an integer related to Hund’s case b and used for the upper level. \(\eta = 1, 2, 3, \ldots\) for \(J' = (N+S), (N+S-1), (N+S-2)\)
- "\(\alpha\)" is an integer related to Hund’s case b and used for the lower level. \(\alpha = 1, 2, 3, \ldots\) for \(J'' = (N+S), (N+S-1), (N+S-2)\)

When \(\eta = \alpha\), only one value is reported

e.g., R\(_1\)(6) line of the (1,0) vibrational band of the \(A^2\Sigma^+ \leftrightarrow X^2\Pi\) of OH

**Rotational line nomenclature:** R-branch; \(N'' = 6\)

**Vibrational band nomenclature:** excitation from \(\nu' = 0\) to \(\nu' = 1\)

**Electronic transition nomenclature:** excitation from the ground (X-) state (a doublet with lambda splitting and \(\Lambda = 1\)) to the first excited electronic (A-) state, which has positive parity and \(\Lambda = 0\)

All of these details are meant to give you a background. However, the specifics change for each molecule and “rules” often are violated.
We will not go into any more spectroscopic details…

Different molecules exhibit different spectral signatures. This stems from the variations in coupling between electrons and nuclear, among other things.

Closing statement: The simpler models that were developed to describe ro-vibrational spectra in IR work very well. When excitation involves an electronic transition, the simple models need to be altered significantly to match observed spectra and become quite complex.

Do you really need to know all of the spectroscopic details to perform an absorption/LIF measurement – NO! For well-known molecules, follow established protocol (but at least know the background).

For “new” molecules/excitations schemes you will need to know a lot about the molecule!