A Quest for the Perfect Mixing Diagnostic

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Advisory Message

- This presentation has been approved by Dave Dickey for post-banquet presentation.
- It does not contain partial derivatives, Rushton turbines, CFD validation plots, or Re to a fractional power.
- It has lots of PICTURES!

There is no “perfect diagnostic”

- What do you want to know?

There is no “perfect diagnostic”

- What do you want to know?
  - Everything

There is no "perfect diagnostic"

- What do you want to know?
  - Nearly everything, but definitely reaction-based, as a function of space and time

There is no "perfect diagnostic"

- What do you want to know?
  - Nearly everything, but definitely reaction-based, as a function of space and time
- What do you really want?
  - engineering insight, or
  - quantitative tests of modeling and CFD

Diagnostics for engineering insight should be ...

- incisive but not necessarily quantitative
- simple to use for iterative runs
- cheap, “simple” chemistry
- colorimetric
- captured on videotape

Diagnostics for engineering insight

examples...

- DISMT (dual indicator system for mixing time)
  - red/yellow/blue-green; acid/base reactions
- FOB (formation of byproduct)
  - clear, green, blue, purple, red; complexation reactions

DISMT

Dual Indicator System for Mixing Time

- Colors can provide quantitative information.

- Mix red liquid with blue liquid
- Obtain yellow liquid only when mixture is within ±5% of ideal mixing
- Acid-base reaction with two indicators (methyl red and thymol blue)
- Must adjust initial pH's carefully

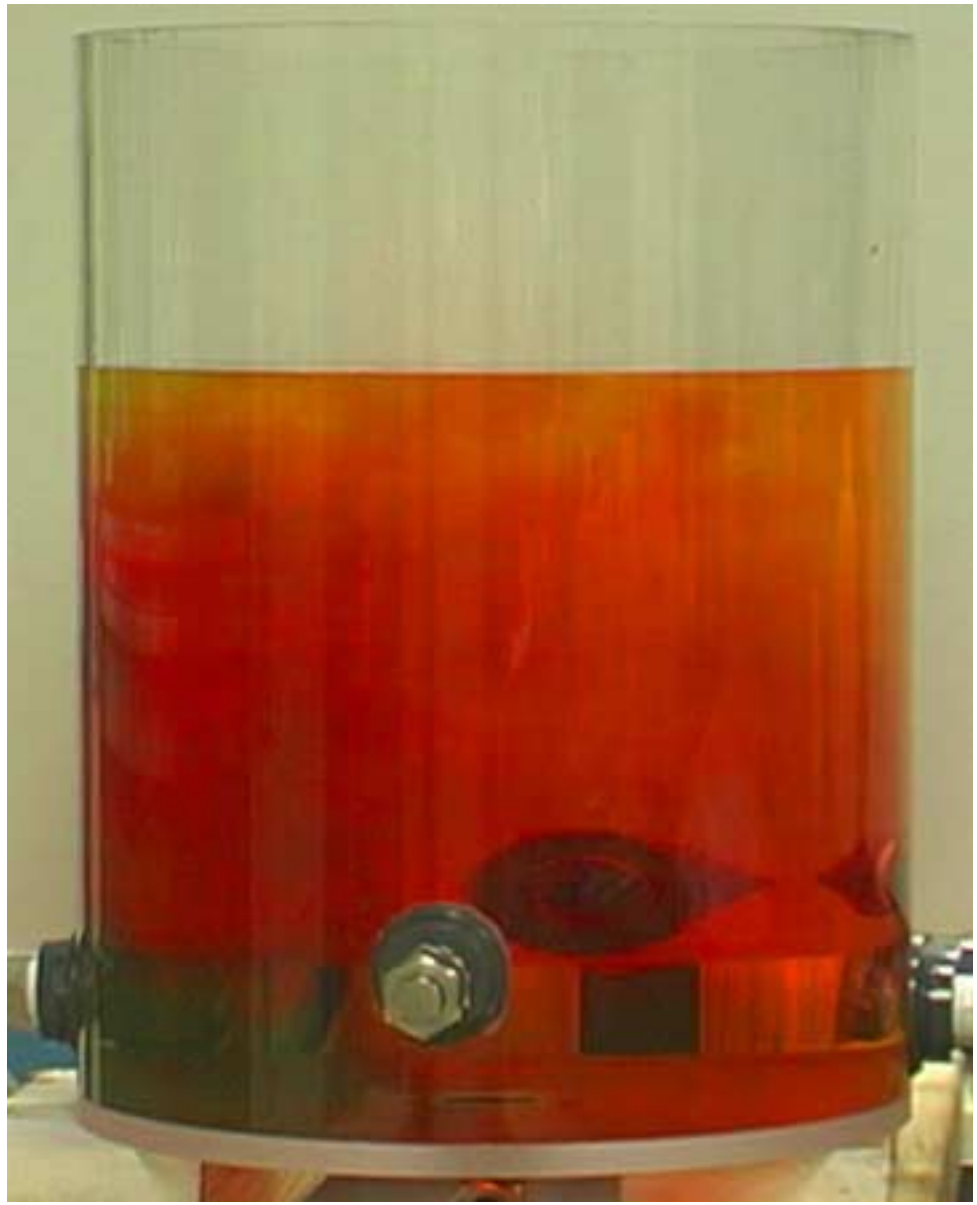
- MIXING TIME = time for entire solution to turn yellow

Jet mixing

(1) Jet of base (blue) from lower right into acid (red)

Base accumulates at lower left

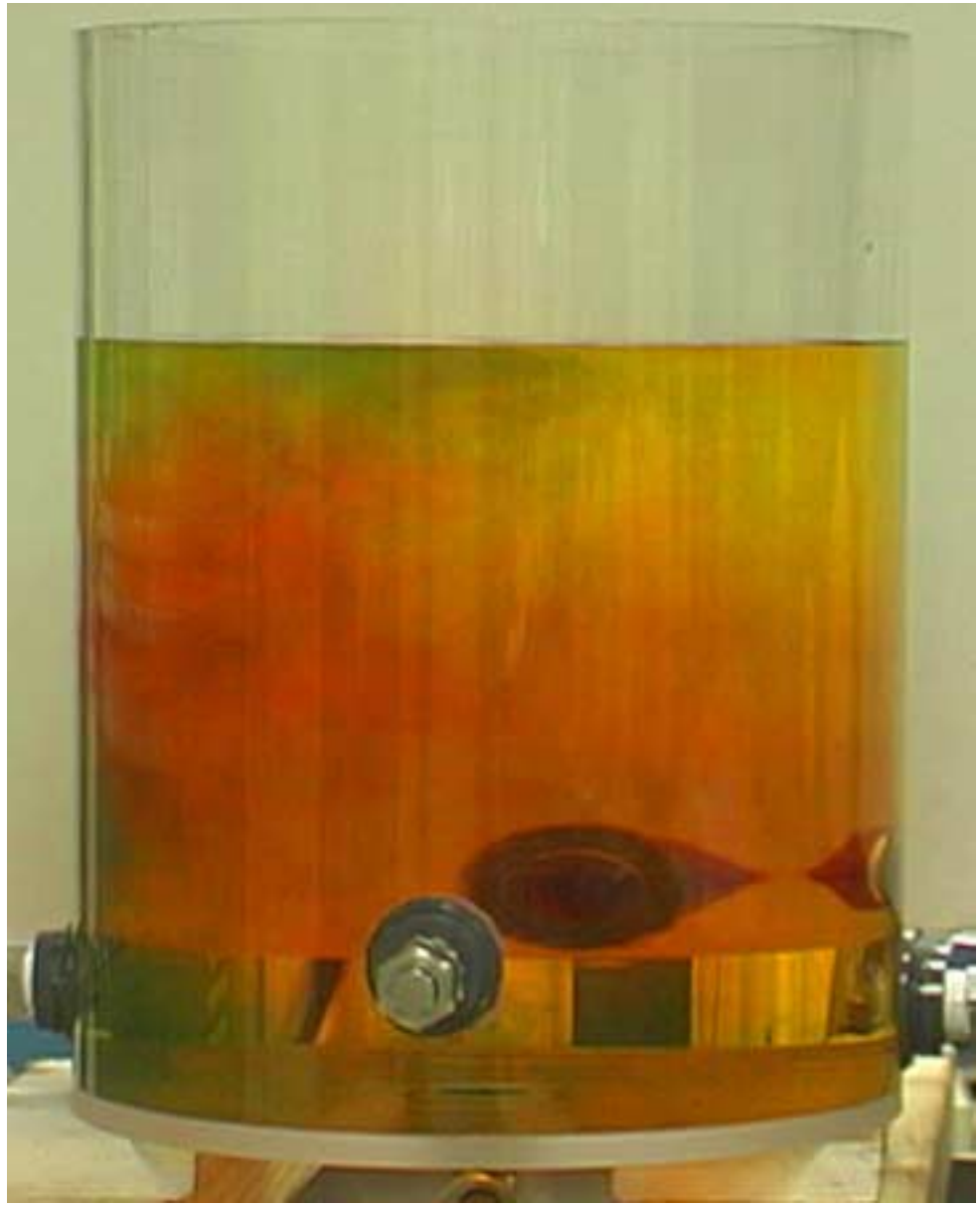
Where will yellow first appear?



Jet mixing

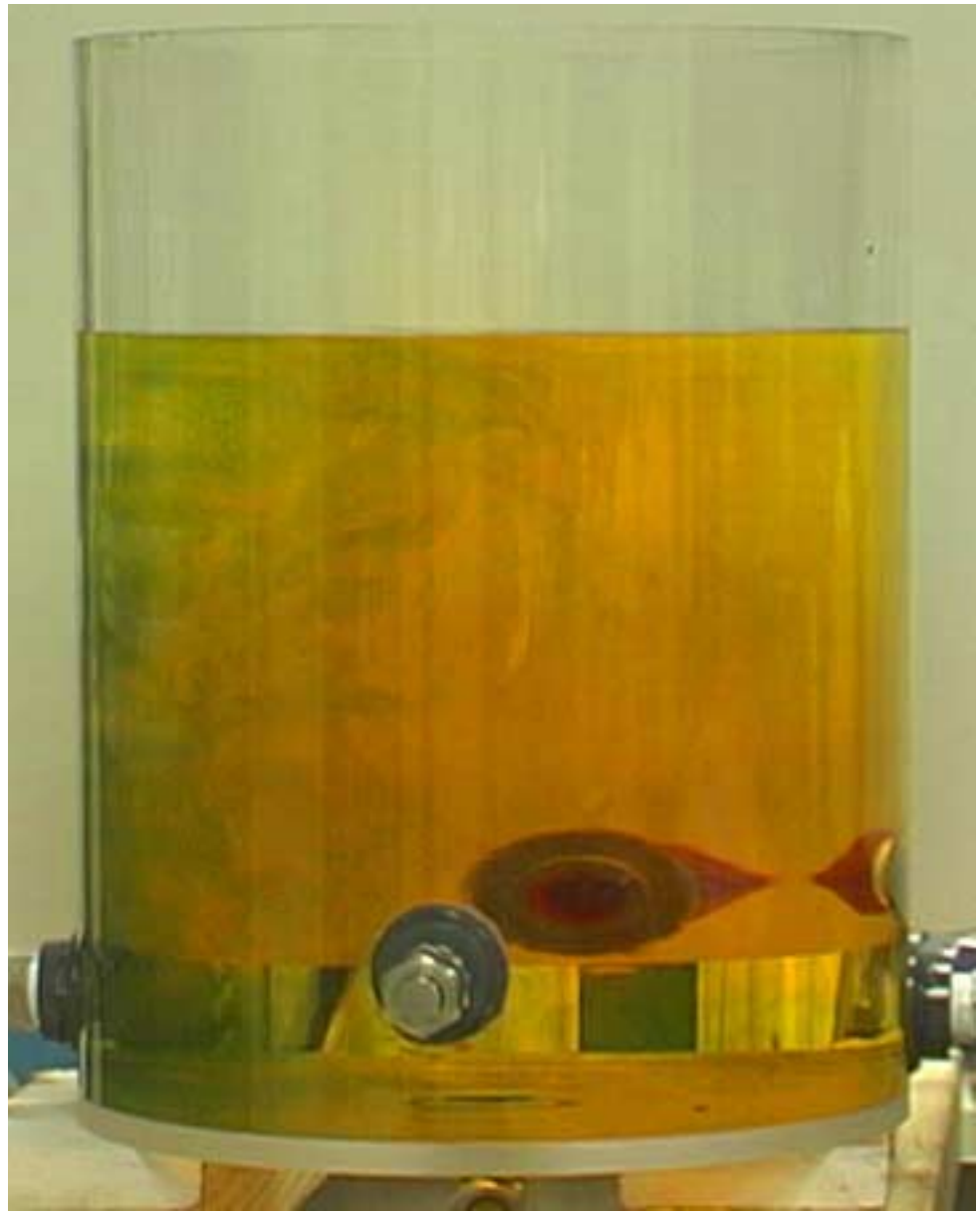
(2) Acid core (red); base circulates clockwise

Yellow first appears at top right.



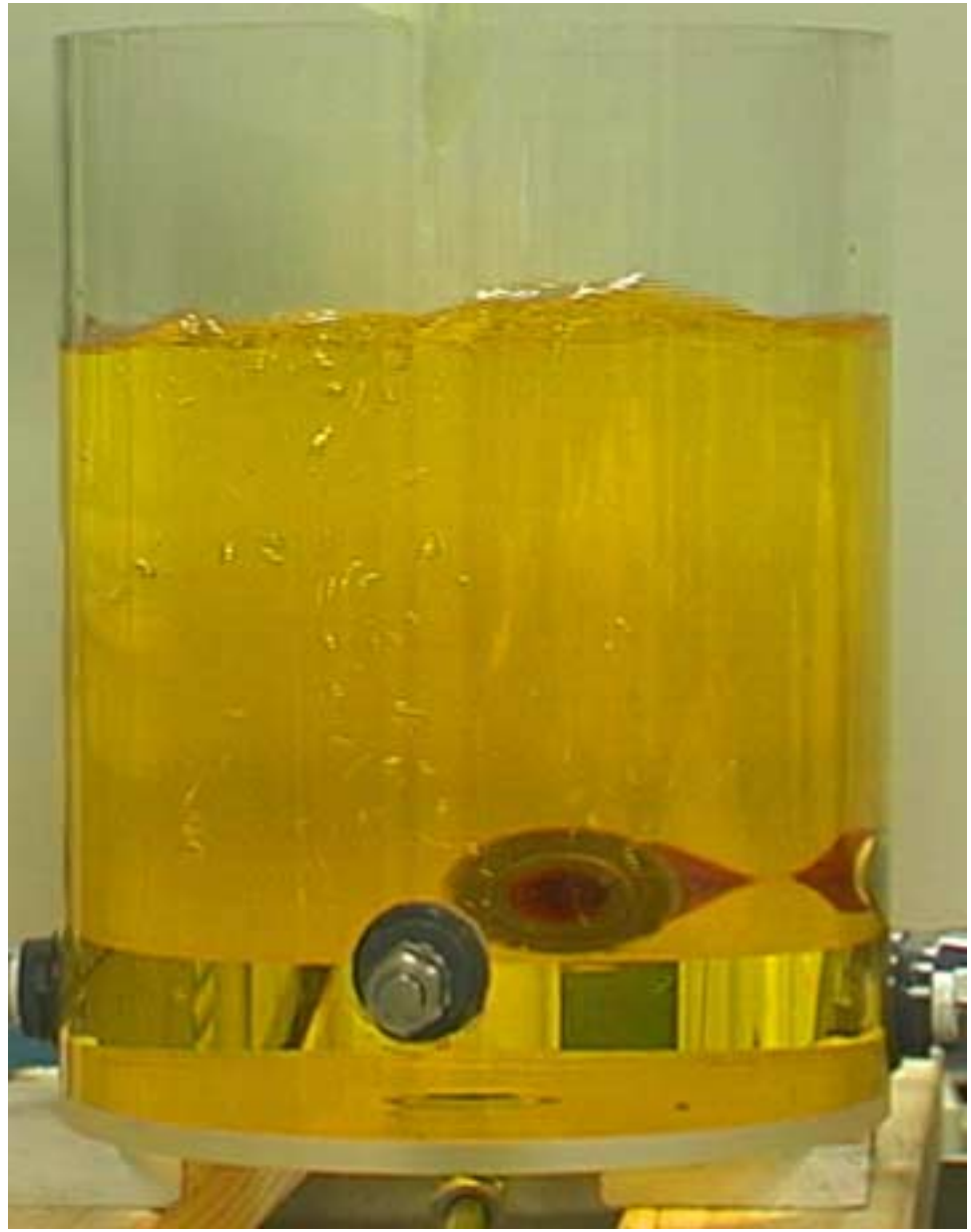
Jet mixing

(3) Acid core (orange) mixes slowly with zone of base (blue) at left



Jet mixing

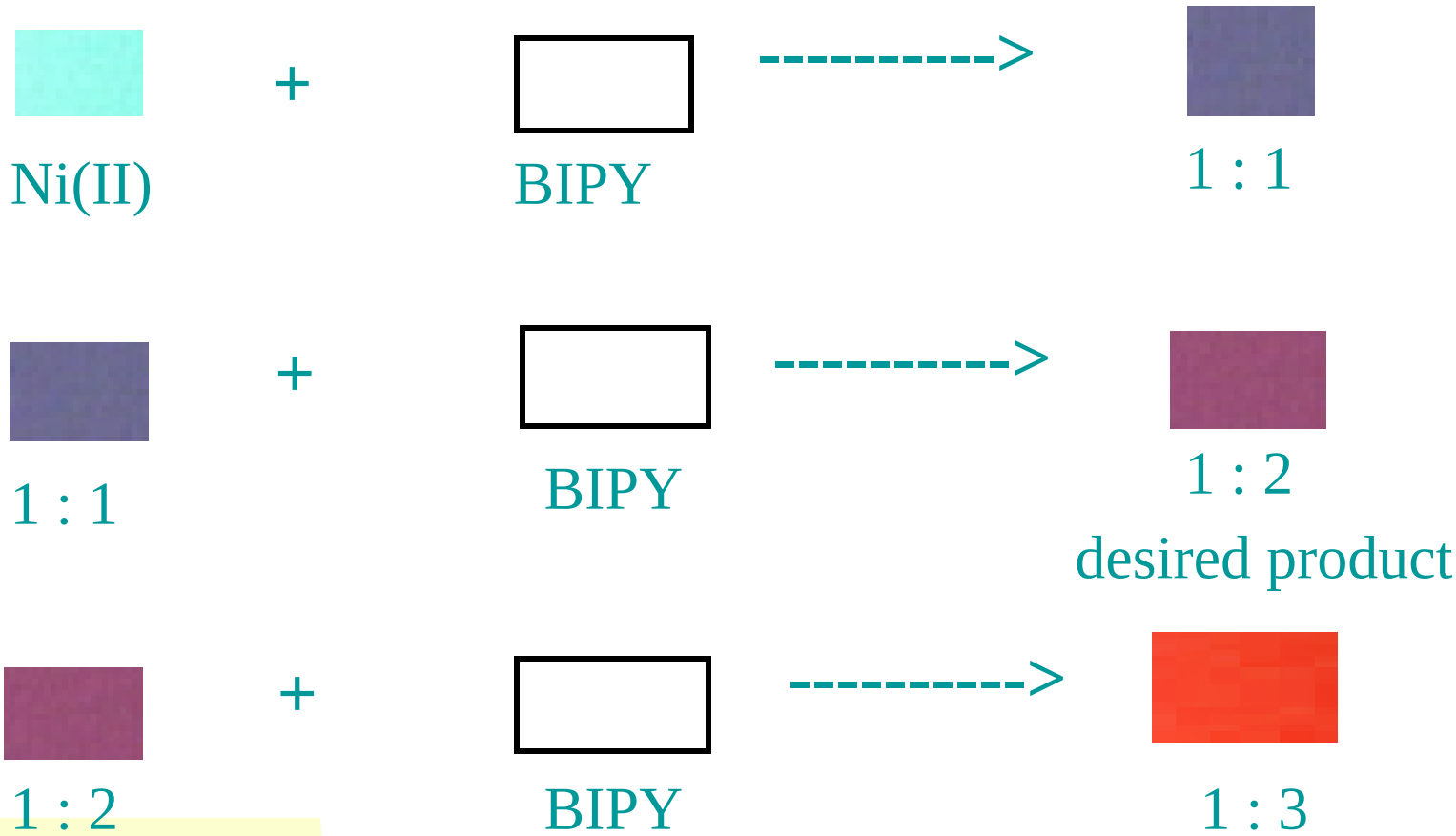
(4) After external mixing, solution is uniformly yellow.



FOB
Formation of Byproduct

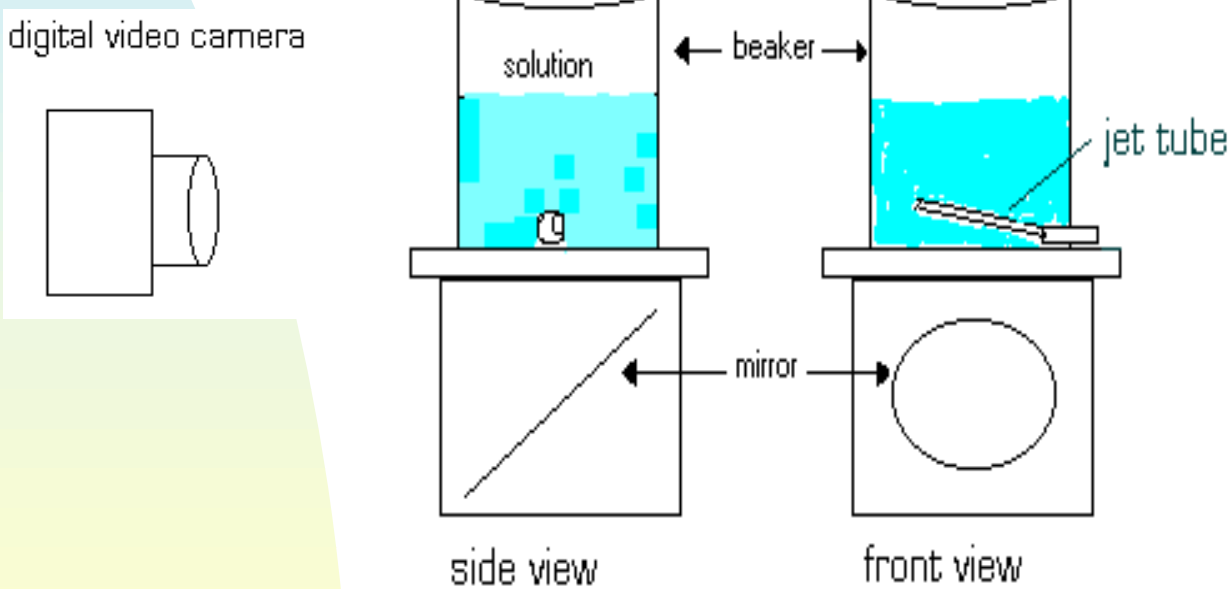
- Form successive complexes of Ni(II) [=M] with 2,2'-bipyridine (BIPY)[=L]
- Colors: clear(L), light green (M), blue (ML), purple (ML_2), red (ML_3)
- The complexation reactions are reversible; equilibrium composition can be obtained.

FOB Reactions
(sequential)

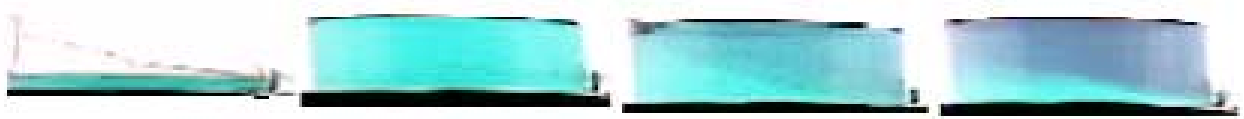


Jet Mixing Demonstration

Apparatus

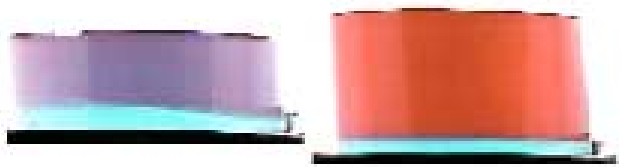


Jet Mixing Demonstration



Ni(II)

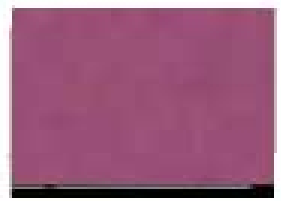
byproduct



1 : 2

poor mixing

product



1 : 2

complete mixing

Quantitative tests of CFD should be ...

- a ternary effort
  - CFD
  - flows
  - diagnostics
- iterative and interactive
- carefully designed and rigorously evaluated.

Diagnostics for quantitative tests of CFD

should be ...

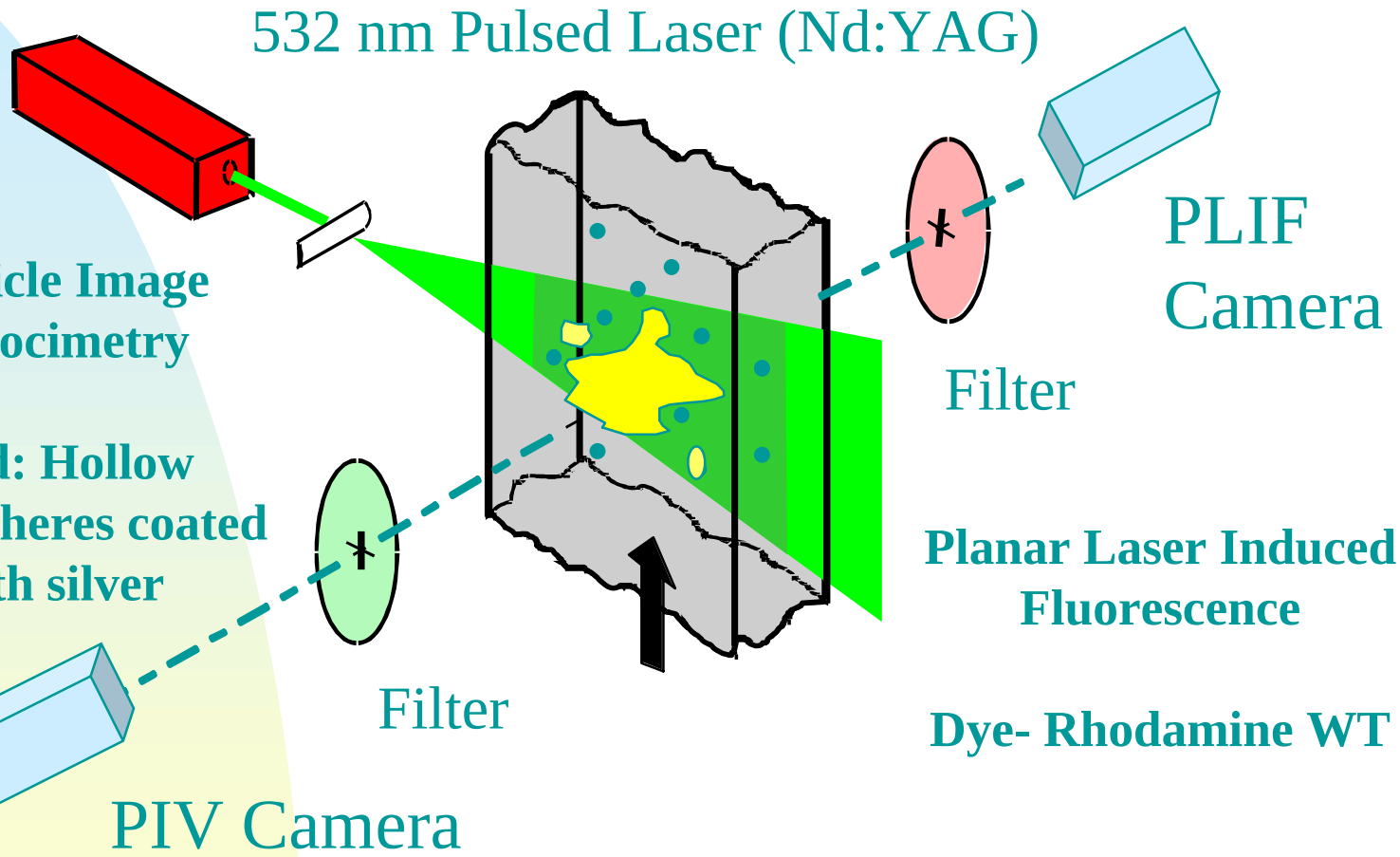
- quantitative (what level??)
- simultaneous PIV/PLIF (correlated velocity and concentration fields)
- known, tunable reaction rates
- high spatial resolution
- captured on digital cameras

Diagnostics for quantitative tests of CFD

at Dow Mixing Lab...

- ✔ quantitative (5% ?)
- ✔ ✔ simultaneous PIV/PLIF (correlated velocity and concentration field)
- ? known, tunable reaction rates
- ✔ high spatial resolution
- ✔ captured on digital cameras

Simultaneous PIV/PLIF



PLIF Advice

- ALWAYS run “optically thin” so that the laser intensity is not attenuated by absorption in the flow.
- $A = \varepsilon\, c\, l < 0.04$ yields less than 10% change in laser intensity across the flow.
- Many non-idealities either disappear or can be ratioed out.

Rhodamine-WT

- Strong absorption at 532 nm
- Fluorescence maximum at 590 nm
- High quantum yield
- Cheap
- Very low toxicity (much lower than Rh-B)
- Fluorescence has weak dependence on pH.

Reacting PLIF

- $Fe(II) + H_2O_2 \Longrightarrow Fe(III) + OH^- + OH^\bullet$ (Fenton's Reagent)
- $OH^\bullet$ + Rh-WT ==> non-fluorescent
- Plus more reactions
- Irreversible kinetics
- Rh-WT disappears with time constant of 1-20 ms (??)
- Currently working on simplified kinetic scheme

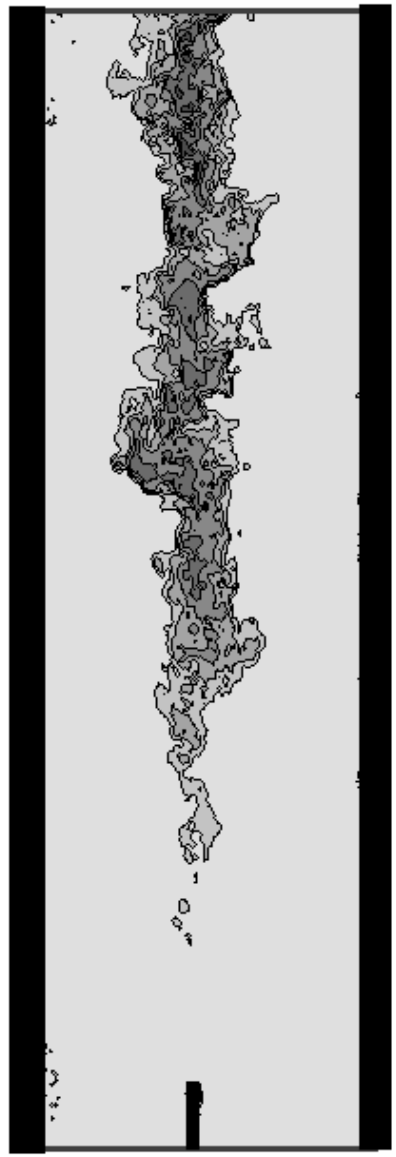
Rhodamine-WT and Fenton's Reagent

- Solution A: Rh-WT + Fe(II)
  fluorescent
- Solution B: Rh-WT + H_2O_2
  fluorescent
- Both solutions are stable over an hour.
- "on" + "on" ==> "off"
  (different but not a problem)

Reactive PLIF measurements in shear flow

Pulsed PLIF images of $Fe(II)/H_2O_2$ reaction zone. Lightest contour corresponds to 10% reaction; darkest to 80%.

Reaction time constant is 10-20 ms; flow time through cell is 200 ms.



ZOMM
zone of molecular mixing

- “off - on - off” with a tunable “time on” of 2-20 ms (pulse in pH)
- fluorescence image shows where mixing/reaction is taking place
- modest kinetic scheme
- might be ready in Fall 2001

Formation of Byproduct

- Capture PLIF images of byproduct formation (and also primary product ?)
- Would like to have tunable ratio of byproduct rate to primary rate
- At least a year away

Reaction rate

- Make fluorescence intensity at particular wavelength proportional to overall reaction rate
- Currently in the concept stage

Back to the Quest...

- Do not limit yourself by asking “What has been used previously?”
- Instead, ask “For my work, what reaction/concentration quantity would provide the most incisive test?
- I love to collaborate.

…for the perfect diagnostic

- PIV and reactive PLIF-FOB with
  - tunable, simple kinetics
  - detection of both the primary product and the byproduct
  - variable viscosities
- CFD would be tested against the flow pattern and two reactions.

Acknowledgements

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