Simulation of light propagation into microfluidic devices and prediction of the absorption profile of substances

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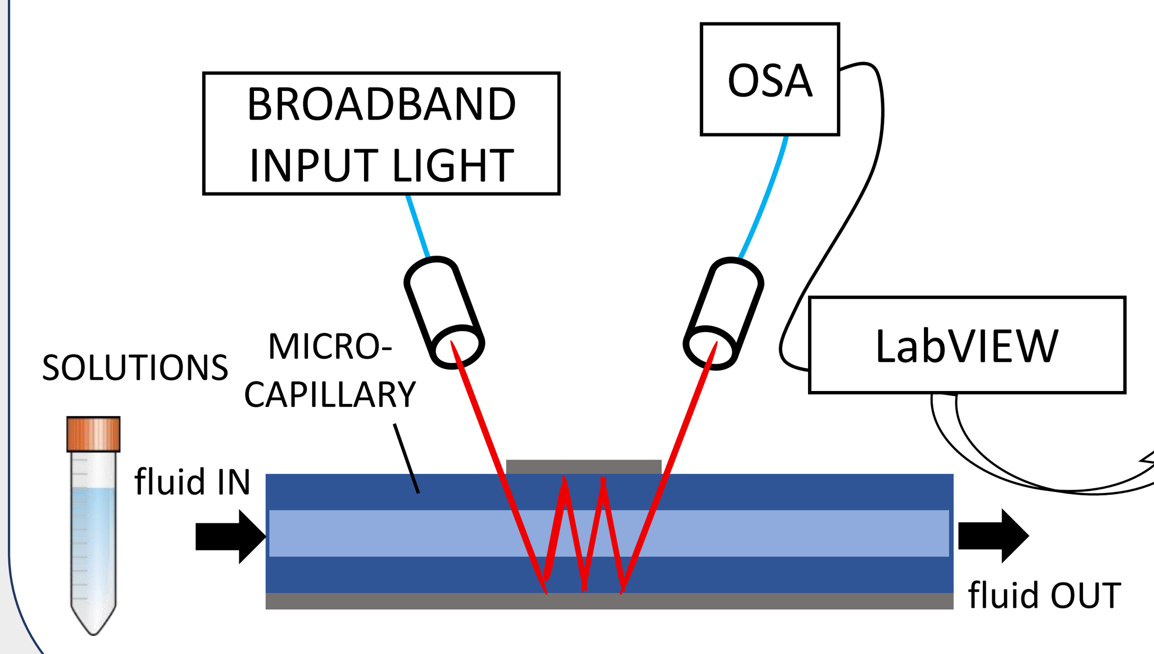
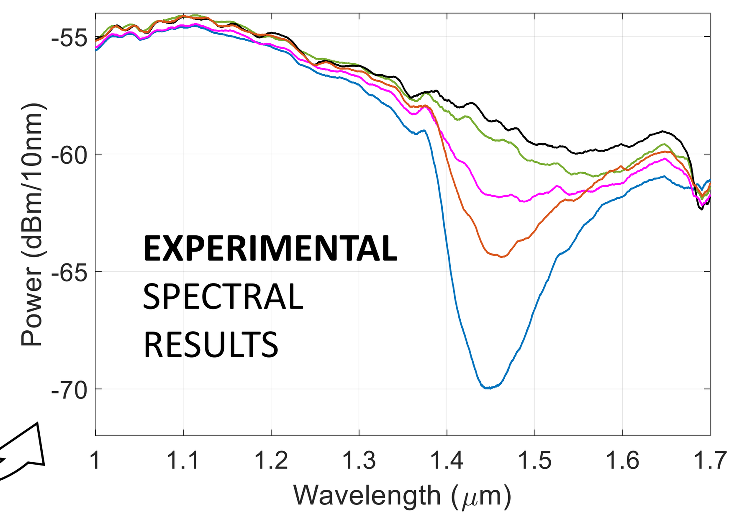
Aim of the work

- Study of the propagation of light travelling into a rectangular-section glass micro-capillary provided with integrated reflectors
- Theoretical analysis of the absorption profile of fluids using the values of the real part and imaginary part of the refractive indices
- Validation of the experimental results





ACQUISITION: Labview interface

DATA ELABORATION: MATLAB environment

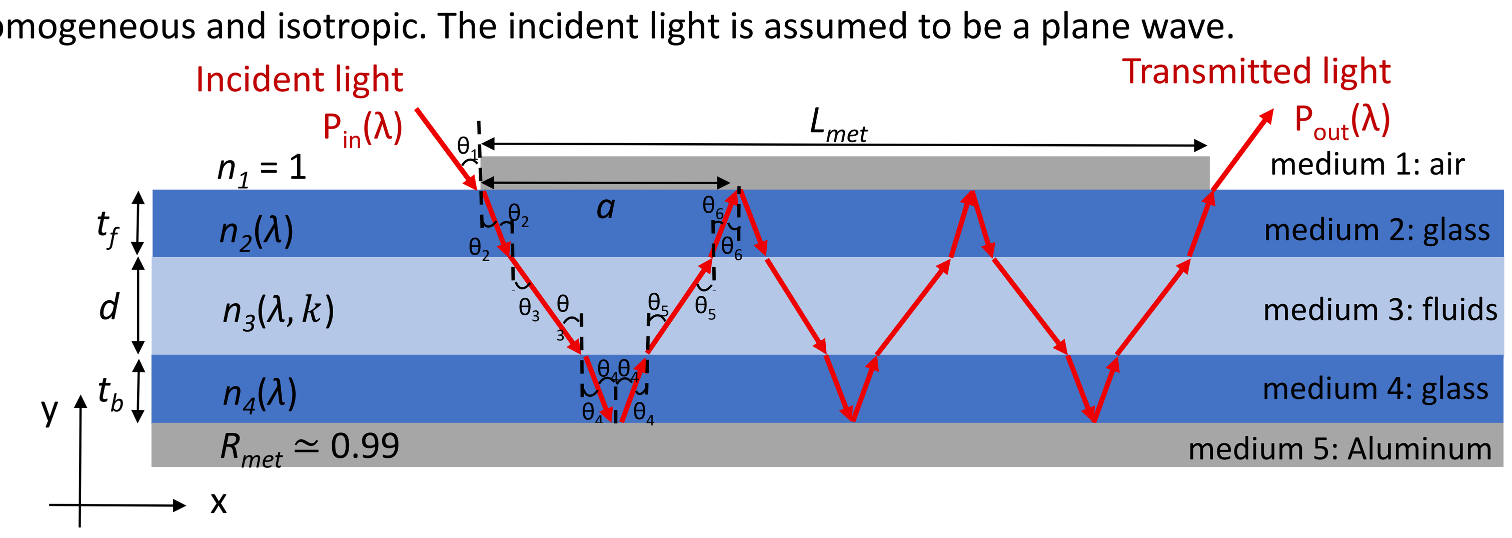
Validation

Simulations implemented in **MATLAB** environment

to obtain predictions that could be compared with the experimental spectral results

Theoretical Model - 1

A sophisticated theoretical model based on **geometrical ray optics approximation** was developed to describe light propagation into the capillary, that can be view as a multi-layer structure composed by different layers with finite thickness (top and bottom glass walls and the channel in which the liquid flows) immersed in air and provided with top and bottom reflectors. The dimensions of the capillary and the refractive indices of air, glass and fluid sample are taken into account. The equations assume that the interface between media is flat and that media are homogeneous and isotropic. The incident light is assumed to be a plane wave.



When the light beam crosses the separation surface between two different media, it is deflected according to **Snell law**:

$$n_j \cdot \sin\theta_j = n_m \cdot \sin\theta_m \qquad j, m\text{: origin and destination media}$$

When the radiation encounters the bottom Aluminum layer, it undergoes a specular reflection and light crosses the capillary twice (**single bounce configuration**). If the light beam encounters also the top reflectors, it is zig-zag guided inside the fluidic channel and it crosses the sample multiple times (**multiple bounce configuration**). The **number of bounces *N*** into the capillary is calculated as:

$$N = L_{met}/a$$

The total geometrical path *L* into the channel is calculated as:

$$L = 2 \cdot N \cdot d / \cos\theta_3 \qquad d\text{: channel depth}$$

Theoretical Model - 2

At each interface, the electrical field is partially transmitted and partially reflected.
The transmission coefficient for the field at each interface is retrieved by recursively applying **Fresnel equations**.

$$t_{s,jm} = 2 \cdot n_j \cdot \cos\theta_j \;/\; [n_j \cdot \cos\theta_j + n_m \cdot \cos\theta_m] \qquad \text{s-polarized field}$$

$$t_{p,jm} = 2 \cdot n_j \cdot \cos\theta_j \;/\; [n_m \cdot \cos\theta_j + n_j \cdot \cos\theta_m] \qquad \text{p-polarized field}$$

Overall field transmission coefficient: $t_{jm} = (t_{s,jm} + t_{p,jm})/2$

Power transmission coefficient at each interface: $T_{jm} = [n_m \cdot cos\theta_m / n_j \cdot cos\theta_j] \cdot |t_{jm}|^2$

Effect of fluid absorption: **Beer-Lambert law** for solution.

$$T_{abs}(\lambda) = e^{-\alpha(\lambda)\cdot x} \qquad \alpha(\lambda) = 4 \cdot \pi \cdot k(\lambda)/\lambda \qquad \text{k(λ): imaginary part of fluid refractive index}$$

Absoprtion for **mixtures:** law of additivity of absorbance.

$$T_{abs,mixt}(\lambda) = 1/10\text{^}A_{mixture}(\lambda) \qquad A_{mixture}(\lambda) = \Sigma_z A_z \cdot p_z$$

A_z: absorbance of each substance $\quad p_z$: fractional volume concentration of each substance

The overall spectral transmission is calculated by multiplying all the contribution of transmission:

$$T_{sample}(\lambda) = P_{out,sample}(\lambda)/P_{in}(\lambda) = T_{12} \cdot T_{23}^N \cdot T_{34}^N \cdot T_{43}^N \cdot T_{32}^N \cdot T_{21} \cdot R_{met}^{2N-1} \cdot T_{abs}(\lambda)$$

$$T_{air}(\lambda) = P_{out,air}(\lambda)/P_{in}(\lambda) = T_{12} \cdot T_{23}^N \cdot T_{34}^N \cdot T_{43}^N \cdot T_{32}^N \cdot T_{21} \cdot R_{met}^{2N-1} \cdot T_{abs}(\lambda)$$

Sim. Results – Single bounce configuration

The model has been implemented to study the theoretical spectral transmission of isopropanol, water, ethanol and air filling the channel. The values of refractive indices in the spectral region of interest (1-1.7 μm) are tabulated in the literature [1,2].

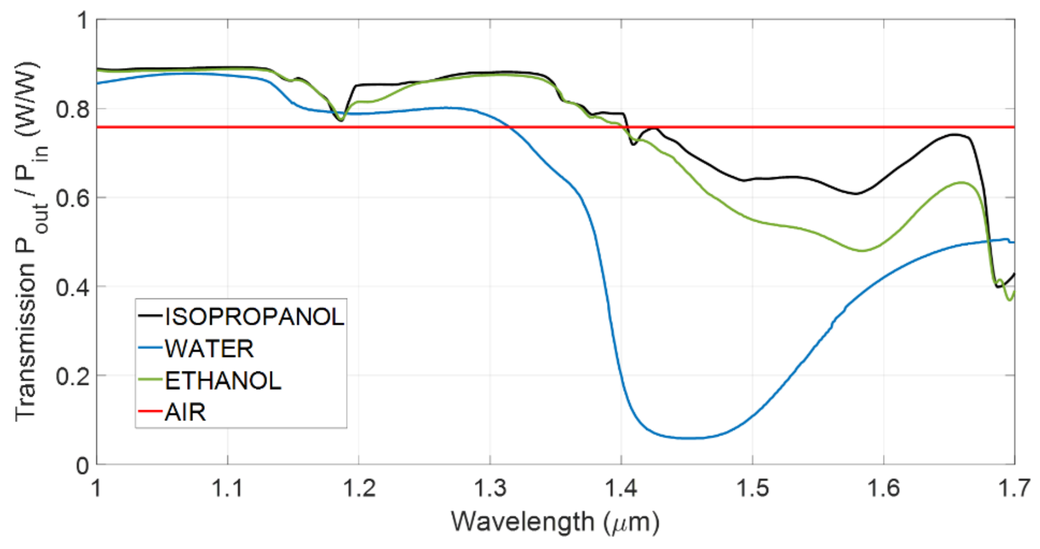
Results obtained for a capillary in single bounce configuration:

$N = 1$

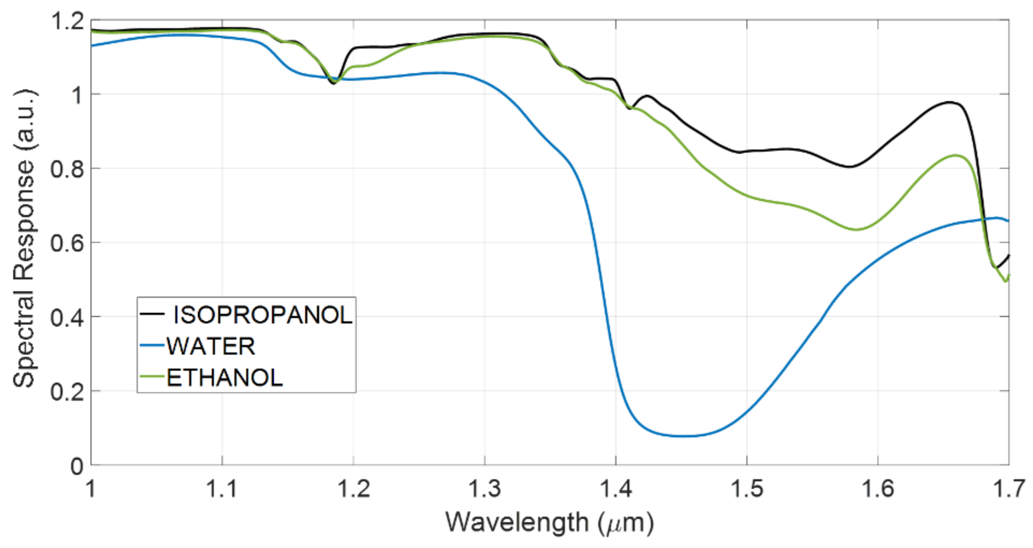
$d = 440\ \mu m$

$t_f = t_b = 280\ \mu m$

$\theta_1 = 35°$



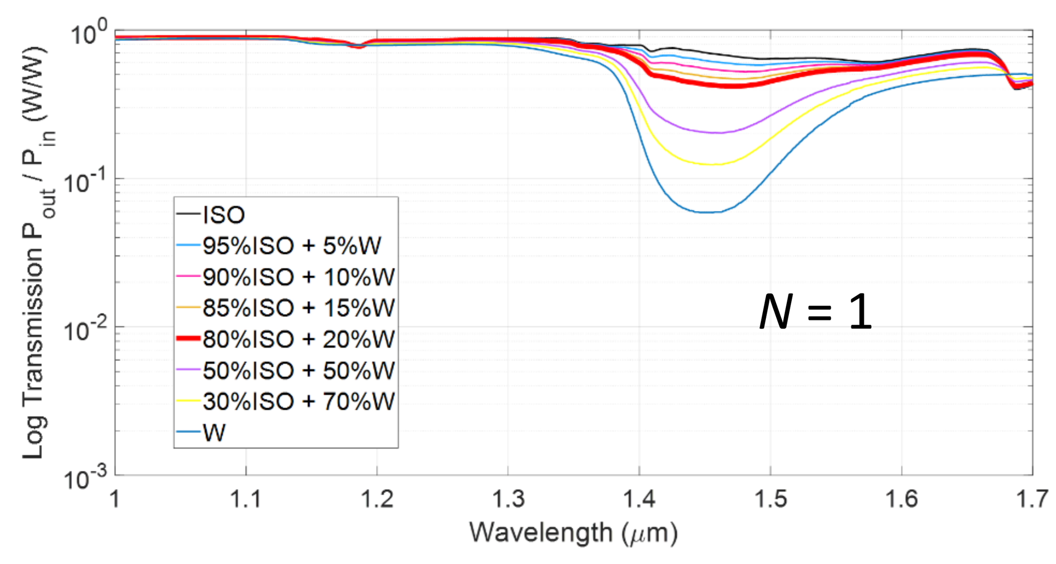
$$\text{Spectral response}(\lambda) = T_{sample}(\lambda)/T_{air}(\lambda)$$



Sim. Results – Multiple bounce configuration

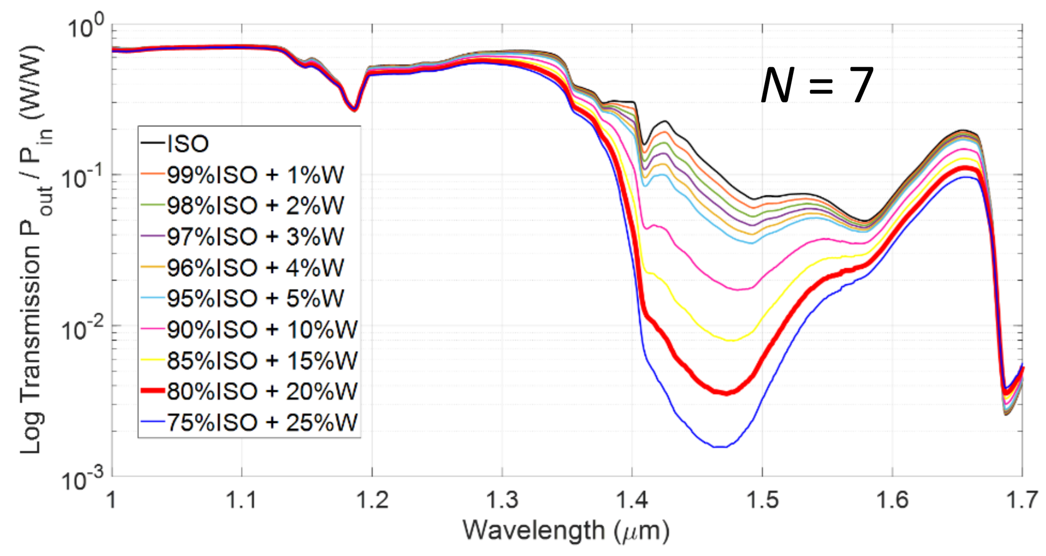
In case of multiple bounce configuration, simulations were performed by changing the length of the top Aluminum layer L_{met}. By considering L_{met} = 5 cm, a number of bounces *N* = 7 was found.

Figures show the theoretical spectral transmission obtained considering solutions of isopropanol ('ISO') and water ('W') at different volume concentrations in case of single bounce configuration and multiple bounce configuration with *N* = 7.



In multiple bounce configuration, the optical path into the channel increases, thus the effect of fluid absorption is enhanced.

NOTE: same y-axis for direct comparison



References

[1] S. Kedenburg, M. Vieweg, T. Gissibl, and H. Giessen. Linear refractive index and absorption measurements of nonlinear optical liquids in the visible and near-infrared spectral region, Opt. Mat. Express 2, pp. 1588-1611, 2012.

[2] E. Sani and A. Dell'Oro, Spectral optical constants of ethanol and isopropanol from ultraviolet to far infrared, Opt. Mater., vol. 60, pp. 137–141, 2016.