NANOANDES 2017

22 al 29 de noviembre

Modelado y simulación de circuitos de microfluídica

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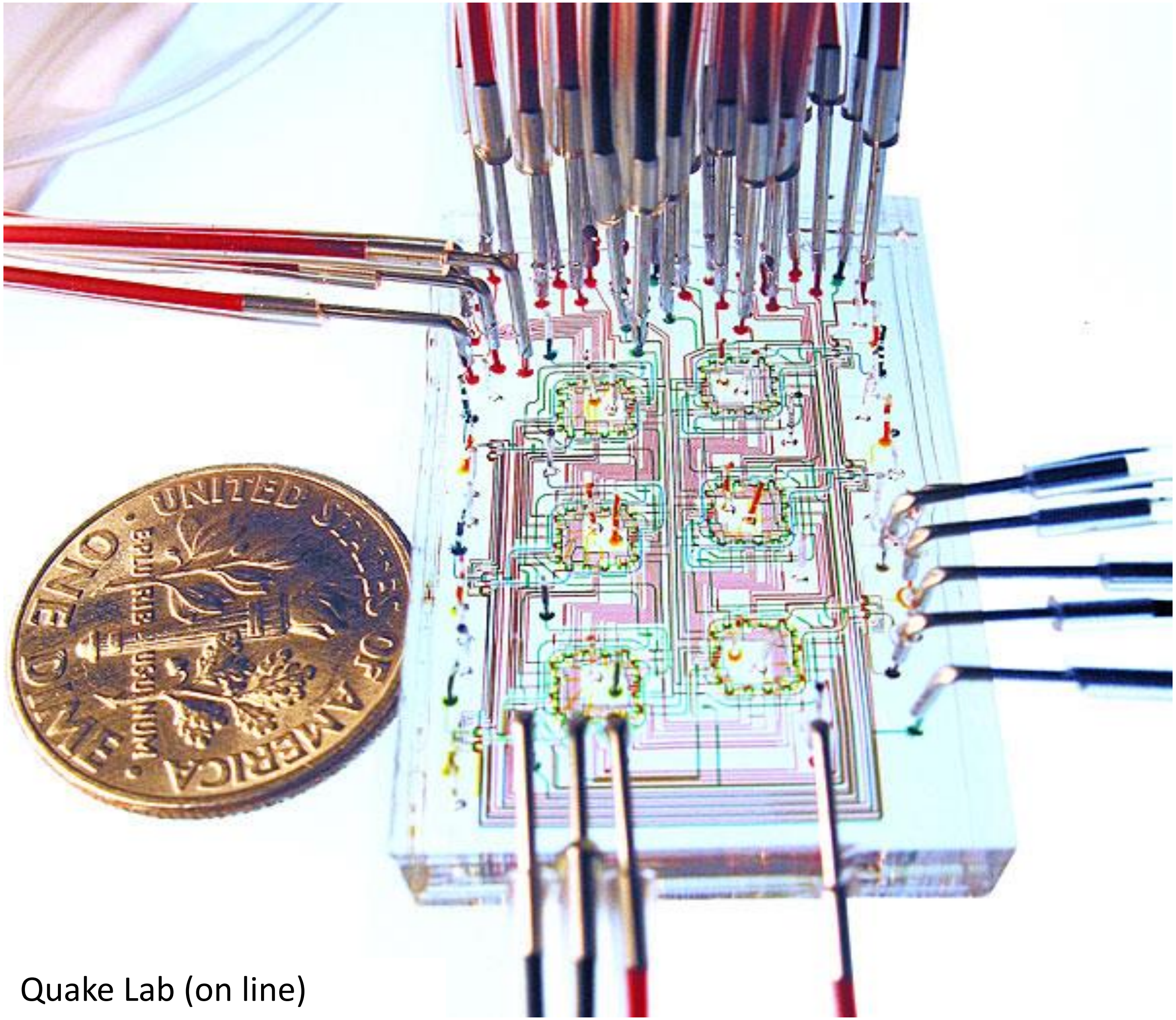
Primera parte

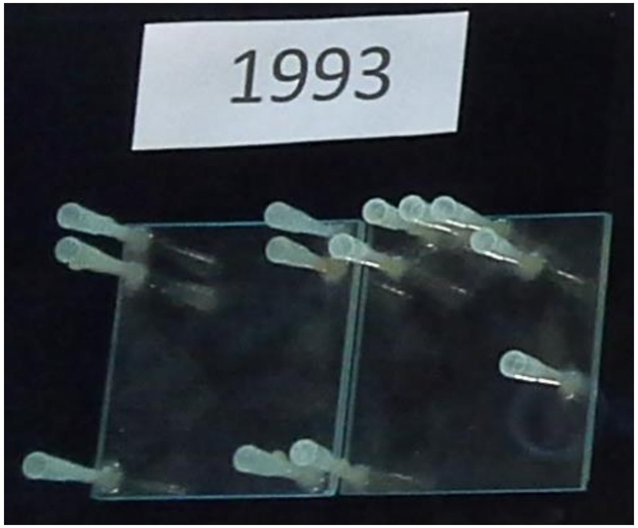
- ***i.*** **Introducción**
  - Definición/laboratorios en chips
  - Breve historia, evolución y presente
  - Publicaciones y mercado (ciencia y tecnología)
  - La Microfluídica como herramienta
- ***ii.*** **Circuitos de microcanales**
- ***iii.*** **Ejemplo: nuevos materiales**

i. Microfluídica



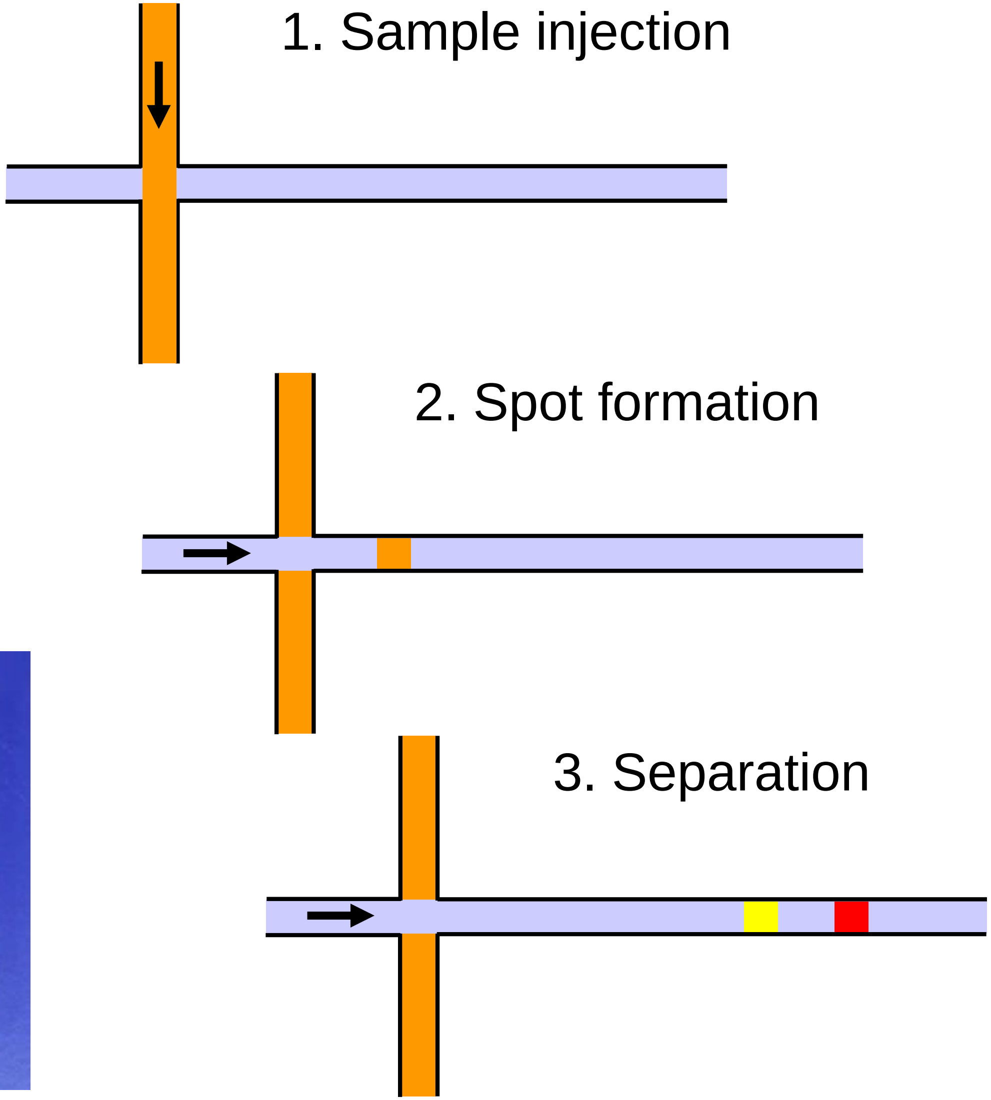
Quake Lab (on line)

i. Breve historia



Harrison et al., *Science* **261** (1993) 895

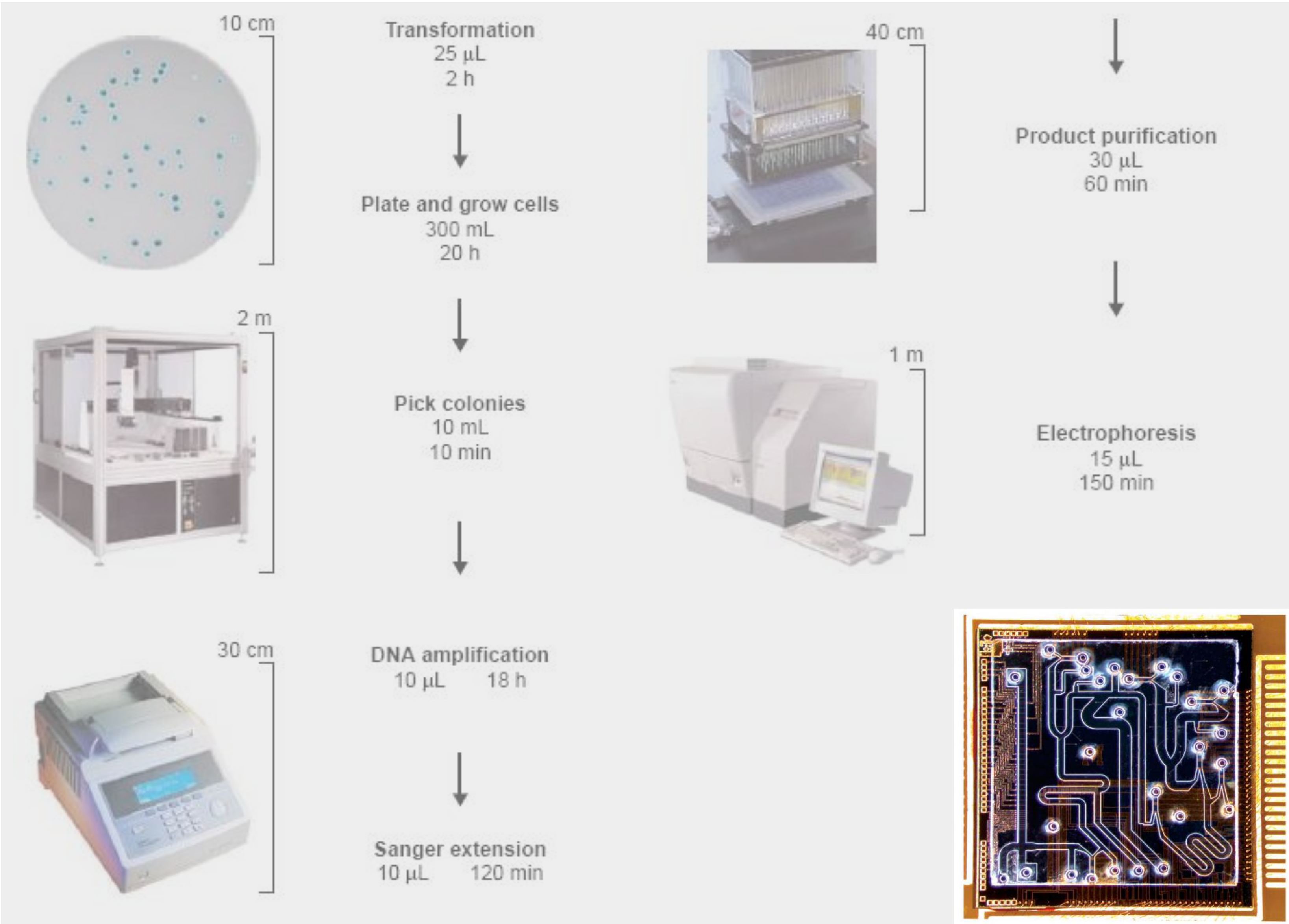
micronit.com



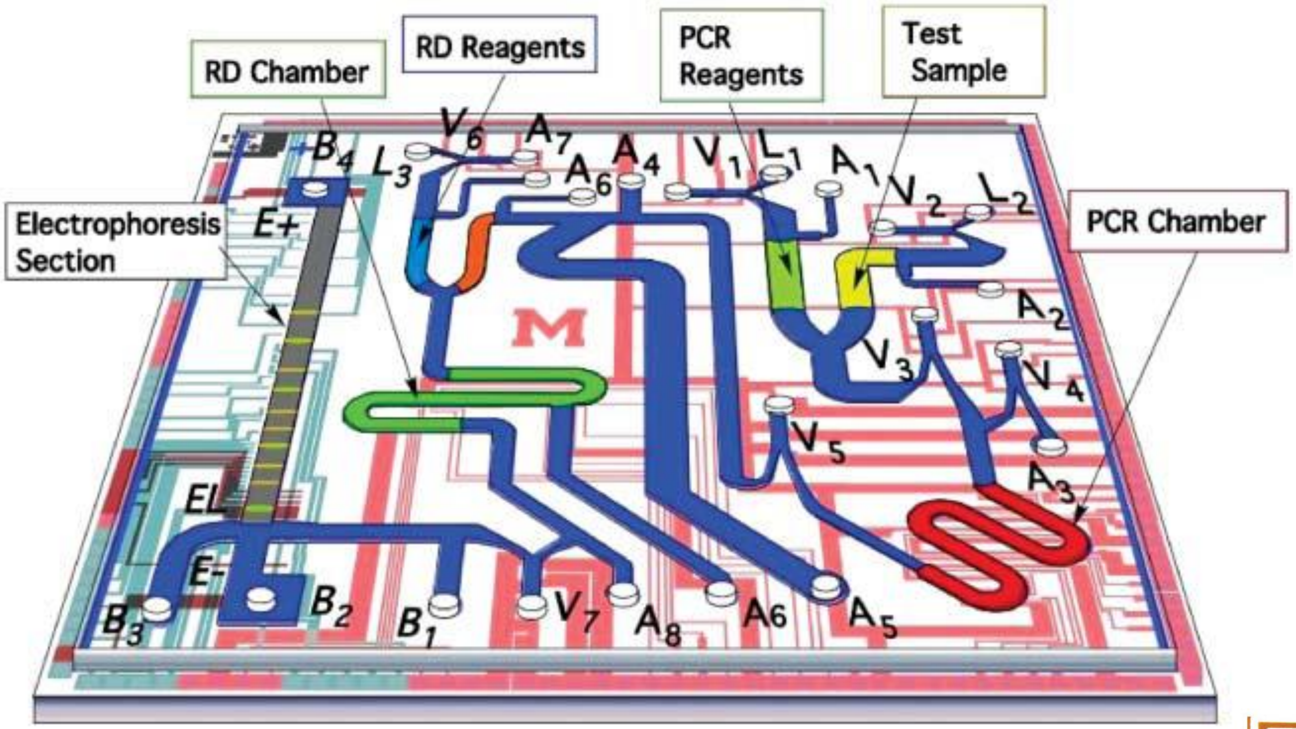
i. Breve historia

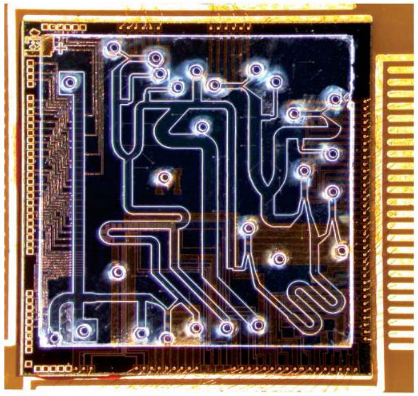
Caliper/Agilent Technologies (1998)

i. Todo el laboratorio...



¡…en un chip!





Pal et al., *Lab Chip* **5** (2005) 1024

i. Ensamble de micro y nanotecnologías

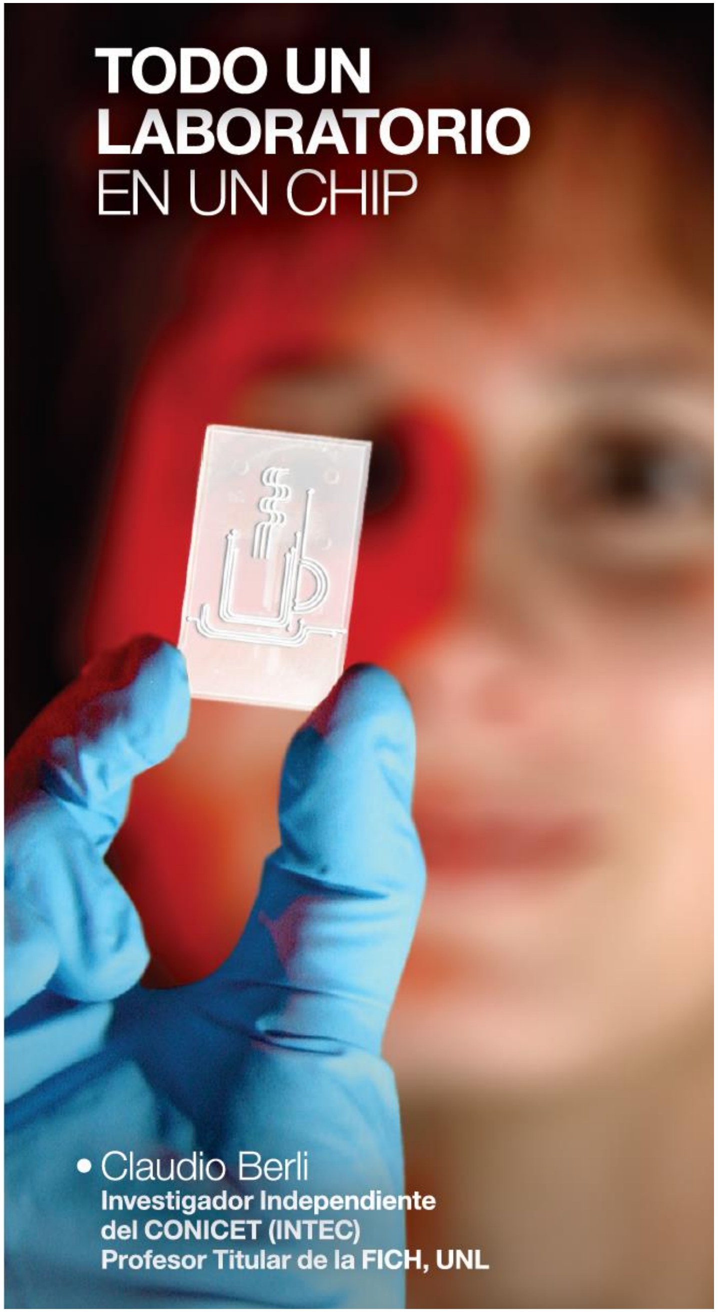
lab-on-a-chip

µTAS

nanotechnology

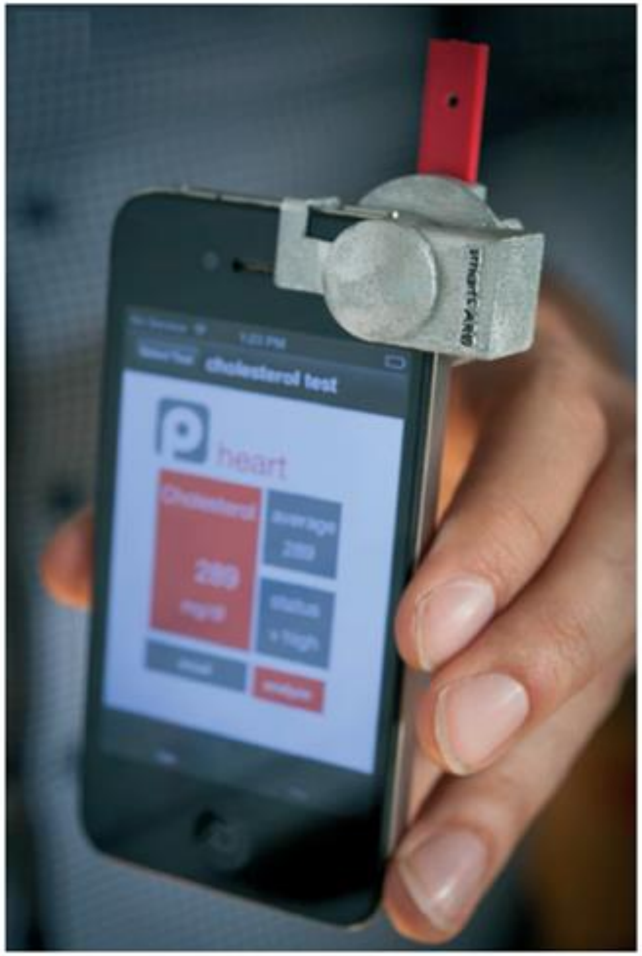
MEMS

biosensors

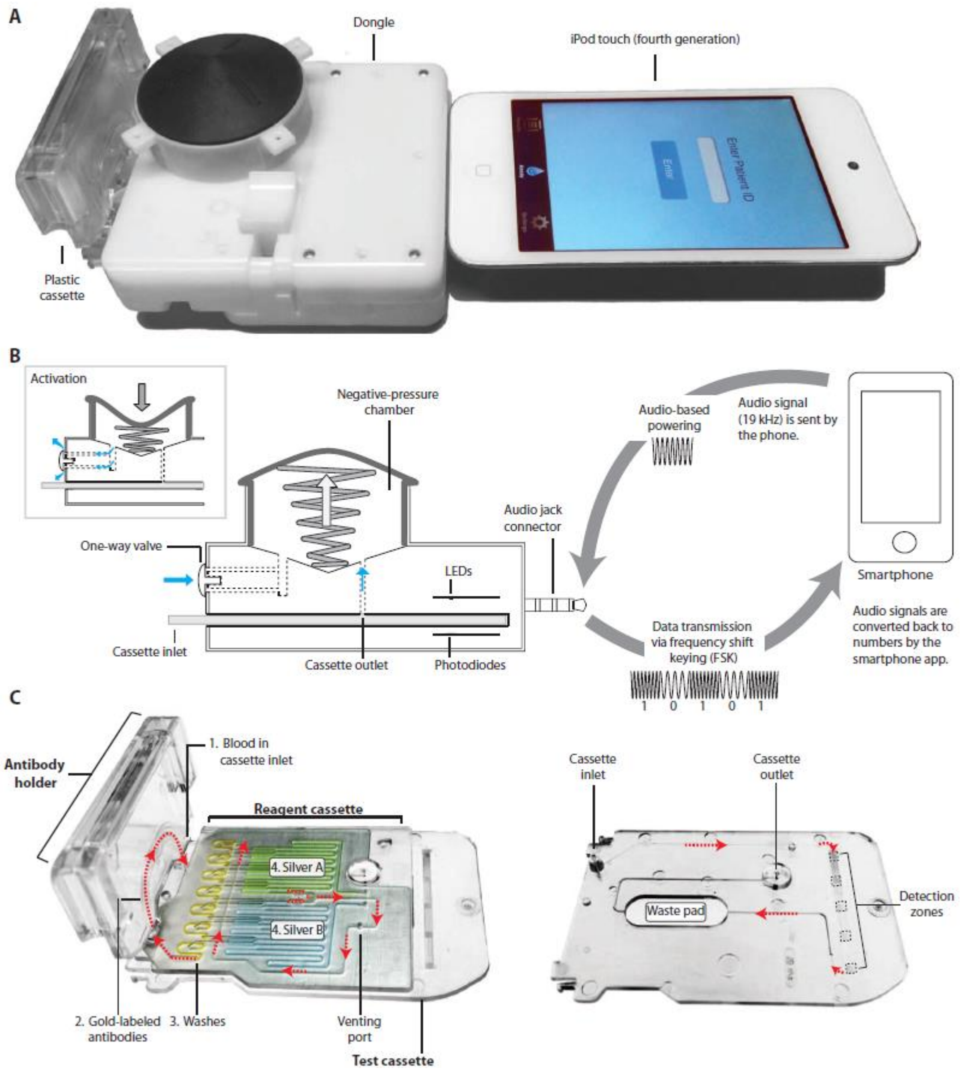


i. Chips “listos para usar” (POC, *health care*)

i. POC + telefonía móvil: *mHealth*

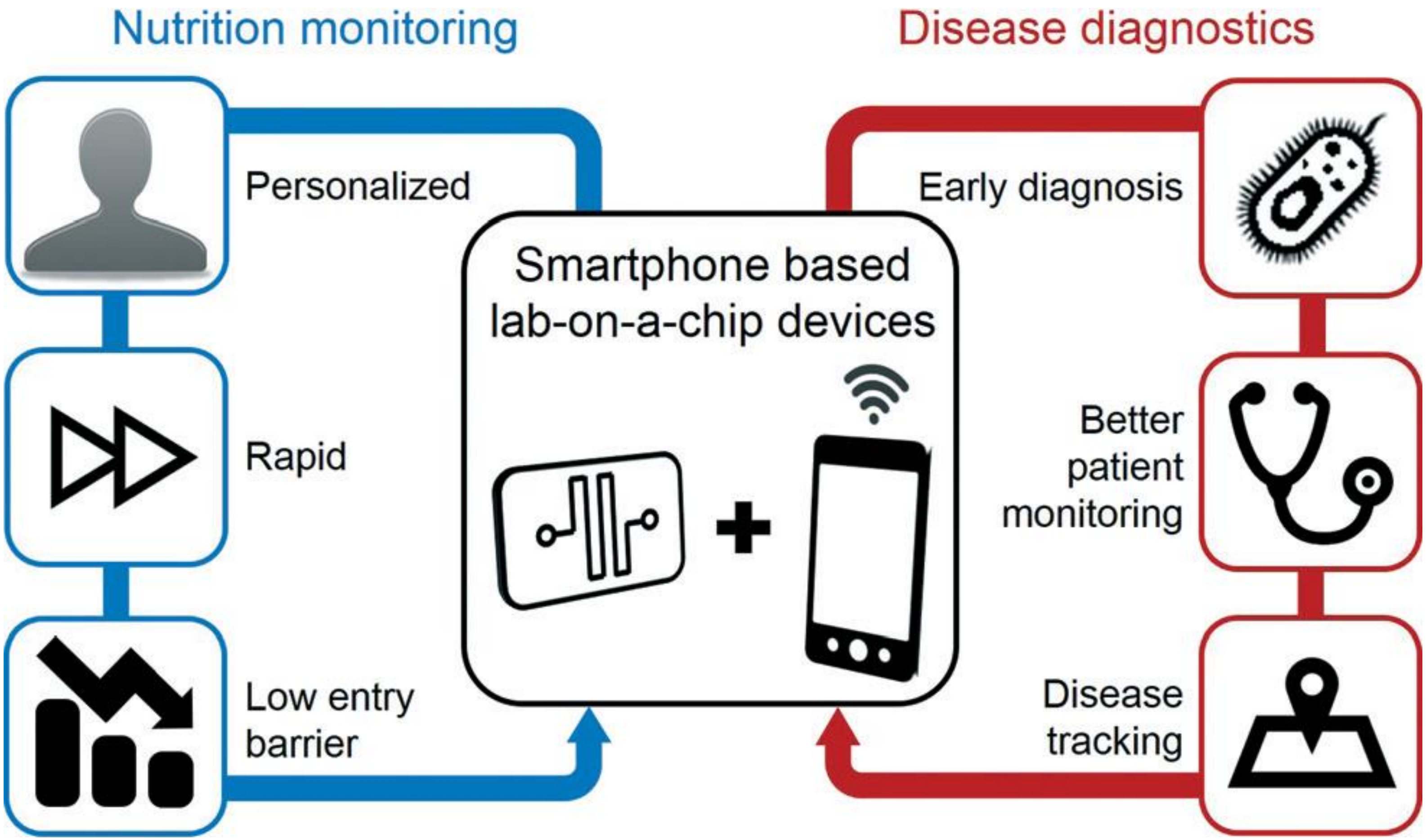


Erickson et al.,
Lab Chip **14** (2014) 3159



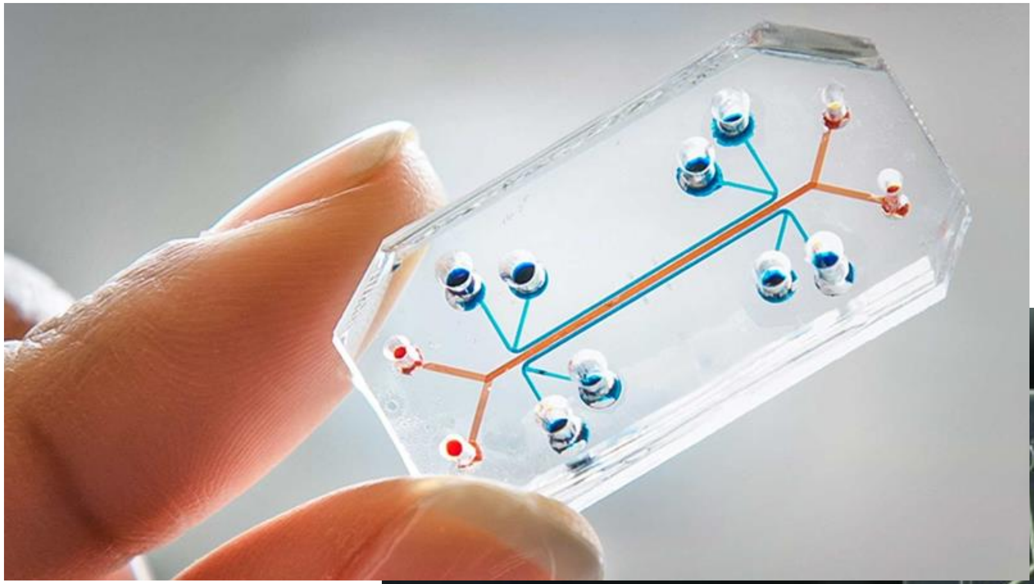
Laksanasopin et al., *Science Trans Med* **7** (2015) 273

i. Microfluídica y *mHealth*



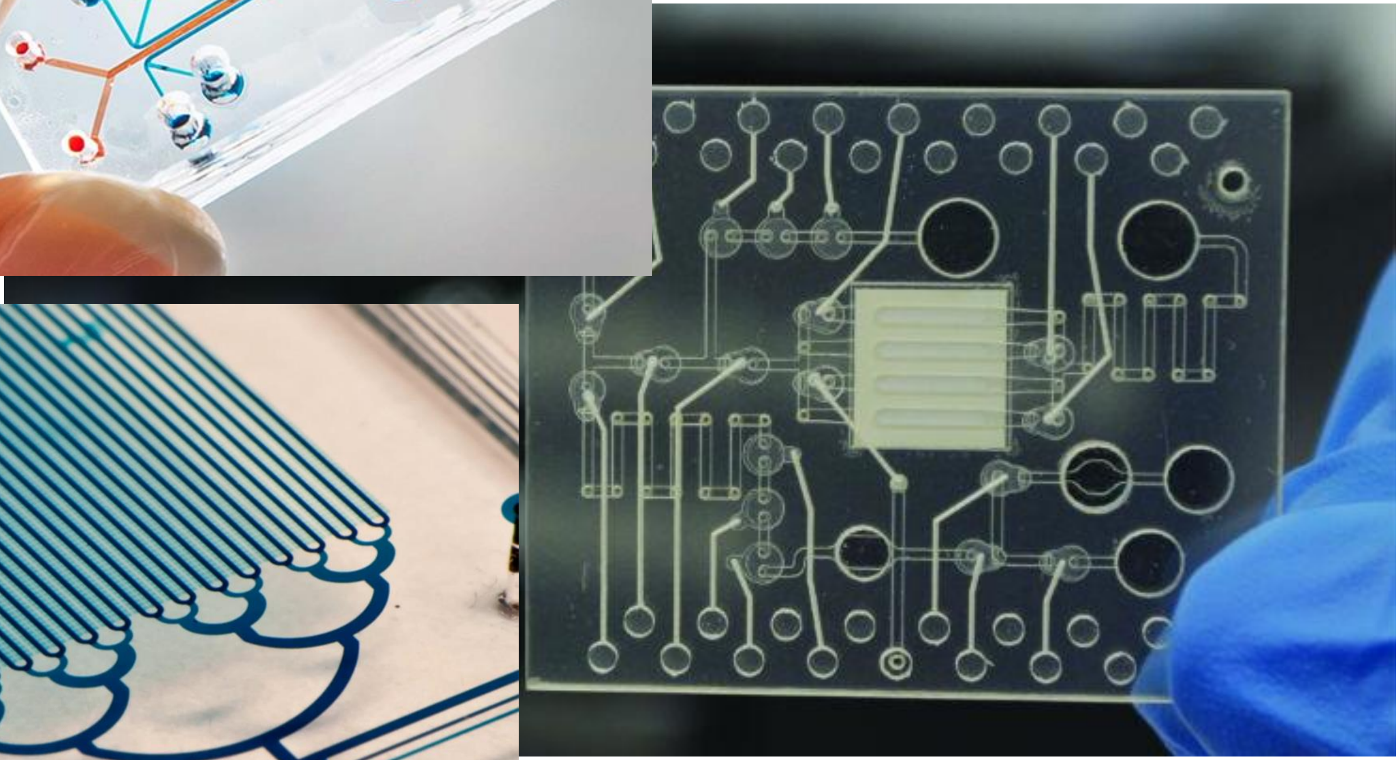
Erickson et al., *Lab Chip* **14** (2014) 3159

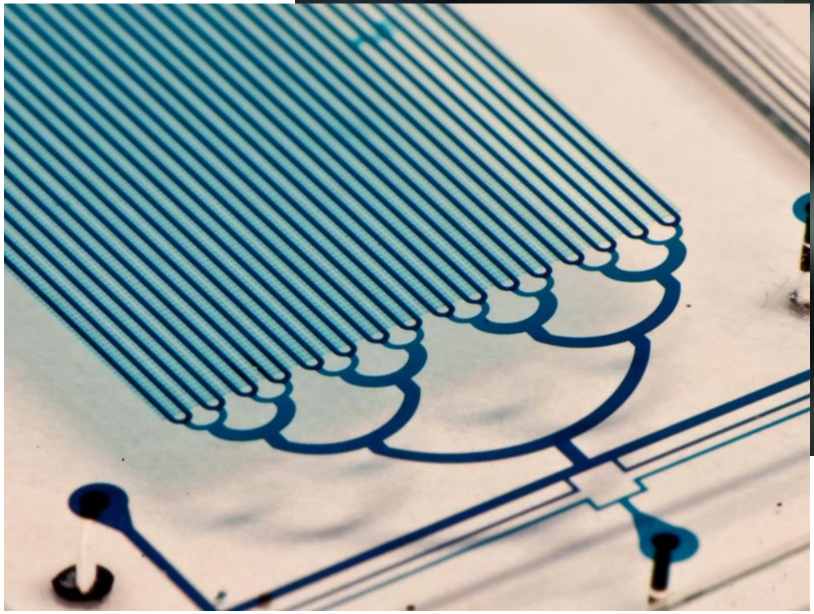
i. Chips para especialistas (labs)



Elveflow

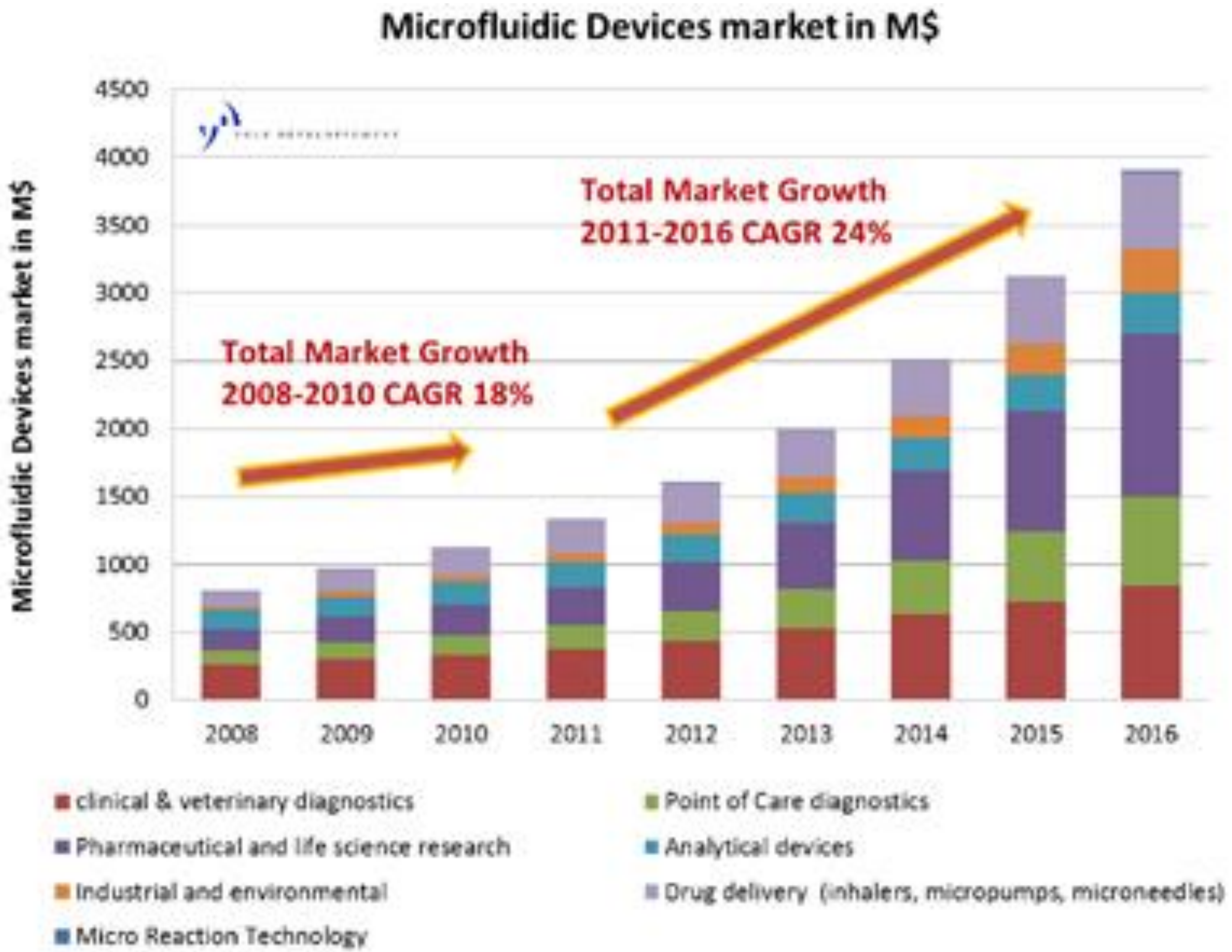
CytoFluidix





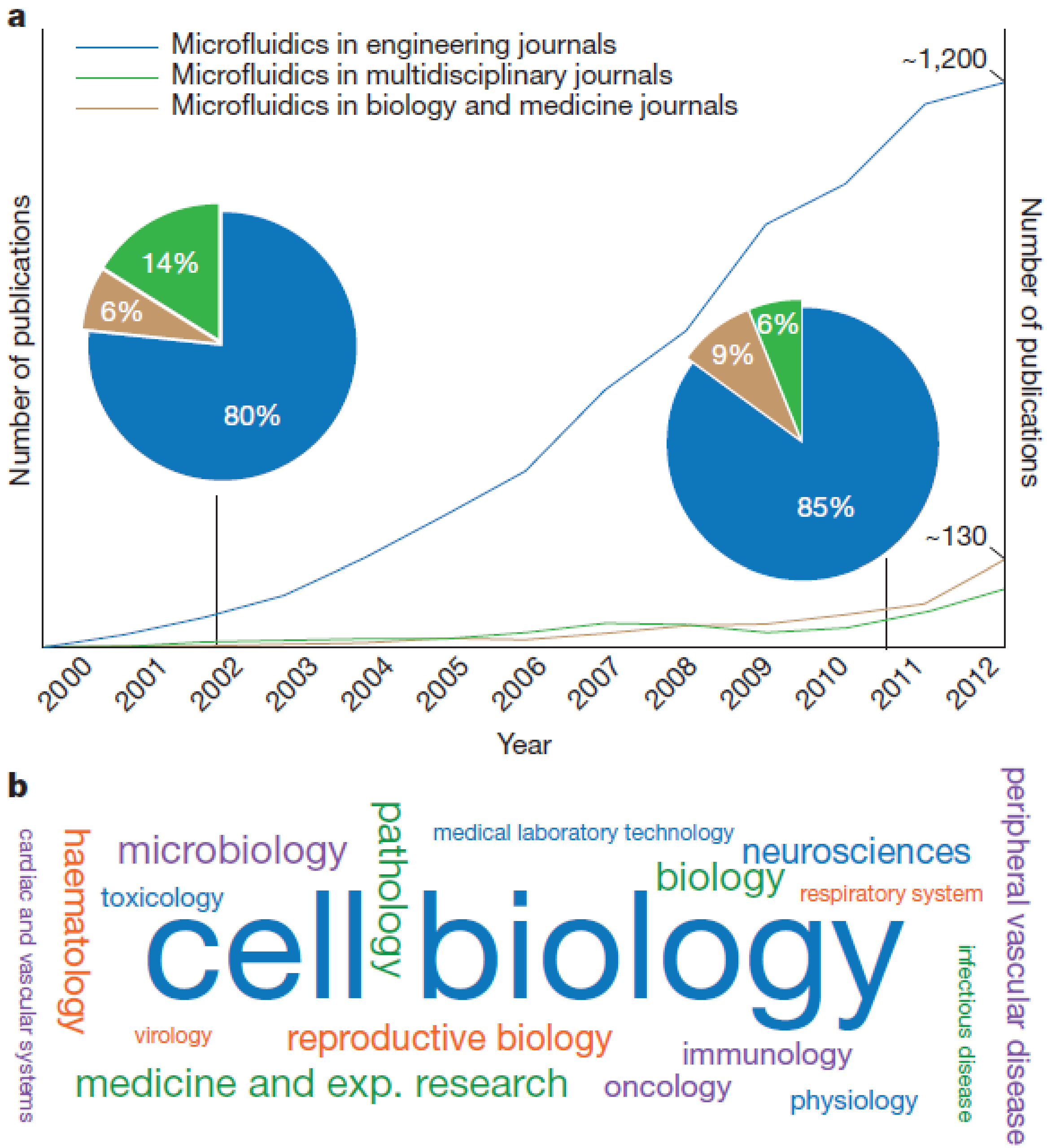
Dolomite

i. Mercado asociado a la microfluídica



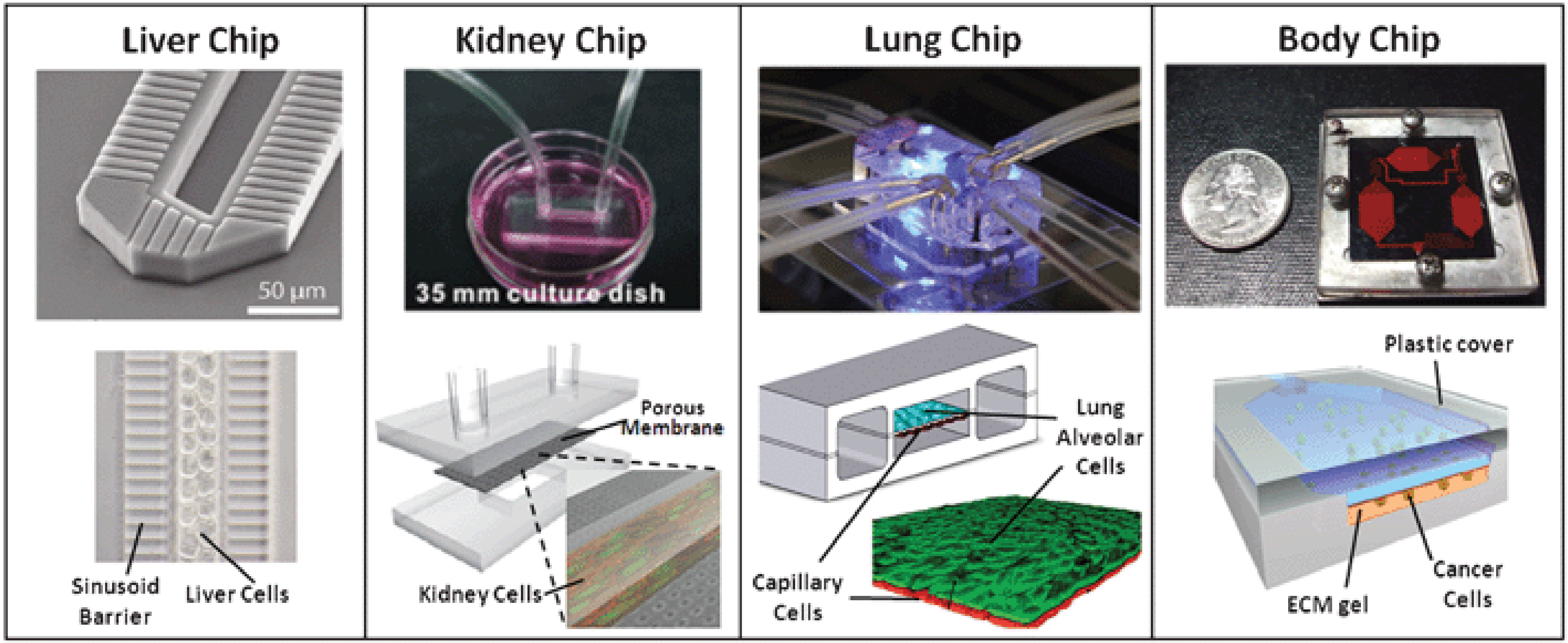
www.psmarketresearch.com/press-release/microfluidic-devices-market

i. Publicaciones en microfluídica



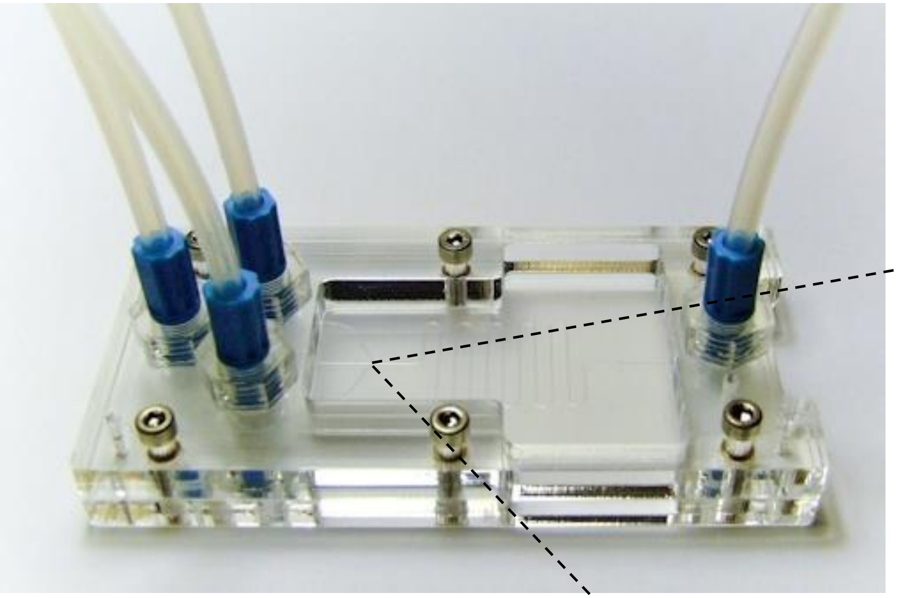
Nature **507**, March 2014

i. Hot topic: órganos en chips

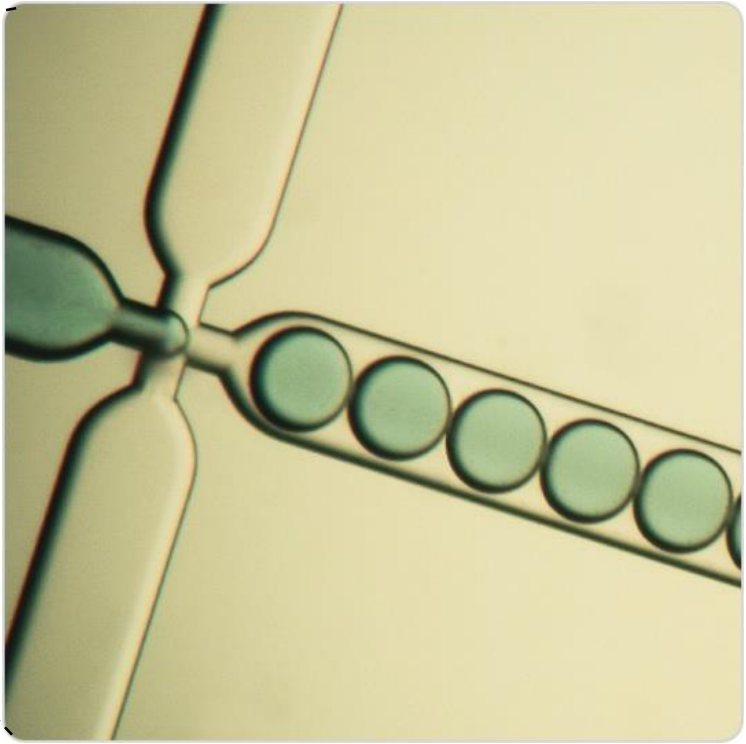


Huh et al., *Lab Chip* **12** (2012) 2156

i. Microgotas: una gran ventaja de la microfluídica



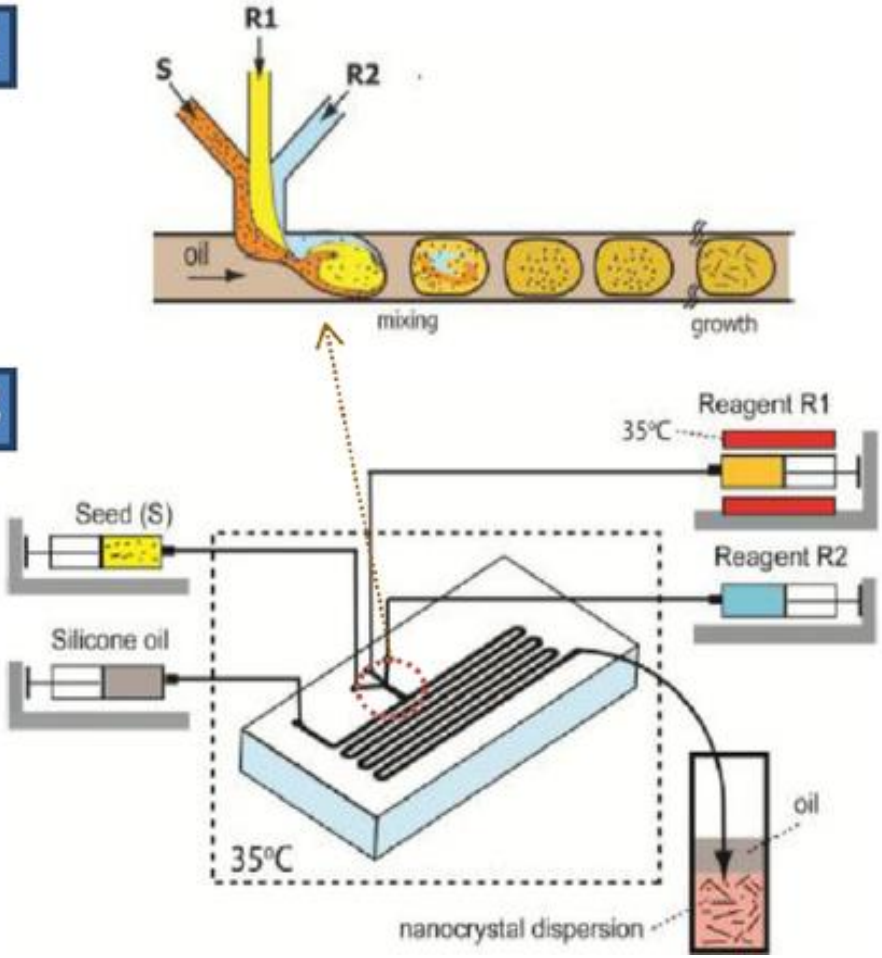
dolomite-microfluidics.com



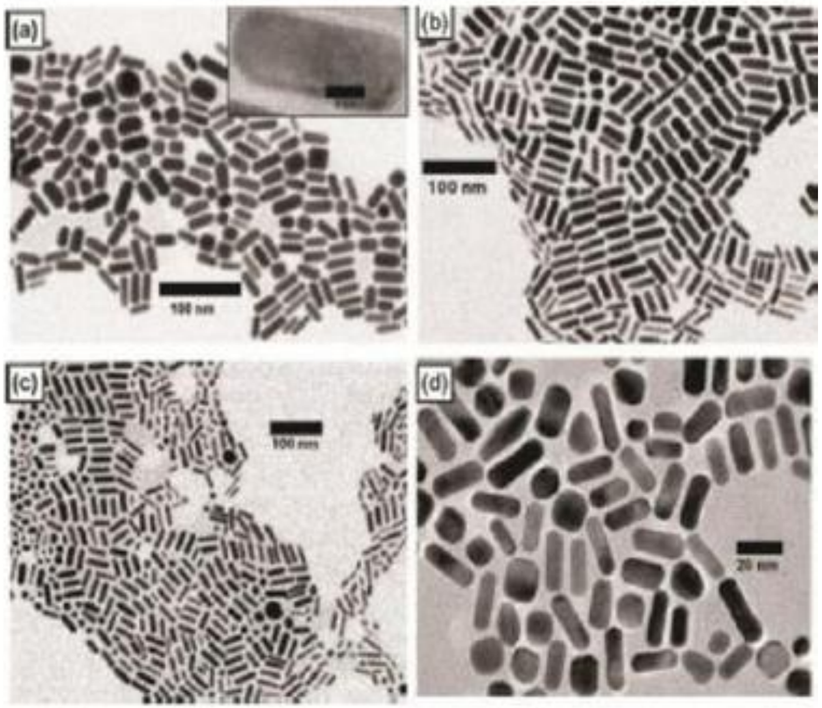
i. Nanopartículas/nanocristales

1

3

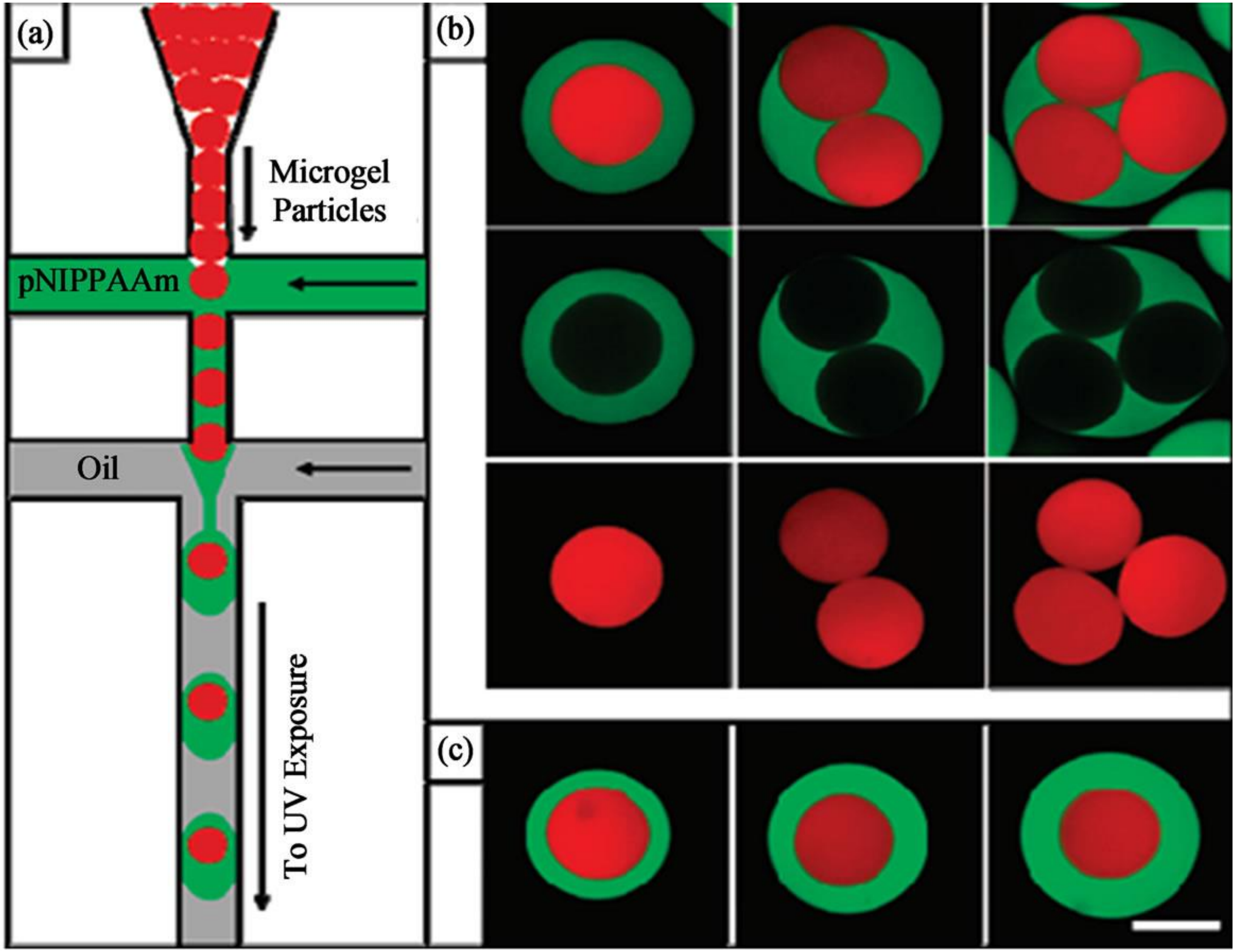


2



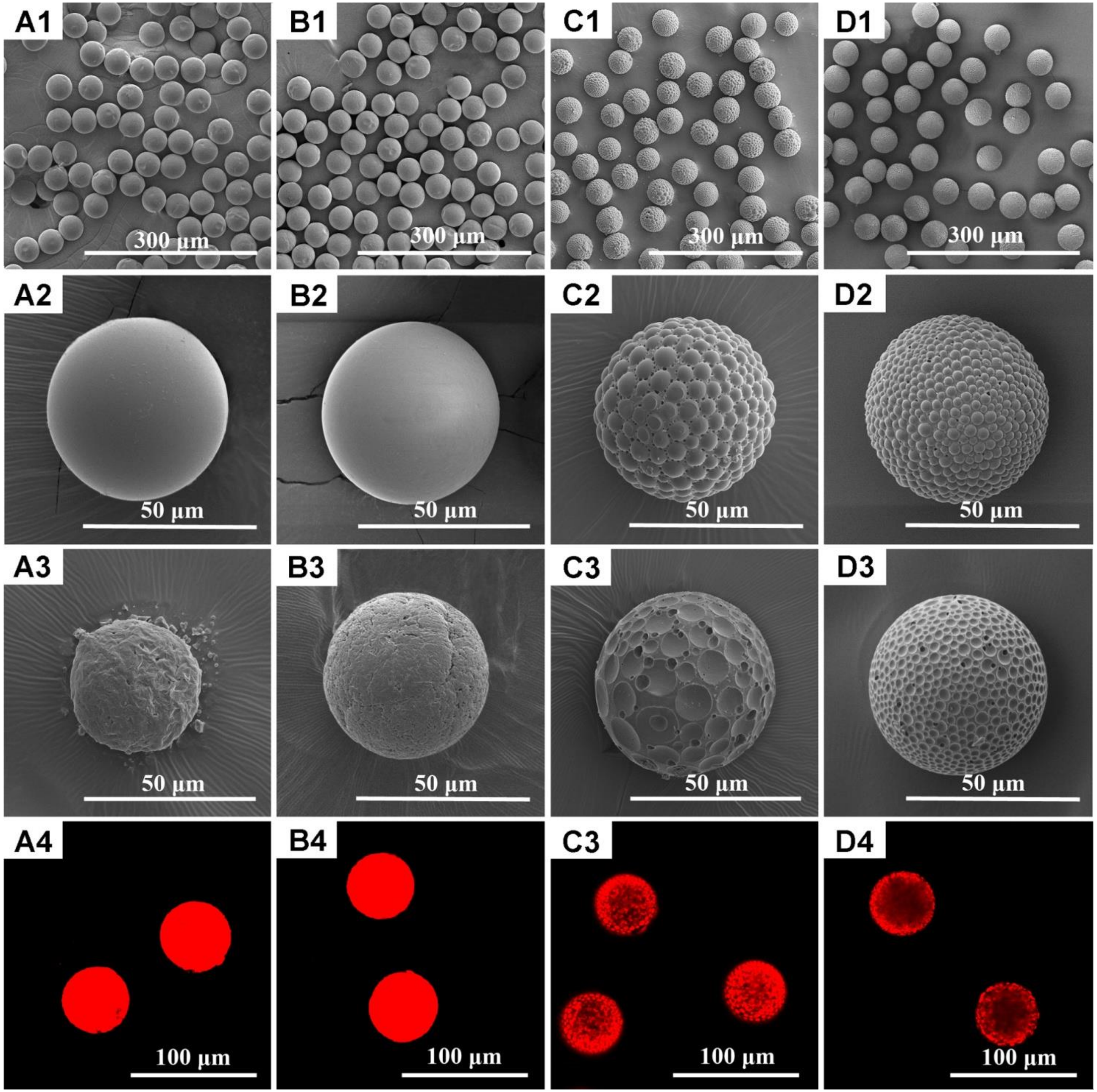
Duraiswamy and Khan, *Small* **5** (2009) 2828

i. Partículas: microgeles, cápsulas, múltiples



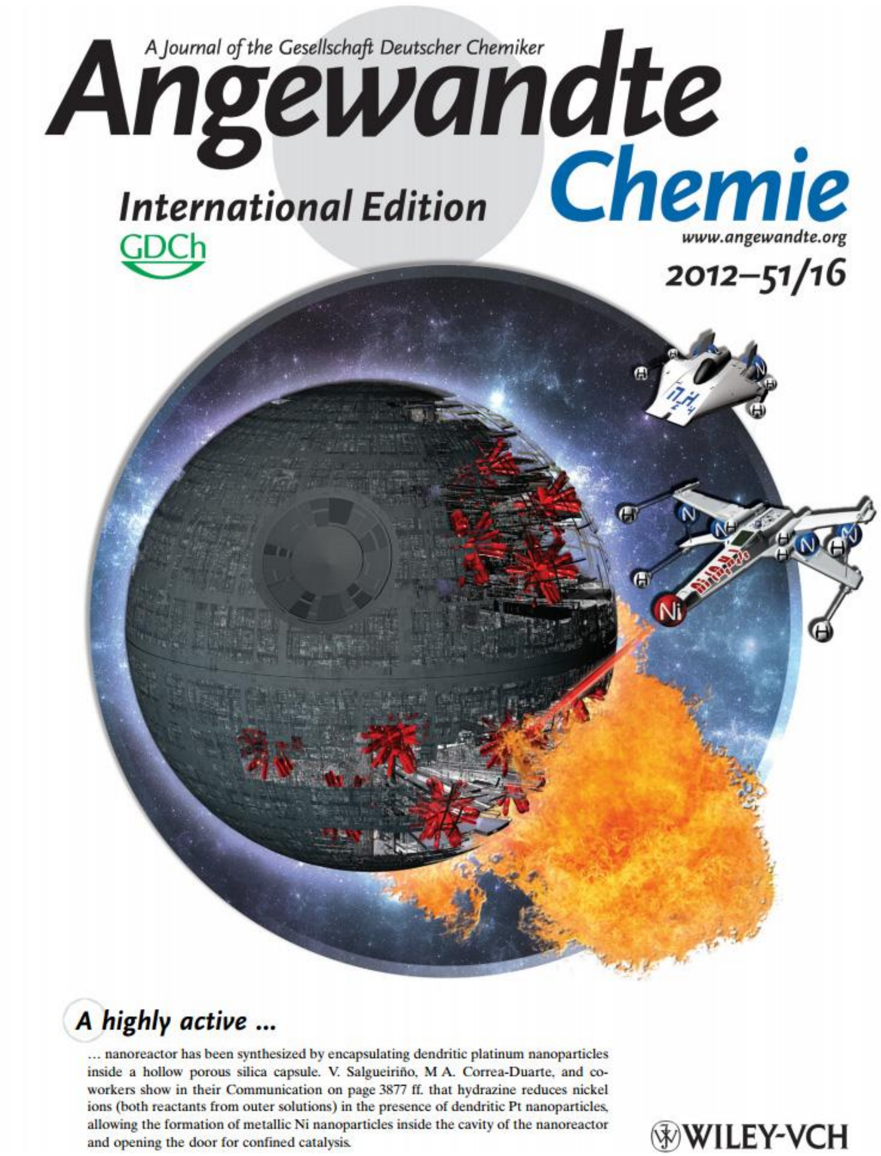
Seiffert et al, *JAOCS* **132** (2010) 6606

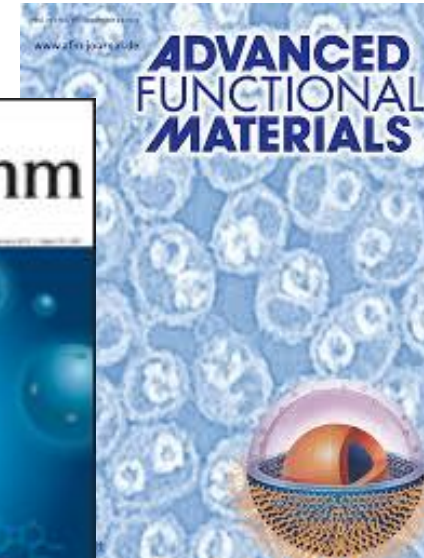
i. Partículas con gran precisión



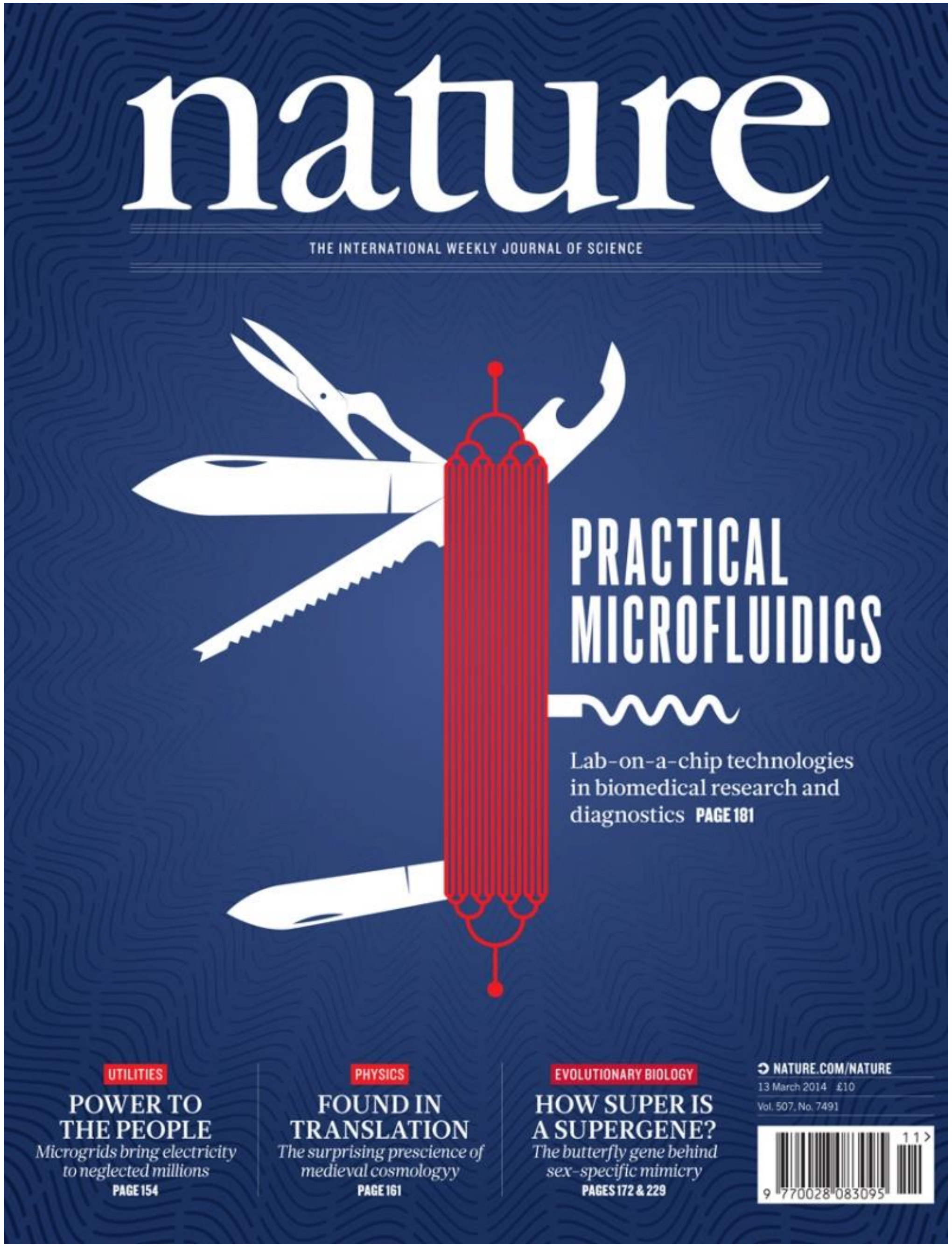
Cao et al, *RSC Adv* **5** (2015) 79969

¡. Partículas activas!



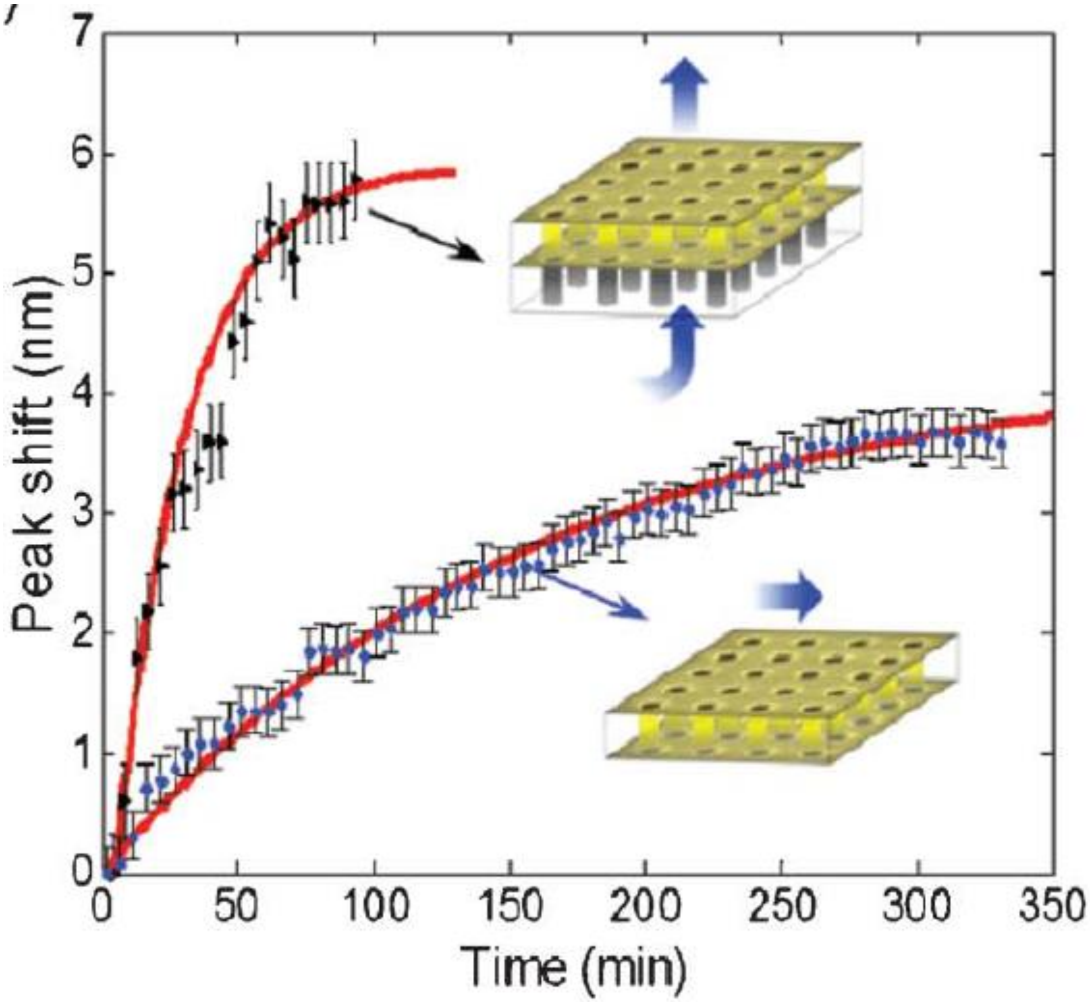


¡. Microfluídica: una herramienta de laboratorio!



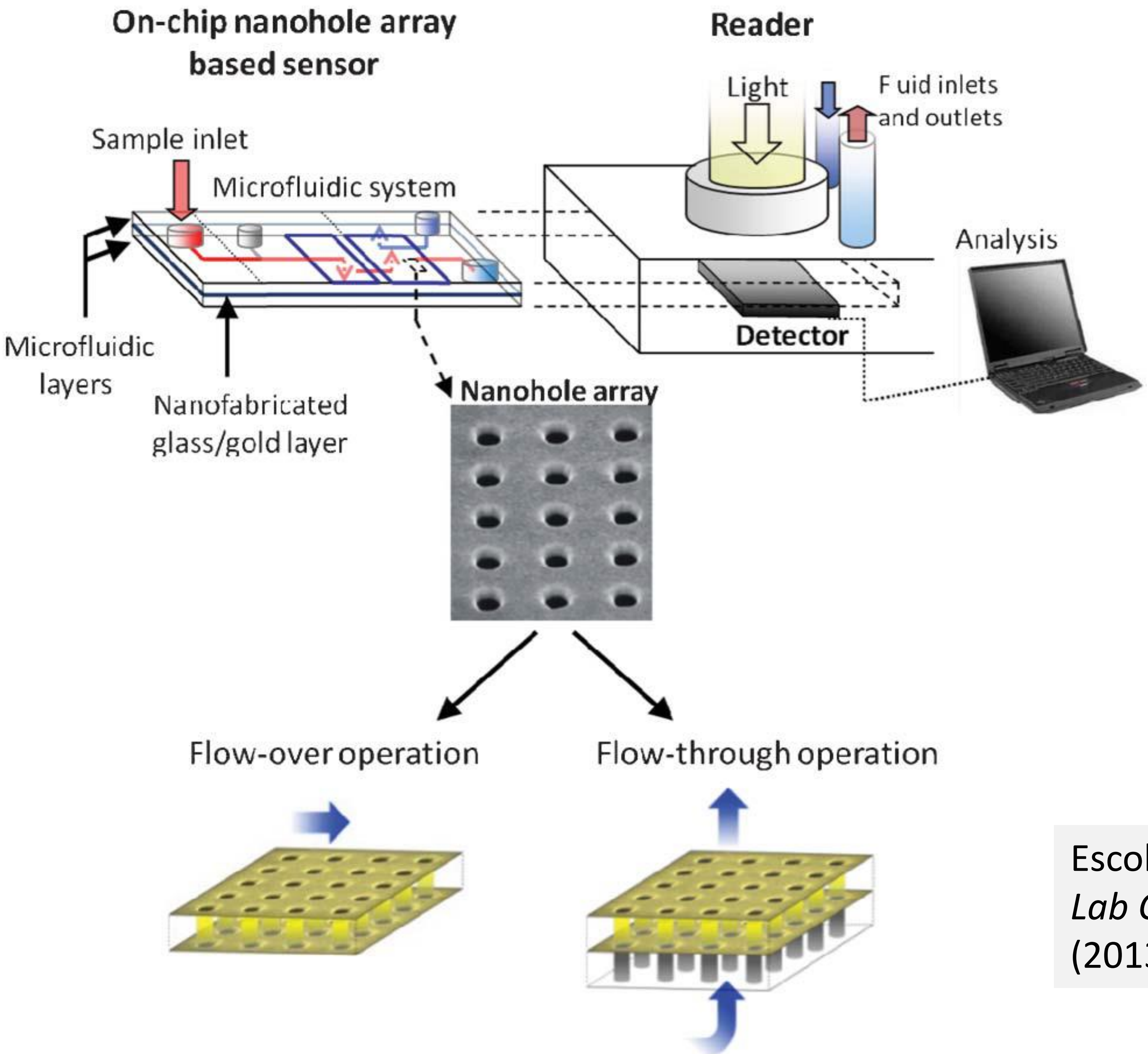
Nature **507**, March 2014

¿Por qué microfluídica en nano-ciencia/tecnología?



Escobedo,
Lab Chip **13**
(2013) 2445

i. Porque es la conexión con el mundo macro…



Escobedo, *Lab Chip* **13** (2013) 2445

Segunda parte

- *i.* **Introducción**
- *ii.* **Circuitos de microcanales**
  - Fundamentos y abordaje académico
  - Navier-Stokes, regímenes de flujo
  - Perfiles de velocidad 1D
  - Relaciones flujo-fuerza
  - Redes de microcanales
  - Co-flujos (juntura Y, juntura X, aplicaciones)
  - Flujos 2D y 3D: simulación
- *iii.* **Ejemplo: nuevos materiales**

ii. ¿Para qué estudiar los fundamentos?

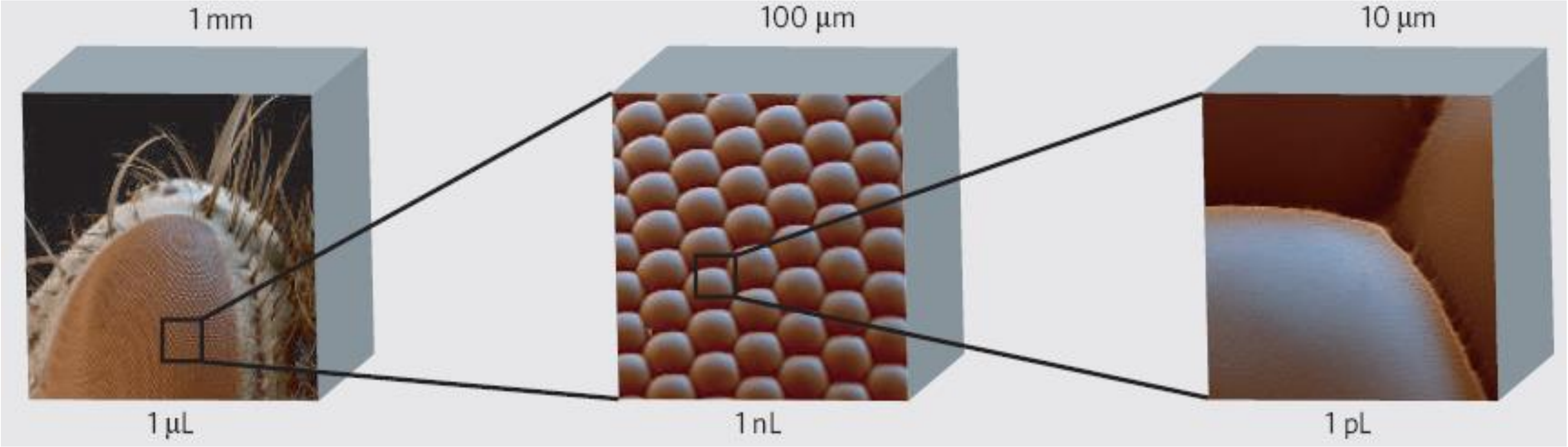
fundamentos y modelado

simulación, diseño y fabricación

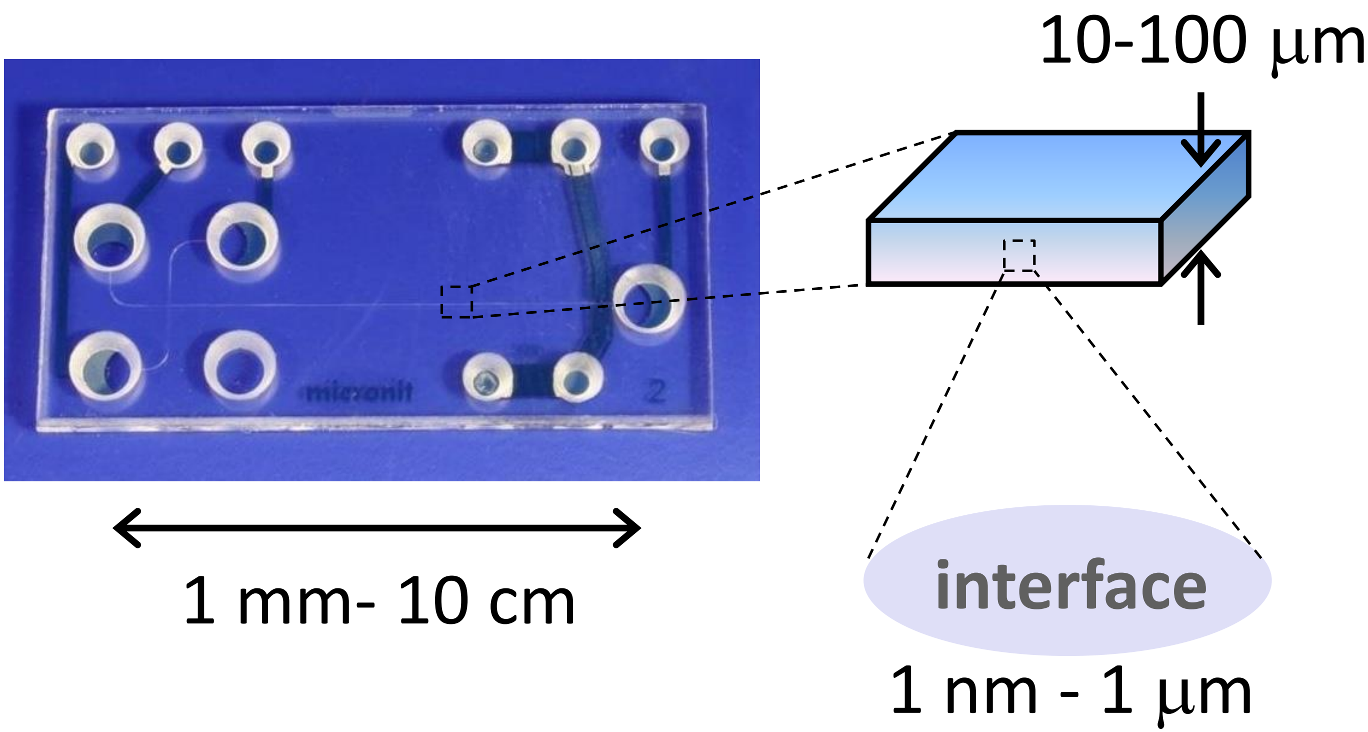
operación de los chips

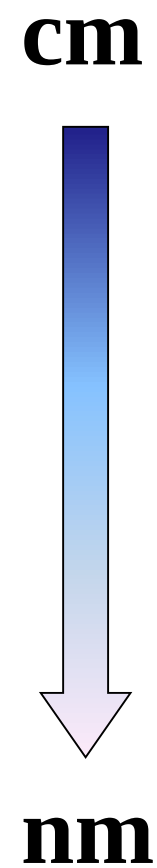
nuevos conocimientos

ii. Escalas de la microfluídica



ii. Dimensiones características





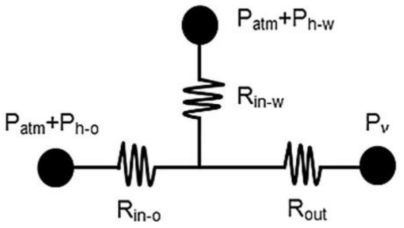
Multi-escala

Multi-física

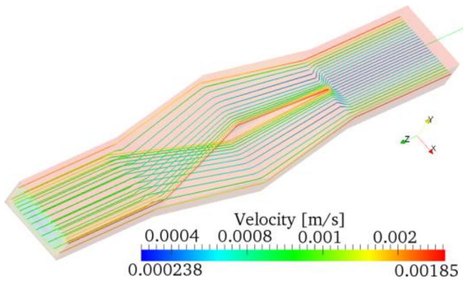
cm

nm

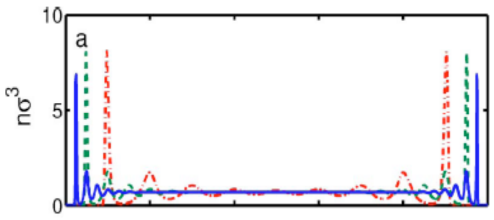
System level
Equivalent circuit theory



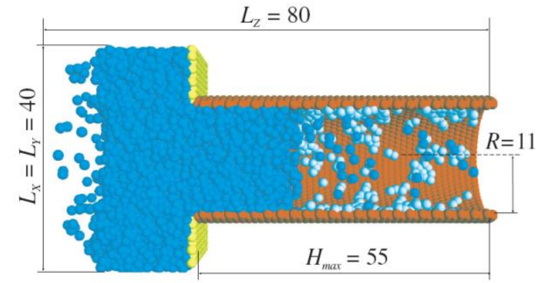
Macroscopic
Continuum equations
Transport phenomena



Mesoscopic
Lattice Boltzmann
Dissipative dynamics



Microscopic
Molecular dynamics
Monte Carlo



ii. Breve historia académica

Happel and Brenner (1965) **Low Re Number Hydrodynamics**

Batchelor (1977) **Microhydrodynamics**

Probstein (1989) **Physicochemical Hydrodynamics**

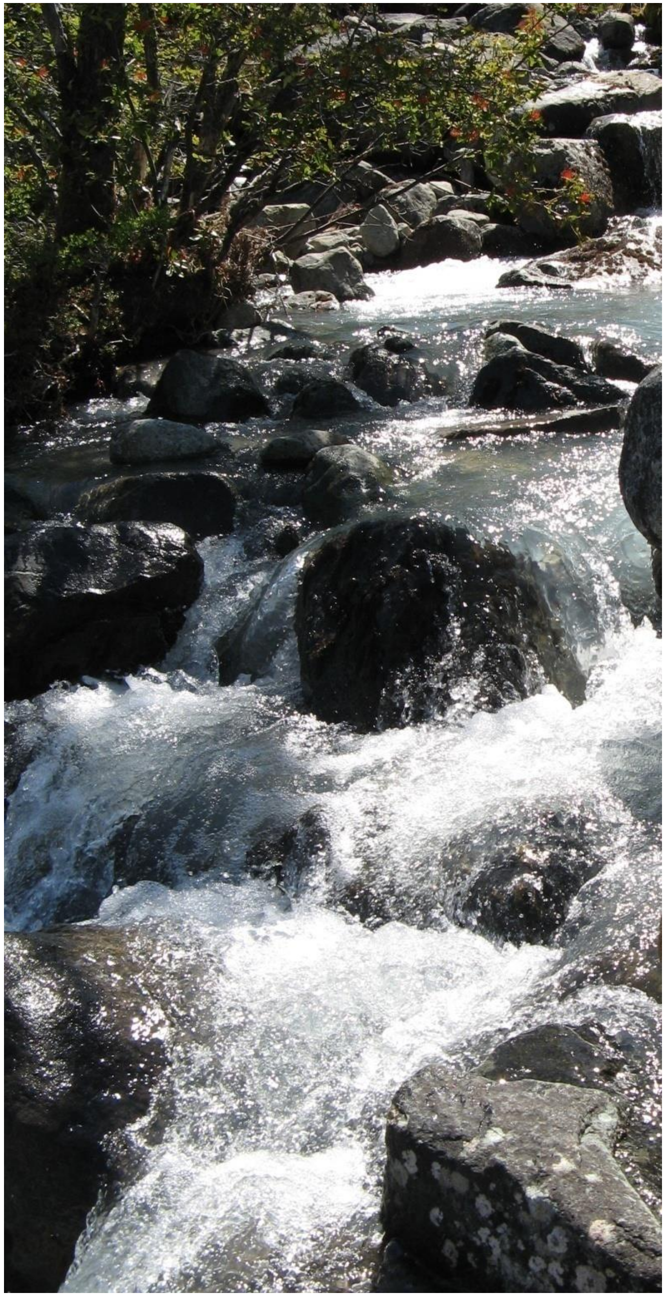
Karnidiakis and Beskok (2002) **Microflows**

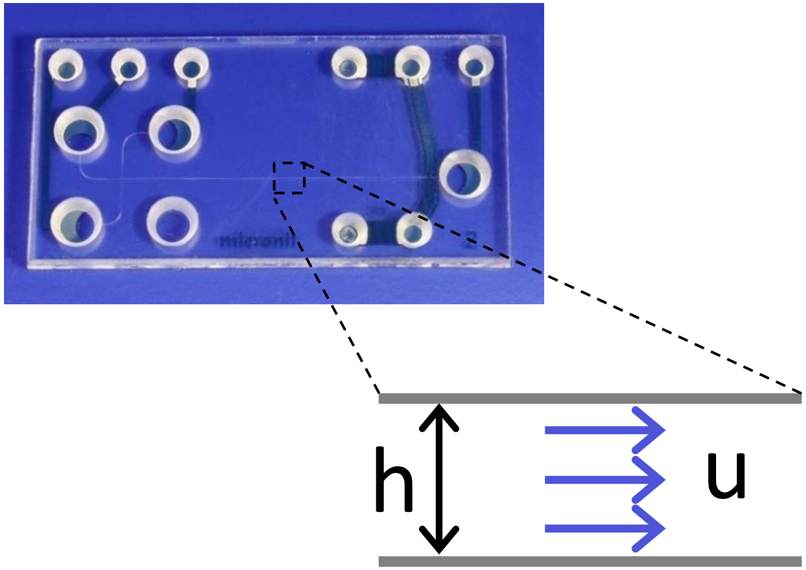
Tabeling (2005) **Introduction to Microfluidics**

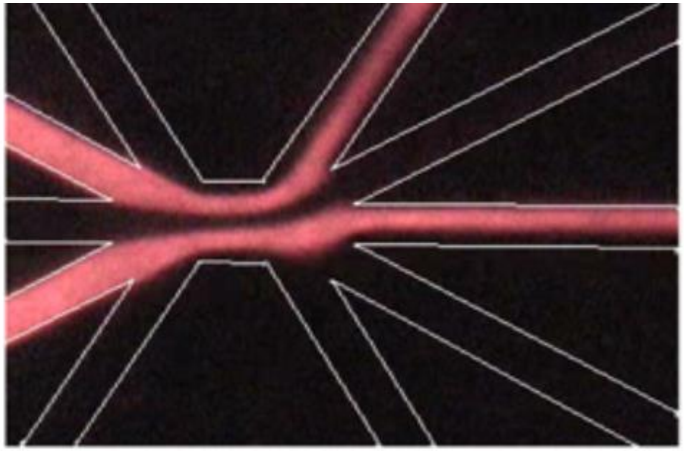
Bruus (2008) **Theoretical Microfluidics**

Lab-on-a-Chip	(RCS, 2000)
Microfluidics and Nanofluidics	(Springer, 2004)
Biomicrofluidics	(AIP, 2007)

ii. Propiedades de los flujos confinados







Pan et al, *JMM* **17** (2007) 820

ii. Reynolds, Navier y Stokes

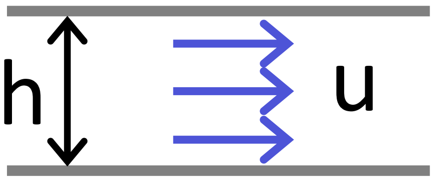
Newtoniano
incompresible
isotérmico

$$\nabla.\mathbf{u} = 0$$

Navier, 1785-1836
Stokes, 1819-1903

$$\rho\left(\frac{d\mathbf{u}}{dt} + \mathbf{u}.\nabla\mathbf{u}\right) = -\nabla P + \mu\nabla^2\mathbf{u}$$

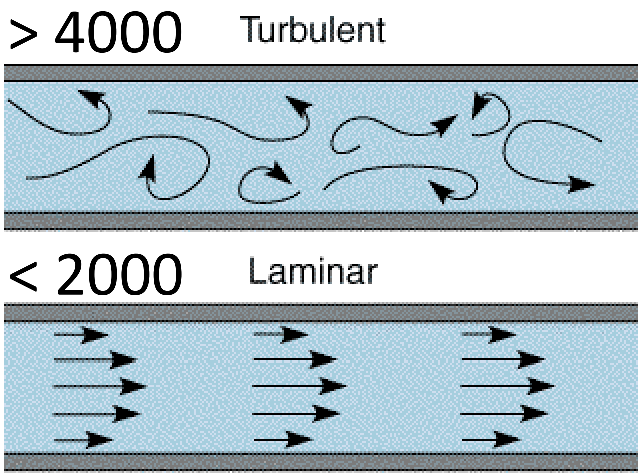
Reynolds, 1842-1912

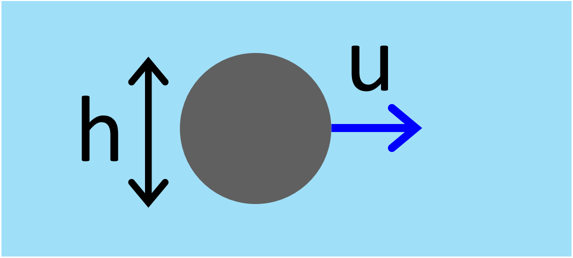


$$Re = \frac{\rho u h}{\mu}$$

ii. Reynolds, Navier y Stokes

$$Re = \frac{\rho u h}{\mu}$$





> 90 separated
> 5 unseparated
< 1 creeping

Re < 1

→ Regimen de Stokes
→ Sin aceleración, reversible
→ Alta viscosidad, baja velocidad
→ → o altamente confinado

ii. Regímenes de flujo

$Re \sim 10^3$

→ Inviscido
→ Energía mecánica
→ En tuberías: Bernulli, 1739

$Re \sim 10^{-5}$

→ Velocidad constante
→ Microorganismos
→ Microcanales

ii. Regímenes de flujo

$$\tau_s = \frac{\rho h^2}{\mu} \sim \text{ms}$$

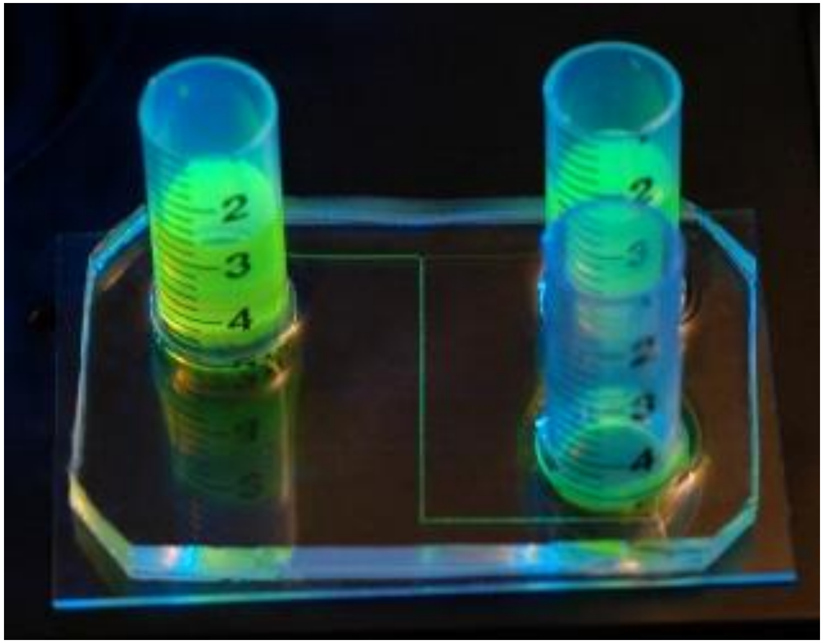
$Re \sim 10^{-2}$

ii. El sello de la microfluídica

Kenis et al.,
Science **285**
(1999) 83

COVER
Seven aqueous streams, each colored with a different dye, converge in a microchannel and proceed in parallel laminar flow, without turbulent mixing.
[© F. Frankel]

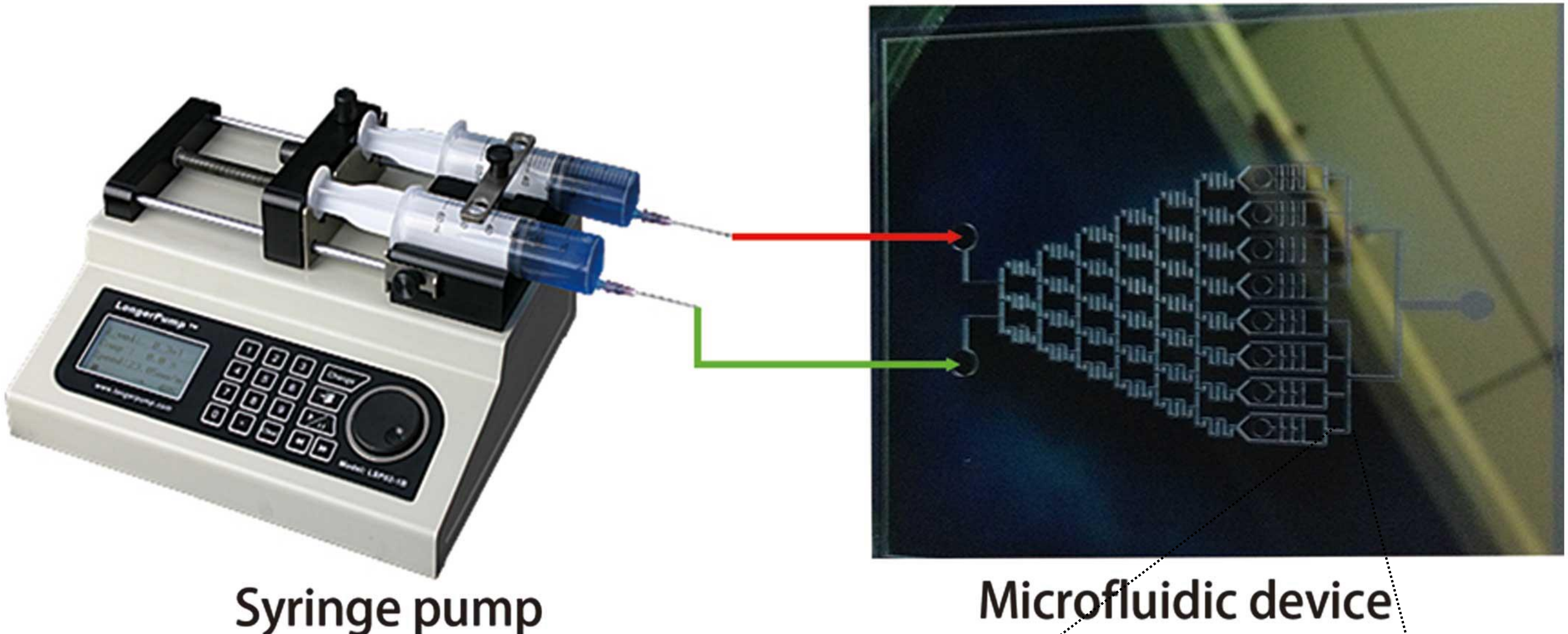
ii. Bombeo elemental: control la presión



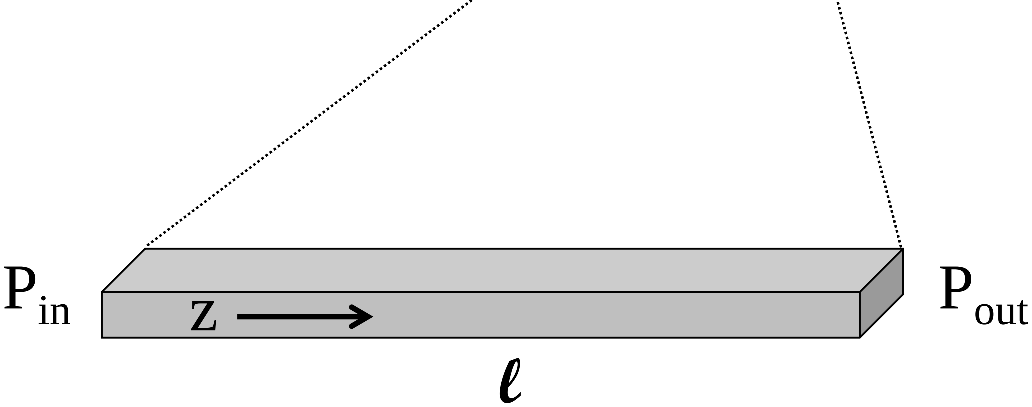
umech.mit.edu

elveflow.com

ii. Flujos inducidos por presión



$$-\frac{\partial P}{\partial z} = \frac{\Delta P}{\ell}$$

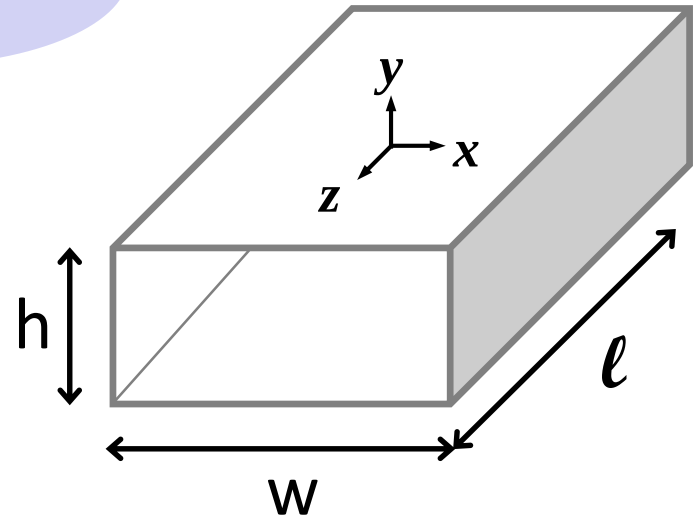


ii. Flujo en canales rectangulares

$$\nabla P = \mu \nabla^2 \mathbf{u}$$

Re << 1, ftd

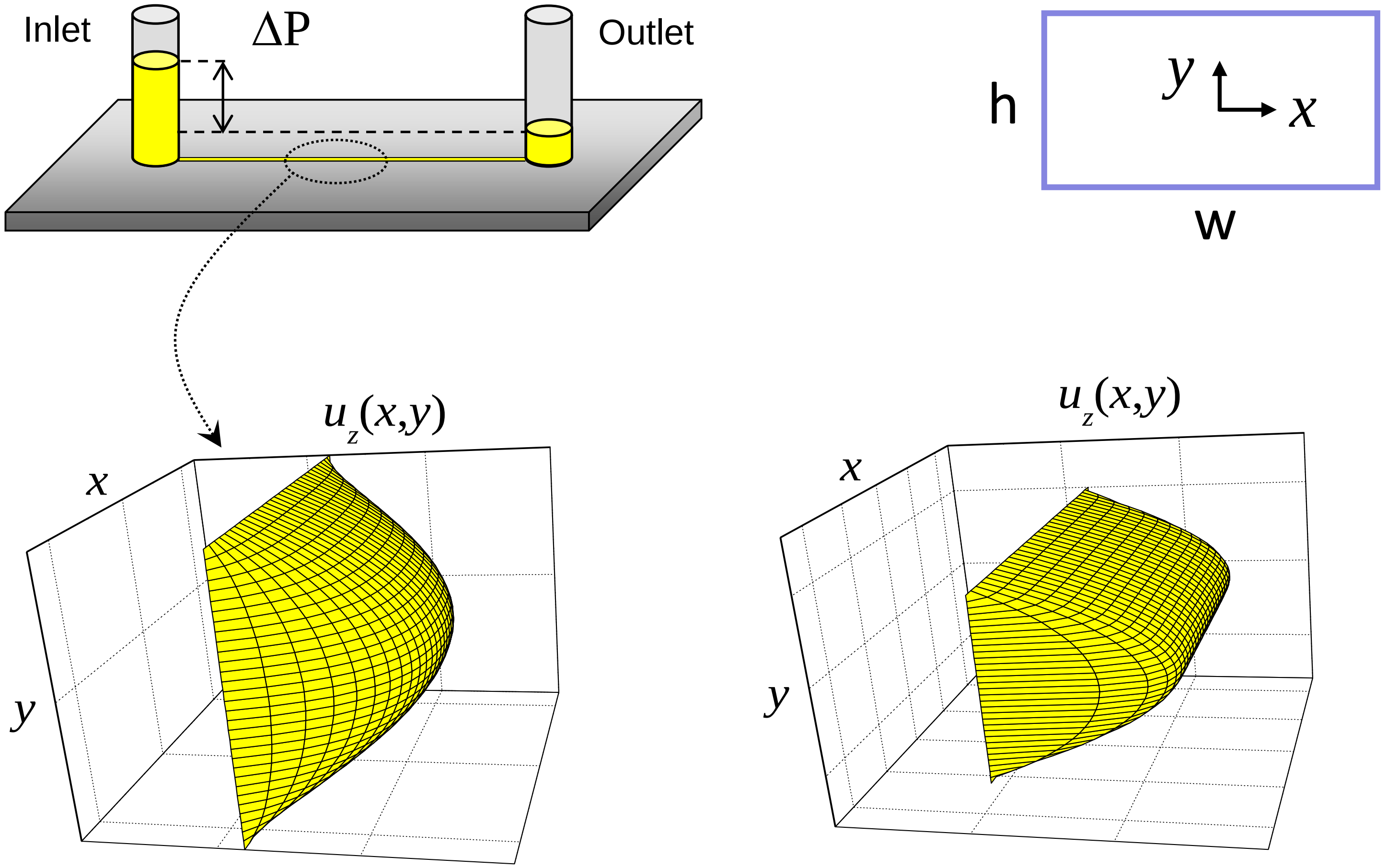
$$\frac{\partial P}{\partial z} = \mu\left(\frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2}\right)$$



$$\Rightarrow \quad u_z(x,y) = \frac{h^2 \Delta P}{8\mu \ell} G(x,y)$$

$$G(x,y) = 32\sum_{m=1}^{\infty}\frac{(-1)^{m+1}}{\beta_m^3}\left(1 - \frac{ch(\beta_m x/h)}{ch(\beta_m w/2h)}\right)\cos(\beta_m y/h)$$

ii. Perfiles de velocidad

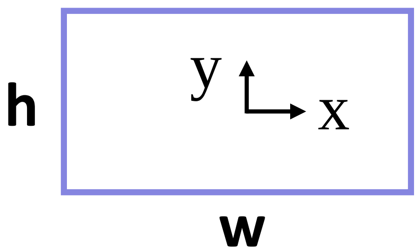


h/w = 2/5

h/w = 1/10

ii. Caudal volumétrico

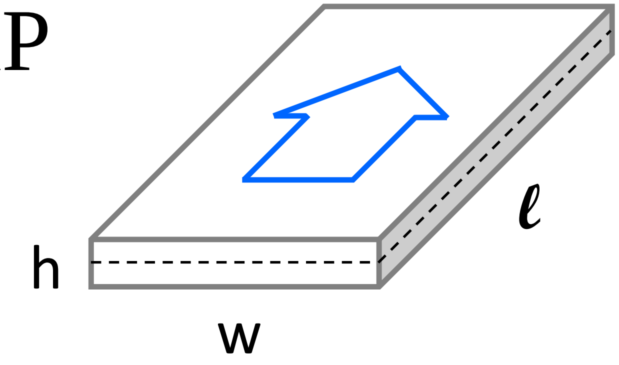
$$Q = \iint u_z(x,y)\,dx\,dy$$



$$= \frac{wh^3 \Delta P}{12\mu\ell} \sum_{m=1}^{\infty} \frac{96}{\beta_m^4}\left[1 - \frac{\tanh\left(\beta_m w/2h\right)}{\beta_m w/2h}\right]$$

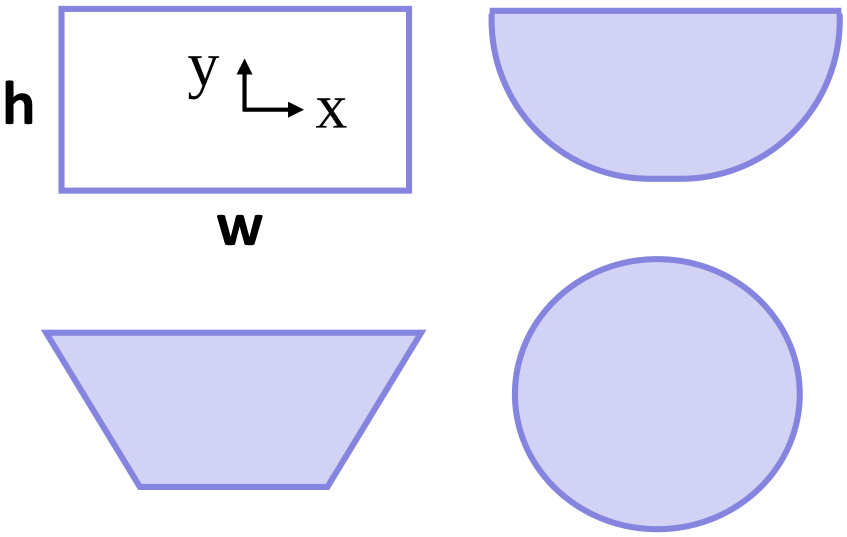
	h/w
0.42	1/1
0.75	2/5
0.99	1/60

$$Q \approx \frac{wh^3}{12\mu\ell}\Delta P$$



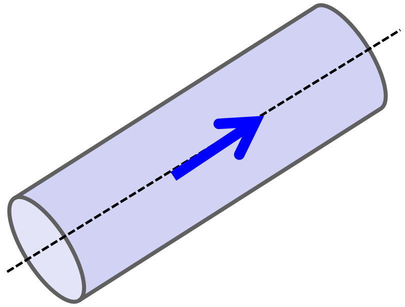
ii. Caudal vs presión

$$Q = \frac{wh^3 f_G}{12\mu\ell} \Delta P$$



$$Q = L \; \Delta P$$

$$\Delta P = R \; Q$$



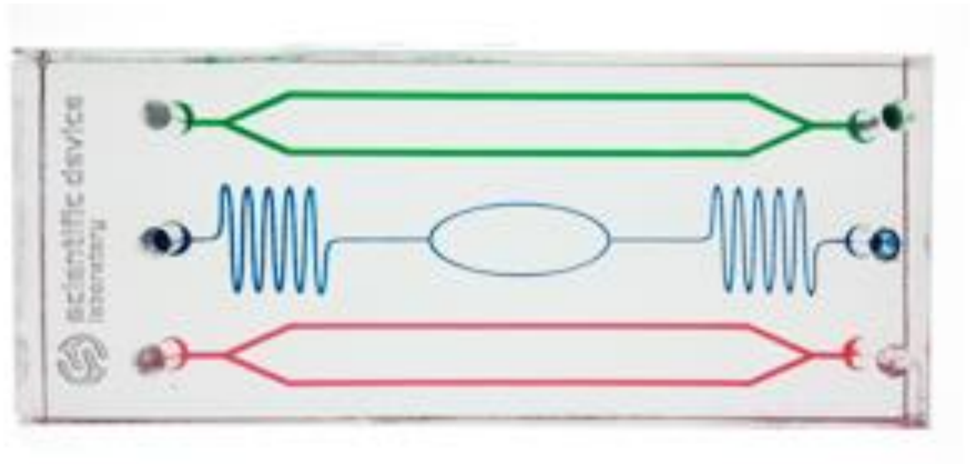
$$R = \frac{8\mu l}{\pi r^4}$$

Hagen, 1838
Poiseuille, 1839

ii. Microcanales en serie/paralelo

Caso más simple: **un puerto de entrada y uno de salida**

$$Q = L_{tot} \; \Delta P$$



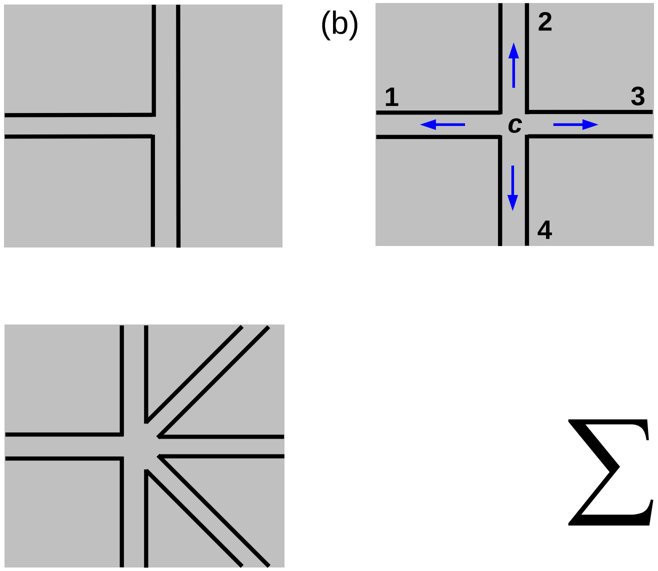
$$\Delta P = R_{tot} \; Q$$

$$R_{ser} = \sum_i R_i \qquad\qquad R_{par}^{-1} = \sum_i R_i^{-1}$$

ii. Redes de microcanales

(a) (b)

(c)



N canales/nodo

→ **1 incógnita**

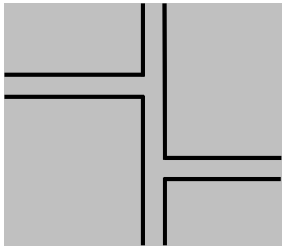
$$\sum_{i=1}^{N} Q_i = 0$$

$$\sum_{i=1}^{N} L_i \left(P_i - P_c\right) = 0$$

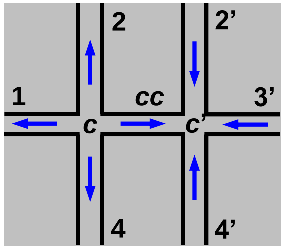
$$P_c = \sum_{i=1}^{N} L_i P_i \Big/ \sum_{i=1}^{N} L_i$$

ii. Redes de microcanales

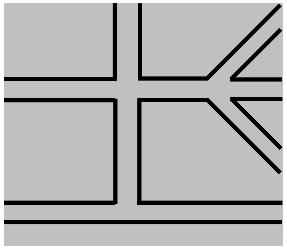
(d)



(e)



(f)



N canales/nodo

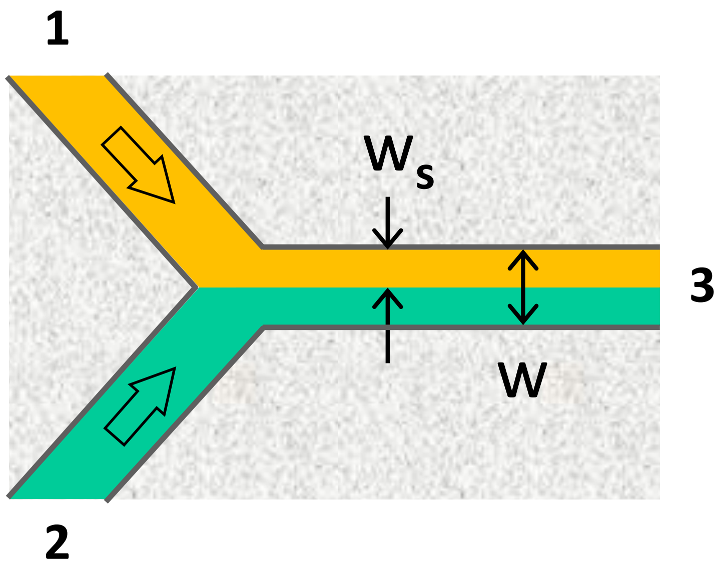
M nodos/red

→ **M incógnitas**

$$\sum_{i=1}^{N} Q_i = 0, \quad j = 1 \text{ a } M$$

$$\begin{bmatrix} \sum_{i=1}^{N} L_{11,i} & -L_{11,cc} \\ -L_{11,cc} & \sum_{i'=1'}^{N'} L_{11,i'} \end{bmatrix} \begin{bmatrix} P_c \\ P_{c'} \end{bmatrix} = \begin{bmatrix} \sum_{i \neq cc}^{N} L_{11,i} P_i \\ \sum_{i' \neq cc}^{N'} L_{11,i'} P_{i'} \end{bmatrix}$$

ii. Co-flujos, juntura Y

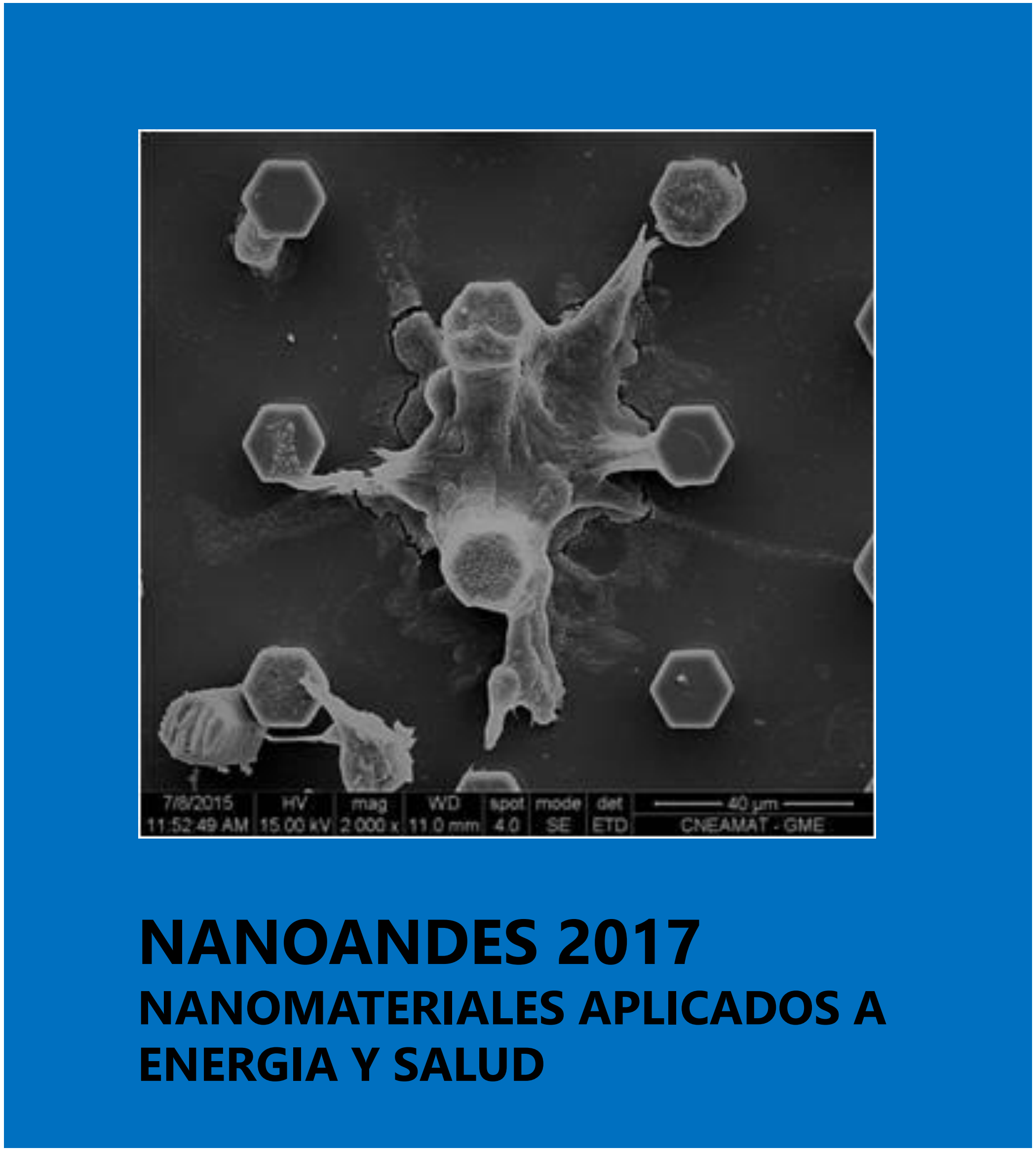


$$\frac{w_s}{w} = \frac{Q_1/Q_2}{1 + Q_1/Q_2}$$

$$P_3 = P_{atm},$$
$$L_1 = L_2 = L_3$$
$$1/2 \leq P_1/P_2 \leq 2$$

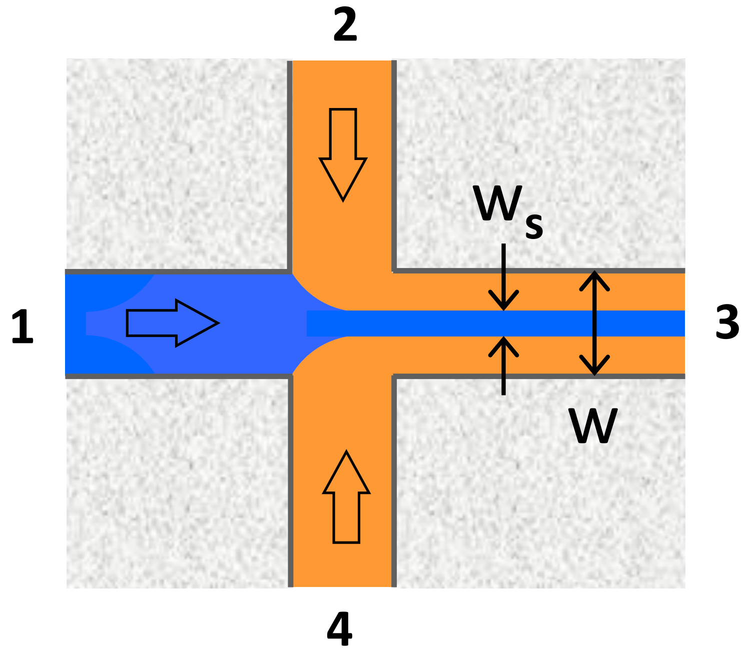
$$\Rightarrow \quad \frac{w_s}{w} = \frac{2 - P_2/P_1}{P_2/P_1 + 1}$$

ii. Co-flujos, juntura Y: aplicaciones



Takayama et al., *Chem. Biol.* **10** (2003) 123

ii. Co-flujos, juntura X

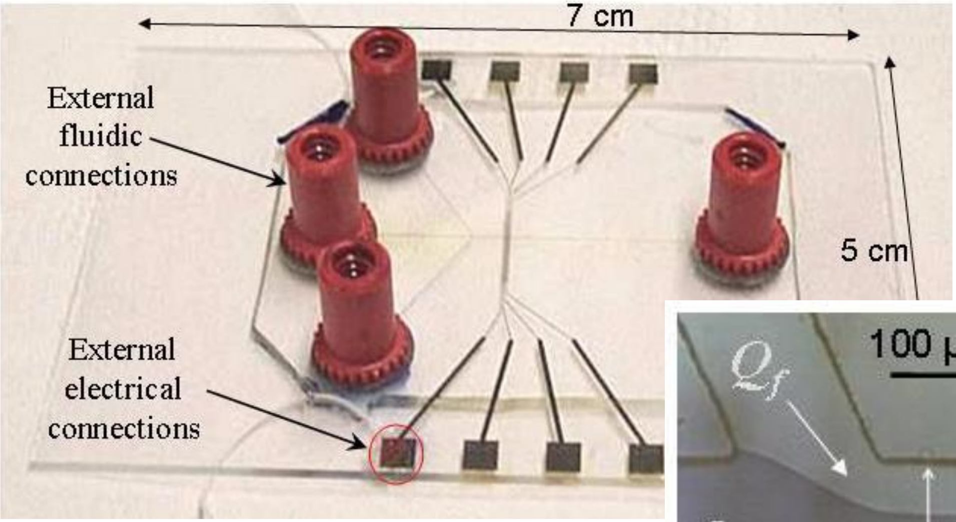


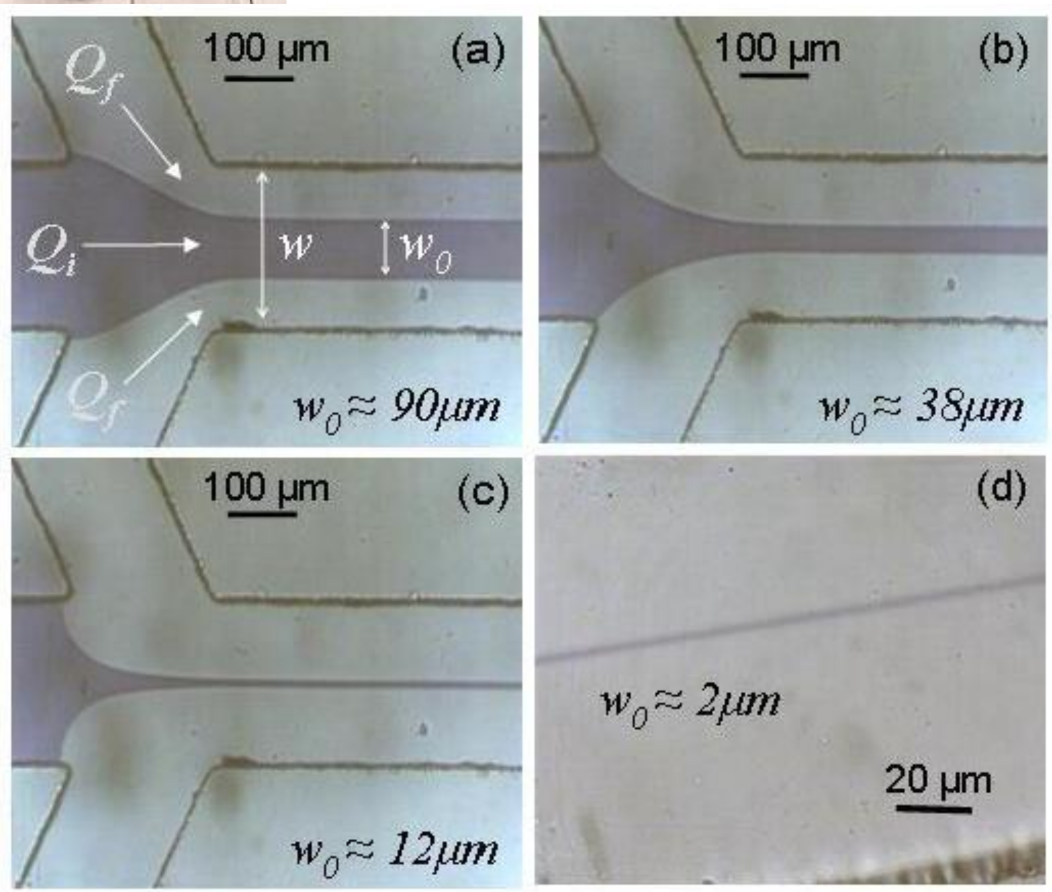
$$\frac{w_s}{w} = \frac{1}{1 + 2Q_{2,4}/Q_1}$$

$$P_3 = P_{atm},$$
$$L_1 = L_2 = L_3 = L_4$$
$$2/3 \leq P_{2,4}/P_1 \leq 3/2$$

$$\frac{w_s}{w} = \frac{3/2 - P_{2,4}/P_1}{1/2 + P_{2,4}/P_1}$$

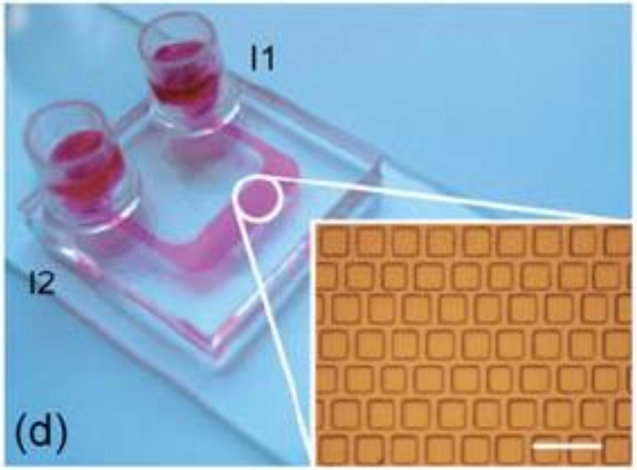
ii. Co-flujos, juntura X: aplicaciones

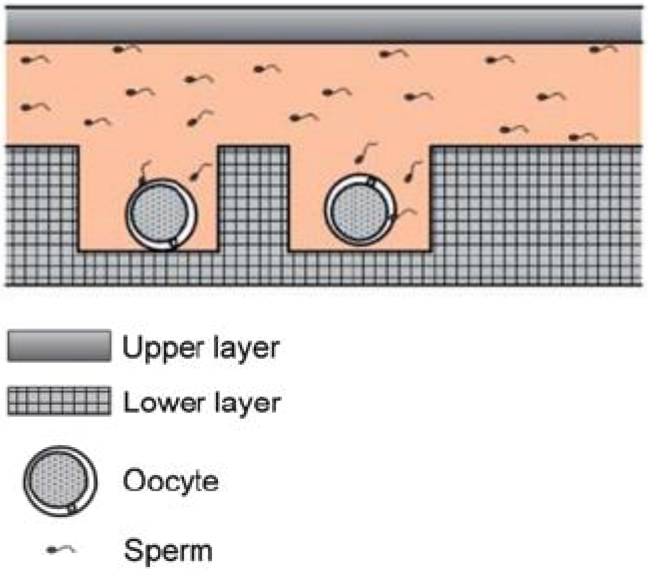




Rodriguez et al.,
Microfluid Nanofluid **3** (2007) 171

ii. Flujos 2D y 3D: simulación

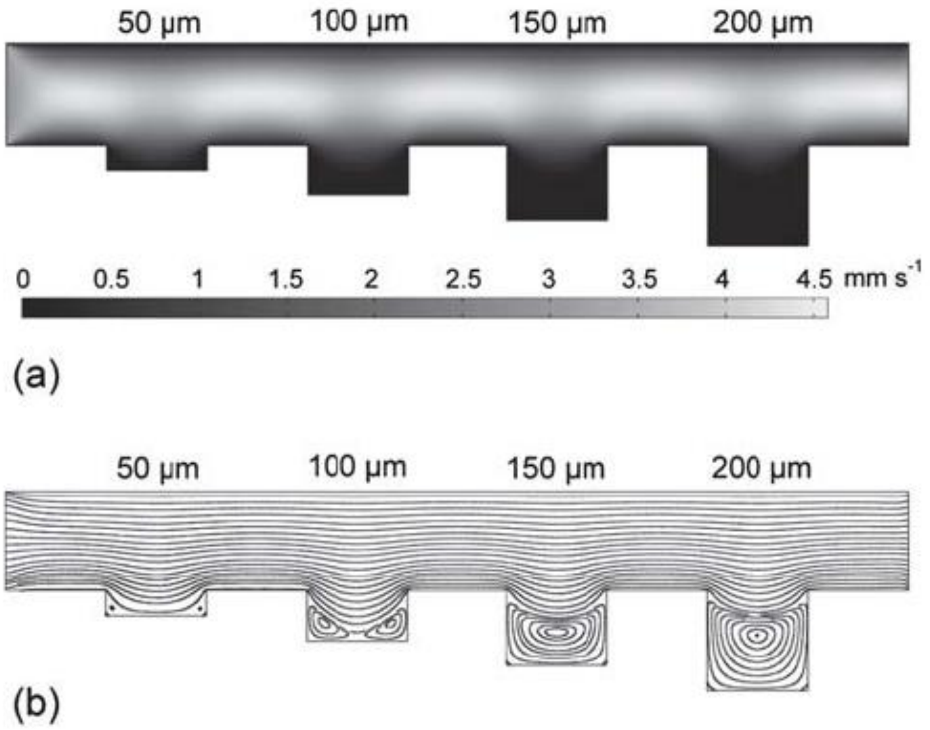




$$\nabla.\mathbf{u} = 0$$

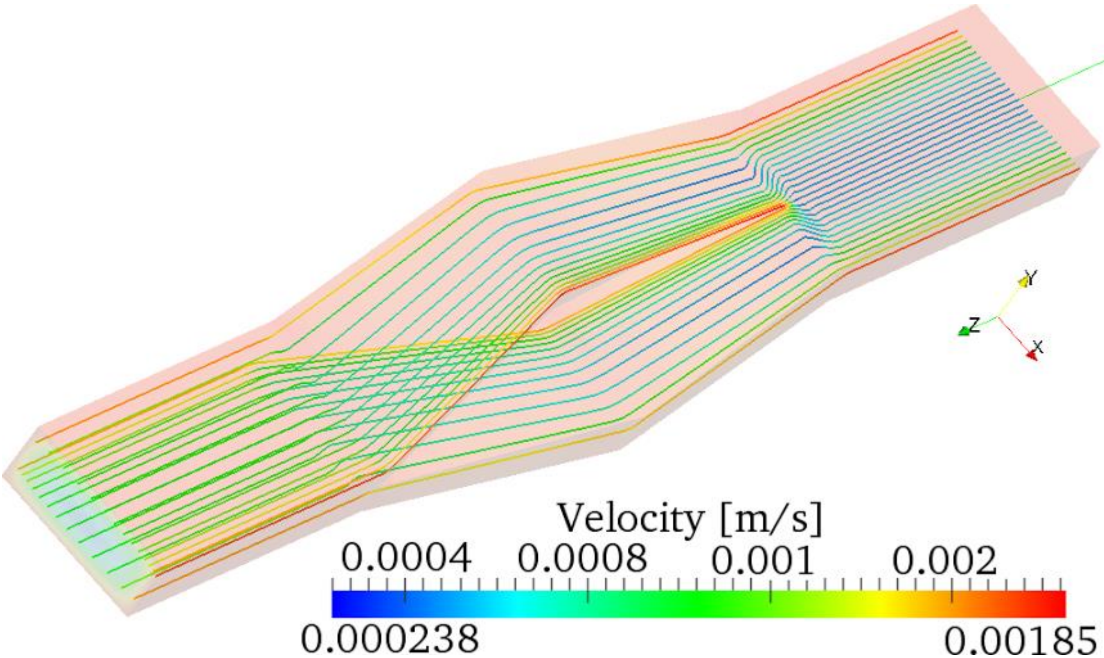
Newtoniano
incompresible
isotérmico

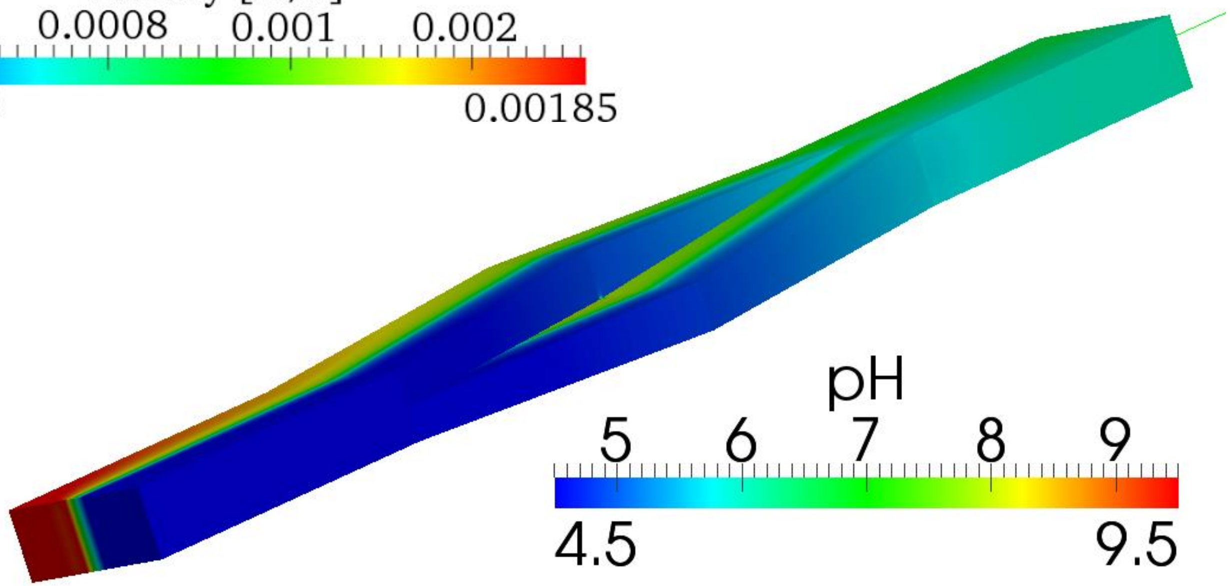
$$\rho\left(\frac{d\mathbf{u}}{dt} + \mathbf{u}.\nabla\mathbf{u}\right) = -\nabla P + \mu\,\nabla^2\mathbf{u}$$



Han et al., *Lab Chip* **10** (2010) 2848

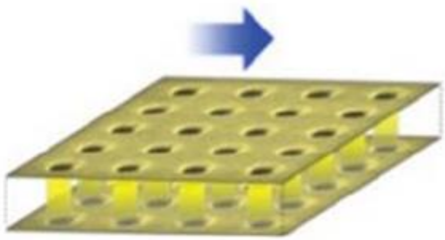
ii. Flujos 2D y 3D: simulación

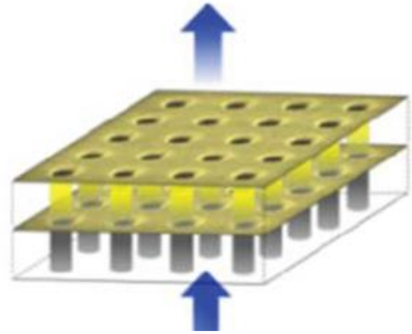


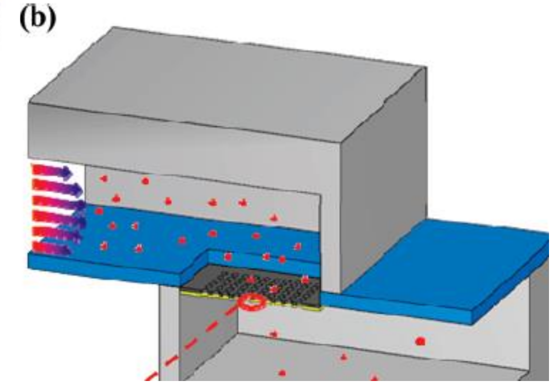


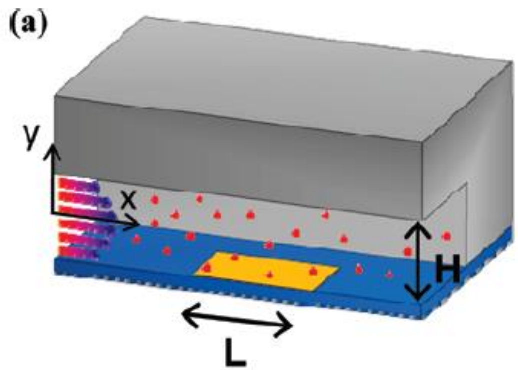
Kler et al.
Comp Mech
51 (2013) 171

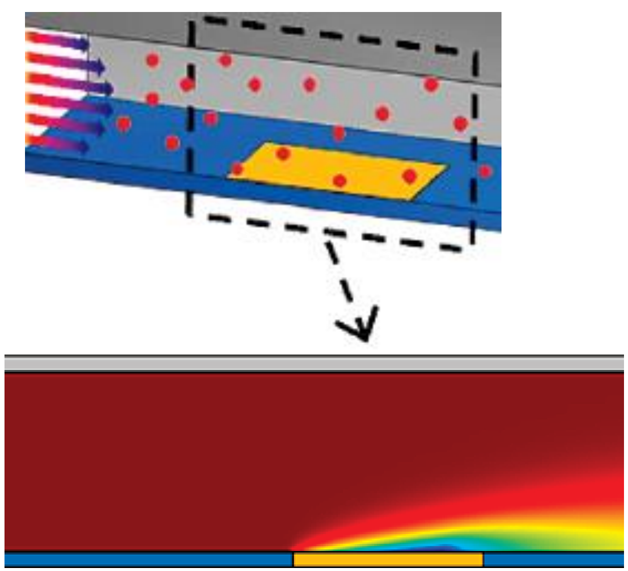
ii. Flujos 2D y 3D: simulación

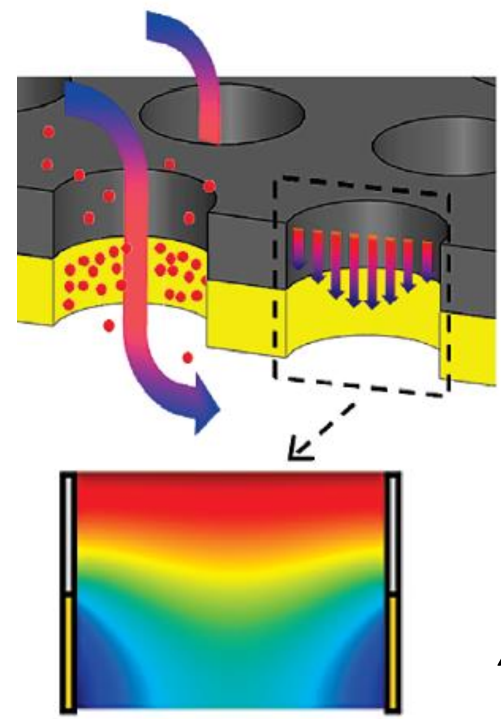










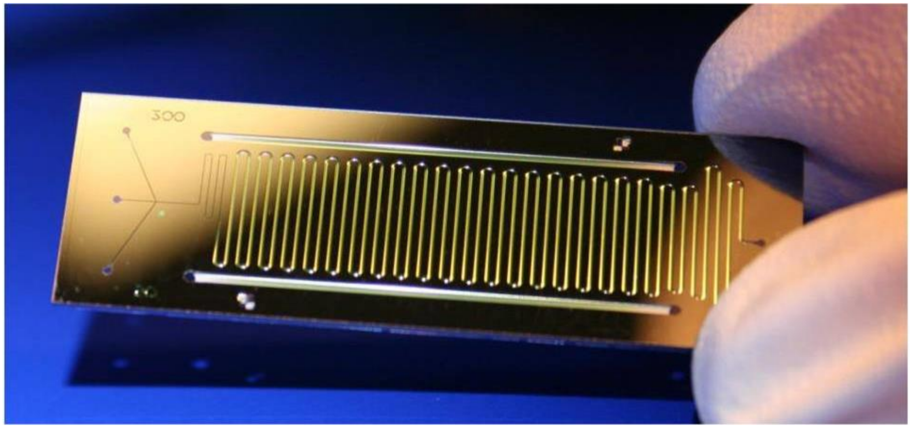


Escobedo et al,
Anal Chem **82**
(2010) 10015

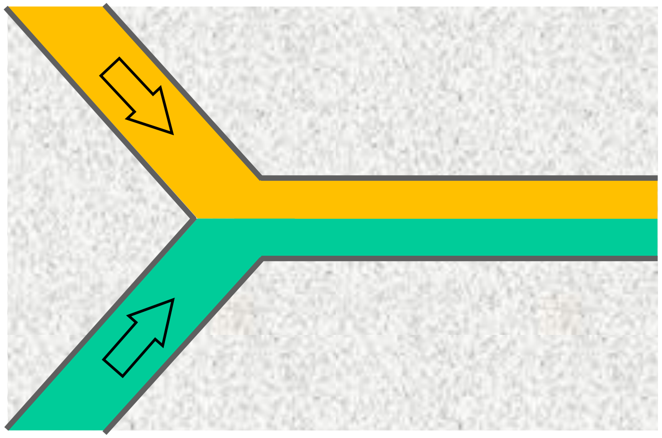
Tercera parte

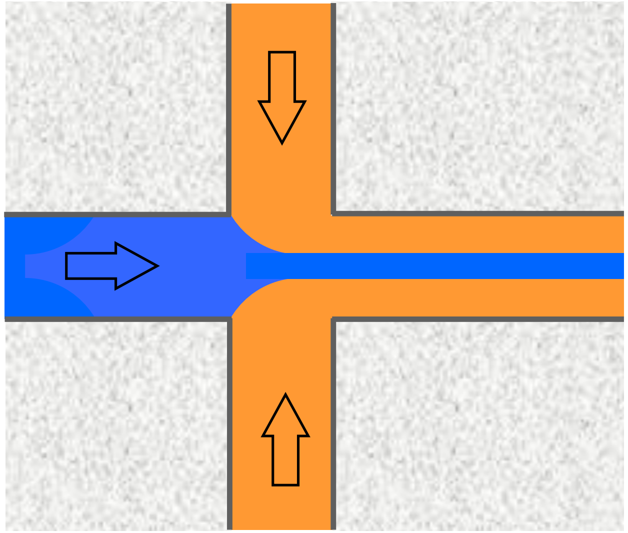
- *i.* Introducción
- *ii.* Circuitos de microcanales
- *iii.* Ejemplo: nuevos materiales
  - Reacciones en co-flujo
  - El problema básico: difusión molecular
  - Difusión transversal
  - Síntesis de nanomateriales
  - Un ejemplo del mundo natural

iii. Aplicaciones del problema básico: co-flujos

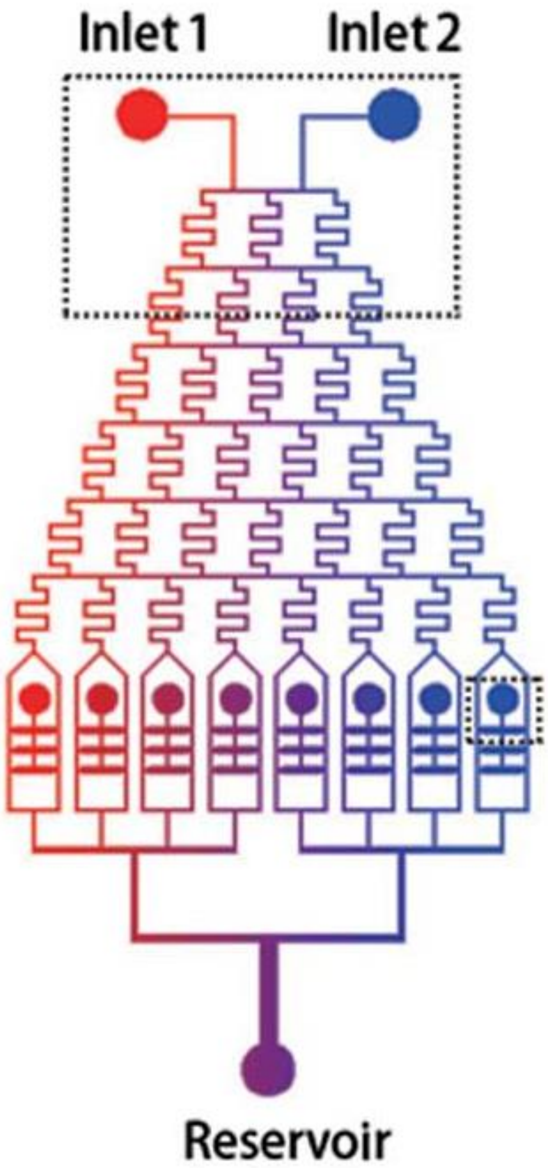


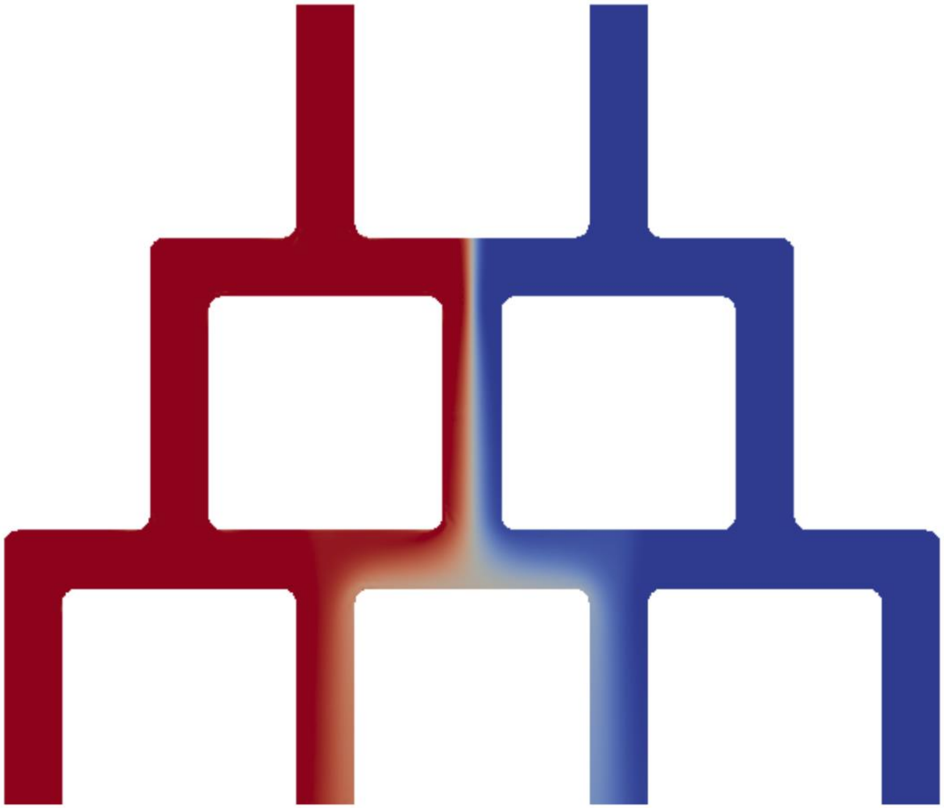
micronit.com





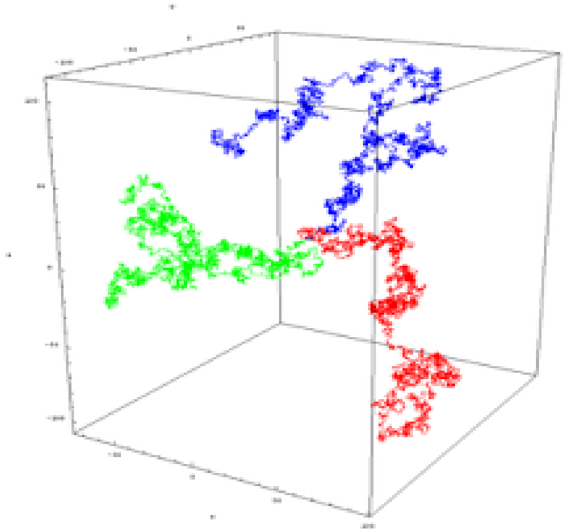
iii. Gradientes de concentración





Schaumburg et al (2017)

iii. Difusión molecular



$$\sigma^2 = 6Dt$$

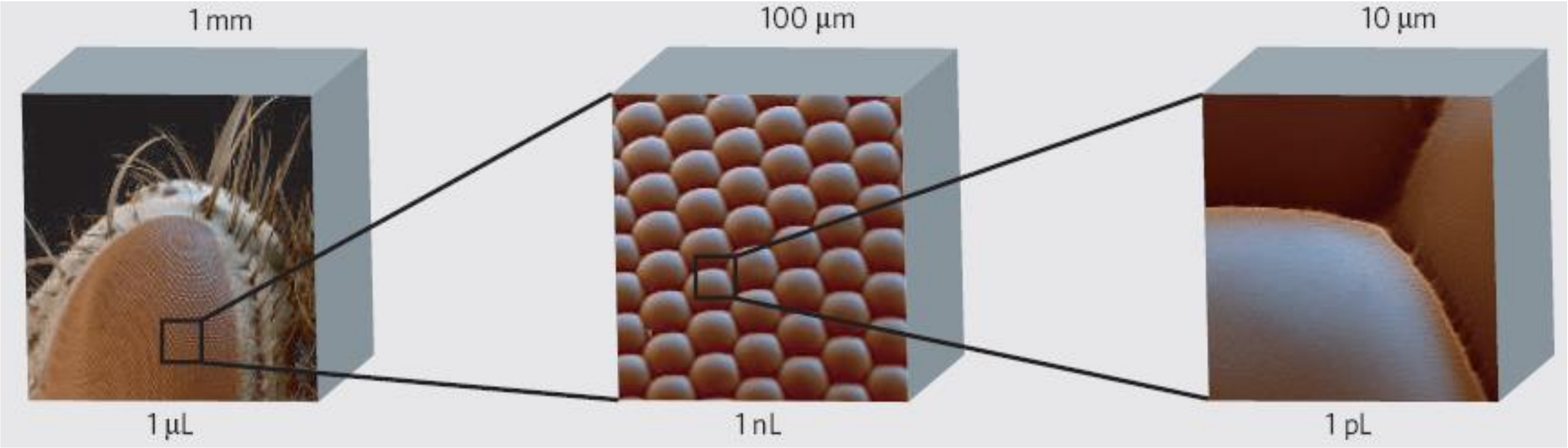
$$D = k_B T / 6\pi\mu r$$

iii. Tiempos característicos de difusión

$$z \rightarrow \sigma_z = (2Dt)^{1/2}$$

$D = 5\ 10^{-10}\ m^2/s$

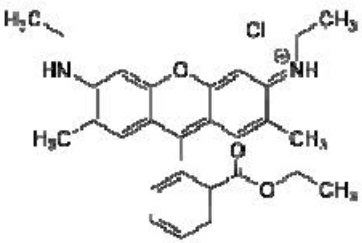
$t = z^2/2D$



1000 s **10 s** **0,1 s**

iii. Tiempos característicos de difusión

$D \approx 10^3\ \mu m^2/s$

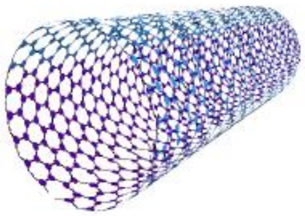


< 1 nm

$D \approx 40\ \mu m^2/s$

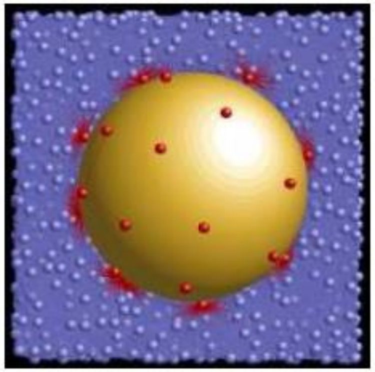
5 nm

$D \approx 2\ \mu m^2/s$



100 nm

$D \approx 0.2\ \mu m^2/s$



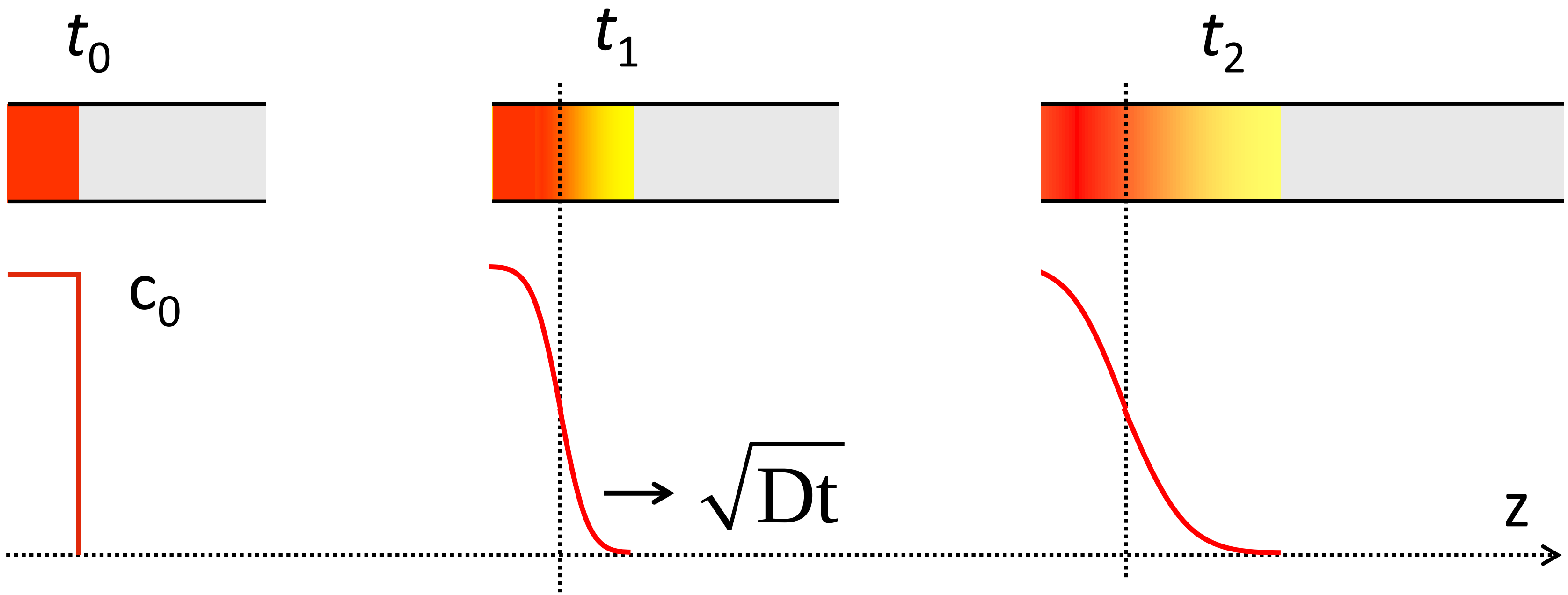
1 μm

$t \sim (100\ \mu m)^2/2D$

---

5 s **2 min** **42 min** **7 h**

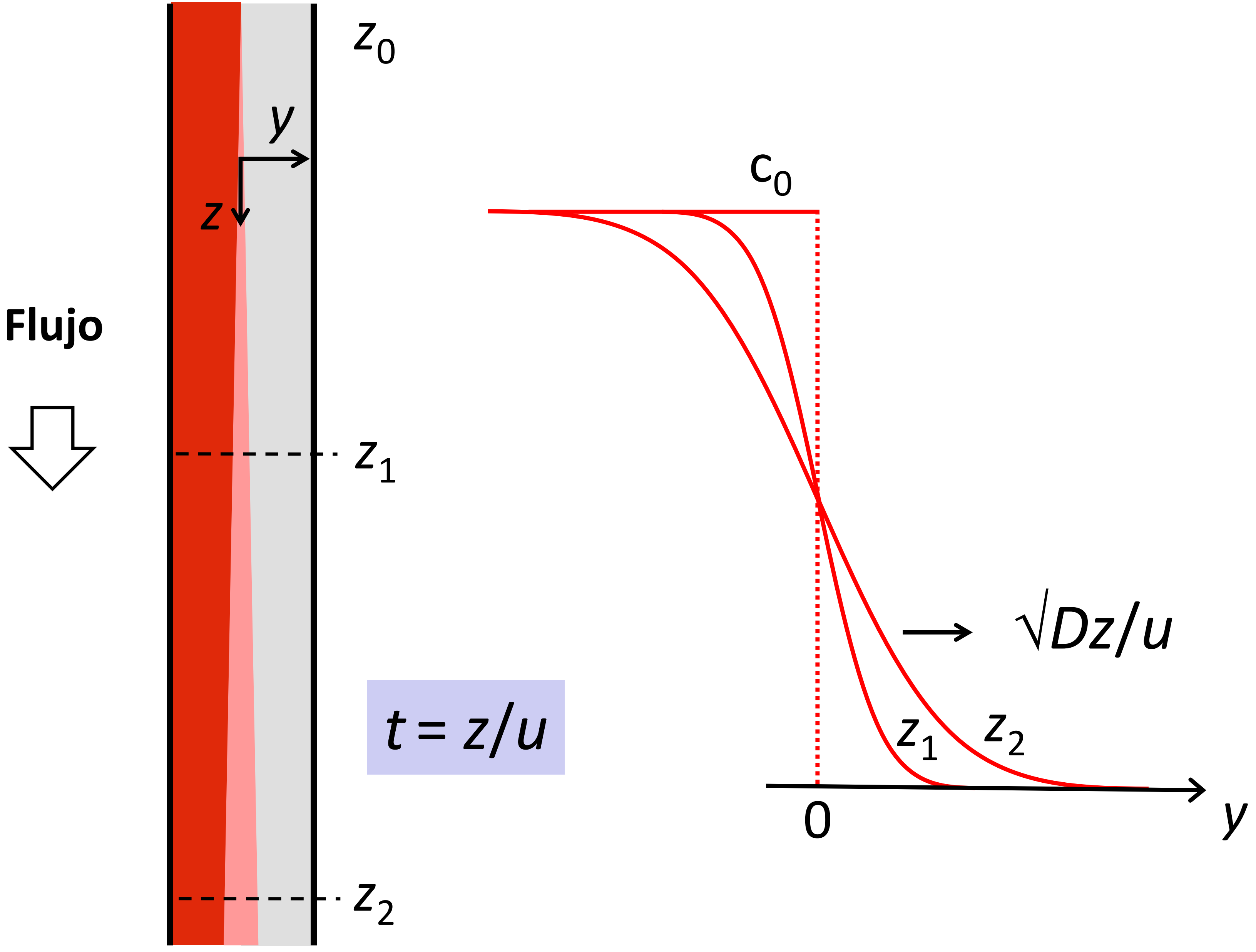
iii. Transporte difusivo, fluido estanco



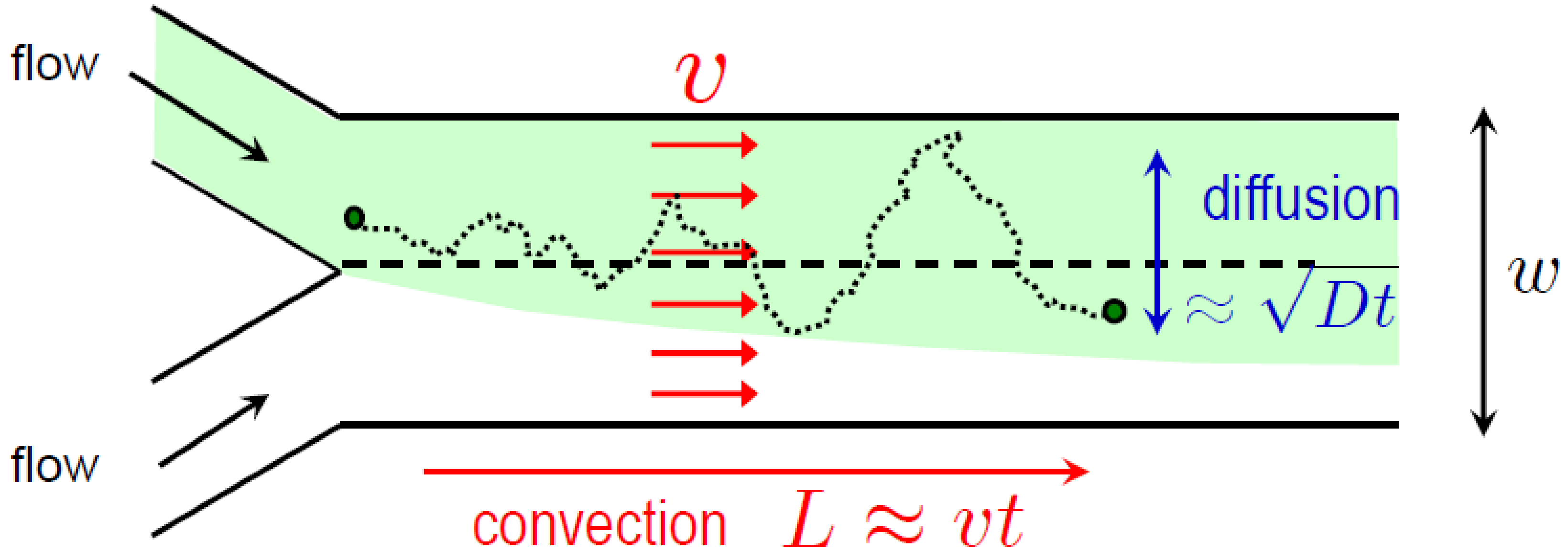
$$\frac{dc}{dt} = D\frac{d^2c}{dz^2}$$

$$c(z,t) = \frac{c_0}{2}\,\mathrm{cerf}\left(-\frac{z}{2\sqrt{Dt}}\right)$$

iii. Transporte difusivo, flujo transversal



iii. Difusión en co-flujo



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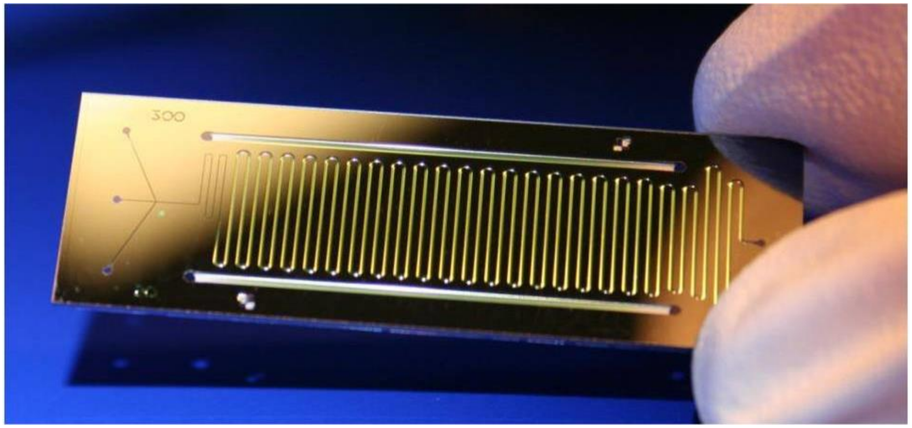
www.lof.cnrs.fr



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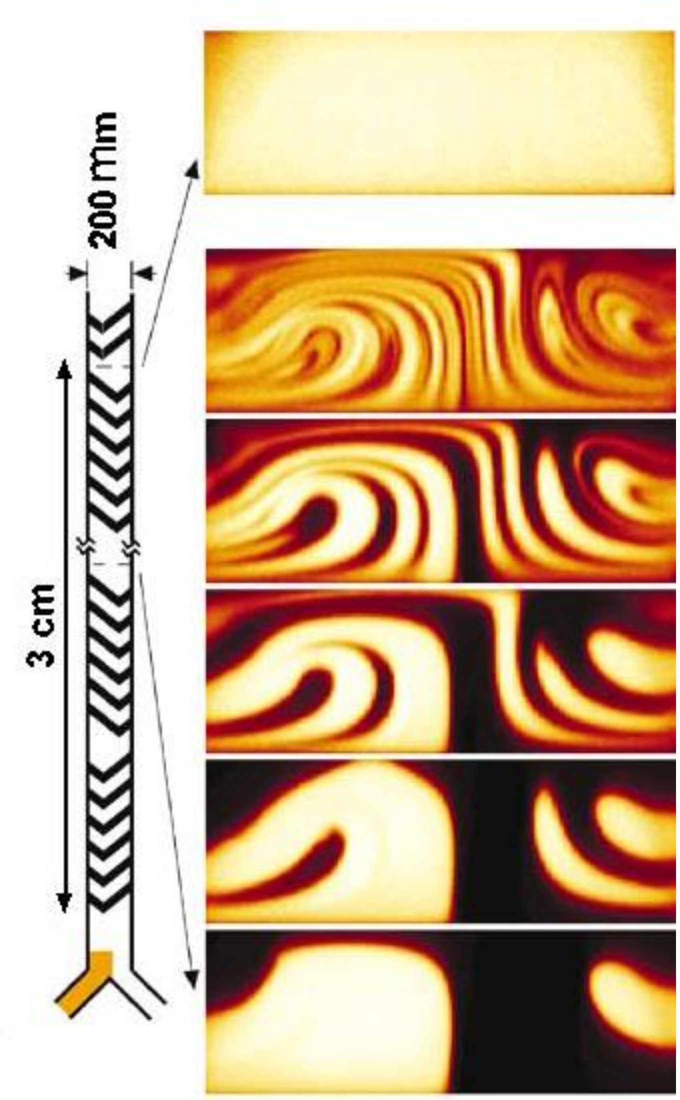
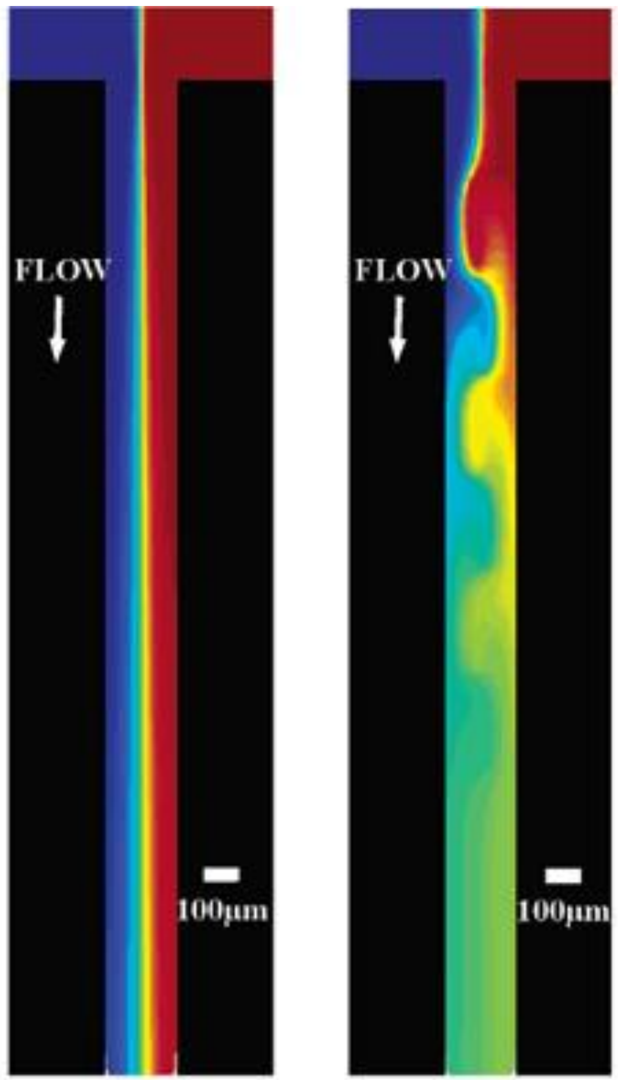
iii. La difusión como problema: mezclado

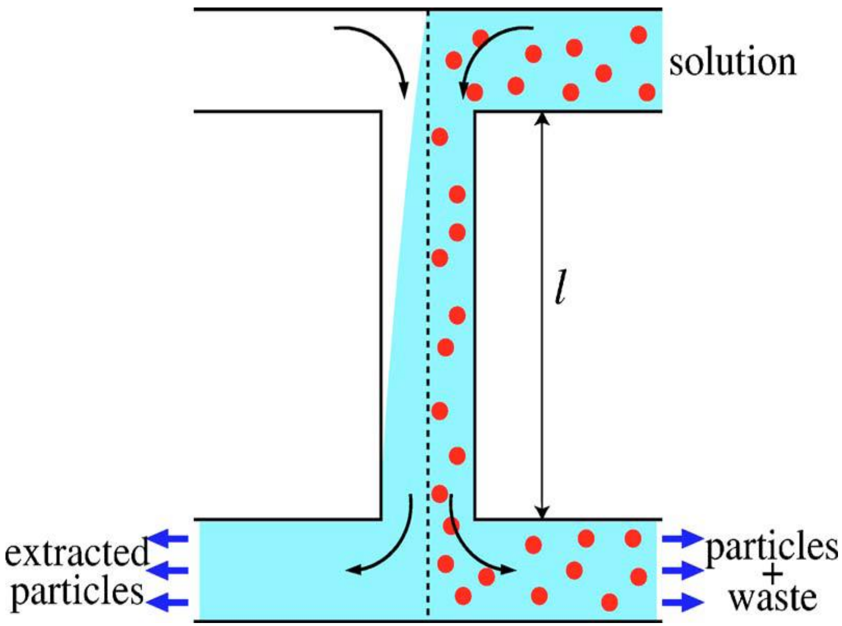


Strook et al., *Anal Chem* **74** (2002) 7306

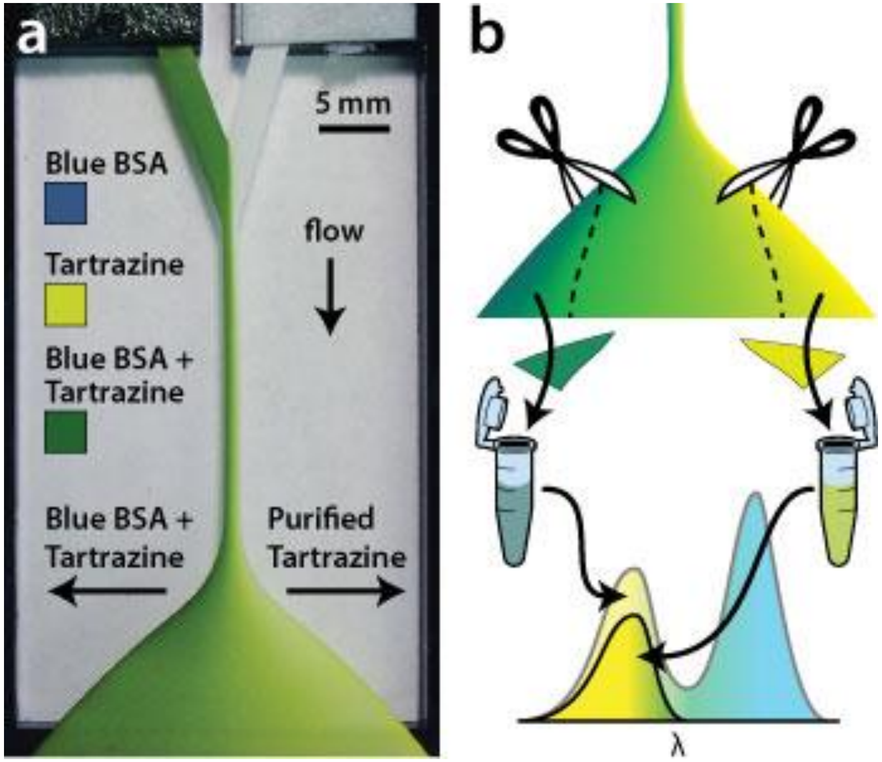


Biddis et al., *Anal Chem* **76** (2004) 3208

iii. La difusión en positivo: filtros sin membranas

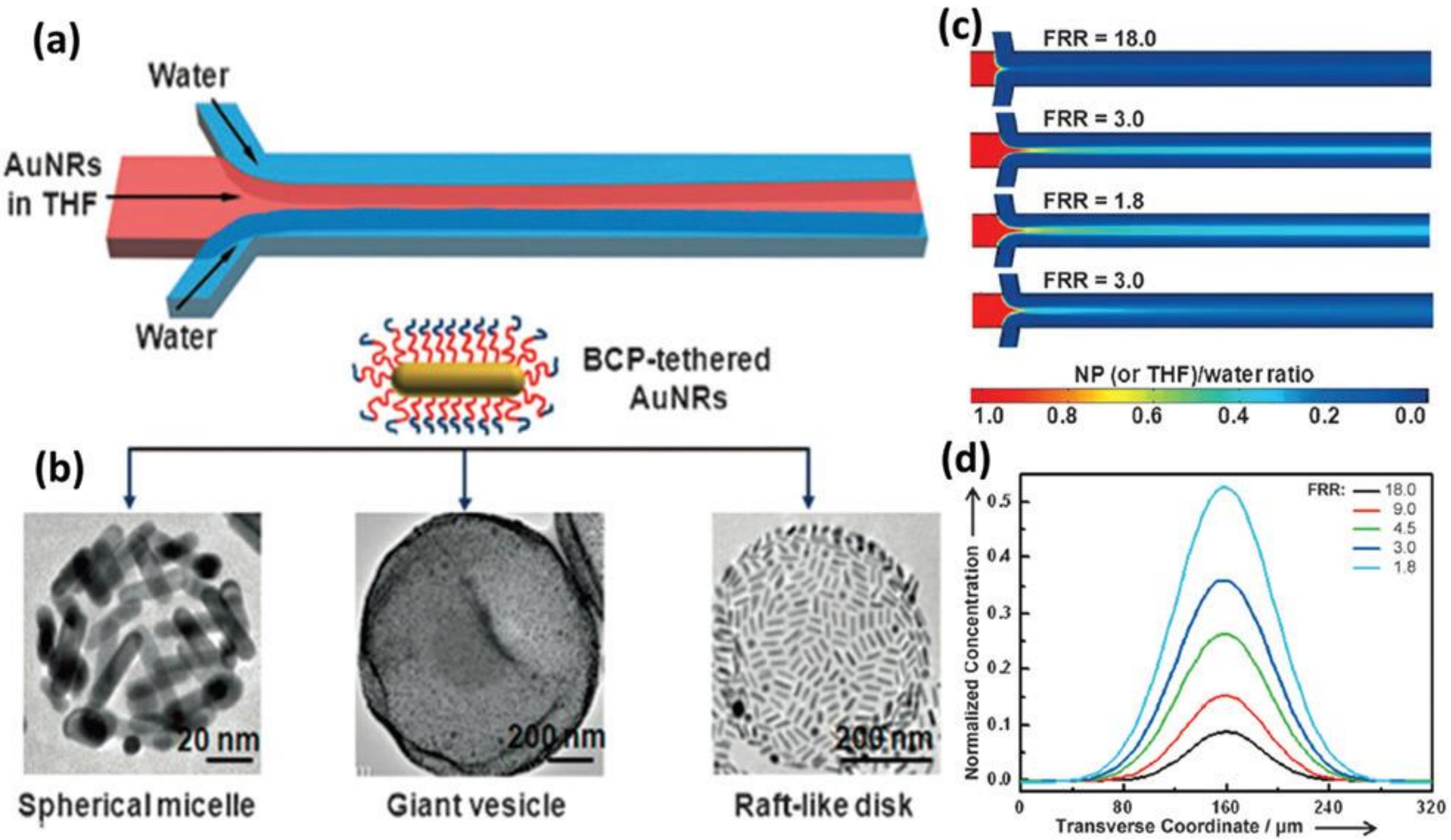


Brody and Yager,
Sens. Actuators A **58** (1997) 13



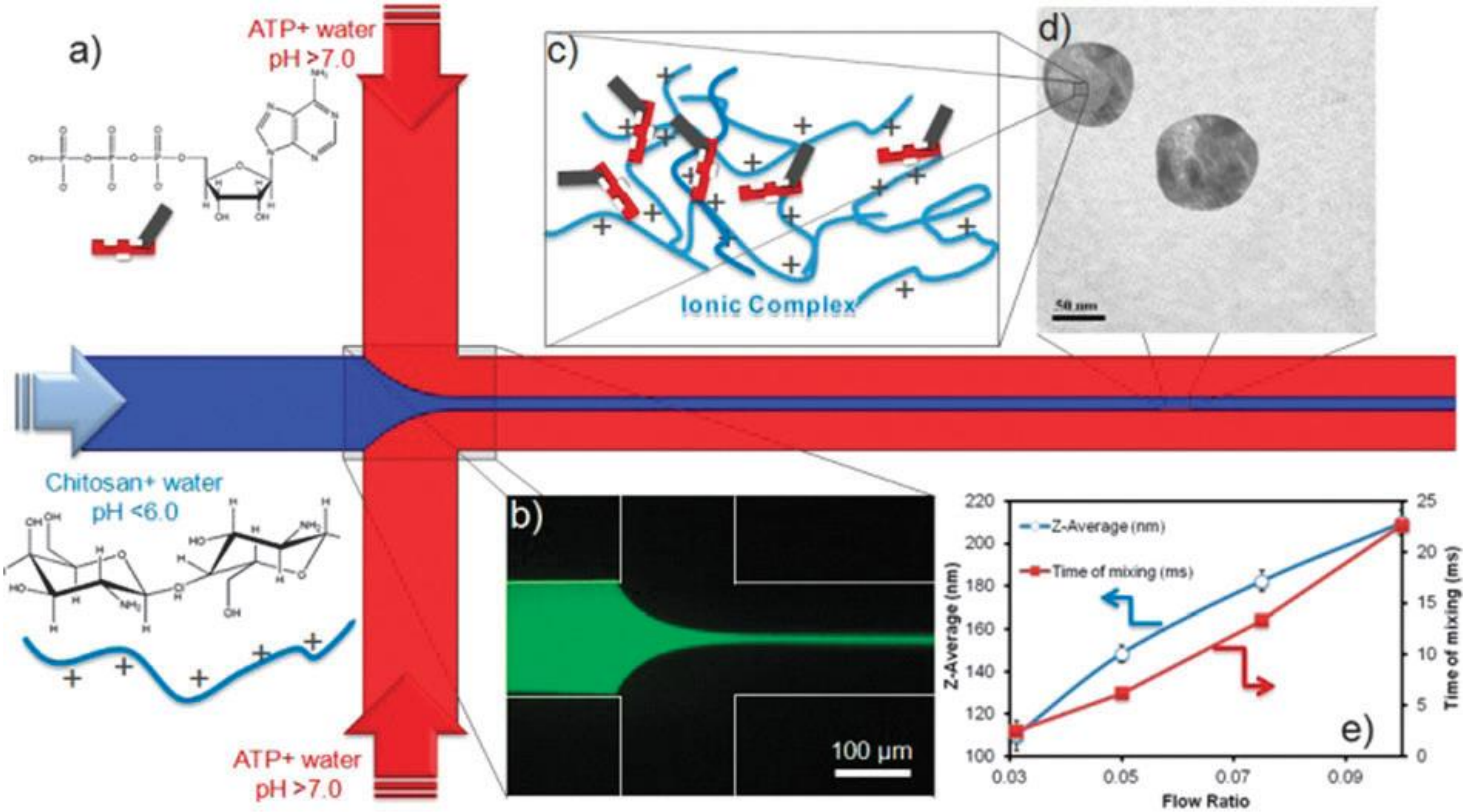
Osborn et al,
Lab Chip **10** (2010) 2659

iii. Reacciones en co-flujo: auto-ensamblados



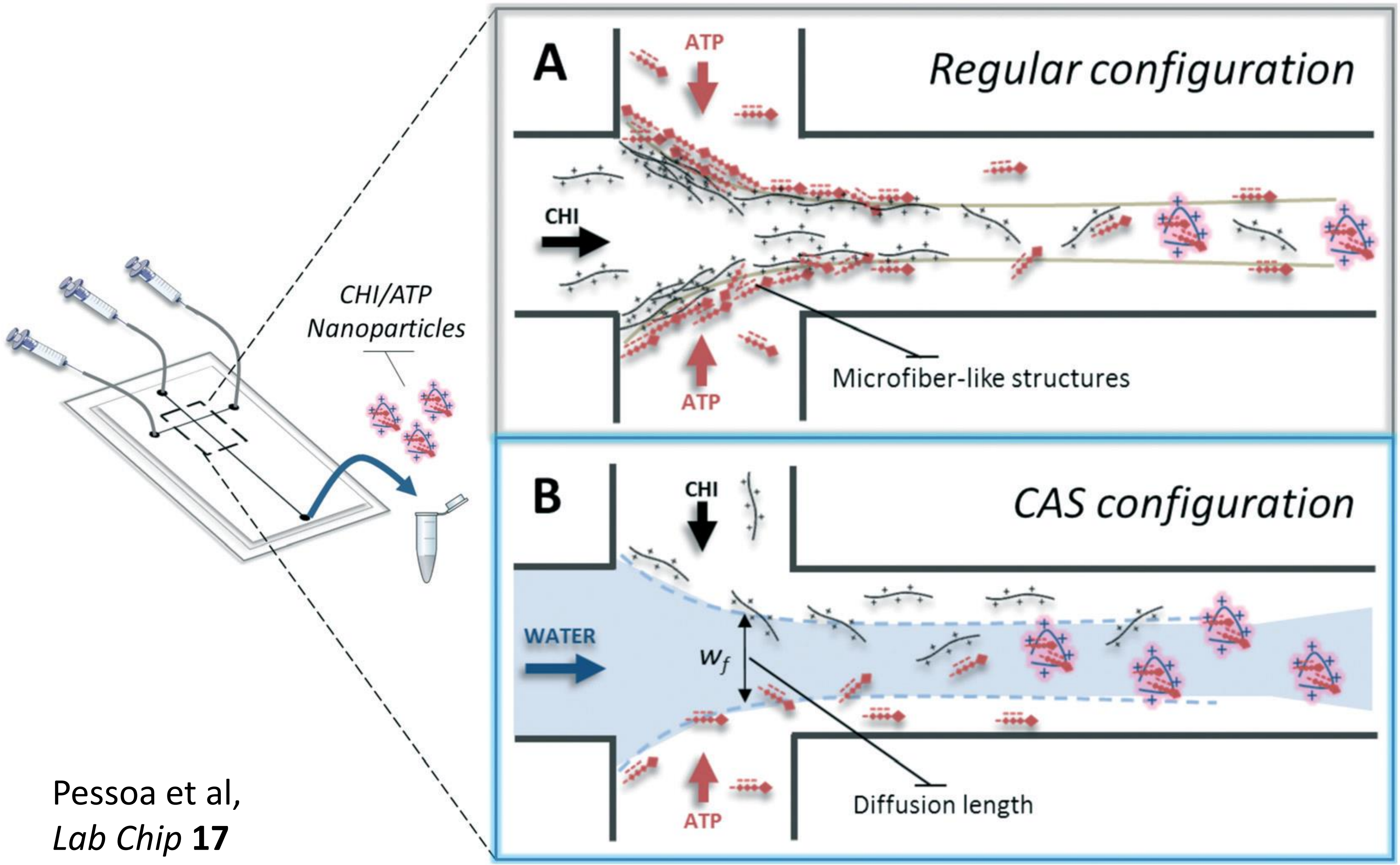
He et al., *Angew. Chem., Int. Ed.*, **52** (2013) 2463

iii. Reacciones en co-flujo: auto-ensamblados



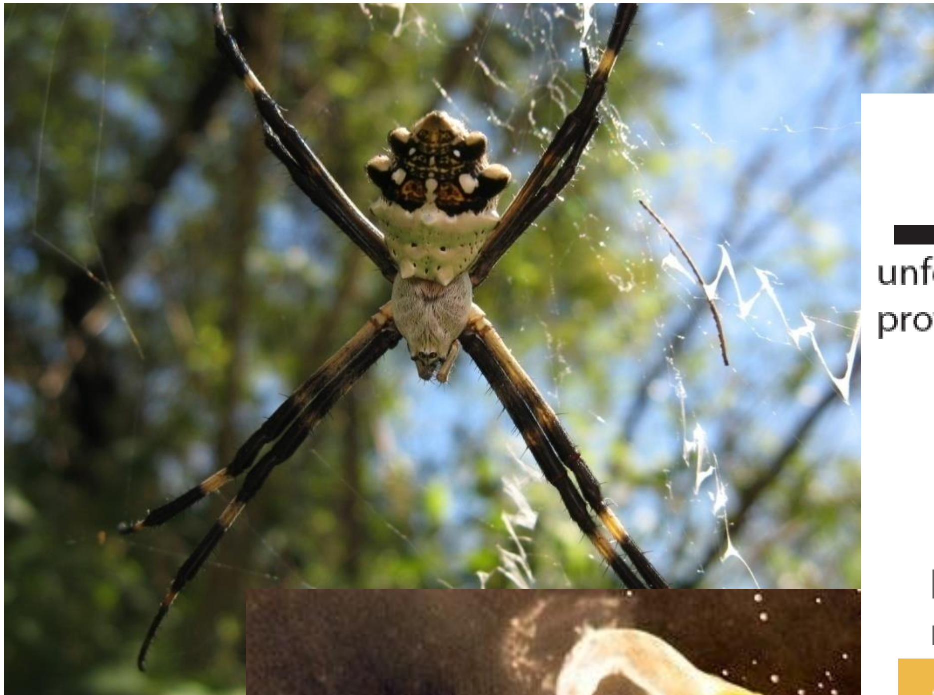
Majedi et al., *Chem. Commun.* **48** (2012) 7744

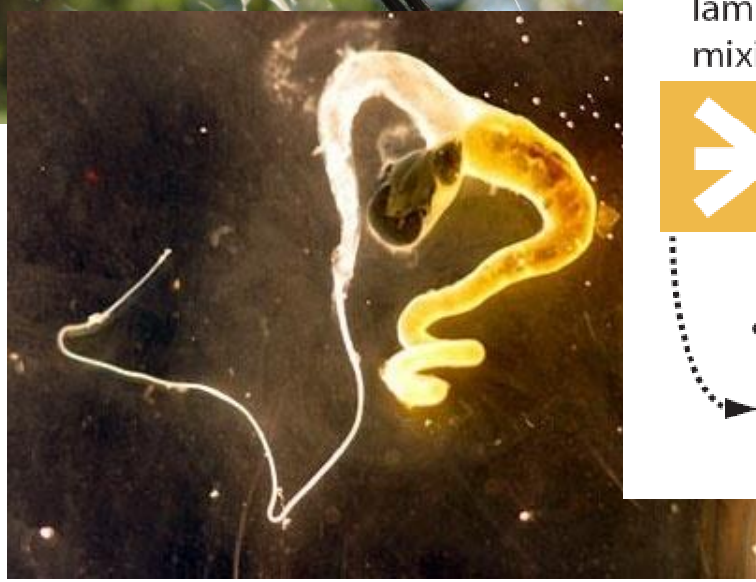
iii. Reacciones en co-flujo: auto-ensamblados

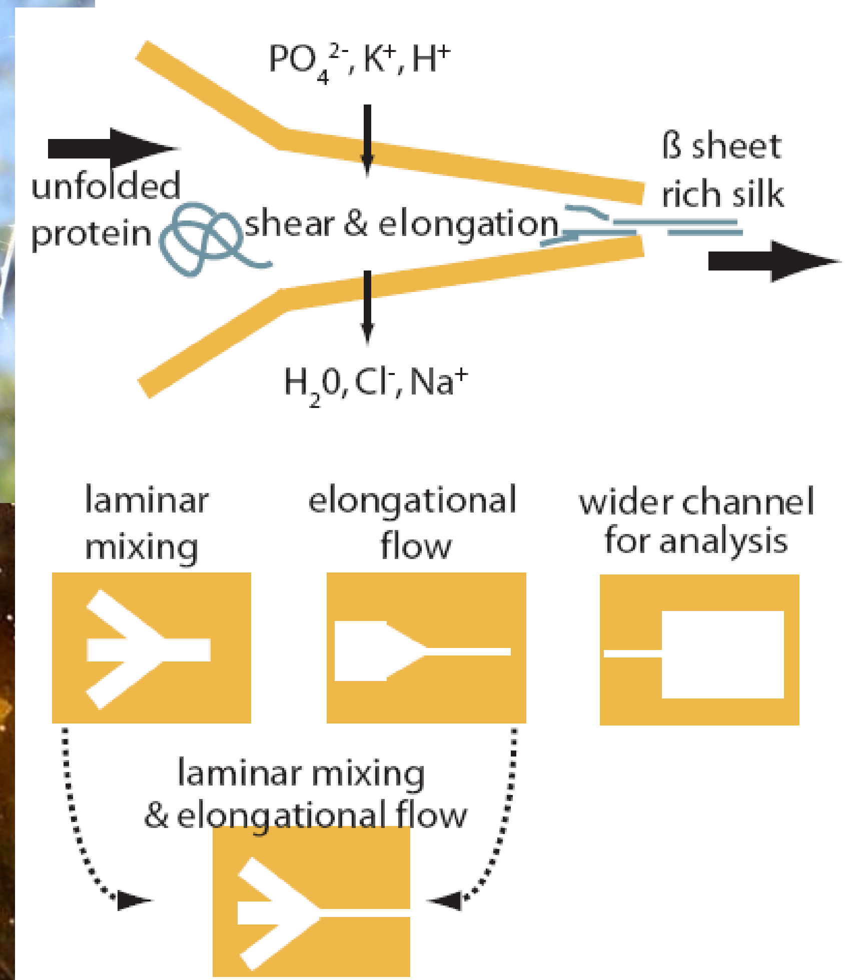


Pessoa et al,
Lab Chip **17**
(2017) In press

iii. ¿Hasta dónde podemos con esta configuración?

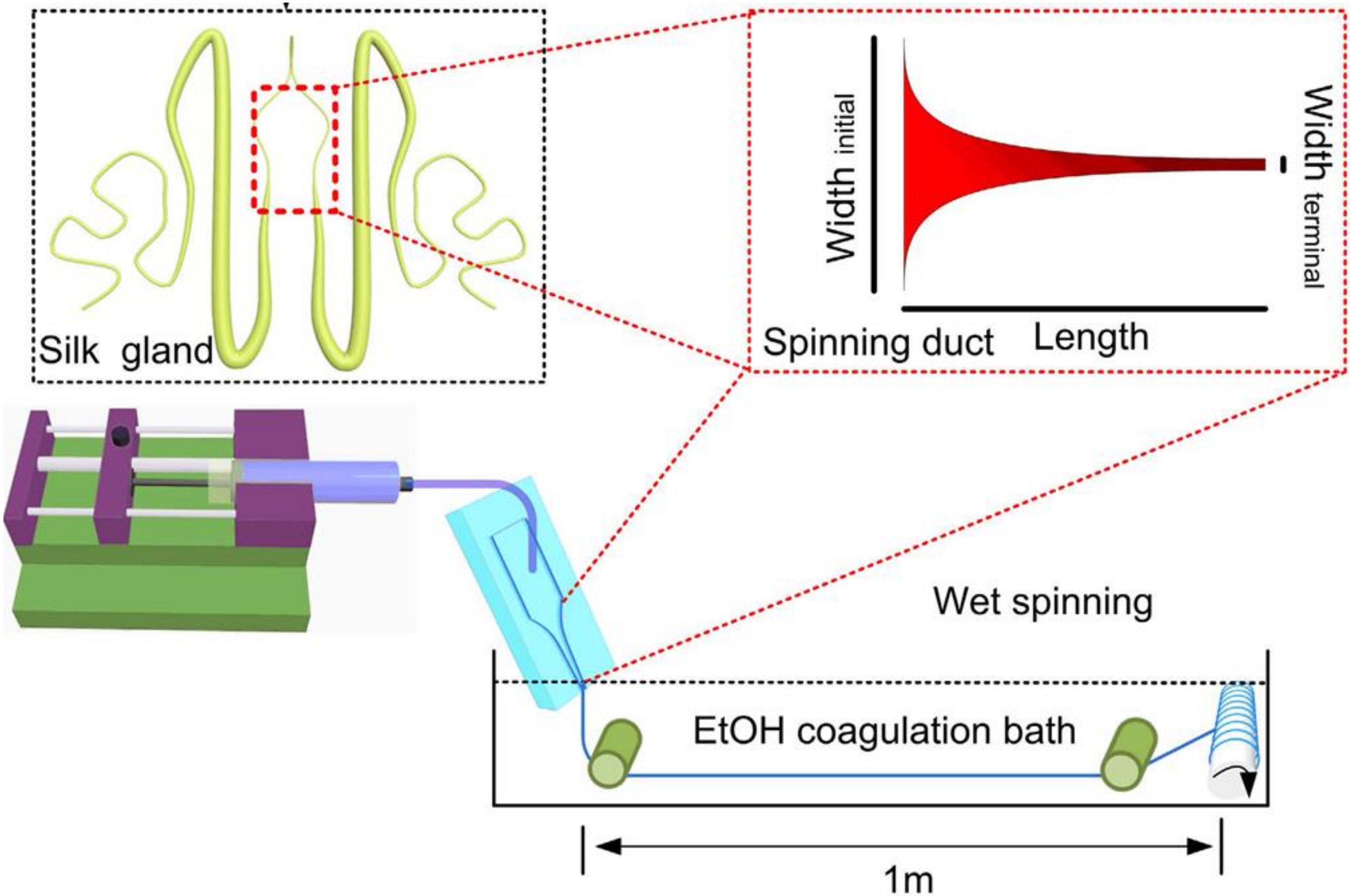






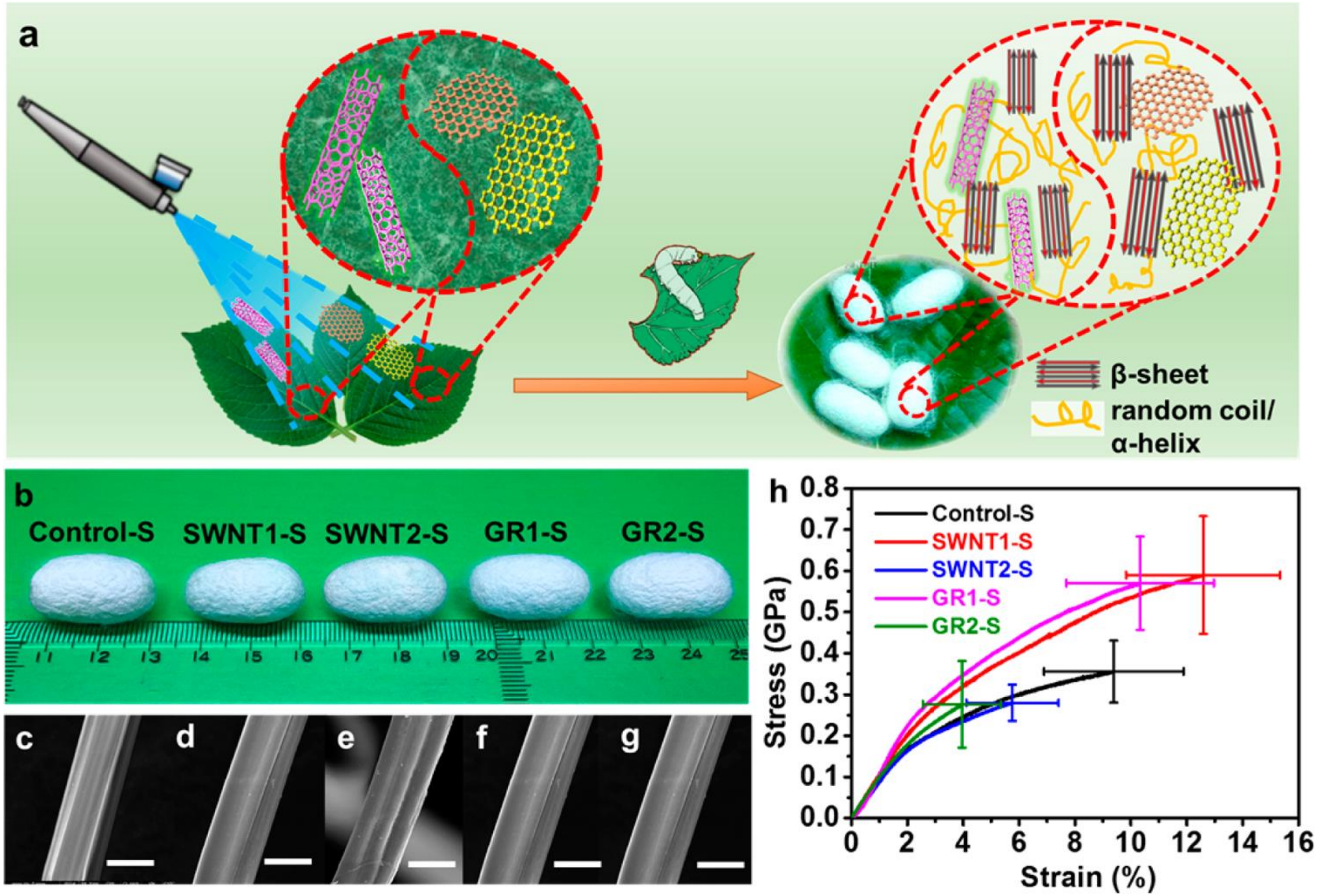
Rammensee et al,
PNAS **105** (2008) 6590

iii. Nuevos materiales imitando la naturaleza



Peng et al, *Sci Reports*
6 (2016) 36473

iii. Nuevos materiales con la naturaleza



Wang et al, *Nano Lett* **105** (2016) 6695

Muchas gracias:

A los organizadores por su amable invitación,
al CELFI por la ayuda financiera,
y a todos los presentes por su atención!

Claudio Berli
23/11/2017

NANO ANDES

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