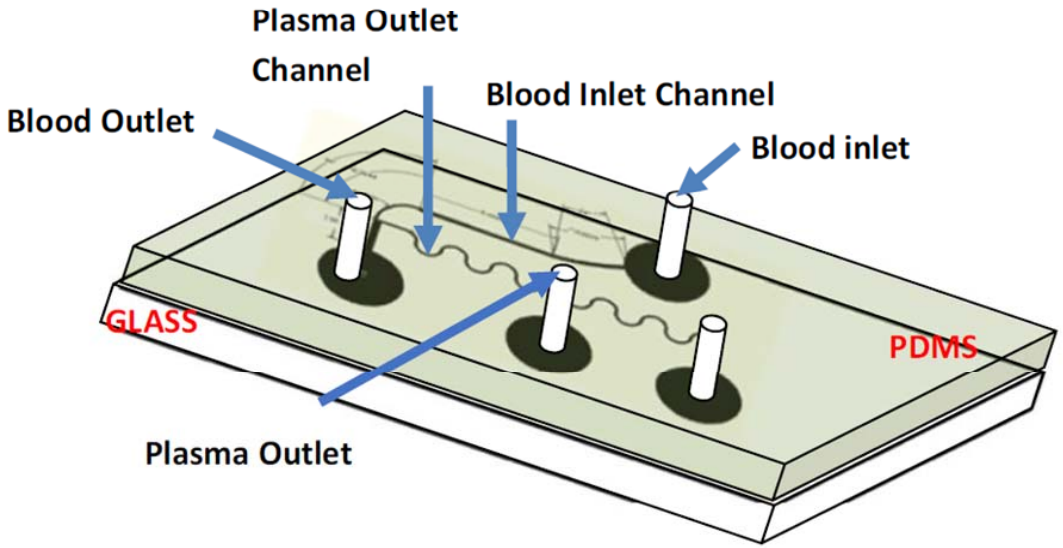
Development of Innovative Bio-Microdevices



Amit Agrawal

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Prof. H.H. Mathur Award for Excellence in Applied Sciences

IIT Bombay, 27 February 2018

Outline of the talk

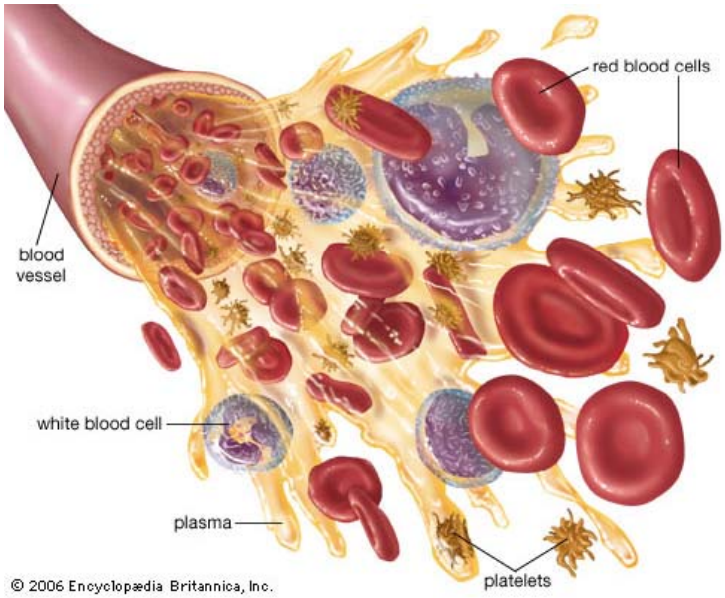
- Development of Innovative Bio-microdevices
  - Blood plasma separation microdevice
  - Three-dimensional hydrodynamic focusing device
- Looking beyond the Navier-Stokes equations
  - First analytical solution of Burnett equations
  - Derivation of Onsager-Burnett equations
- Conclusions

Development of Blood-Plasma-Separation Microdevice

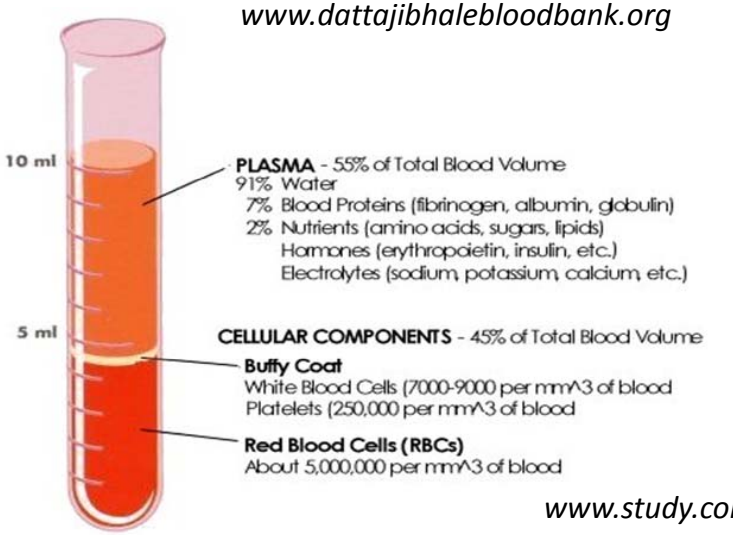
Why separate plasma from blood?

- Many blood tests are carried out on plasma
- Plasma has plenty of biomarkers and analytes – indicators of human body functioning
- Efficient detection of these analytes requires separation of cells – as cells may interfere with analysis
- Separation of plasma from blood is an indispensable process for disease diagnostics

Constituents of Human Blood



www.dattajibhalebloodbank.org



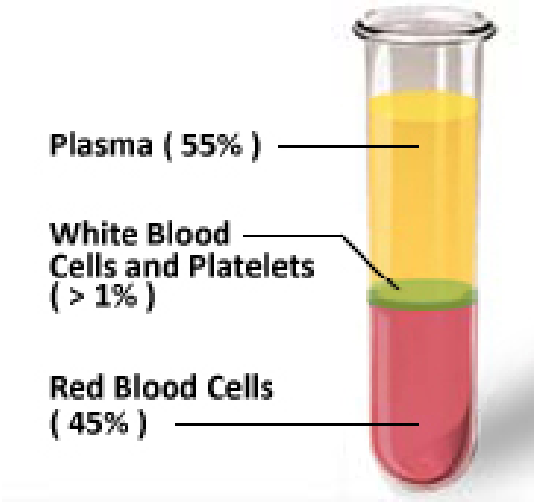
www.study.com

Constituents	% of whole blood	Typical size (µm)	Normal count (per µL)
RBC	45-50	7-9	4.5 – 5.5 million
WBC	1	8-18	5000 - 8000
Platelets		2.5	250,000 - 300,000
Plasma	Rest	NA	NA

Conventional Method for Separating Plasma from Blood

Centrifuge

www.pocdscientific.com.au



www.pennmedicine.org

- Centrifugation

  Issues: Labor intensive, time consuming, multiple stages of blood handling, prone to errors

Microfluidics offers a platform to bring all stages of processing (plasma separation, tests, etc) into a single micro-device!

Lab-on-a-Chip device

Blood-plasma separation microdevice @ IIT Bombay

Advantages of point-of-care micro-device

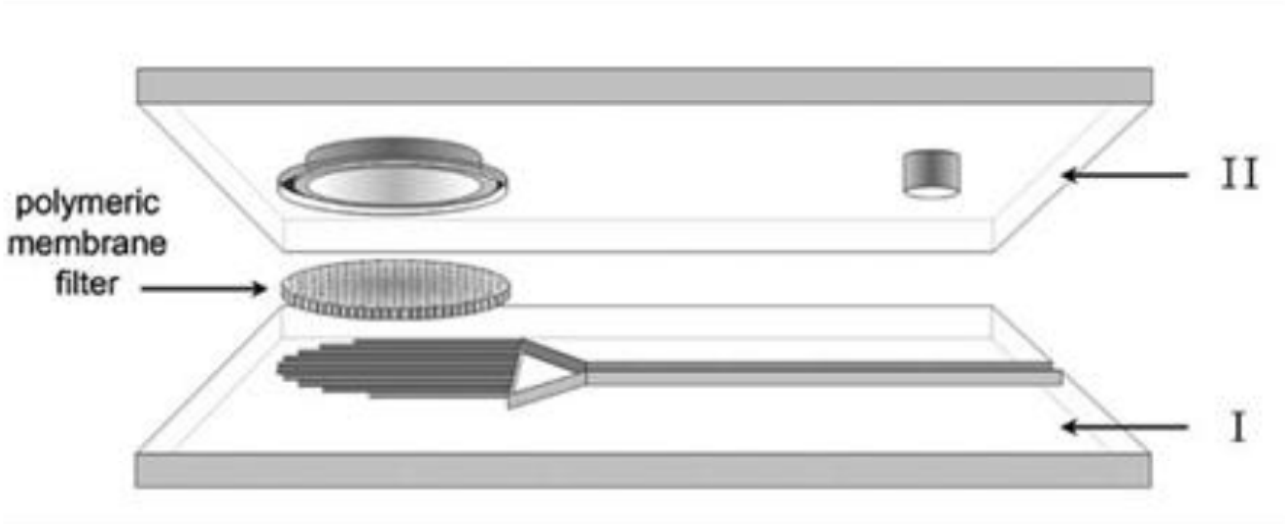
- Reduces size of functionally critical components of analytical systems
- Small sample amount/ less consumption of costly reagents
- Quick and accurate analysis – reduces multiple stages of manual handling, minimal errors
- Portability – Can be used even in very remote areas – carry in your pocket!
- Bed site testing – reduction in transportation time

Filtration based devices in Literature

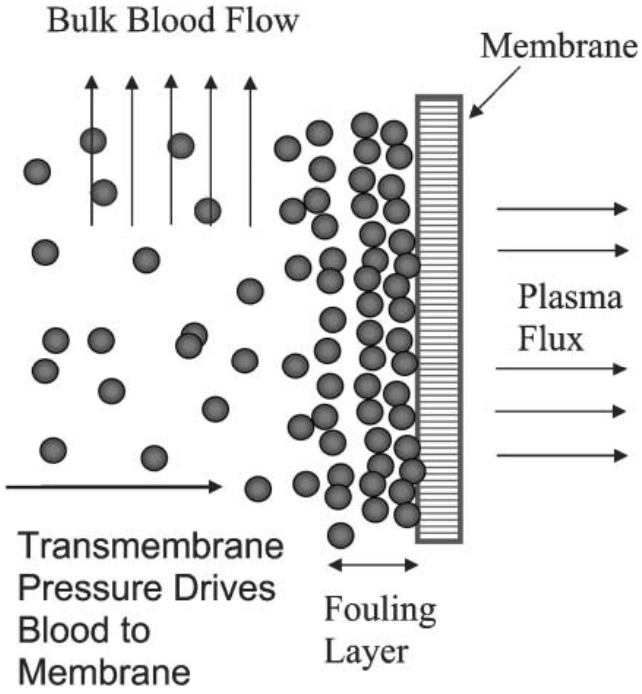
If particles are rigid – will not be able to pass through pores smaller than their size

Depending upon the point of plasma extraction

- Dead End Filtration
- Cross Flow Filtration

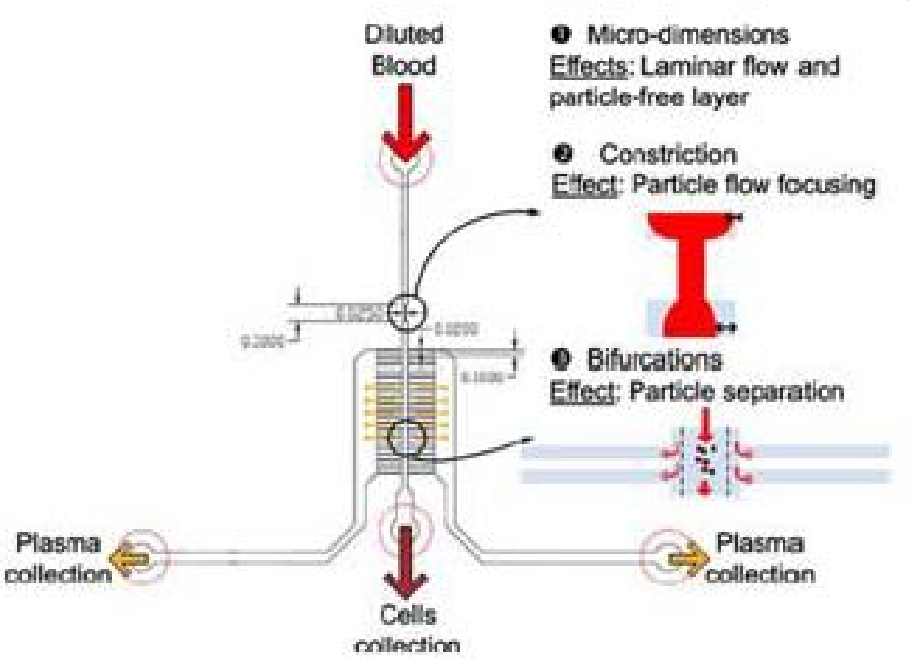


Thorslund, S., Klett, O., Nikolajeff, F., Markides, K., & Bergquist, J. (2006). A hybrid poly (dimethylsiloxane) microsystem for on-chip whole blood filtration optimized for steroid screening. Biomedical Microdevices, 8(1), 73-79.

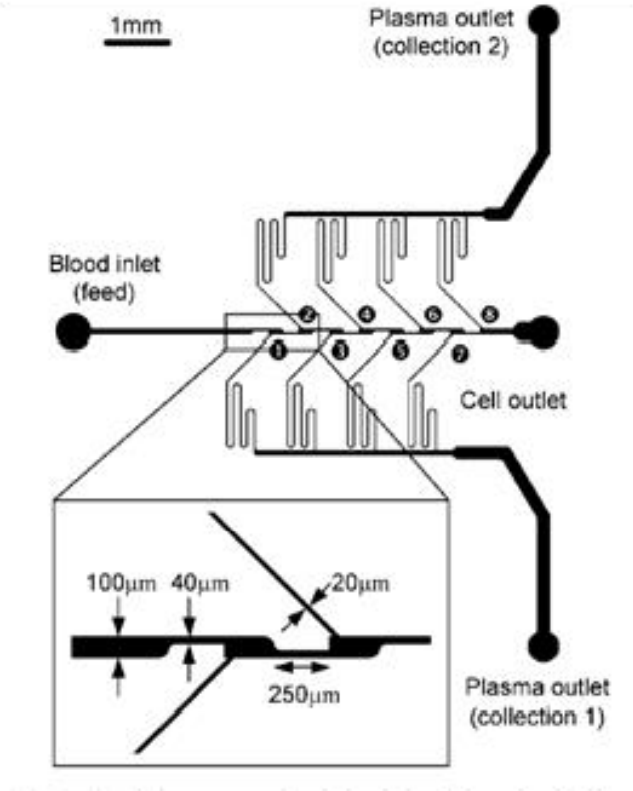


Crowley, T. A., & Pizziconi, V. (2005). Isolation of plasma from whole blood using planar microfilters for lab-on-a-chip applications. Lab on a Chip, 5(9), 922-929.

Hybrid Designs (from Literature)



Kersaudy-Kerhoas, M., Dhariwal, R., Desmulliez, M. P., & Jouvet, L. (2010). Hydrodynamic blood plasma separation in microfluidic channels. Microfluidics and Nanofluidics, 8(1), 105-114.



Kersaudy-Kerhoas, M., Kavanagh, D. M., Dhariwal, R. S., Campbell, C. J., & Desmulliez, M. P. (2010). Validation of a blood plasma separation system by biomarker detection. Lab on a Chip, 10(12), 1587-1595.

Issues with the existing designs

- Most designs demonstrated on diluted blood

- Small feature sizes
  - Dimensional tolerances become critical
  - Difficult to manufacture
  - Prone to clogging

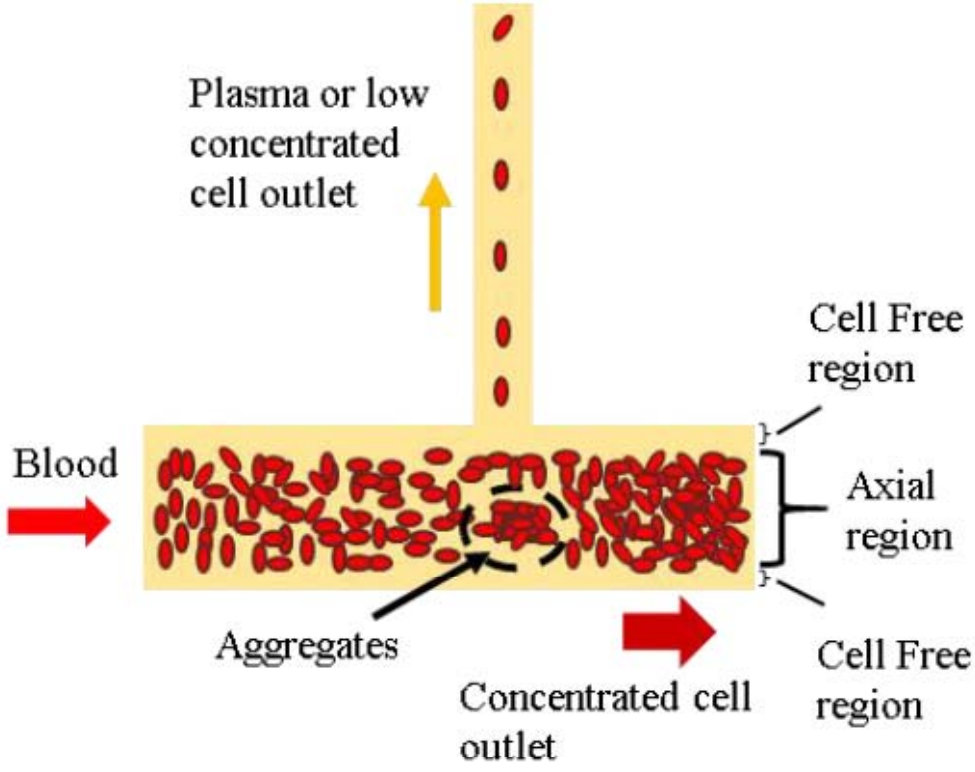
- Low rate of plasma extraction

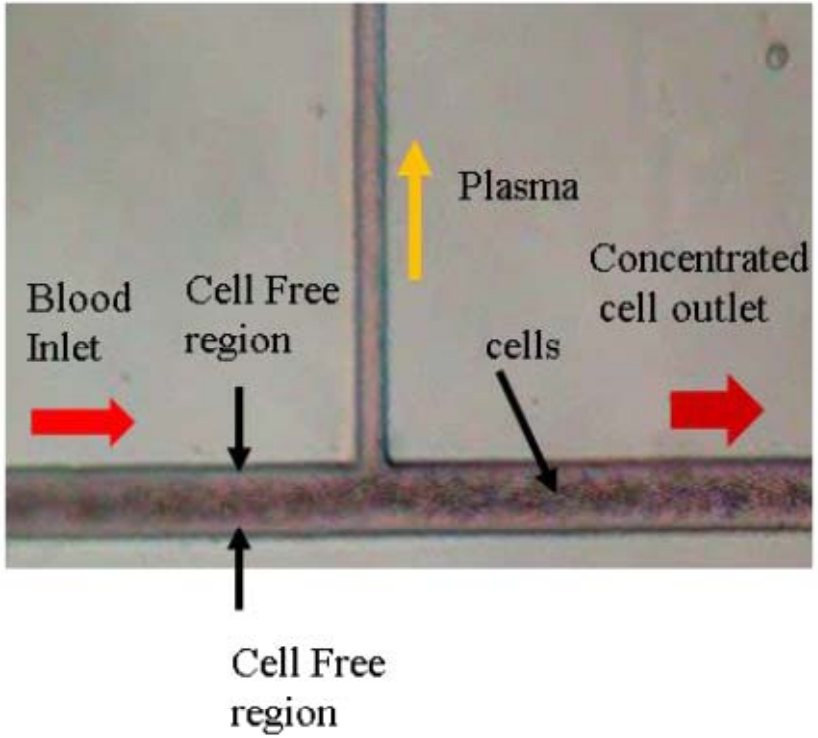
Can the design be simplified?

Tripathi et al., **J Micromechanics and Microengineering**, Vol. 25, 083001, 2015. **(Invited review)**

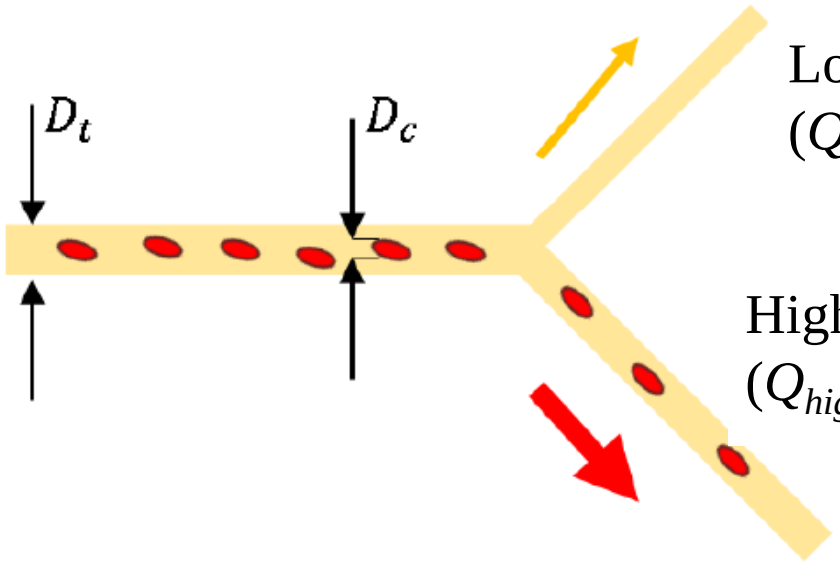
Bio-Physical effects: Fahraeus effect

Fahraeus effect in a simple T shaped microchannel





Bio-Physical effect: Zweifach – Fung Bifurcation Law

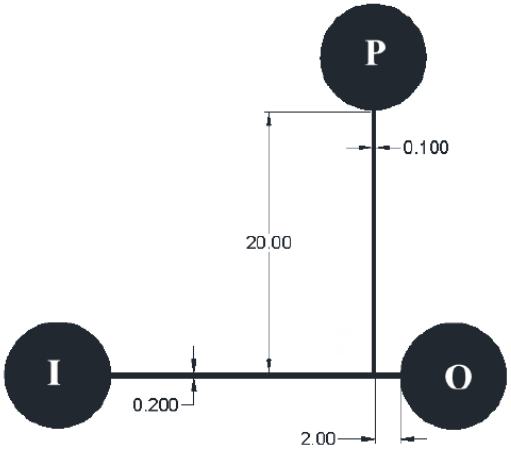


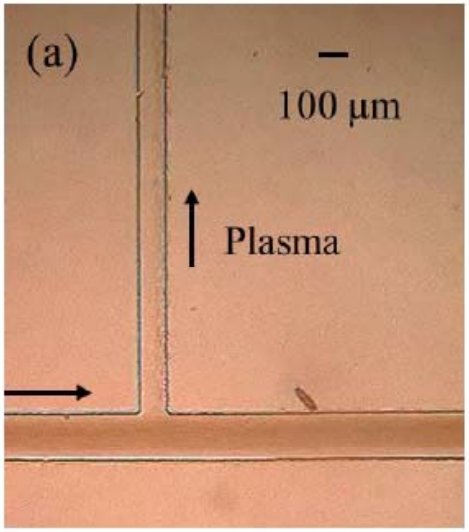
Conditions for all cells to favor high flow rate branch

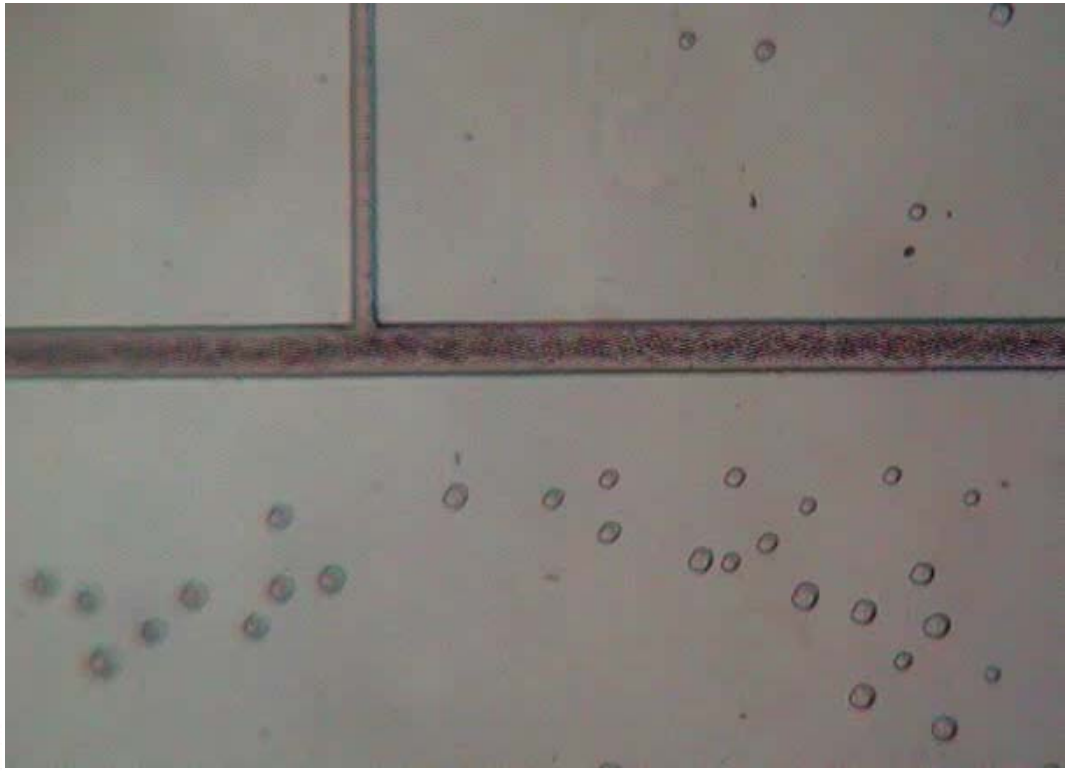
$$\frac{Q_{high}}{Q_{low}} \geq 2.5 \text{ and } \frac{D_c}{D_t} \sim 1$$

- Corner stone of most hydrodynamic based microfluidic devices

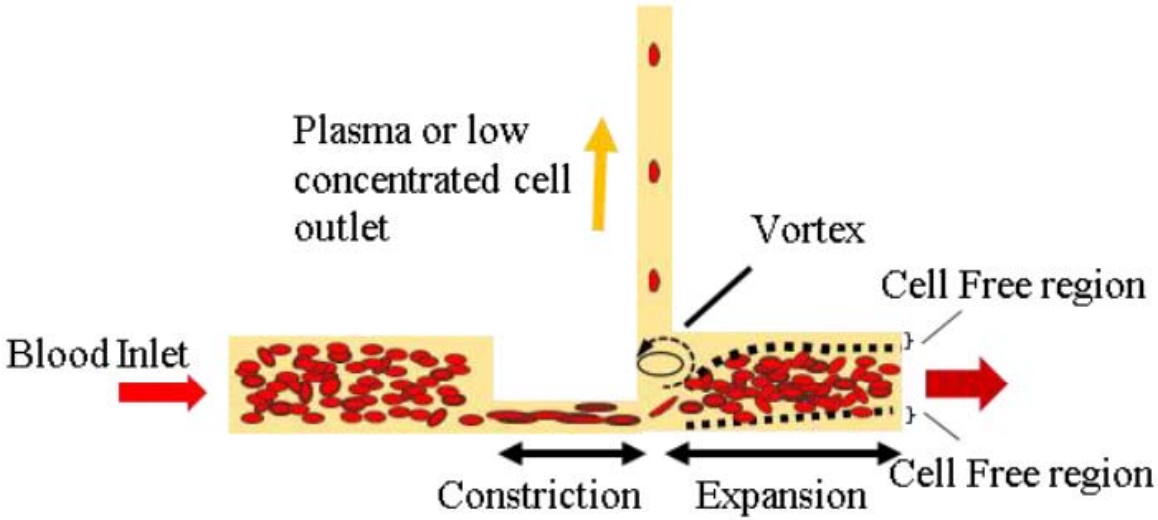
Separation using a simple T-microchannel

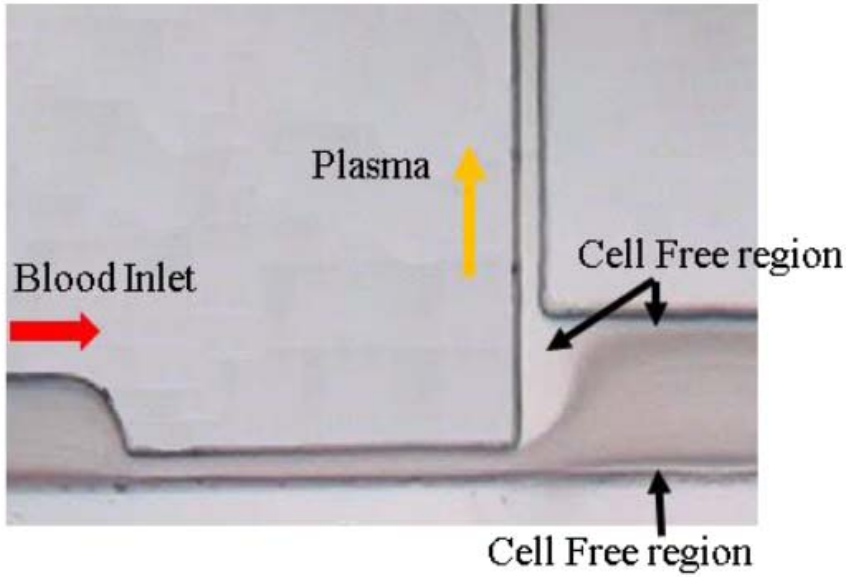






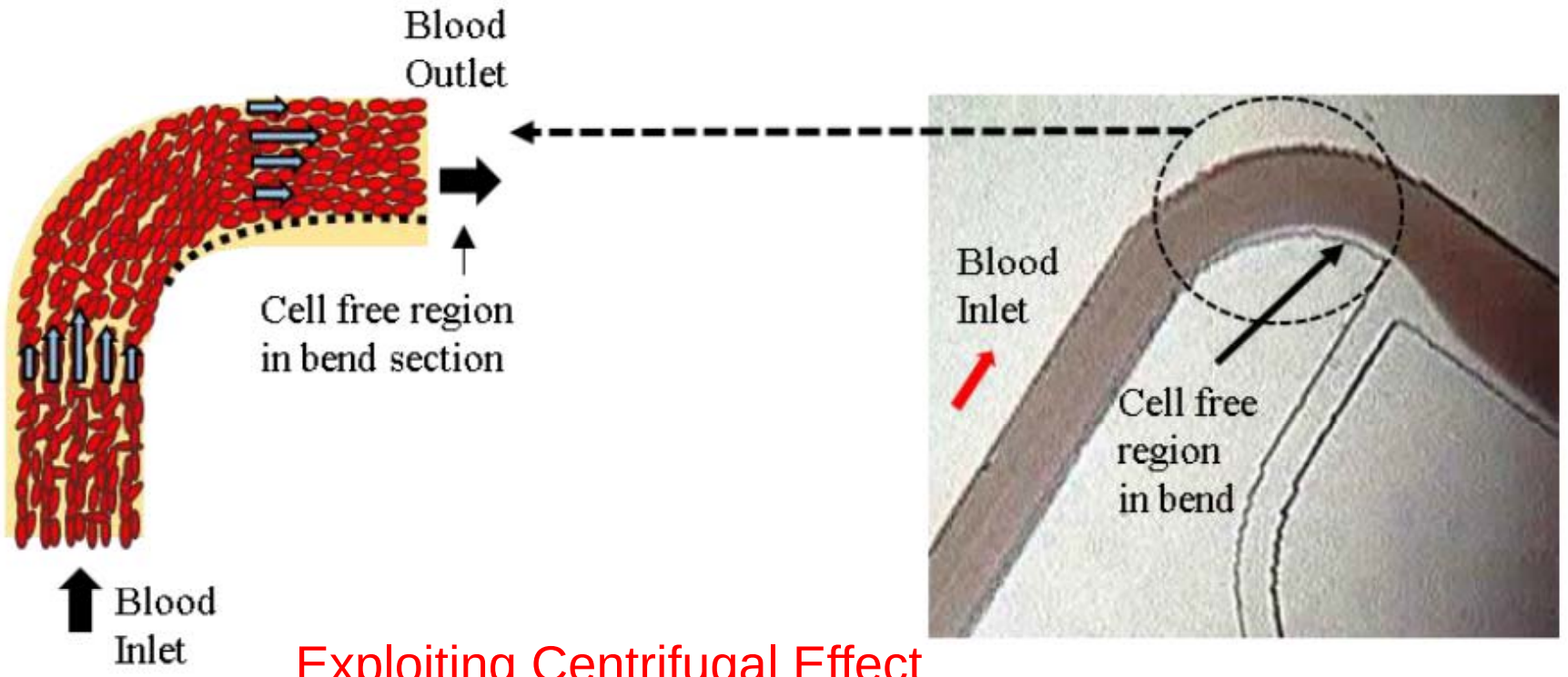
Geometric effect: Constriction-Expansion





Incorporating Constriction-Expansion in a Microchannel

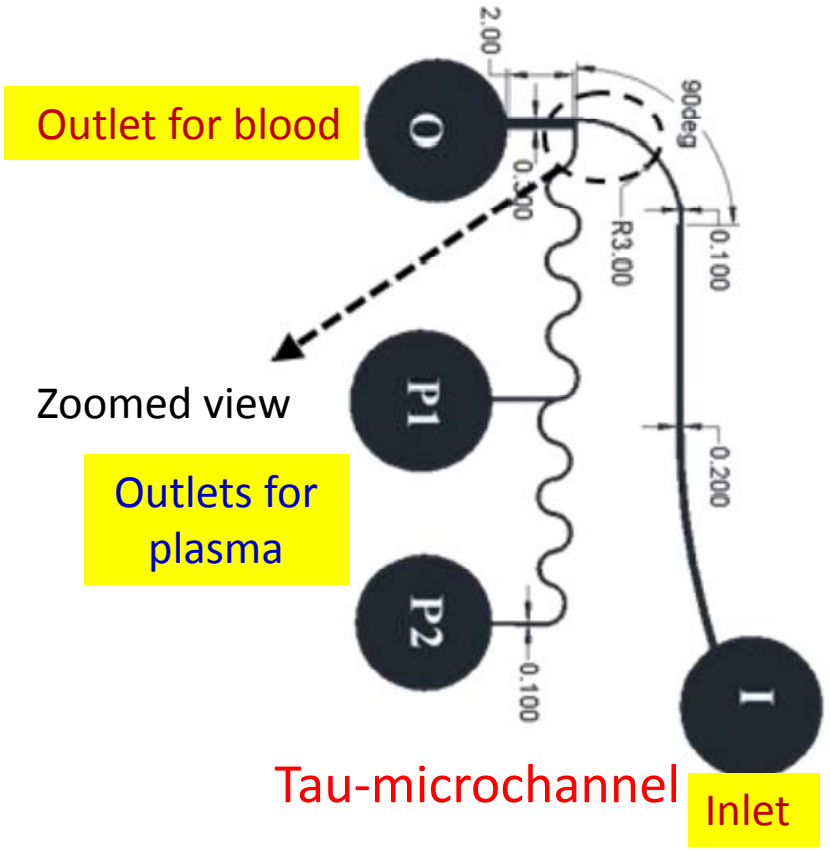
Geometric effect: Centrifugal force

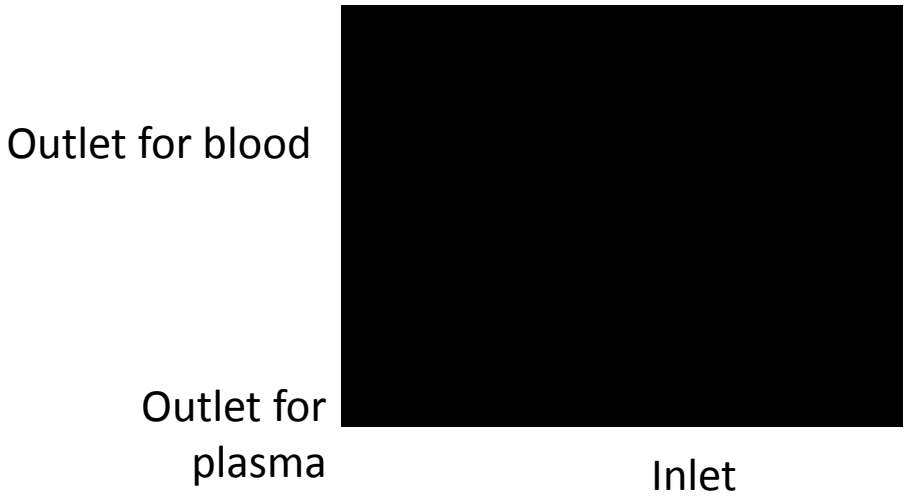


Exploiting Centrifugal Effect

Tripathi, S., Kumar, Y. B. V., Prabhakar, A., Joshi, S. S., & Agrawal, A. (2015). Passive blood plasma separation at the microscale: a review of design principles and microdevices. ***Journal of Micromechanics and Microengineering*, *25*(8), 083001.**

Movie (showing complete separation of plasma)





Prabhakar et al. (2015) ***Microfluidics and Nanofluidics,*** 18, 995-1006

Tripathi et al. (2015) ***J. Micromechanics and Microengineering***, 25, 084004

Patent pending

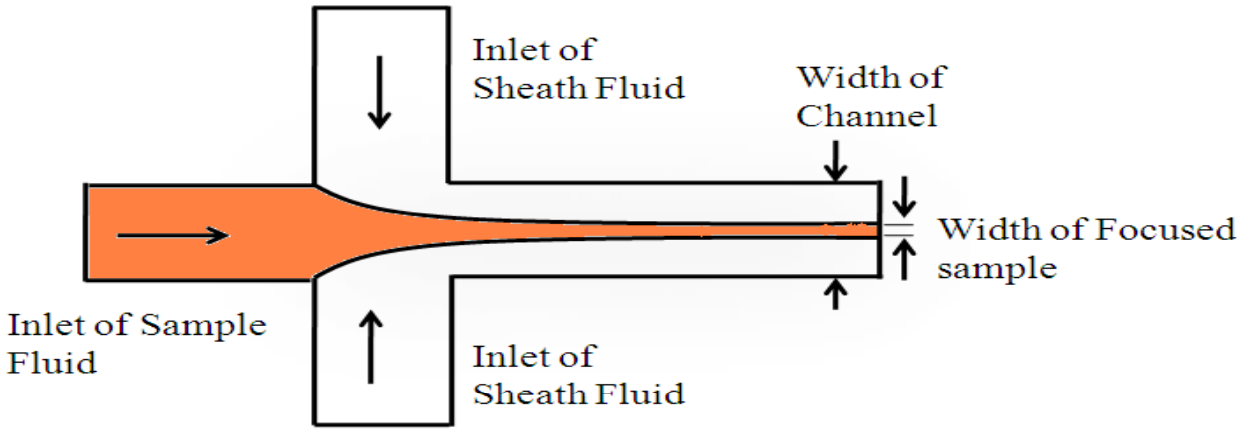
Unique features of our design

- Achieves almost 100% separation efficiency with whole blood
  - Demonstrated in hematocrit of 62% (found in polycythemia – a disease)
- Low separation time (relatively large flow rate: 0.3-0.5 ml/min)
- Elevated dimensions (> 100 μm)
  - Avoids problem of clogging!
  - Does not require tight dimensional tolerances
  - Reduces cost of manufacturing
- Biological characterization of plasma shows proteins are unaffected
  - Random-blood glucose test, Hemolysis free, Protein test
- Extensively tested (same microdevice used up to 1 year!)

Device licensed to Embryyo Bio-micordevices, Pune

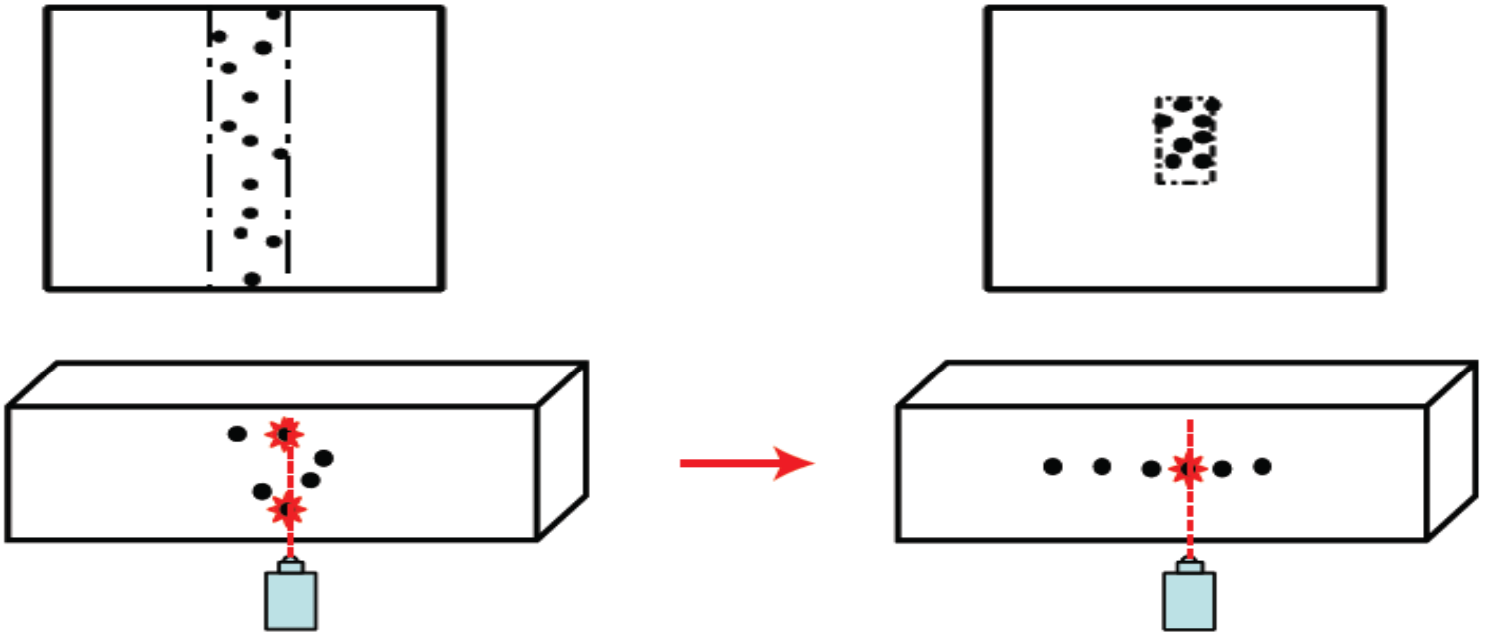
Hydrodynamic focusing microdevice

Hydrodynamic Focusing



Hydrodynamic Flow Focusing: Squeezing of a sample fluid using a sheath fluid.
Simple & effective technique for flow focusing and manipulating the sample flow

2D and 3D HF

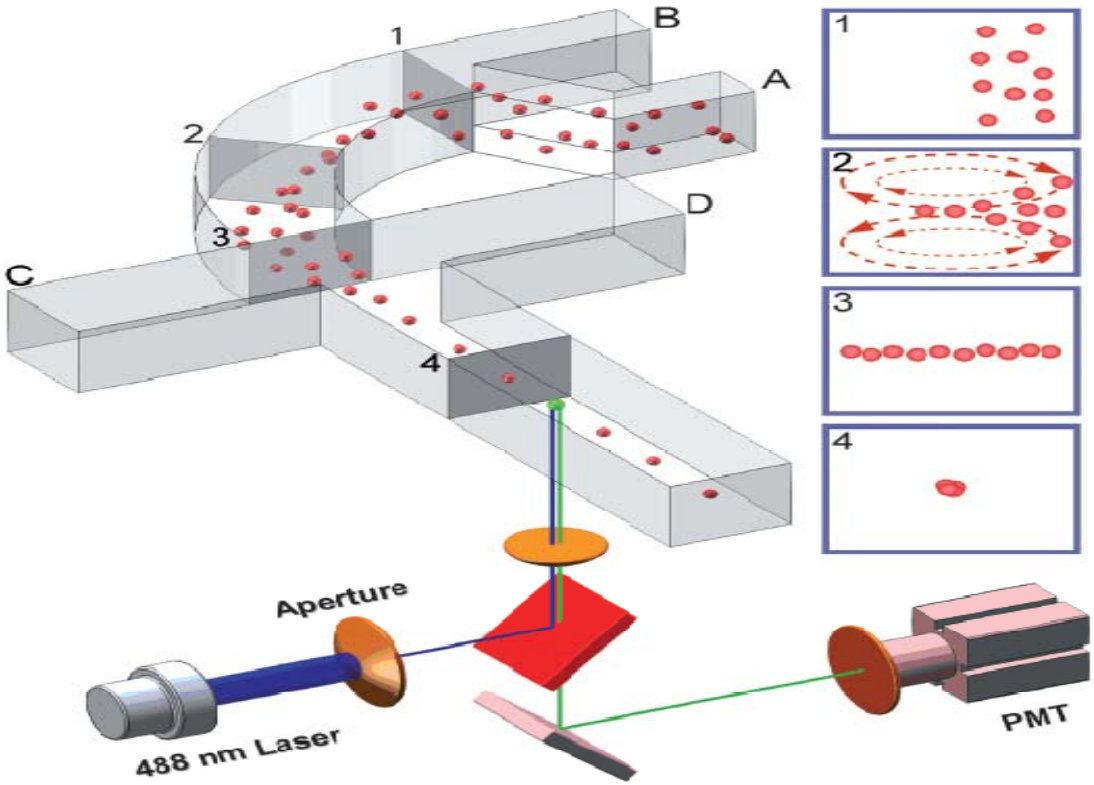


2D HF 3D HF

Disadvantages of 2-D focusing

- 2 or more cells can pass through the interrogation region
- Large cells can clog the microchannel
- Integration with optics
- Less uniform velocities

3D-Hydrodynamic Focusing Microdevice (from literature)

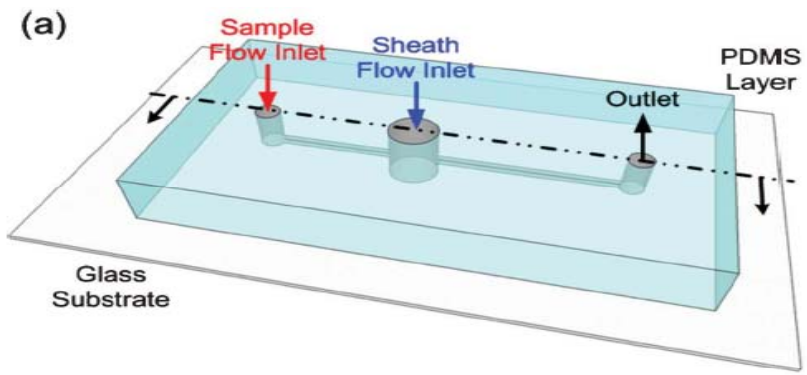


Use of Dean Forces
The device is 75 µm high
The main channel is 100 µm wide and 1 cm long,
Radius of the curve (average of inner and outer portion) is
250 µm.
A=51.9 µl/min,B=337.5 µl/min
C=225.5 µl/min,D=225.5 µl/min
Used LIF
Fluorescent polystrene 7.32 & 8.32 µm in SDS soln, with De-Ionized Water as sheath
CCD/Side view imaging
Focused region 14µm X 12 µm
Rate 1700 cells /sec

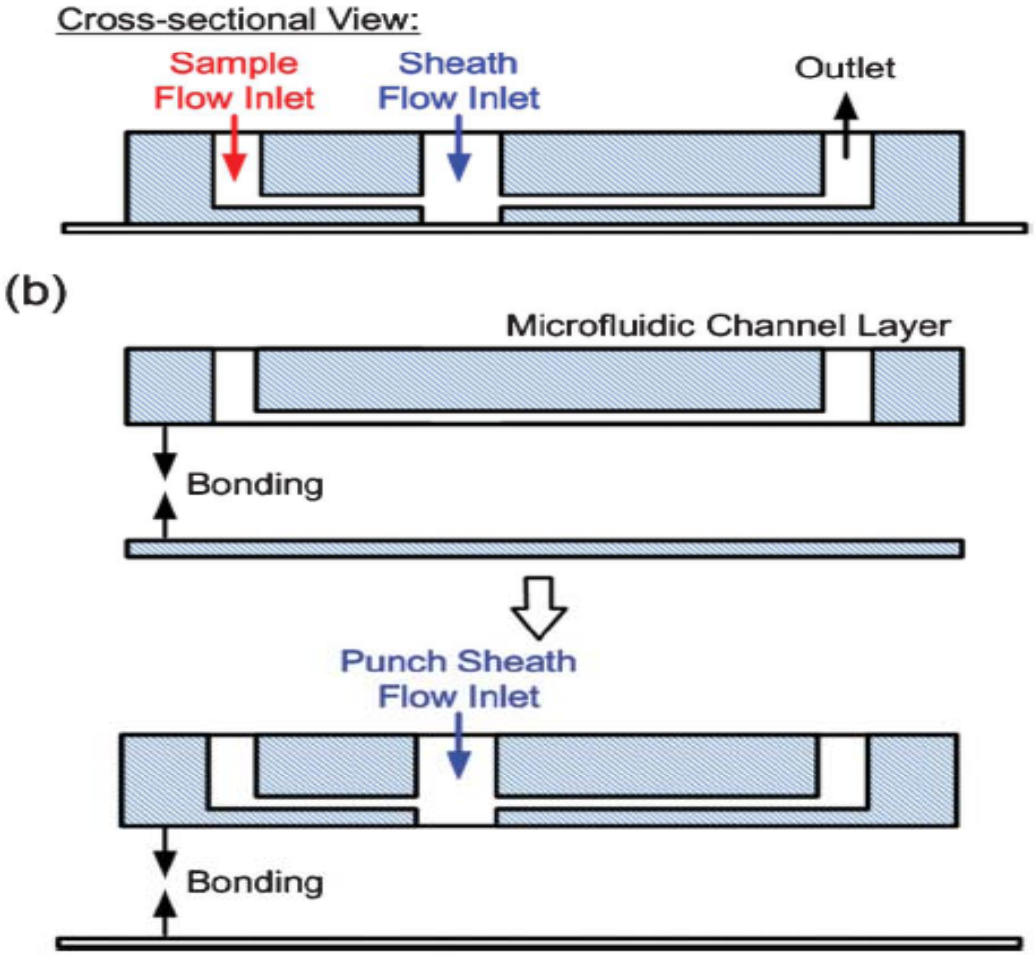
Schematic of the device setup and microfluidic drifting mechanism. Inlet A: cells or particles; inlet B: vertical focusing sheath flow; lnlets C and D: horizontal focusing sheath flows. Insets (1–4) on the right show the particle distribution in the cross-sectional planes 1–4 during the 3D hydrodynamic focusing process..

Mao et al, Single-layer planar on-chip flow cytometer using microfluidic drifting based three-dimensional (3D) hydrodynamic focusing, Lab Chip, 9, 1583-1589, 2009

3D Focusing-Single Sheath

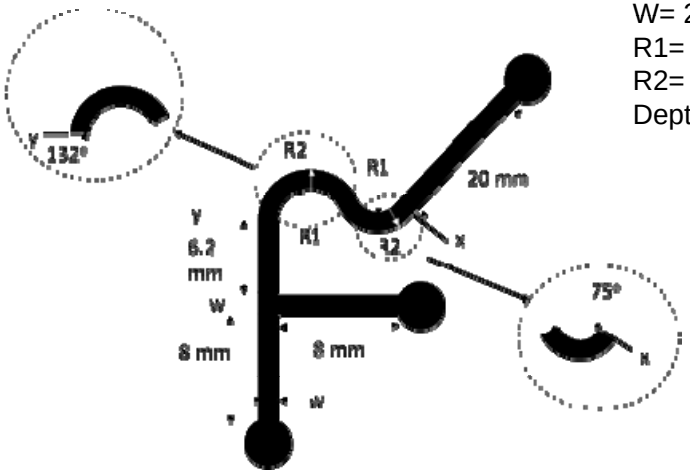


Width =200 µm,Thickness =150 µm
Thickness bottom PDMS film =600 µm
Inlet and outlet hole dia= 1mm
Sheath dia=1.5,2,3 mm
Water: Sample
Sheath: fluorescein chloride salt
Total flow rate of 100 µl/min
to 600 µl/min , and sheath/sample flow rate ratios of 1 : 1 to 1 : 4 are tested



Lin et.al, Single channel layer, single sheath-flow inlet microfluidic flow cytometer with three-dimensional hydrodynamic focusing, Lab Chip, 12, 3135-3141, 2012,

Three-dimensional Hydrodynamic Focusing

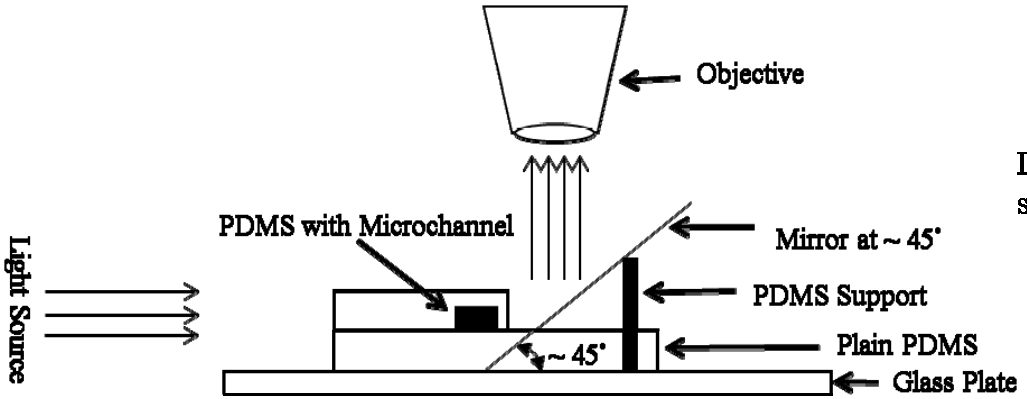


W= 200 µm
R1= 200 µm
R2= 400 µm
Depth= 100 µm

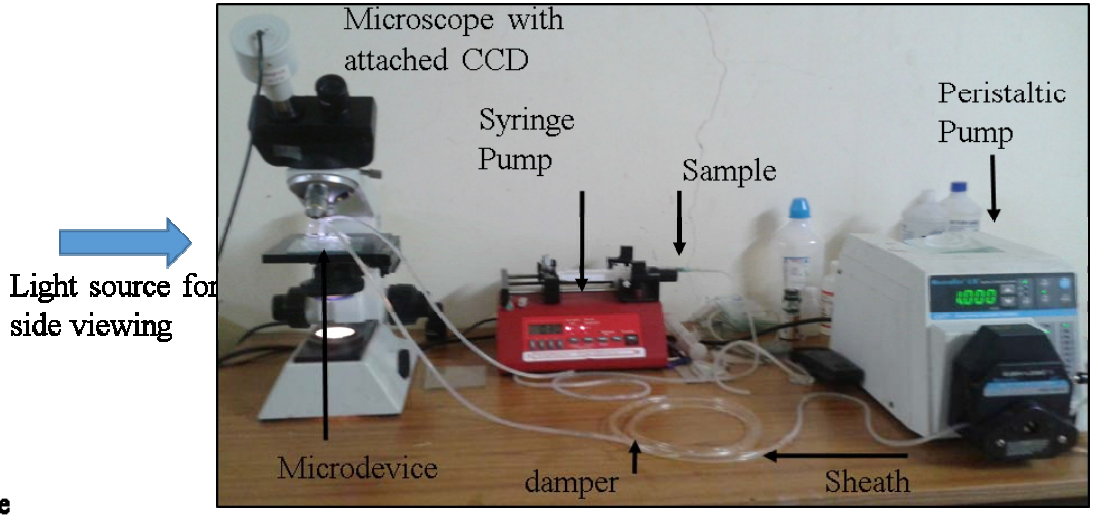
Schematic showing geometrical details of the fabricated microdevice

Experiment Details

Experiment	#1	#2
Sample	FITC Dye and Particles	Blood (Hct 5%)
Sheath	DIW	Saline
Detection	Confocal Microscopy	Microscope and CCD with side view imaging technique

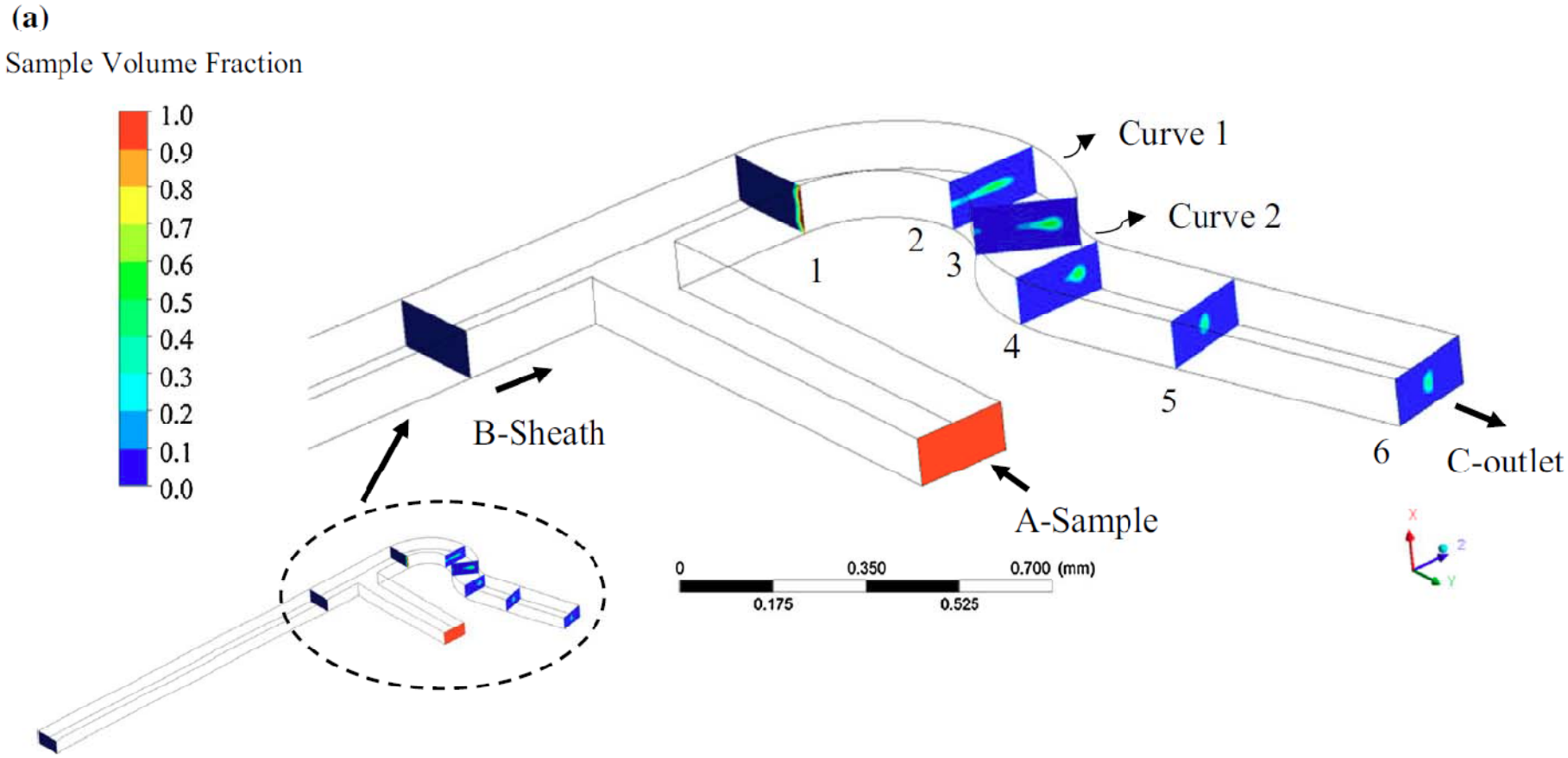


Home made-Side view imaging technique

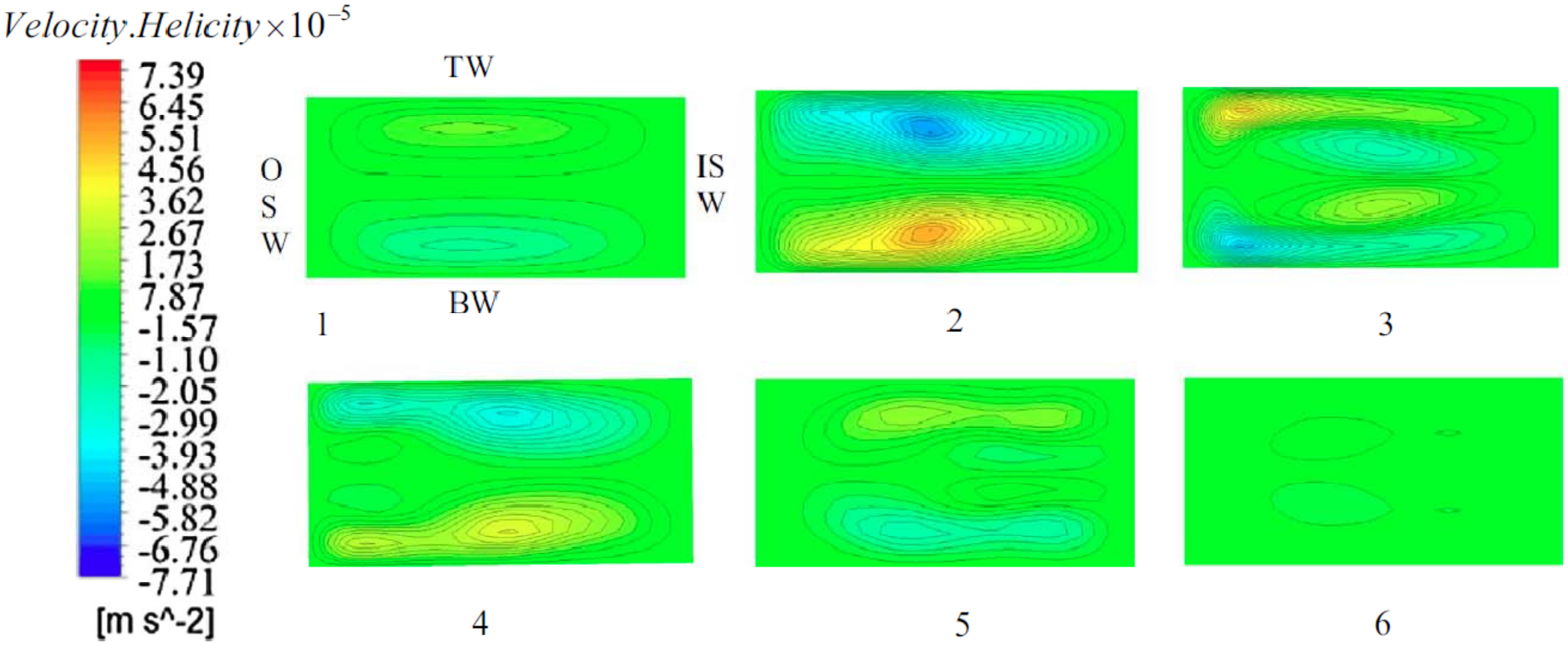


Experimental setup

Three-dimensional Hydrodynamic Focusing (Proposed Device)

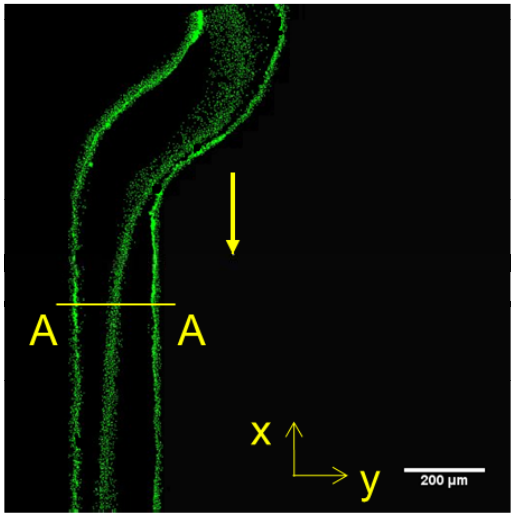


Working of the Microdevice



Cross-sectional view of the microdevice showing formation of Dean's vortices

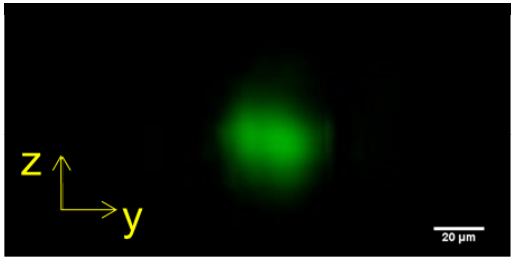
Experimental Results-FITC Dye and Particles



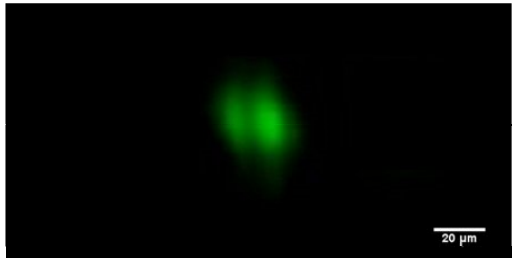
(a)

(b)

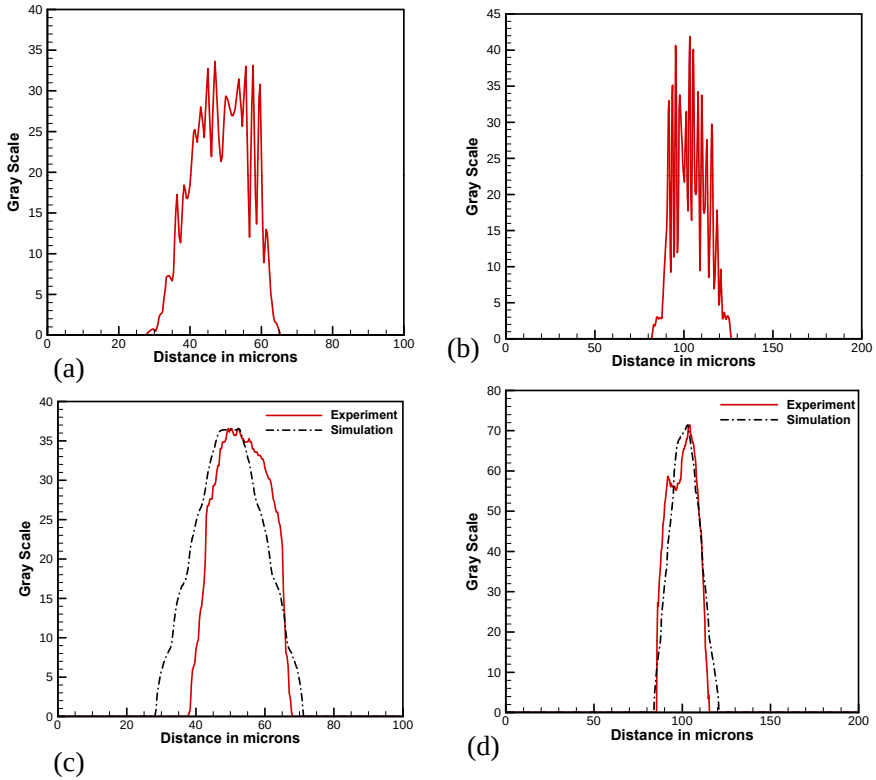
(c)



(d)



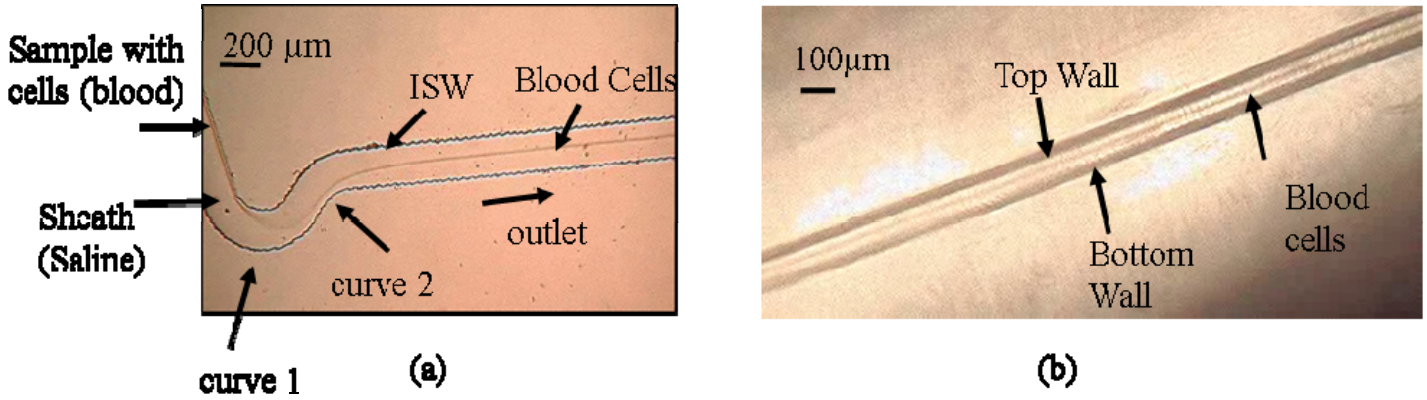
(e)



Intensity profiles for sample and sheath flow rate – **comparison between experiments and simulations**

Experimental results using confocal microscopy
Showing three-dimensional hydrodynamic focusing

Experimental Results-Human blood as sample fluid

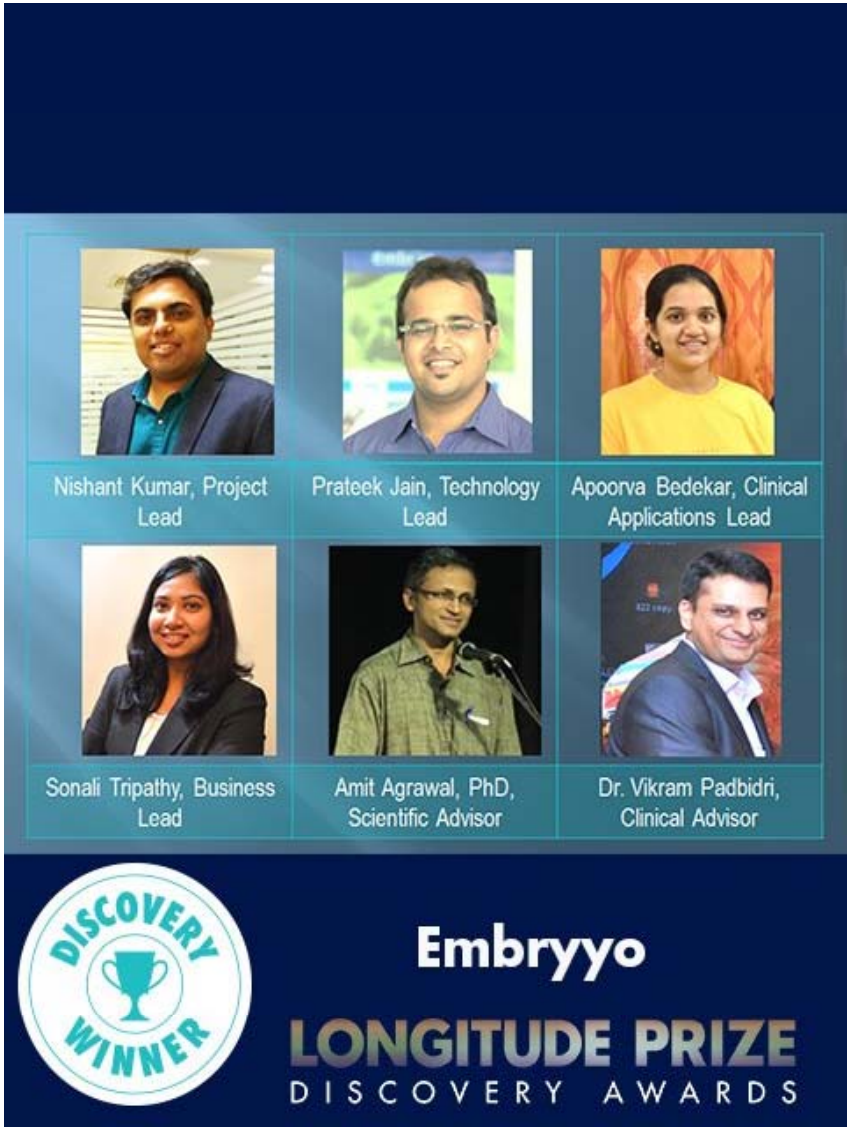


Experimental result of flow focusing using cells, Sample and sheath flow rate of 0.12 ml/min and 1.8 ml/min respectively (a) Horizontal focusing (b) Vertical focusing of cells

Tripathi, S., Kumar, A., Kmar, B.V., and Agrawal, A., "Three-dimensional hydrodynamic focusing of dye, particles and cells in a microfluidics device by employing two bends of opposite curvature," **Microfluidics and Nanofluidics**, Vol. 20, pp. 1-14, 2016

Device licensed to Embryyo Bio-micordevices, Pune

Extension to further challenging microdevices …



Looking beyond the Navier-Stokes equations

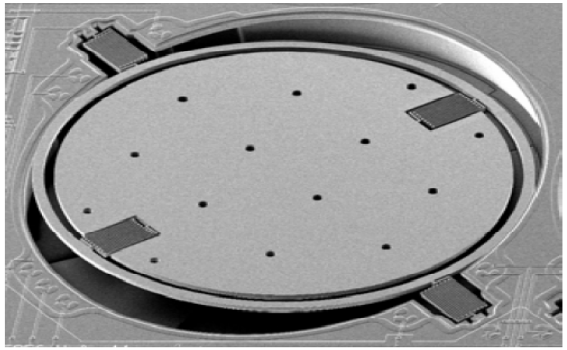
Primary Question

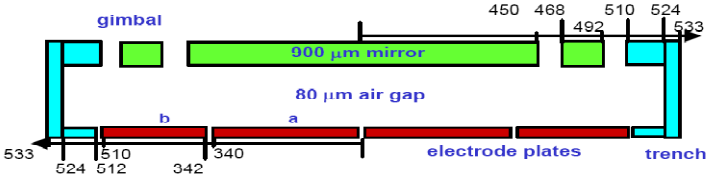
- What is the more general form of the Navier-Stokes equation?

- Recall
  - Navier-Stokes equations represent Conservation of Momentum for a differential fluid element
  - Navier-Stokes equations are 2nd order, non-linear, coupled partial differential equations

Practical Relevance

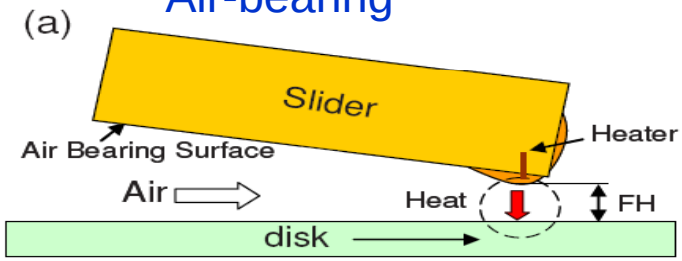
Flow in MEMS devices





Chu et al., (JMEMS, 2004)

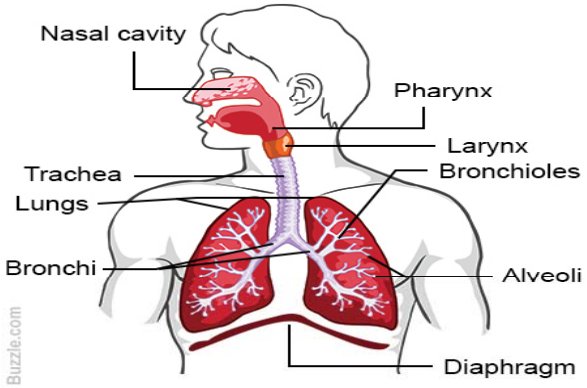
Air-bearing



Zhou et al. (PRE, 2010)

Aeration of Soil

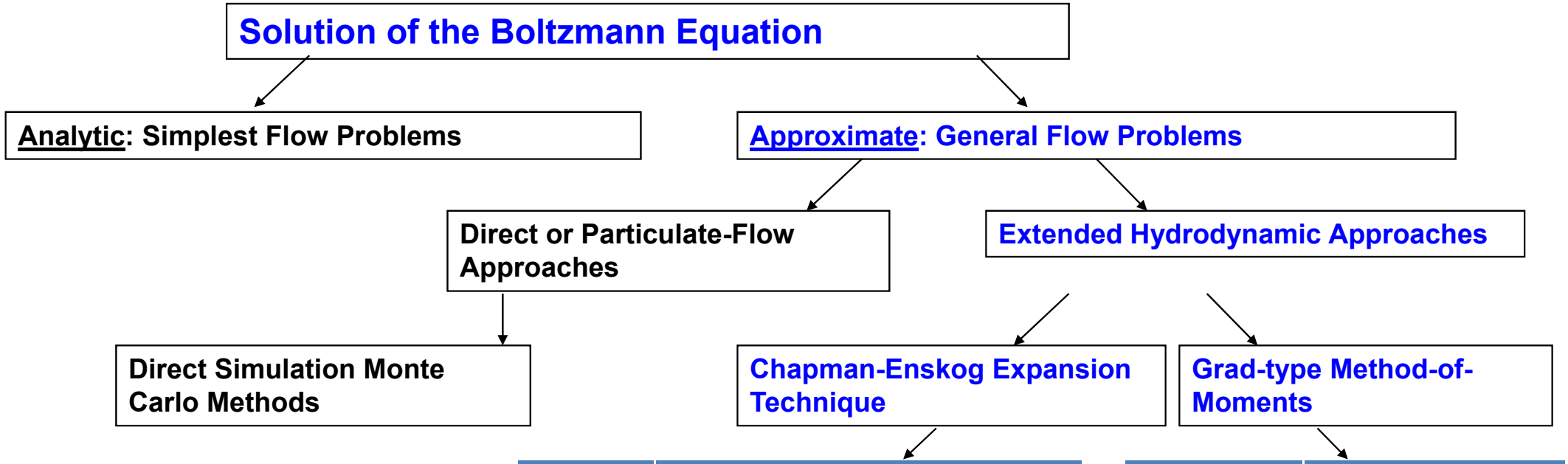
Flow in lungs



High altitude aircraft flight

Derivation of Hydrodynamic Equations

Adapted from: Balakrishnan, PhD Thesis, Univ. of WSU (1999)



O(Kn)	Resulting Equation
0	Euler Equations
1	Navier-Stokes Equations
2	Burnett Equations
3	Super-Burnett Equations

No. of moments	Resulting Equation
13	Grad Equations
26	26 Equations

From ‘atomistic view’ to fluid dynamics

Boltzmann equation:

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + G_i \frac{\partial f}{\partial c_i} = J(f, f)$$

$$\rho(r,t) = m \int f(r,c,t)\, dc$$

$$u(r,t) = \frac{1}{n} \int c f(r,c,t)\, dc$$

$$e(r,t) = \frac{1}{n} \int \frac{m}{2} C^2 f(r,c,t)\, dc$$

Multiplying by $\psi_i(\mathbf{x}, \mathbf{c}, t) = \{1, \mathbf{c}, C^2\}_i$ and integrating over velocity space, we get the conservation equations.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_k}{\partial x_k} = 0$$ Continuity equation

$$\rho \frac{\partial u_i}{\partial t} + \rho u_k \frac{\partial u_i}{\partial x_k} + \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = \rho G_i,$$ Cauchy’s equation of motion

$$\rho \frac{\partial \epsilon}{\partial t} + \rho u_k \frac{\partial \epsilon}{\partial x_k} + p \frac{\partial u_k}{\partial x_k} + \frac{\partial q_k}{\partial x_k} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} = 0,$$ Energy equation

System of equations is not closed.

The Chapman-Enskog method

Perturbative method based on an expansion in terms of Kn,

$$f = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \epsilon^3 f^{(3)} + \ldots$$

$$\sigma_{ij} = m \int C_{<i} C_{j>} f \; d\mathbf{c}, \quad q_i = \frac{m}{2} \int C^2 C_i f \, d\mathbf{c}$$

$$\sigma_{ij} = \sigma_{ij}^{(0)} + \epsilon \sigma_{ij}^{(1)} + \epsilon^2 \sigma_{ij}^{(2)} + \epsilon^3 \sigma_{ij}^{(3)} + \ldots,$$

$$q_i = q_i^{(0)} + \epsilon q_i^{(1)} + \epsilon^2 q_i^{(2)} + \epsilon^3 q_i^{(3)} + \ldots$$

In increasing order of Knudsen number,

- $O(Kn^0)$: Euler
- $O(Kn^1)$: Navier-Stokes-Fourier
- $O(Kn^2)$: Burnett
- $O(Kn^3)$: Super-Burnett

Burnett (1935) obtained the distribution function to second order.

Burnett stress and heat flux

Burnett

$$\sigma_{ij}^{(2)} = \frac{\mu^2}{p}\left[\overline{\omega_1}\frac{\partial v_k}{\partial x_k}S_{ij} - \overline{\omega_2}\left(\frac{\partial}{\partial x_{\langle i}}\left[\frac{1}{\rho}\frac{\partial p}{\partial x_{j\rangle}}\right] + \frac{\partial v_k}{\partial x_{\langle i}}\frac{\partial v_{j\rangle}}{\partial x_k} + 2\frac{\partial v_k}{\partial x_{\langle i}}S_{j\rangle k}\right)\right.$$
$$\left. + \overline{\omega_3}\frac{\partial^2\theta}{\partial x_{\langle i}\partial x_{j\rangle}} + \overline{\omega_4}\frac{\partial\theta}{\partial x_{\langle i}}\frac{\partial \ln p}{\partial x_{j\rangle}} + \overline{\omega_5}\frac{1}{\theta}\frac{\partial\theta}{\partial x_{\langle i}}\frac{\partial\theta}{\partial x_{j\rangle}} + \overline{\omega_6}S_{k\langle i}S_{j\rangle k}\right]$$

$$q_i^{(2)} = \frac{\mu^2}{\rho}\left[\theta_1\frac{\partial v_k}{\partial x_k}\frac{\partial \ln\theta}{\partial x_i} - \theta_2\left(\frac{2}{3}\frac{\partial^2 v_k}{\partial x_k\partial x_i} + \frac{2}{3}\frac{\partial v_k}{\partial x_k}\frac{\partial \ln\theta}{\partial x_i} + 2\frac{\partial v_k}{\partial x_i}\frac{\partial \ln\theta}{\partial x_k}\right)\right.$$
$$\left. + \theta_3 S_{ik}\frac{\partial \ln p}{\partial x_k} + \theta_4\frac{\partial S_{ik}}{\partial x_k} + 3\theta_5 S_{ik}\frac{\partial \ln\theta}{\partial x_k}\right]$$

Super-Burnett

Computation extremely complicated, hence three dimensional equations are still not known

Burnett Stress term in Cylindrical Coordinates ($\sigma_{r\theta}$)

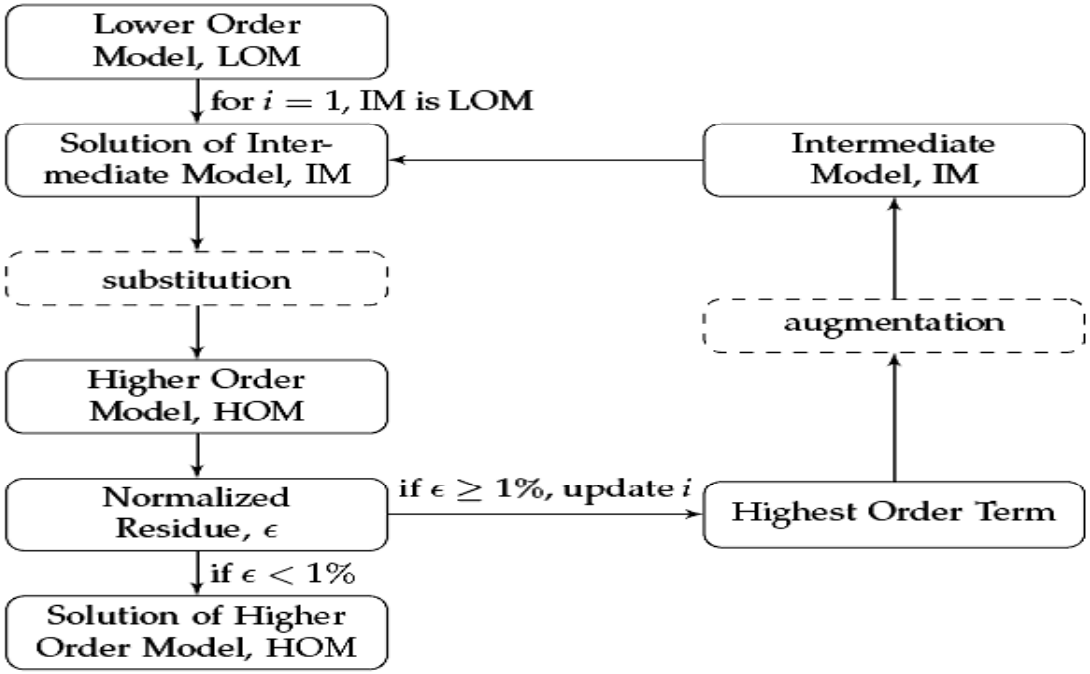
$$\sigma^B_{r\theta} = \sigma^B_{\theta r} = \frac{\mu^2}{p}\Bigg[-\left(\frac{\omega_1}{2}-\frac{5\omega_2}{3}+\frac{\omega_6}{6}\right)\left(\frac{v}{r}\frac{\partial u}{\partial r}\right)+\left(\frac{\omega_1}{2}-\frac{2\omega_2}{3}+\frac{\omega_6}{6}\right)\left(\frac{u}{r^2}\frac{\partial u}{\partial \theta}\right)$$
$$-\left(\frac{\omega_1}{2}-\frac{2\omega_2}{3}-\frac{\omega_6}{6}\right)\left(\frac{uv}{r^2}\right)+\left(\frac{\omega_1}{2}-\frac{5\omega_2}{3}+\frac{\omega_6}{6}\right)\left(\frac{u}{r}\frac{\partial v}{\partial r}\right)$$
$$-\left(\frac{\omega_1}{2}-\frac{2\omega_2}{3}+\frac{\omega_6}{6}\right)\left(\frac{v}{r^2}\frac{\partial v}{\partial \theta}\right)-\left(\frac{\omega_1}{2}+\frac{\omega_2}{3}-\frac{\omega_6}{3}\right)\left(\frac{v}{r}\frac{\partial w}{\partial z}\right)$$
$$+\left(\frac{\omega_1}{2}+\frac{\omega_2}{3}-\frac{\omega_6}{3}\right)\left(\frac{1}{r}\frac{\partial u}{\partial \theta}\frac{\partial w}{\partial z}\right)+\left(\frac{\omega_1}{2}-\frac{5\omega_2}{3}+\frac{\omega_6}{6}\right)\left(\frac{1}{r}\frac{\partial u}{\partial r}\frac{\partial u}{\partial \theta}\right)$$
$$+\left(\frac{\omega_1}{2}+\frac{\omega_2}{3}-\frac{\omega_6}{3}\right)\left(\frac{\partial v}{\partial r}\frac{\partial w}{\partial z}\right)+\left(\frac{\omega_1}{2}-\frac{2\omega_2}{3}+\frac{\omega_6}{6}\right)\left(\frac{\partial u}{\partial r}\frac{\partial v}{\partial r}\right)$$
$$+\left(\frac{\omega_1}{2}-\frac{2\omega_2}{3}+\frac{\omega_6}{6}\right)\left(\frac{1}{r^2}\frac{\partial u}{\partial \theta}\frac{\partial v}{\partial \theta}\right)+\left(\frac{\omega_1}{2}-\frac{5\omega_2}{3}+\frac{\omega_6}{6}\right)\left(\frac{1}{r}\frac{\partial v}{\partial r}\frac{\partial v}{\partial \theta}\right)$$
$$-\left(\omega_2-\frac{\omega_6}{4}\right)\left(\frac{\partial v}{\partial z}\frac{\partial w}{\partial r}\right)-\left(\omega_2-\frac{\omega_6}{4}\right)\left(\frac{1}{r}\frac{\partial u}{\partial z}\frac{\partial w}{\partial \theta}\right)-\left(\omega_2-\frac{\omega_6}{4}\right)\left(\frac{1}{r}\frac{\partial w}{\partial r}\frac{\partial w}{\partial \theta}\right)$$
$$+\omega_3\frac{R}{r}\frac{\partial^2 T}{\partial r\partial\theta}-\omega_3\frac{R}{r^2}\frac{\partial T}{\partial\theta}+\frac{\omega_4}{2}\frac{R}{r}\frac{1}{p}\frac{\partial p}{\partial\theta}\frac{\partial T}{\partial r}+\frac{\omega_4}{2}\frac{1}{r}\frac{R}{p}\frac{\partial p}{\partial r}\frac{\partial T}{\partial\theta}$$
$$+\omega_5\frac{1}{T}\frac{R}{r}\frac{\partial T}{\partial r}\frac{\partial T}{\partial\theta}+\frac{\omega_6}{4}\frac{\partial u}{\partial z}\frac{\partial v}{\partial z}+\omega_2\frac{1}{r^2}\frac{1}{\rho}\frac{\partial p}{\partial\theta}-\omega_2\frac{1}{r}\frac{1}{\rho}\frac{\partial^2 p}{\partial r\partial\theta}+\frac{\omega_2}{2}\frac{1}{r}\frac{1}{\rho^2}\frac{\partial p}{\partial\theta}\frac{\partial\rho}{\partial r}+\frac{\omega_2}{2}\frac{1}{r}\frac{1}{\rho^2}\frac{\partial p}{\partial r}\frac{\partial\rho}{\partial\theta}\Bigg]$$

Just one of the stress terms!

Question: Is it possible to obtain an analytical solution of the Burnett equations?

Proposed Approach to Solve Burnett Equations

- Start with solution of Navier-Stokes equations
- Substitute in Burnett equations
  - evaluate order of magnitude of additional terms
- Identify highest order term
  - augment governing equation with this additional term
- Re-solve the resulting equations
- Repeat above steps, till convergence achieved



Note: Requirement of additional boundary condition deferred till third-order term gets added in the governing equation!

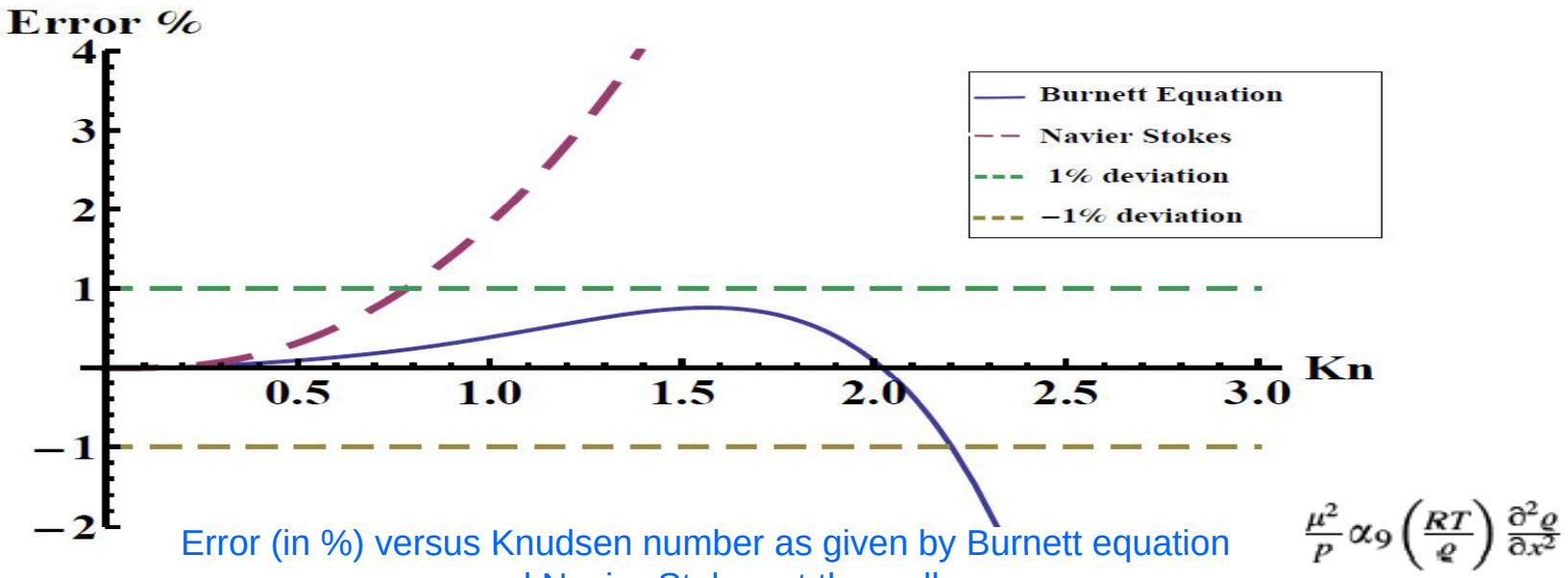
Singh and Agrawal, Journal of Fluid Mechanics, 2014

Solution of Burnett Equation for plane Poiseuille Flow

- **Streamwise Velocity**
  - $$u(x,y) = \left(\frac{Re\mu RT}{pD_h}\right)\frac{\left[\frac{y}{H}-\left(\frac{y}{H}\right)^2+2C_1Kn+8C_2Kn^2\right]}{\left(\frac{1}{6}+2C_1Kn+8C_2Kn^2\right)}$$
- **Cross-Stream Velocity**
  - $$v(x,y) = \frac{(12C_1Kn+96C_2Kn^2)}{(1+12C_1Kn+48C_2Kn^2)}\left(\frac{Re\mu RT}{D_h}\right)\left(\frac{1}{p^2}\right)\left(\frac{dp}{dx}\right)\times\left\{y\left[1-\frac{\frac{3y}{H}-2\left(\frac{y}{H}\right)^2+12C_1Kn+48C_2Kn^2}{(1+12C_1Kn+48C_2Kn^2)}\right]\right\}$$
- **Pressure**
  - $$\left(\frac{p}{p_o}\right)^2-1+Re^2\omega\frac{\mu^2RT}{(D_h{}^2p_o{}^2)}\left\{12C_1Kn_o\left(\frac{p_o}{p}-1\right)+24C_2Kn_o{}^2\left[\left(\frac{p_o}{p}\right)^2-1\right]+\log\left(\frac{p_o}{p}\right)\right\}$$
    $$+96C_2Kn_o{}^2\log\left(\frac{p}{p_o}\right)+24C_1Kn_o\left(\frac{p}{p_o}-1\right)=96Re\frac{\mu^2RT}{(D_h{}^2p_o{}^2)}\frac{(x_o-x)}{D_h}$$

Validation of Proposed Solution

Normalized error upon substituting the solution in governing equation is evaluated



Error (in %) versus Knudsen number as given by Burnett equation and Navier-Stokes at the wall

Normalized error less then 1% till Kn = 2.2

Solution satisfies governing equation (and boundary conditions)

N. Singh, N. Dongari, A. Agrawal (2014) Analytical solution of plane Poiseuille flow within Burnett hydrodynamics, **Microfluidics and Nanofludics**, Vol. 16, pp. 403-412

Critiques against Burnett equations

- Requires additional boundary conditions
  - Due to presence of the higher order derivatives
  - Additional boundary conditions are generally not available
- The convergence properties of the Chapman-Enskog series are not known.
- The equations suffer from instabilities in transient processes and from unphysical oscillations in steady state processes (Bobylev's instability)
- So far, there is *no proof that the Burnett equations follow positive definite entropy production*

Variants of Burnett equations: BGK-Burnett, Augmented Burnett, simplified Burnett, Dadzie-Burnett

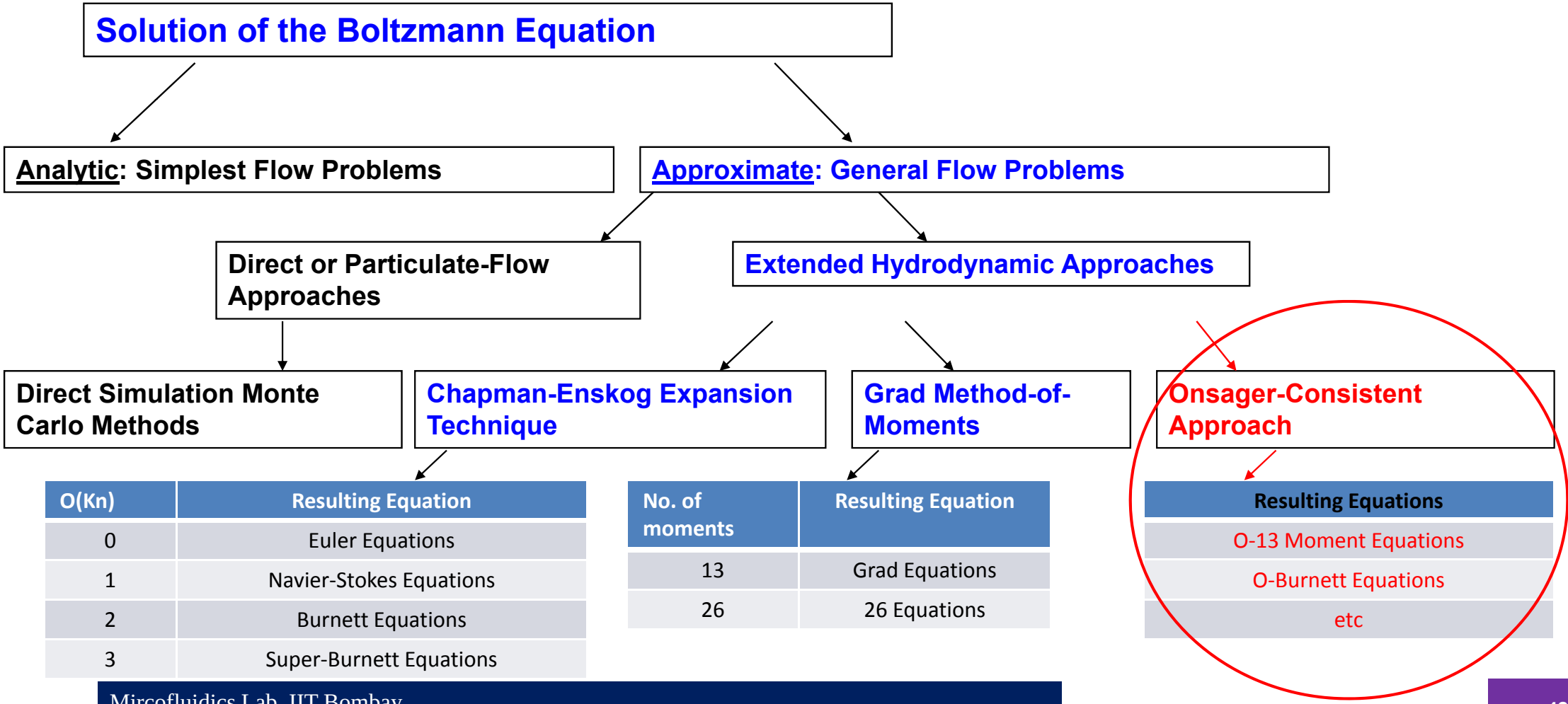
All these variants are inconsistent!

In general, Burnett and Grad's equations do not perform well at high Knudsen numbers!

Ref: Agarwal et al., PoF (2001); Garcia-Colin et al., Physics Reports (2008); Dadzie, JFM (2012)

Derivation of (Better?) Higher Order Moment Equations

Our Approach



O(Kn)	Resulting Equation
0	Euler Equations
1	Navier-Stokes Equations
2	Burnett Equations
3	Super-Burnett Equations

No. of moments	Resulting Equation
13	Grad Equations
26	26 Equations

Resulting Equations
O-13 Moment Equations
O-Burnett Equations
etc

Proposed distribution function

Phase density function casted in terms of thermodynamic forces X_i and fluxes Y_i

Satisfies Onsager's symmetry principle

$$f' = f_0 - (\Upsilon_\tau : X_\tau + \Upsilon_q \cdot X_q + (\Upsilon'_{\tau\tau} \odot X_\tau) : X_\tau + (\Upsilon'_{qq} \odot X_q) \cdot X_q)$$

Final form of distribution function satisfies

- Linearized Boltzmann equation
- Collision invariance property
- Onsager's symmetry principle

Therefore, consistent with principles of non-equilibrium thermodynamics

Note, no reference to Knudsen number in the derivation

- Expect to capture relatively strong non-equilibrium effects in slip and transition regimes

A. Mahendra, Meshless method for slip flows, *Ph.D. thesis*, Homi Bhabha National Institute, Mumbai (2011)
N. Singh and A. Agrawal, Onsager's principle consistent 13-moment transport equations, *Physical Review E* **93**, 063111 (2016)

Derivation of Onsager-Burnett Equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_k}{\partial x_k} = 0$$

$$\rho \frac{\partial u_i}{\partial t} + \rho u_k \frac{\partial u_i}{\partial x_k} + \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = \rho G_i,$$

$$\rho \frac{\partial \epsilon}{\partial t} + \rho u_k \frac{\partial \epsilon}{\partial x_k} + p \frac{\partial u_k}{\partial x_k} + \frac{\partial q_k}{\partial x_k} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} = 0,$$

Utilize the Onsager-consistent distribution function to evaluate σ_{ij} and q_i and obtain Burnett-type equations.

Proposed Onsager-Burnett equations

Euler/NSF/O-Burnett

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_k}{\partial x_k} = 0, \quad \text{Continuity equation}$$

$$\rho \frac{\partial u_i}{\partial t} + \rho u_k \frac{\partial u_i}{\partial x_k} + \frac{\partial p}{\partial x_i} + \left[\frac{\partial \sigma_{ik}}{\partial x_k} \right] = \rho G_i, \quad \text{Cauchy's equation of motion}$$

$$\rho \frac{\partial \epsilon}{\partial t} + \rho u_k \frac{\partial \epsilon}{\partial x_k} + p \frac{\partial u_k}{\partial x_k} + \left[\frac{\partial q_k}{\partial x_k} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} \right] = 0, \quad \text{Energy equation}$$

Constitutive relationships: Singh et al., Derivation of stable Burnett equations for rarefied gas flows, PRE (2017)

$$\sigma_{xx} = \sigma_{xx}^{NS} + \sigma_{xx}^{B} = \left[\mu \left(\delta_1 \frac{\partial u}{\partial x} + \delta_2 \frac{\partial v}{\partial y} + \delta_2 \frac{\partial w}{\partial z} \right) \right] + 4 \frac{\mu^2 \beta}{\rho} \left[\alpha_1 \left(\frac{\partial u}{\partial x} \right)^2 + \alpha_2 \left(\frac{\partial u}{\partial y} \right)^2 + \alpha_3 \left(\frac{\partial u}{\partial z} \right)^2 \right.$$
$$+ \alpha_4 \frac{\partial u}{\partial y} \frac{\partial v}{\partial x} + \alpha_5 \frac{\partial u}{\partial z} \frac{\partial w}{\partial x} + \alpha_6 \left(\frac{\partial w}{\partial x} \right)^2 + \alpha_7 \left(\frac{\partial v}{\partial x} \right)^2 + \alpha_8 \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} + \alpha_9 \left(\frac{\partial v}{\partial y} \right)^2 + \alpha_{10} \left(\frac{\partial w}{\partial z} \right)^2$$
$$\left. + \alpha_{11} \frac{\partial v}{\partial y} \frac{\partial w}{\partial z} + \alpha_{12} \frac{\partial u}{\partial x} \frac{\partial w}{\partial z} + \alpha_{13} \frac{\partial v}{\partial z} \frac{\partial w}{\partial y} + \alpha_{14} \left(\frac{\partial w}{\partial y} \right)^2 + \alpha_{15} \left(\frac{\partial v}{\partial z} \right)^2 \right],$$

$$\sigma_{xy} = \sigma_{xy}^{NS} + \sigma_{xy}^{B} = \left[\mu \delta_3 \frac{\partial u}{\partial y} + \mu \delta_3 \frac{\partial v}{\partial x} \right] + 4 \frac{\mu^2 \beta}{\rho} \left[\beta_1 \frac{\partial u}{\partial x} \frac{\partial u}{\partial y} + \beta_2 \frac{\partial v}{\partial x} \frac{\partial v}{\partial y} + \beta_3 \frac{\partial u}{\partial z} \frac{\partial v}{\partial z} + \beta_4 \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} \right.$$
$$\left. + \beta_5 \frac{\partial u}{\partial y} \frac{\partial v}{\partial y} + \beta_6 \frac{\partial w}{\partial x} \frac{\partial w}{\partial y} + \beta_7 \frac{\partial v}{\partial z} \frac{\partial w}{\partial x} + \beta_8 \frac{\partial u}{\partial z} \frac{\partial w}{\partial y} + \beta_9 \frac{\partial u}{\partial y} \frac{\partial w}{\partial z} + \beta_{10} \frac{\partial v}{\partial x} \frac{\partial w}{\partial z} \right],$$

Proposed Onsager-Burnett equations

Euler/NSF/O-Burnett

$$q_x = q_x^{NS} + q_x^B = \delta_4 \kappa \frac{1}{2R\beta^2}\frac{\partial \beta}{\partial x} + 4\frac{\mu^2\beta}{\rho}\left[\gamma_1 \frac{1}{\beta}\frac{\partial g}{\partial x}\frac{\partial u}{\partial x} + \gamma_2 \frac{1}{\beta^2}\frac{\partial \beta}{\partial x}\frac{\partial v}{\partial y} + \gamma_3 \frac{1}{\beta^2}\frac{\partial \beta}{\partial x}\frac{\partial w}{\partial z} + \gamma_4 \frac{1}{\beta}\frac{\partial g}{\partial y}\frac{\partial u}{\partial y}\right.$$
$$+ \gamma_5 \frac{1}{\beta}\frac{\partial g}{\partial y}\frac{\partial v}{\partial x} + \gamma_6 \frac{1}{\beta}\frac{\partial g}{\partial z}\frac{\partial w}{\partial x} + \gamma_7 \frac{1}{\beta^2}\frac{\partial \beta}{\partial x}\frac{\partial u}{\partial x} + \gamma_8 \frac{1}{\beta^2}\frac{\partial \beta}{\partial y}\frac{\partial u}{\partial y} + \gamma_9 \frac{1}{\beta^2}\frac{\partial \beta}{\partial z}\frac{\partial u}{\partial z} + \gamma_{10} \frac{1}{\beta^2}\frac{\partial \beta}{\partial y}\frac{\partial v}{\partial x}$$
$$\left. + \gamma_{11} \frac{1}{\beta^2}\frac{\partial \beta}{\partial z}\frac{\partial w}{\partial x} + \gamma_{12} \frac{1}{\beta}\frac{\partial g}{\partial x}\frac{\partial v}{\partial y} + \gamma_{13} \frac{1}{\beta}\frac{\partial g}{\partial x}\frac{\partial w}{\partial z}\right] + \left(\frac{2\kappa(\gamma-1)}{R\gamma}\right)^2 \frac{1}{\rho\beta}\left[\gamma_{14}\frac{\partial \beta}{\partial y}\frac{\partial v}{\partial x} + \gamma_{15}\frac{\partial \beta}{\partial z}\frac{\partial w}{\partial x}\right.$$
$$\left. + \gamma_{16}\frac{\partial \beta}{\partial x}\frac{\partial u}{\partial x} + \gamma_{17}\frac{\partial \beta}{\partial y}\frac{\partial u}{\partial y} + \gamma_{18}\frac{\partial \beta}{\partial z}\frac{\partial u}{\partial z} + \gamma_{19}\frac{\partial \beta}{\partial x}\frac{\partial v}{\partial y} + \gamma_{20}\frac{\partial \beta}{\partial x}\frac{\partial w}{\partial z}\right],$$

$$\text{where, } \beta = \frac{1}{2RT}, \qquad g = \log\left(\frac{\rho}{\beta}\right)$$

Singh et al., Derivation of stable Burnett equations for rarefied gas flows, PRE (2017)

Advantages of Proposed Approach

- Additional boundary conditions not required
  - OBurnett equations are 2nd order!
- Stress terms are not dependent on temperature gradient
- Derived equations are unconditionally stable
- Accounts for non-unity Prandtl number

Proposed equations appear to be physically more consistent

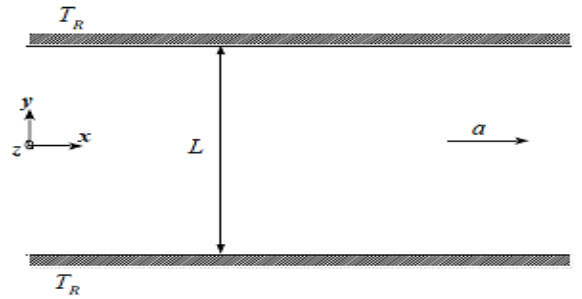
Validation of Proposed OBurnett Equations

- Couette flow
- Force driven Poiseuille flow
- Pressure driven Poiseuille flow

Forced driven Poiseuille flow using OBurnett equations

Assumptions

- The velocity normal to the stationary walls, *v* is zero.
- The third component of velocity, *w* is zero, owing to the flow being two-dimensional.
- All the flow variables are functions of *y*-direction only.



Schematic of plane Poiseuille flow driven by external force, '*a*'

Ref: Uribe and Garcia, PRE 1999

Governing Equations

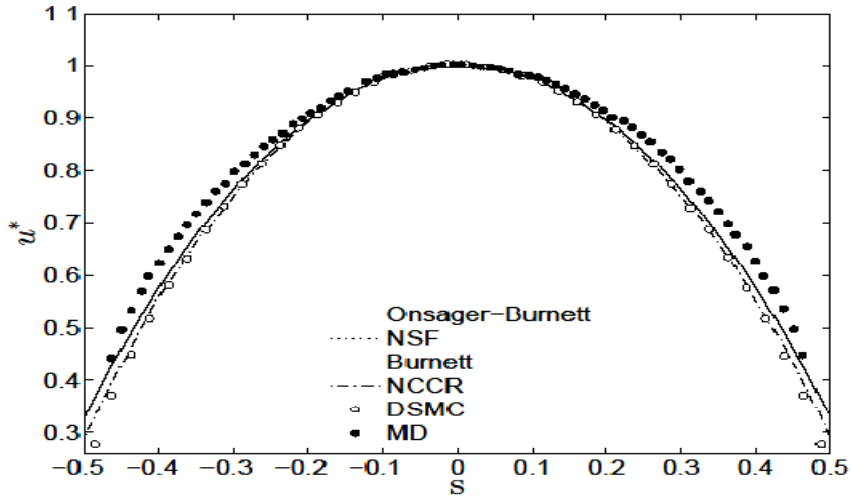
$$\frac{d^2u^*}{ds^2} = -\frac{1}{2T^*}\frac{dT^*}{ds}\frac{du^*}{ds} + \frac{b_0' p^*}{T^{*3/2}},$$

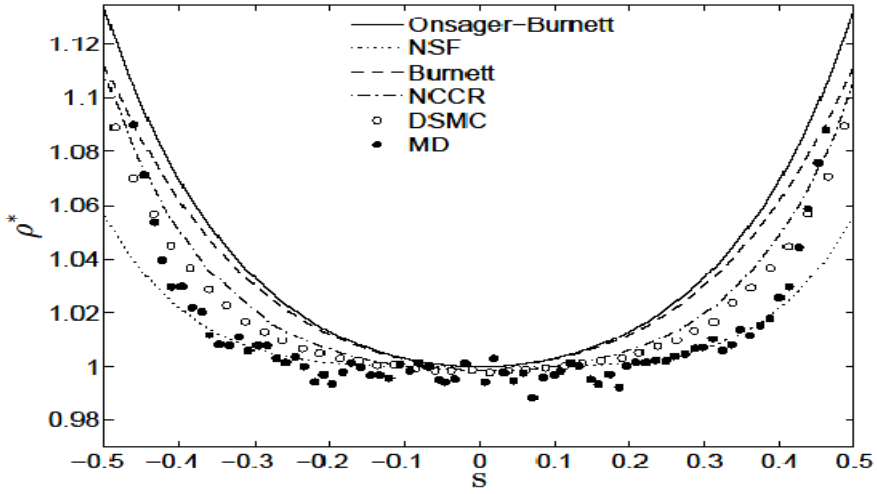
$$\frac{dp^*}{ds} = \frac{\left\{ -\frac{2T^*}{p^*}\frac{du^*}{ds}\left[-\frac{1}{2T^*}\frac{dT^*}{ds}\frac{du^*}{ds} + \frac{b_o' p^*}{T^{*3/2}} \right] + \left(\frac{du^*}{ds}\right)^2 \frac{1}{p^*}\frac{dT^*}{ds} \right\}}{\left\{ b_2' - \frac{T^*}{p^{*2}}\left(\frac{du^*}{ds}\right)^2 \right\}},$$

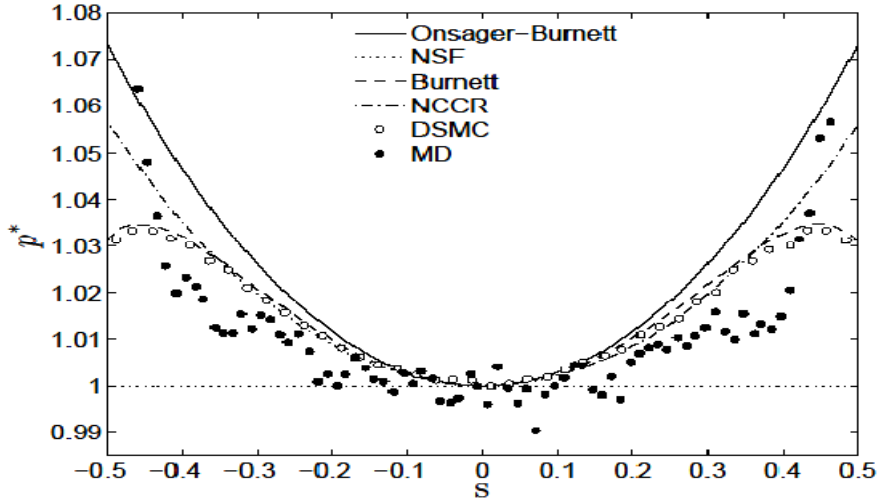
$$\frac{d^2T^*}{ds^2} = -\frac{8c_\mu}{15c_\lambda}\left(\frac{du^*}{ds}\right)^2 - \frac{1}{2T^*}\left(\frac{dT^*}{ds}\right)^2.$$

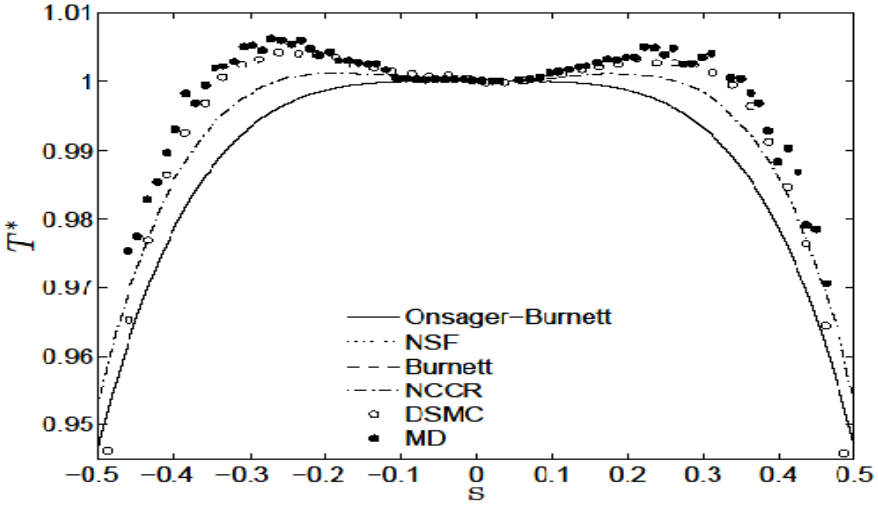
Jadhav et al., Force-driven compressible plane Poiseuille flow by Onsager-Burnett equations, PoF (2017) (**Editor's pick** article)

Conserved variables: u^*, ρ^*, p^* and T^*

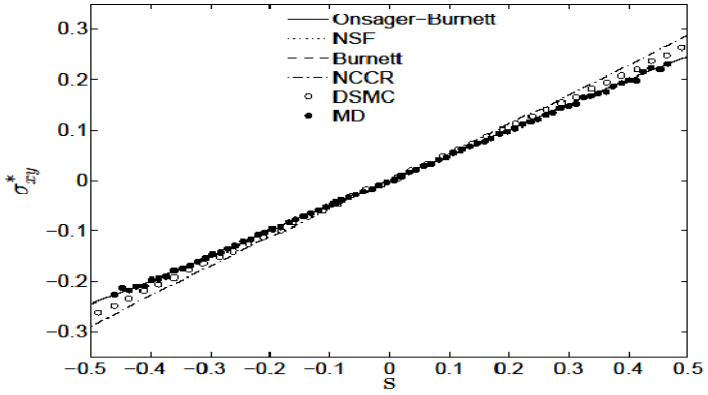


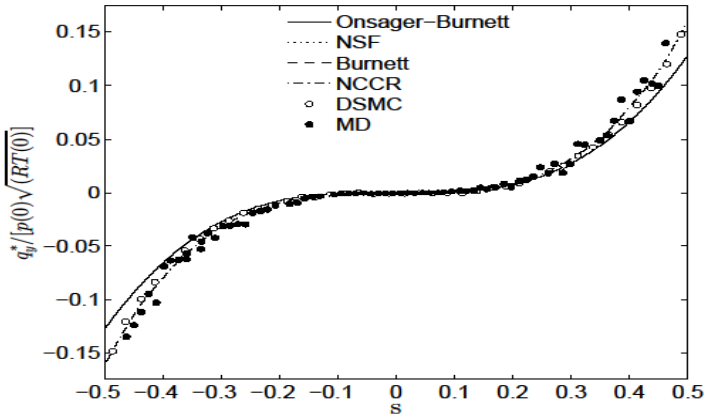


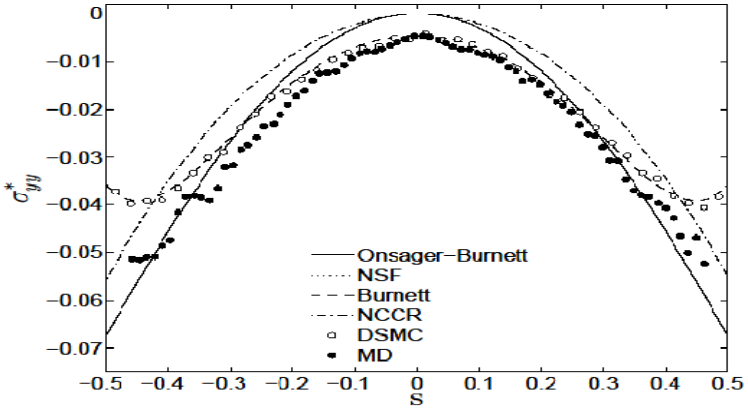


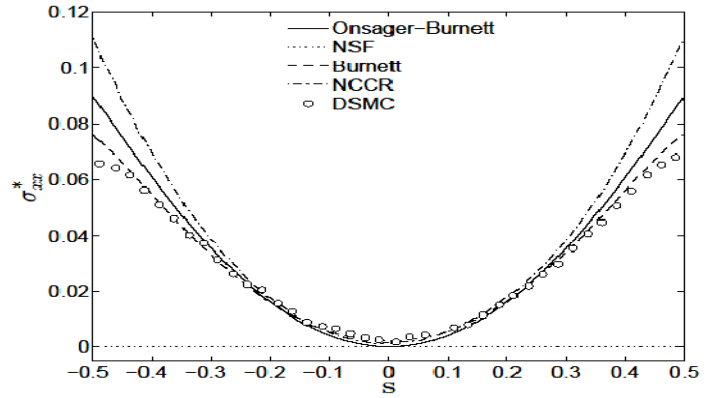


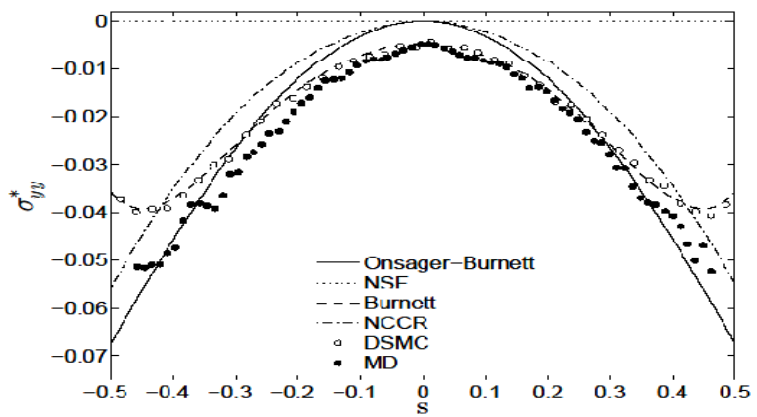
Non-conserved variables: σ^*_{xy}, q^*_y, σ^*_{yy}, σ^*_{xx}, σ^*_{zz} and q^*_x

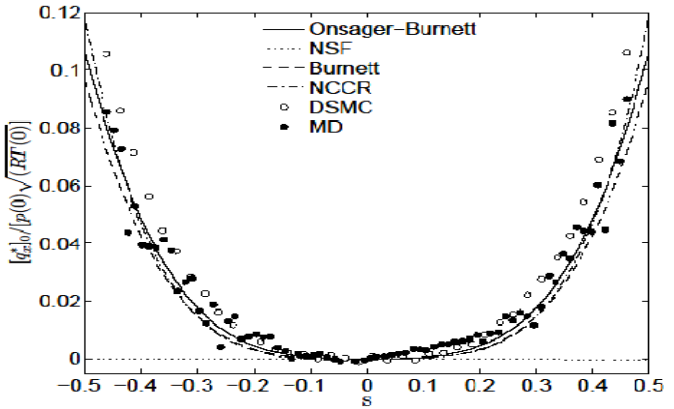












Jadhav et al., Force-driven compressible plane Poiseuille flow by Onsager-Burnett equations, PoF (2017) (**Editor's pick** article)

Summary

Blood plasma separation microdevice

- eliminates the need for centrifugation
- demonstrated on whole blood

Three-dimensional hydrodynamic focusing microdevice

- simple design
- requires fewer number of accessories

Beyond Navier-Stokes equations

- Possible to solve Burnett equations analytically (Kn ~ 2.2)
- Proposed new set of Burnett-type higher-order continuum transport equations (super-set of Navier-Stokes equations)

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