Numerical Optimization Strategy for Determining 3D Flow Fields in Microfluidics

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Introduction: We present a hybrid experimental-numerical method for the generation of 3D flow information from 2D particle image velocimetry (PIV) experimental data and finite element simulations. An optimization algorithm is applied to a theory-based simulation of an ac electrothermal (ACET) micromixer in conjunction with 2D PIV data to generate an improved estimation of 3D steady state flow conditions.

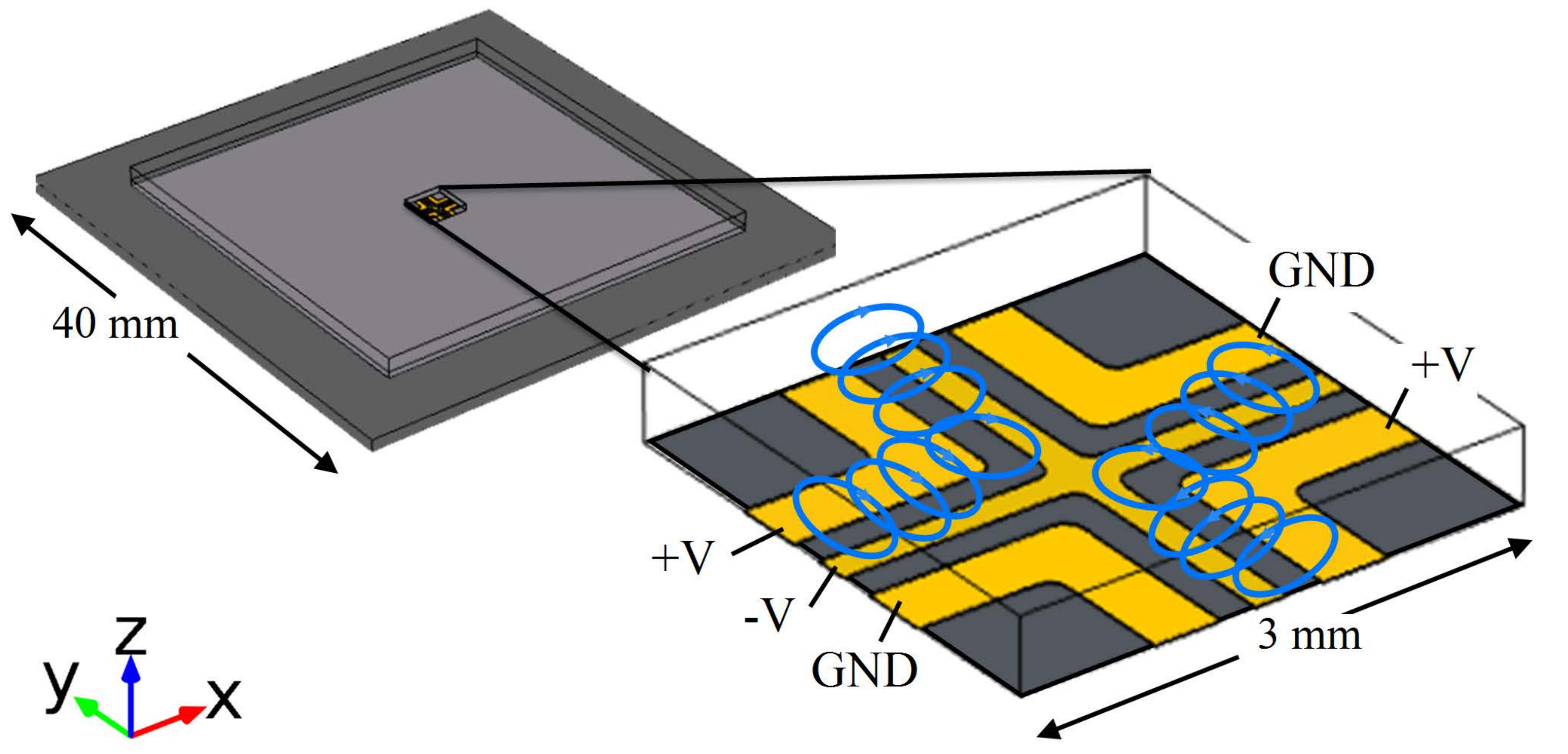

Figure 1. The experimental ACET mixing device, depicting the electrode geometry and general flow patterns for the applied voltages shown (*f* = 1 MHz, V_{pp} = 26 V)

Computational Methods:

- Numerical simulations performed using *COMSOL Multiphysics* v5.1
- Governing equations based on theoretical model [1],[2]
  - Electric field (Gauss's Law) solved using *coefficient form PDE*
  - Temperature field (Joule heating equation) solved using *heat transfer in fluids*
  - Velocity field (Stokes equations) solved using *laminar single-phase flow*
  - Nelder-Mead optimization algorithm used to minimize error by scaling several parameters to fit experimental data

$$\begin{cases} \boldsymbol{\nabla}^2\tilde{V} = c_\sigma \boldsymbol{\nabla} T \cdot \boldsymbol{\nabla}\tilde{V}, \qquad \widetilde{\boldsymbol{E}} = -\boldsymbol{\nabla}\tilde{V} \\ \rho(T)C_p(T)\boldsymbol{u}\cdot\boldsymbol{\nabla}T = \boldsymbol{\nabla}\cdot(k_m\boldsymbol{\nabla}T) + \dfrac{\sigma_m(T)}{2}\left|\widetilde{\boldsymbol{E}}\right|^2 \\ \boldsymbol{\nabla}\cdot\left(\mu_m(T)(\boldsymbol{\nabla u} + (\boldsymbol{\nabla u})^T)\right) + \boldsymbol{F} = \boldsymbol{\nabla}P, \qquad \boldsymbol{\nabla}\cdot\boldsymbol{u} = 0 \end{cases}$$

$$Objective = \frac{\sum\,(u_{PIV} - u_{Model})^2 + (v_{PIV} - v_{Model})^2}{\sum\,(u_{PIV})^2 + (v_{PIV})^2}$$

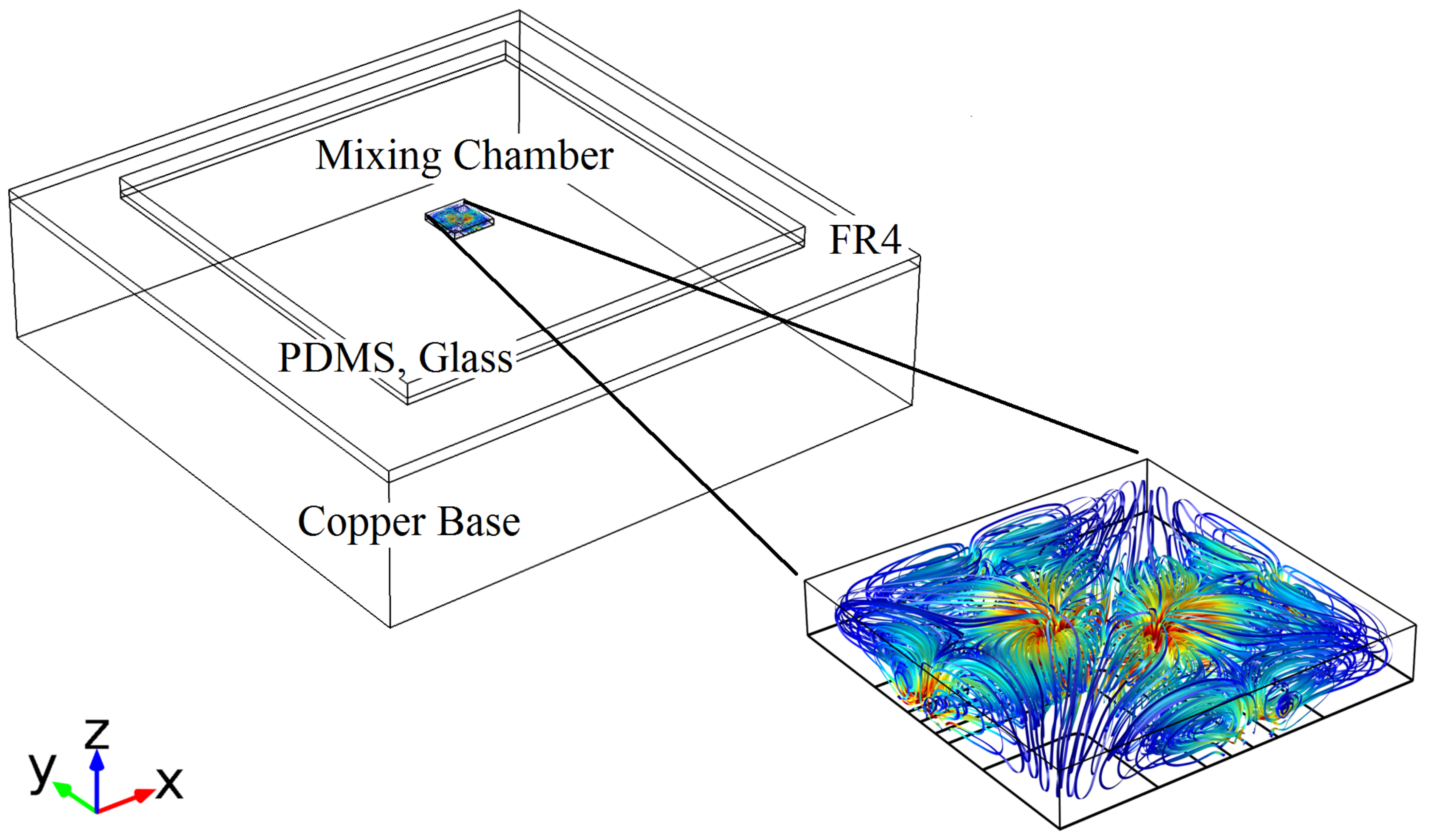

Figure 2. The modeled device with theoretical 3D streamlines for the optimized flow conditions

Results:

- Objective function reduced by more than a factor of 250
  - Velocity relative error reduced by 244%
- Maximum velocity magnitude reduced by factor of about 5
- Scale & direction of optimized velocity results match PIV data

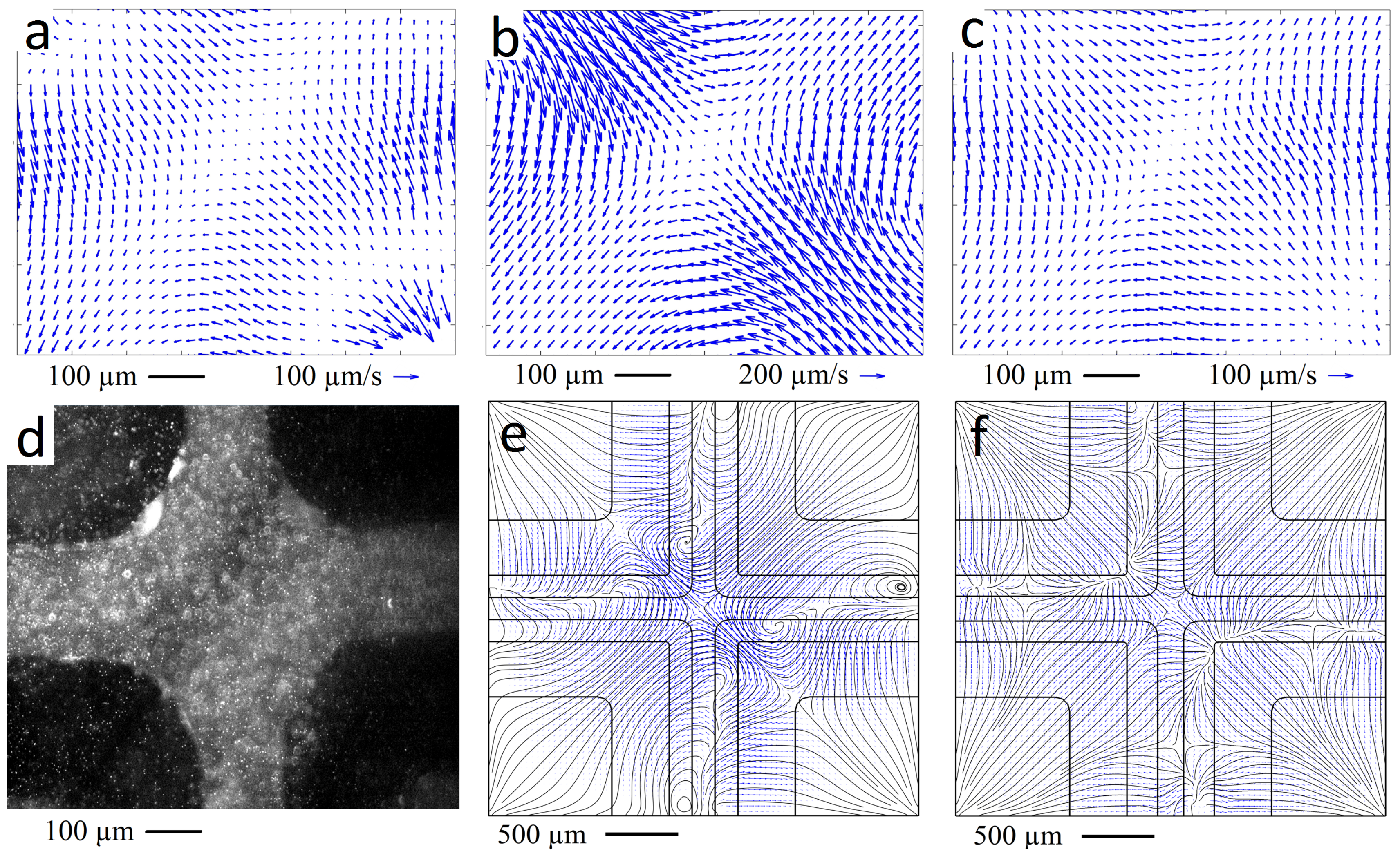

Figure 3. (a) PIV data, (b) original simulation, (c) optimized simulation, (d) PIV experiment image, (e) original flow pattern, (f) optimized flow pattern

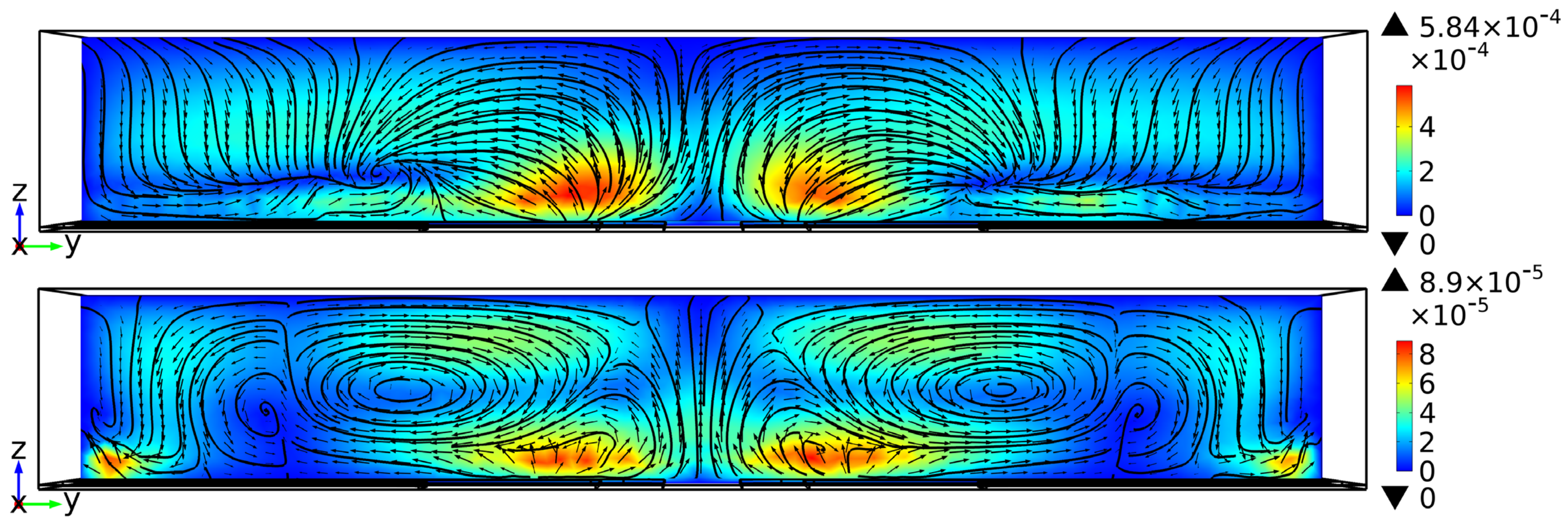

Figure 4. Theoretical velocity field and circulation patterns from a side view of the micromixer for the original (top) and optimized (bottom) flow conditions, in m/s

Parameter	Original	Optimized
Electrothermal Force Scaling	1	0.348
Electric Field Nonlinearity Scaling	1	3.125
Buoyancy Force Scaling	1	4.369
Dielectrophoretic Force Scaling	1	3.539
Fluid Thermal Conductivity	0.61 W $m^{-1}K^{-1}$	0.104 W $m^{-1}K^{-1}$
Fluid Electrical Conductivity	1.6 mS/cm	0.84 mS/cm
Fluid Dynamic Viscosity	$9x10^{-4}$ Pa s	$1.12x10^{-3}$ Pa s
Gaussian Function Width	5 µm	20 µm
Measurement Plane Location Offset	0	-48.25 µm
Center Electrode Width	200 µm	160 µm
Gap Width Between Electrodes	200 µm	205 µm
FR4 Thermal Conductivity, x-direction	0.8 W $m^{-1}K^{-1}$	4.25 W $m^{-1}K^{-1}$
FR4 Thermal Conductivity, y-direction	0.8 W $m^{-1}K^{-1}$	3.26 W $m^{-1}K^{-1}$
FR4 Thermal Conductivity, z-direction	0.3 W $m^{-1}K^{-1}$	0.965 W $m^{-1}K^{-1}$

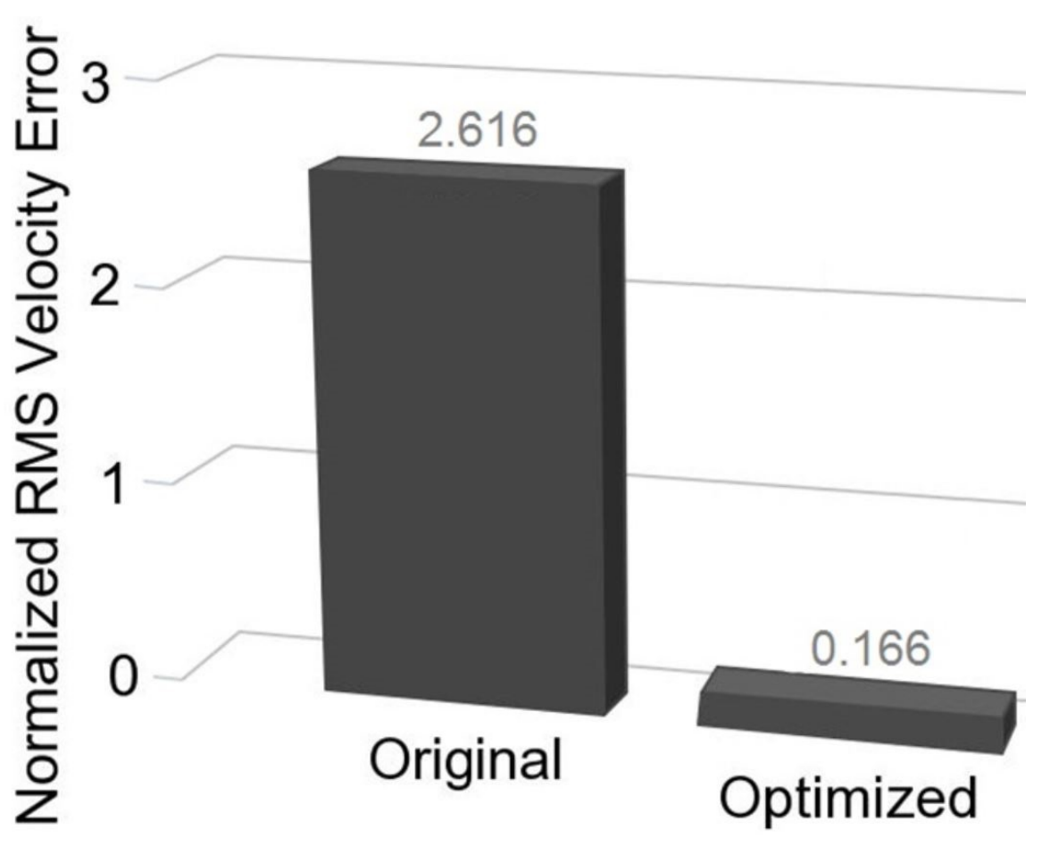

Figure 5. Original and optimized control parameters (left), NRMSE values (right)

Conclusions:

- Normalized RMS velocity error between experiment and simulation results reduced by more than an order of magnitude
- Optimization altered 3D fluid circulation patterns considerably
- Yields a more accurate estimation of 3D experimental flow field
- Approach can be generalized to a wide variety of flow problems

References

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2. S. Loire, P. Kauffman, I. Mezić, and C. D. Meinhart, Ac electrokinetics: A theoretical and experimental study of ac electrothermal flows, *J. Phys. D: Appl. Phys*, 45, 185301 (2012)

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