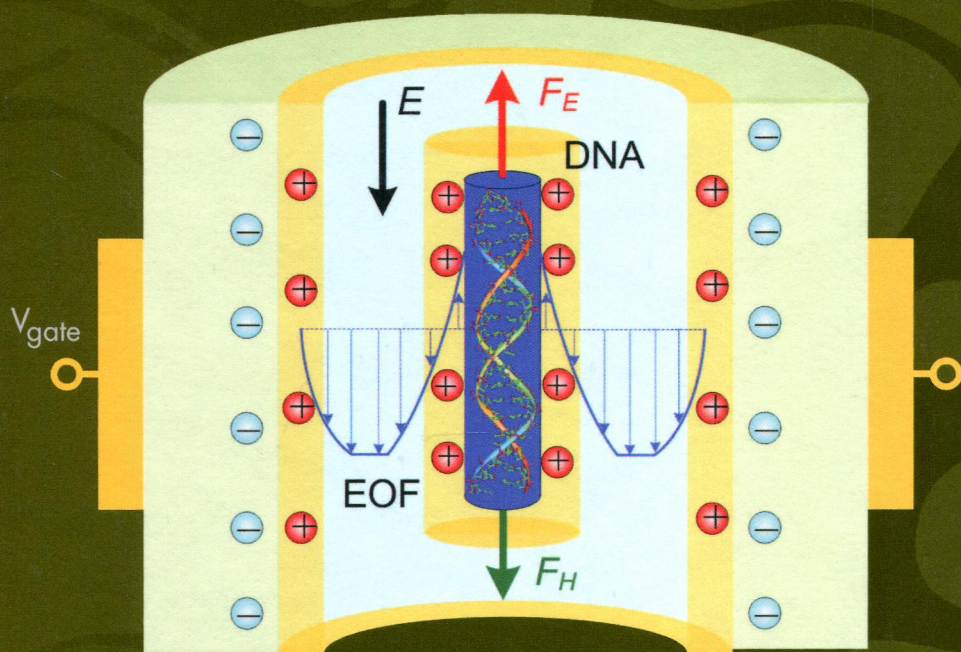


# ELECTROKINETIC PARTICLE TRANSPORT IN MICRO-/NANOFLUIDICS

Direct Numerical Simulation Analysis



Shizhi Qian • Ye Ai

# **ELECTROKINETIC PARTICLE TRANSPORT IN MICRO-/NANOFLUIDICS**

**Direct Numerical Simulation Analysis**

**Shizhi Qian**

*Old Dominion University  
Norfolk, Virginia, U.S.A.*

**Ye Ai**

*Old Dominion University  
Norfolk, Virginia, U.S.A.*



**CRC Press**

Taylor & Francis Group

Boca Raton London New York

---

CRC Press is an imprint of the  
Taylor & Francis Group, an Informa business

CRC Press  
Taylor & Francis Group  
6000 Broken Sound Parkway NW, Suite 300  
Boca Raton, FL 33487-2742

© 2012 by Taylor & Francis Group, LLC  
CRC Press is an imprint of Taylor & Francis Group, an Informa business

No claim to original U.S. Government works

Printed in the United States of America on acid-free paper  
Version Date: 20120409

International Standard Book Number: 978-1-4398-5438-9 (Hardback)

This book contains information obtained from authentic and highly regarded sources. Reasonable efforts have been made to publish reliable data and information, but the author and publisher cannot assume responsibility for the validity of all materials or the consequences of their use. The authors and publishers have attempted to trace the copyright holders of all material reproduced in this publication and apologize to copyright holders if permission to publish in this form has not been obtained. If any copyright material has not been acknowledged please write and let us know so we may rectify in any future reprint.

Except as permitted under U.S. Copyright Law, no part of this book may be reprinted, reproduced, transmitted, or utilized in any form by any electronic, mechanical, or other means, now known or hereafter invented, including photocopying, microfilming, and recording, or in any information storage or retrieval system, without written permission from the publishers.

For permission to photocopy or use material electronically from this work, please access [www.copyright.com](http://www.copyright.com) (<http://www.copyright.com/>) or contact the Copyright Clearance Center, Inc. (CCC), 222 Rosewood Drive, Danvers, MA 01923, 978-750-8400. CCC is a not-for-profit organization that provides licenses and registration for a variety of users. For organizations that have been granted a photocopy license by the CCC, a separate system of payment has been arranged.

**Trademark Notice:** Product or corporate names may be trademarks or registered trademarks, and are used only for identification and explanation without intent to infringe.

---

**Library of Congress Cataloging-in-Publication Data**

---

Qian, Shizhi.

Electrokinetic particle transport in micro-/nanofluidics : direct numerical simulation analysis / Shizhi Qian, Ye Ai.  
p. cm. -- (Surfactant science)

Includes bibliographical references and index.

ISBN 978-1-4398-5438-9 (hardback)

1. Electrophoresis. 2. Electrokinetics. 3. Nanofluids. 4. Microfluidics. 5. Molecular biotechnology. I. Ai, Ye, 1983- II. Title.

QP519.9.E434Q24 2012

541.372--dc23

2011049955

---

Visit the Taylor & Francis Web site at  
<http://www.taylorandfrancis.com>

and the CRC Press Web site at  
<http://www.crcpress.com>

---

# Contents

Preface.....	xv
<b>Chapter 1</b> Basics of Electrokinetics in Micro-/Nanofluidics .....	1
1.1 Introduction to Micro-/Nanofluidics .....	1
1.2 Particle Transport and Manipulation in Micro-/Nanofluidics .....	3
1.3 Basics of Electrokinetics .....	3
1.3.1 Electrical Double Layer.....	3
1.3.2 Electroosmosis .....	6
1.3.3 Electrophoresis .....	8
1.3.4 Dielectrophoresis.....	10
1.3.5 Induced-Charge Electrokinetics.....	12
1.4 Organization of This Book.....	13
References .....	14
<b>Chapter 2</b> Numerical Simulations of Electrical Double Layer and Electroosmotic Flow in a Nanopore.....	23
2.1 Electrical Double Layer.....	23
2.2 Electroosmotic Flow in a Nanopore .....	36
2.3 Concluding Remarks .....	50
References .....	51
<b>Chapter 3</b> Transient Electrokinetic Motion of a Circular Particle in a Microchannel.....	53
3.1 Introduction .....	54
3.2 Mathematical Model.....	55
3.3 Numerical Implementation in COMSOL .....	60
3.4 Results and Discussion .....	91
3.4.1 In a Straight Microchannel.....	91
3.4.2 In a Converging-Diverging Microchannel .....	97
3.4.2.1 Lateral Motion .....	98
3.4.2.2 Effect of Electric Field.....	100
3.4.2.3 Effect of Particle Size .....	103
3.4.3 In a Y-Shaped Microchannel with a Hurdle.....	103
3.4.3.1 Effect of Particle Size .....	105
3.4.3.2 Effect of Particle's Zeta Potential .....	105
3.4.3.3 Effect of Electric Field.....	105
3.4.3.4 Effect of Channel Geometry.....	107

3.4.4	In an L-Shaped Microchannel.....	107
3.4.4.1	Experimental Setup .....	108
3.4.4.2	Experimental Results.....	111
3.4.4.3	Comparison between Experimental and Numerical Results.....	112
3.4.4.4	Particle Rotation .....	114
3.4.4.5	Effect of Particle Size .....	117
3.4.4.6	Effect of Electric Field.....	117
3.5	Concluding Remarks .....	118
	References .....	119
<b>Chapter 4</b>	<b>Electrokinetic Transport of Cylindrical-Shaped Cells in a Straight Microchannel.....</b>	<b>123</b>
4.1	Introduction .....	124
4.2	Experimental Setup .....	125
4.3	Mathematical Model.....	126
4.4	Numerical Implementation in COMSOL .....	130
4.5	Results and Discussion .....	141
4.5.1	Experimental Results .....	141
4.5.2	Effect of Channel Wall.....	143
4.5.3	Effect of Electric Field .....	145
4.5.4	Effect of Zeta Potential Ratio.....	147
4.5.5	Effect of Particle's Aspect Ratio .....	148
4.5.6	Effect of Particle's Initial Angle.....	150
4.6	Concluding Remarks .....	151
	Appendix .....	151
	References .....	154
<b>Chapter 5</b>	<b>Shear- and Electrokinetics-Induced Particle Deformation in a Slit Channel.....</b>	<b>157</b>
5.1	Introduction .....	157
5.2	Shear-Induced Particle Deformation .....	158
5.2.1	Mathematical Model .....	158
5.2.2	Numerical Implementation.....	160
5.2.3	Results and Discussion.....	173
5.3	Electrokinetic-Induced Particle Deformation .....	173
5.3.1	Mathematical Model .....	173
5.3.2	Numerical Implementation and Code Validation.....	178
5.3.3	Results and Discussion .....	190
5.3.3.1	DEP Effect .....	191
5.3.3.2	Effect of Particle's Shear Modulus .....	193
5.3.3.3	Effect of Electric Field.....	194

	5.3.3.4	Effect of Particle's Zeta Potential .....	196
	5.3.3.5	Effect of Rigid Channel Boundary .....	196
	5.4	Concluding Remarks .....	199
		References .....	199
<b>Chapter 6</b>	<b>Pair Interaction between Two Colloidal Particles under DC Electric Field.....</b>		<b>201</b>
	6.1	Introduction .....	202
	6.2	Mathematical Model.....	203
	6.3	Numerical Implementation in COMSOL .....	206
	6.4	Results and Discussion .....	218
	6.4.1	Comparison between DEP Particle-Particle Interaction and Brownian Motion .....	218
	6.4.2	Parallel Orientation, $\theta = 0^\circ$ .....	220
	6.4.3	Perpendicular Orientation, $\theta = 90^\circ$ .....	220
	6.4.4	Intermediate Orientation, $0^\circ < \theta < 90^\circ$ .....	223
	6.5	Concluding Remarks .....	226
		References .....	227
<b>Chapter 7</b>	<b>Electrokinetic Translocation of a Cylindrical Particle through a Nanopore: Poisson-Boltzmann Approach.....</b>		<b>229</b>
	7.1	Introduction .....	230
	7.2	Mathematical Model.....	232
	7.2.1	Dimensional Form of Mathematical Model .....	233
	7.2.2	Dimensionless Form of Mathematical Model.....	235
	7.3	Numerical Implementation in COMSOL and Code Validation .....	236
	7.4	Results and Discussion .....	251
	7.4.1	Effect of Particle's Initial Orientation .....	252
	7.4.2	Effect of Particle's Initial Lateral Offset .....	255
	7.4.3	Effect of Nanopore's Surface Charge Density ....	260
	7.5	Concluding Remarks .....	262
		References .....	263
<b>Chapter 8</b>	<b>Electrokinetic Translocation of a Cylindrical Particle through a Nanopore: Poisson-Nernst-Planck Multi-Ion Model .....</b>		<b>267</b>
	8.1	Introduction .....	268
	8.2	Mathematical Model.....	269
	8.2.1	Dimensional Form of Mathematical Model .....	270
	8.2.2	Dimensionless Form of Mathematical Model.....	273

8.3	Numerical Implementation in COMSOL and Code Validation .....	274
8.4	Results and Discussion .....	288
8.4.1	Comparison between PB Model and PNP Model.....	289
8.4.2	Effect of Ratio of Particle Radius to Debye Length .....	291
8.4.3	Effect of Particle's Initial Orientation .....	294
8.4.4	Effect of Initial Lateral Offset from Nanopore's Centerline .....	297
8.4.5	Effect of Nanopore's Surface Charge Density ....	297
8.5	Concluding Remarks .....	302
	References .....	303
<b>Chapter 9</b>	<b>Field Effect Control of DNA Translocation through a Nanopore.....</b>	<b>307</b>
9.1	Introduction .....	307
9.2	Mathematical Model.....	310
9.3	Implementation in COMSOL Multiphysics and Code Validation .....	314
9.4	Results and Discussion .....	326
9.4.1	Effect of Gate Potential .....	327
9.4.2	Effect of Ratio of Particle Radius to Debye Length .....	332
9.4.3	Effect of Nanopore's Permittivity .....	333
9.5	Concluding Remarks .....	335
	References .....	336
<b>Chapter 10</b>	<b>Electrokinetic Particle Translocation through a Nanopore Containing a Floating Electrode .....</b>	<b>339</b>
10.1	Introduction .....	339
10.2	Mathematical Model.....	340
10.3	Implementation in COMSOL Multiphysics.....	344
10.4	Results and Discussion .....	353
10.4.1	Effect of Electric Field .....	353
10.4.2	Effect of Ratio of Particle Radius to Debye Length .....	357
10.5	Concluding Remarks .....	362
	References .....	363
<b>Index.....</b>		<b>365</b>