

# A Molecular Dynamics Study of Flow Regimes with Effects of Wall Properties in 2-D Nano-Couette Flows

by

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Thesis submitted for the degree of  
Doctor of Philosophy

in

The University of Adelaide  
School of Chemical Engineering  
Faculty of Engineering, Computer & Mathematical Sciences

February 22, 2010



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# Acknowledgments

I would like to thank several individuals for their support and guidance throughout this work.

To Dr. Chris Colby and A/Prof. Brian O'Neill for their valuable supervision. Without their encouragement and advice, the implementation of this thesis would not have been possible. To Dr. Dzuy Nguyen and Dr. Yung Ngothai for taking the time to edit this thesis and suggest useful changes.

Special thanks to eResearchSA for access to their parallel computing centre to conduct Molecular Dynamics simulations.

Financial support was granted by the Australian Government (in the form of the Australian Postgraduate Award) and CRC for Tissue Growth and Repair. I am thankful for their scholarship and contribution towards the operating expenses incurred.

Last, and by no means least, I would like to thank my family. Their love, continual support and encouragement have been my inspiration.

# Abstract

The transitional Reynolds number and range for macrochannel flows are around 1200 and 1000 respectively. Several studies have shown that for microchannel flows, the transitional Reynolds number drops to around 500 and the transitional range around 300. This thesis provides some data on the laminar to turbulent transition for nano-channel flows through molecular dynamic simulations.

The Lennard-Jones potential is used for fluid-fluid and wall-fluid interactions, and a non-linear spring potential is used for wall-wall interactions. The mixing is characterised by averaging the maximum transverse movement for all fluid molecules. Six nano-separations were simulated and the flow and mixing behaviours examined. The results show that the transitional Reynolds number and the range increase with increasing diameter.

The effects of wall properties on flow regimes were also investigated using molecular dynamic simulations. The results show that the transitional Reynolds number and range increased with increasing wall density. For increasing wall interaction strength, the effect on the transitional Reynolds number was inconclusive. However, the transitional range increased. With an increase in wall wettability, which corresponds to an increase in hydrophilicity, there was an increase in both the transition Reynolds number and range.

The wall roughness was modeled as sinusoidal. For an increase in the amplitude of the wall

roughness, there was a decrease in the transitional Reynolds number. The effect on the transitional range was inconclusive. For an increase in the period of the wall roughness, both the transitional Reynolds number and range increased.

Errors involved in MD simulations arise from several sources. They include the size of the time-step, thermostat model, wall model, and viscosity calculation method. No experimental results at the nano-scale are available for direct comparison however they provide a basis for future work. As computation power improves, MD simulations at higher Reynolds numbers may be compared with experimental results of flows through microchannels. Also, as laboratory technology and measurement accuracy improves, experimental results of flows through nano-channels may be conducted and used for comparison.

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D. To, C. Colby, B. O'Neill, Y. Ngothai, and D. Nguyen. A Molecular Dynamics Study of Laminar-Turbulent Transition in 2-D Nano-Couette Flows : Part I. *Submitted to Physical Review E*, 2009a.

D. To, C. Colby, B. O'Neill, Y. Ngothai, and D. Nguyen. A Molecular Dynamics Study of Laminar-Turbulent Transition in 2-D Nano-Couette Flows : Part II - Wall Effects. *Submitted to Physical Review E*, 2009b.

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